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Tese de Doutorado

Combinação de Cálculos de Estrutura Eletrônica e Espectroscopia Rovibracional para o Aprimoramento do Potencial Lennard-Jones na Descrição de Complexos de van der Waals Envolvendo Gases-Nobres

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Brasília, 15 de Agosto de 2018

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Por

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Tese apresentada ao Instituto de Física da Universidade de Brasília como parte dos requisitos necessários para a obtenção do título de Doutor em Física.

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Dedico esta tese a meu pai
Carlos Alberto Mendes de Almeida e
aos meus avós José Mendes da Paz e
Maria Almeida.

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Resumo

As propriedades de sistemas envolvendo gases nobres têm auxiliado muito no desenvolvimento de técnicas de modelagem e de valores padrão para estudos experimentais. Sistemas diatômicas formados por gases nobres, no estado fundamental, representam protótipos ideais de complexos do tipo van der Waals, e suas propriedades espectroscópicas e termodinâmicas têm sido extensivamente estudadas tanto teórica como experimentalmente. Neste trabalho, determinamos as energias eletrônicas no estado fundamental considerando um conjunto amplo de configurações nucleares para todos os sistemas diatômicos possíveis envolvendo os átomos de He, Ne, Ar, Kr, Xe e Rn. Estas energias foram obtidas utilizando o método *coupled cluster* e os conjuntos de funções de base aug-cc-pVTZ, aug-cc-pVQZ e aug-cc-pV5Z. Em seguida, estas energias foram ajustadas para a forma analítica denominada Improved Lennard Jones (ILJ) com o objetivo de obter o valor específico β para cada sistema molecular estudado, pois experimentalmente, ele é estimado para ser β=9 para todo complexo envolvendo gás nobre. A determinação acurada deste parâmetro é importante pois ele leva em consideração a dureza/maciez dos átomos envolvidos no complexo. Observou-se nos ajustes realizados que o parâmetro β se aproxima mais do valor experimental quando o conjunto de base aug-cc-pV5Z é usado. A qualidade da forma analítica ILJ (usando o parâmetro β ajustado para cada complexo) foi testada com o cálculo das propriedades espectroscópicas rovibracionais. Verificou-se a partir destes cálculos que as constantes espectroscópicas determinadas via ILJ (com o β ajustado) concordam mais com os dados experimentais que outros resultados disponíveis na literatura. Este fato sugere que a forma analítica ILJ torna-se mais acurada para descrever complexos de van der Waals quando o parâmetro β ajustado é usado.

Abstract

The properties of systems involving noble gases have greatly aided the development of modeling techniques and the obtention of standard values for experimental studies. Diatomic systems formed by noble gases in the ground state represent ideal prototypes of van der Waals complexes, and their spectrocopic and thermodynamic properties have been extensively studied both theoretically and experimentally. In this work, we determine the electronic energies in the ground state, considering a broad set of nuclear configurations for all possible diatomic systems involving the atoms of He, Ne, Ar, Kr, Xe and Rn. These energies were obtained using the coupled cluster method with aug-cc-pVTZ, aug-cc-pVQZ and aug-cc-pV5Z basis sets. These energies were then adjusted to the analytical form called Improved Lennard Jones (ILJ) in order to obtain the specific value of the beta parameter for each molecular system studied, since it is experimentally estimated to be the same (β =9) for any complex involving noble gas. The accurate determination of this parameter is important because it takes into account the hardness/softness of the atoms involved in the molecule. It was observed in the fittings made that the parameter approaches more the experimental value when the $aug-cc-pV5Z$ base set is used. The quality of the analytical form ILJ (using the adjusted parameter for each molecule) was tested with the calculation of the rovibrational spectroscopic properties. It has been found from these calculations that the spectroscopic constants determined via ILJ (with fittid β) agree more with the experimental data than other results available in the literature. This fact suggests that the ILJ analytical form becomes more accurate to describe van der Waals complexes when the adjusted β parameter is used

1 Introdução

As propriedades de sistemas atômicos e moleculares envolvendo gases nobres são de grande interesse tanto para o desenvolvimento de técnicas de modelagem como para valores padrão para estudos experimentais. As moleculas diatômicas envolvendo gases nobres em seus estados eletrônicos fundamentais representam protótipos ideais de moléculas do tipo van der Waals. Suas propriedades espectroscópicas e termodinâmicas têm sido estudadas de forma extensiva, tanto teórico [1–13] como experimentalmente [14–22].

As propriedades espectroscópicas fornecem informações da geometria e dinâmica de sistemas moleculares. Isso mostra a grande importância do estudo espectroscópico no campo teórico e experimental para diversos ramos da ciência como biofísica, bioquímica e astrofísica [23]. São essas observações que levam à construção de modelos que proporcionam a compreensão, bem como a predição das propriedades do sistema atômico ou molecular de interesse que usualmente estão associados a conceitos e princípios da mecânica quântica. Dessa forma, esses aspectos importantes motivam o estudo detalhado destas propriedades em sistemas envolvendo gases nobres.

O conhecimento das interações intermoleculares fracas, geralmente determinadas pelos parâmetros de um potencial intermolecular, é uma informação necessária para muitos cálculos de modelagem em sistemas complexos tais como plasmas, lasers, moléculas de interesse biológico, atmosférico e químico [24]. Dessa maneira, a caracterização detalhada desses potenciais e o desenvolvimento de funções analíticas adequadas são imprescindíveis para a descrição das propriedades macroscópicas e microscópicas da matéria.

Dados espectroscópicos de alta resolução em sistemas diatômicos de gases nobres levaram à determinação de energias de ionização e dissociação, distâncias internucleares de equilíbrio, entre outros parâmetros a partir dos quais suas funções de energia potencial podem ser calculadas [25–28]. As principais fontes de dados sobre os sistemas

diatômicos heteronucleares de gases raros são medições por espectroscopia de microondas [14,29,30], medidas das seções transversais de dispersão elástica [31] e medidas dos coeficientes viriais [32]. As funções de energia potencial também foram determinadas usando métodos químicos quânticos *ab initio* [27,28,33], que proporcionaram previsões confiáveis de suas propriedades espectroscópicas. No entanto, o crescente número de elétrons nos sistemas de gases nobres mais pesados torna os cálculos *ab initio* mais dispendiosos sob o ponto de vista computacional.

Em uma série de artigos, vários pesquisadores [34–36] realizaram estudos sistemáticos da força de interação envolvida em sistemas van der Waals por meio de experimentos de dispersão de feixe moleculares a partir de uma função de energia potencial adequada denominada Improved Lennard Jones (ILJ) [37]. Essa forma analítica, introduzida na literatura por Pirani e colaboradores [37], generaliza o modelo de Lennard Jones (LJ) [38]. Além da energia de dissociação e distância de equilíbrio, a função ILJ usa o parâmetro β que está relacionado à dureza dos átomos que interagem no complexo. Alguns estudos têm demonstrado que o modelo ILJ consegue corrigir as deficiências de curto e longo alcance observados no modelo LJ. Com esses recursos foram construídas curvas de energia potencial para vários sistemas moleculares, entre eles os sistemas homonucleares e heteronucleares envolvendo gases nobres.

Esses estudos experimentais estimaram o parâmetro β igual a 9 para todas os complexos estudados. No entanto, espera-se que a curva de energia potencial via modelo ILJ de cada complexo possa ser melhor representada por um valor específico do β, ou seja, que cada complexo possua o seu valor característico para o parâmetro β. Dessa forma, um dos objetivos do presente trabalho é a determinação do parâmetro β para cada complexo estudado. Para tanto, foram determinadas as energias eletrônicas em nível CCSD(T) (do inglês *coupled cluster* com excitações simples, duplas e as triplas por pertubação) [39] e com três diferentes conjuntos de funções de base publicadas por Dunning ($aug-cc-pVTZ$, $aug-cc-pVQZ$ e $aug-cc-pV5Z$) [40] variando as distâncias internucleares desde a região de forte interação (distâncias internucleares menores que a distância de equilíbrio do sistema diatômico) até a região assintótica (distâncias internucleares grandes comparadas à distância de equilíbrio). Em seguida, o parâmetro β para cada complexo foi obtido ajustando estas energias eletrônicas para o modelo ILJ (nesses ajustes tanto a distância de equilíbrio com a energia de dissociação dos complexos foram fixadas). Com

esse procedimento, foi possível determinar o valor específico do parâmetro β para cada sistema diatômico aqui estudada.

Uma vez determinadas as curvas de energia potencial por modelo LJ e ILJ para cada complexo estudado, a partir das energias eletrônicas, passou-se para o segundo objetivo desta tese, que foi o cálculo das constantes espectroscópicas rovibracionais das complexos estudados, usando tanto a forma do modelo LJ quanto a do modelo ILJ, a fim de testar a qualidade dos dois modelos. Os resultados obtidos sugerem que as constantes espectroscópicas rovibracionais determinadas com o modelo ILJ concordam melhor com os dados experimentais do que as obtidas via modelos LJ e ILJ com o β igual a 9.

Dessa forma, organizamos nosso estudo em 5 capítulos; o capítulo 2 é dedicado à fundamentação teórica utilizada no desenvolvimento deste trabalho. No capítulo 3 são apresentados e discutidos os resultados para distâncias internucleares de equilibrio, energias de dissociação, ajustes dos parâmetros β, constantes espectroscópicas rovibracionais e tempo de vida de todos os complexos estudados. No capitulo 4, são apresentadas as conclusões, bem como perspectivas futuras. Por fim, o capítulo 5 apresenta os fatores de convenção utilizados, as energias *ab initio* e trabalhos realizados.

2 Metodologias

2.1 O Sistema Molecular

Para descrever de forma apropriada um sistema molecular qualquer, devemos recorrer à solução da equação de Schrödinger (independente do tempo e sem correções relativísticas) dada por [41]:

$$\hat{H}\Psi(\mathbf{r},\mathbf{R}) = E\Psi(\mathbf{r},\mathbf{R}), \tag{2.1}$$

onde $\Psi(\mathbf{r},\mathbf{R})$ representa a função de onda do sistema, sendo $\mathbf{r}$ o conjunto das coordenadas eletrônicas e $\mathbf{R}$ o conjunto das coordenadas nucleares.

O hamiltoniano $\hat{H}$ não relativístico de um sistema molecular constituído de N elétrons e M núcleos é dado por:

$$\hat{H} = \hat{T}_e(\mathbf{r}) + \hat{T}_n(\mathbf{R}) + \hat{V}_n(\mathbf{R}) + \hat{V}_{ne}(\mathbf{r},\mathbf{R}) + \hat{V}_e(\mathbf{r}), \tag{2.2}$$

onde cada operador desse hamiltoniano, escrito em unidades atômicas ($\hbar = m_e = e = 1$), é definido da seguinte forma:

- $\hat{T}_e(\mathbf{r}) = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2$ representa o operador energia cinética dos elétrons.
- $\hat{T}_n(\mathbf{R}) = -\sum_{A=1}^{M}\frac{1}{2M_A}\nabla_A^2$ representa o operador energia cinética dos núcleos.
- $\hat{V}_n(\mathbf{R}) = \sum_{A=1}^{M-1}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}}$ representa o operador energia potencial da interação núcleo-núcleo.
- $\hat{V}_{ne}(\mathbf{r},\mathbf{R}) = -\sum_{A=1}^{M}\sum_{i=1}^{N}\frac{Z_A}{r_{iA}}$ é o operador que corresponde a interação elétron-núcleo.
- $\hat{V}_e(\mathbf{r}) = \sum_{i=1}^{N-1}\sum_{j>i}^{N}\frac{1}{r_{ij}}$ é o perador energia potencial referente a interação elétron-elétron.

Nos operadores acima, M_A e Z_A correspondem respectivamente à massa e ao número atômico do núcleo A, ∇_A^2 é o Laplaciano em relação às coordenadas nucleares e ∇_i^2 é o Laplaciano em relação às coordenadas eletrônicas.

Substituindo a equacão 2.2 na equacão 2.1 obtêm-se:

$$\left[-\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - \sum_{A=1}^{M}\frac{1}{2M_A}\nabla_A^2 - \sum_{A=1}^{M}\sum_{i=1}^{N}\frac{Z_A}{r_{iA}} + \sum_{A=1}^{M-1}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}} + \sum_{i=1}^{N-1}\sum_{j>i}^{N}\frac{1}{r_{ij}}\right]\Psi(\mathbf{r},\mathbf{R}) = E\Psi(\mathbf{r},\mathbf{R}). \tag{2.3}$$

Contudo, para um sistema quântico de muitos corpos, a equacão (2.3) é complicada de ser solucionada sem a utilização de aproximações. Uma aproximação utilizada frequentemente para aplicação da mecânica quântica à moléculas e sólidos é a aproximação de Born-Oppenheimer [41].

2.2 A Aproximação de Born-Oppenheimer

De acordo com o teorema adiabático, se a pertubação aplicada a um sistema for suficientemente lenta, o sistema é capaz de adaptar-se à nova configuração e assim seu autoestado é consevardo [41]. Assim, expressa-se a função de onda do sistema molecular em termos da expansão adiabática da seguinte forma:

$$\Psi(\mathbf{r},\mathbf{R}) = \phi(\mathbf{r};\mathbf{R})\chi(\mathbf{R}), \tag{2.4}$$

onde $\phi(\mathbf{r};\mathbf{R})$ representa a função de onda eletrônica que depende explicitamente das coordenadas eletrônicas e parametricamente das coordenadas nucleares, $\chi(\mathbf{R})$ representa a função de onda nuclear.

Substituindo a expressão (2.4) na Eq. (2.3), obtêm-se:

$$-\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2[\phi(\mathbf{r};\mathbf{R})\chi(\mathbf{R})] - \sum_{A=1}^{M}\frac{1}{2M_A}\nabla_A^2[\phi(\mathbf{r};\mathbf{R})\chi(\mathbf{R})] - \sum_{A=1}^{M}\sum_{i=1}^{N}\frac{Z_A}{r_{iA}}\phi(\mathbf{r};\mathbf{R})\chi(\mathbf{R}) +$$
$$+\sum_{A=1}^{M-1}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}}\phi(\mathbf{r};\mathbf{R})\chi(\mathbf{R}) + \sum_{i=1}^{N-1}\sum_{j>i}^{N}\frac{1}{r_{ij}}\phi(\mathbf{r};\mathbf{R})\chi(\mathbf{R}) = E\phi(\mathbf{r};\mathbf{R})\chi(\mathbf{R}). \tag{2.5}$$

Analisando o Laplaciano no segundo termo do lado esquerdo da eq. 2.5, temos:

$$\nabla_A^2\left[\phi(\mathbf{r};\mathbf{R})\chi(\mathbf{R})\right] = [\nabla_A^2\phi(\mathbf{r};\mathbf{R})]\chi(\mathbf{R}) + 2\nabla_A\phi(\mathbf{r};\mathbf{R})\cdot\nabla_A\chi(\mathbf{R}) + \phi(\mathbf{r};\mathbf{R})[\nabla_A^2\chi(\mathbf{R})]. \tag{2.6}$$

De acordo com aproximação adiabática a função de onda eletrônica $\phi(\mathbf{r};\mathbf{R})$ varia lentamente com R, logo podemos considerar:

$$\nabla_A^2 \phi(\mathbf{r};\mathbf{R}) \approx 0 \tag{2.7}$$

e

$$\nabla_A \phi(\mathbf{r};\mathbf{R}) \approx 0, \tag{2.8}$$

ou seja:

$$\nabla_A^2 \left[\phi(\mathbf{r};\mathbf{R})\chi(\mathbf{R})\right] \approx \phi(\mathbf{r};\mathbf{R})[\nabla_A^2 \chi(\mathbf{R})]. \tag{2.9}$$

Desta forma, a equação 2.9 representa matematicamente a aproximação de Born-Oppenheimer (ABO).

Substituindo a eq. 2.9 na eq. 2.6, obtém-se:

$$\left[-\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - \sum_{A=1}^{M}\sum_{i=1}^{N}\frac{Z_A}{r_{iA}} + \sum_{i=1}^{N-1}\sum_{j>i}^{N}\frac{1}{r_{ij}}\right]\phi(\mathbf{r};\mathbf{R}) = +\epsilon(\mathbf{R})\phi(\mathbf{r};\mathbf{R}) \tag{2.10}$$

e

$$\left[-\sum_{A=1}^{M}\frac{1}{2M_A}\nabla_A^2 + V(\mathbf{R})\right]\chi(\mathbf{R}) = E\chi(\mathbf{R}), \tag{2.11}$$

onde

$$V(\mathbf{R}) = \sum_{A=1}^{M-1}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}} + \epsilon(\mathbf{R}). \tag{2.12}$$

Sendo assim, através da ABO separou-se a equação de Schrödinger independente do tempo em duas: a parte eletrônica e a parte nuclear. A equação 2.10 descreve o problema eletrônico, cuja solução para um conjunto de configurações nucleares nos fornece um conjunto de funções eletrônicas $\phi(\mathbf{r};\mathbf{R})$ e suas energias eletrônicas $\epsilon(\mathbf{R})$ correspondentes. A Equacão 2.11 é a equação de Schrödinger nuclear, sua solução descreve a dinâmica molecular, dentre os quais os movimentos de translação, vibração e rotação. A seguir, serão descritos os métodos utilizados nesse trabalho para resolver a equação de Schrödinger eletrônica.

2.3 Solução da Equação de Schrödinger Eletrônica

2.3.1 Equação de Hartree-Fock

Para solucionar a equação de Schrödinger eletrônica acuradamente, devem-se ultilizar métodos numéricos altamente eficazes, uma vez que resolver essa equação analiticamente é uma uma tarefa complexa. Por essa razão, concentraram-se esforços no desenvolvimento de métodos computacionais capazes de solucionar essas equações. Como resultado, foi desenvolvido o método de Hartre-Fock [41]. A idéia básica do Hartree-Fock (HF) é combinar o princípio variacional, supondo que a função de onda que descreve o sistema

r deve ser antissimétrica e obtida por meio de um determinante, denominado Determinante de Slater, dado da seguinte forma:

$$\Phi = \frac{1}{\sqrt{N!}} \begin{bmatrix} \psi_1(x_1) & \psi_2(x_1) & \dots & \psi_N(x_1) \\ \psi_1(x_2) & \psi_2(x_2) & \dots & \psi_N(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_1(x_N) & \psi_2(x_N) & \dots & \psi_N(x_N) \end{bmatrix}. \tag{2.13}$$

onde o fator $1/\sqrt{N!}$ é a constante de normalização para Φ e N é o número de elétrons. A solução da equação de Hartree-Fock são os spin-orbitais moleculares que por simplicidade usar-se-á o operador de permutação para reescrever o determinante de Slater. Sendo assim, pode-se escrever a função de onda do HF como segue:

$$\Phi = \frac{1}{\sqrt{N!}} \sum_{i=1}^{N!} (-1)^{p_i} \mathcal{P}_i \psi_1(x_1)\psi_2(x_2)\psi_3(x_3)...\psi_N(x_N) \tag{2.14}$$

sendo que $\mathcal{P}_i$ é o operador que gera a i-ésima permutação dos índices de x, e p_i é o número de trocas realizadas, de tal forma que a i-ésima permutação retorne à sua sequência original. Utilizando o determinante de Slater, escrito com o operador permutação, pode-se calcular o valor esperado da energia do sistema molecular. Levando-se em consideração a indistiguibilidade dos elétrons, tem-se

$$E = \langle \Phi | H | \Phi \rangle = \sum_{a=1}^{N} \langle a|h|a\rangle + \frac{1}{2} \sum_{a,b=1}^{N} (\langle ab|ab\rangle - \langle ab|ba\rangle). \tag{2.15}$$

Na equação acima, a e b variam de 1 até N, bem como nas demais que aparecerão neste capítulo, e representam os spin-orbitais moleculares ψ_a e ψ_b, e h é o hamiltoniano que envolve os núcleos da molécula e é dado por:

$$h(x_1) = -\frac{1}{2}\nabla_1^2 - \sum_{A=1}^{M}\frac{1}{r_{1A}} \tag{2.16}$$

Como mencionado anteriomente, o método HF consiste basicamente em combinar o princípio variacional com a suposição de que a função de onda que descreve o sistema é antissimétrica. Dessa forma, a função de onda que mais se aproxima da solução exata é a que conduz a um mínimo. Como a função de onda é escrita em termos de spin-orbitais, escrever-se-á um funcional energia de acordo com a equação 2.15. Logo a energia é um funcional dos spin-orbitais moleculares, dada por:

$$E[\psi] = \sum_a \langle\psi_a|h|\psi_a\rangle + \frac{1}{2}\sum_{a,b}(\langle\psi_a\psi_b|\psi_a\psi_b\rangle - \langle\psi_a\psi_b|\psi_b\psi_a\rangle). \tag{2.17}$$

Para minimizar $E[\psi]$, os spin-orbitais devem ser ortonormais, ou seja, $\langle\psi_a|\psi_b\rangle - \delta_{ab} = 0$. Utilizando a técnica de multiplicadores de Lagrange para a condição de vínculo, tem-se que:

$$L[\psi] = E[\psi] - \sum_{a,b}\epsilon_{ba}(\langle\psi_a|\psi_b\rangle - \delta_{ab}), \tag{2.18}$$

onde os ϵ_{ba} são os multiplicadores de Lagrange. Minimizando esse funcional, chega-se à equação de HF:

$$\mathcal{F}|\psi_a\rangle = \epsilon_a|\psi_a\rangle, \tag{2.19}$$

onde $\mathcal{F}$ é o operador de Fock dado por:

$$\mathcal{F}(1) = h(1) + \sum_b[\mathcal{J}_b(1) - \mathcal{K}_b(1)], \tag{2.20}$$

com $\mathcal{J}_b$ e $\mathcal{K}_b$ sendo os operadores de coulomb e de troca, respectivamente, definidos da seguinte maneira:

$$\mathcal{J}_b(1)\psi_a(1) = \left\langle\psi_b(2)|\tfrac{1}{r_{12}}|\psi_b(2)\right\rangle\psi_a(1) \tag{2.21}$$

$$\mathcal{K}_b(1)\psi_a(1) = \left\langle\psi_b(2)|\tfrac{1}{r_{12}}|\psi_b(2)\right\rangle\psi_b(1), \tag{2.22}$$

sendo que ϵ_a é o autovalor de energia para o orbital a.

Dessa forma, nota-se que o operador de Fock depende das soluções da equação dos spin-orbitais. Existe uma equação para cada orbital que depende dos outros orbitais através do operador de Fock. Logo, essas equações devem ser resolvidas de forma acoplada, ou seja, através de aproximações sucessivas. Devido a isso o método HF é um método autoconsistente, no final do processo as funções ψ que são soluções da equação de Hartree-Fock devem ser as mesmas a partir dos quais o operador de Fock foi obtido.

Desta forma, os determinantes de Slater são a essência do método Hartree-Fock [39]. Usando um único determinante de Slater (equação 2.13), pode-se escrever as dependências com relação a parte espacial e de spin dos spin-orbitais moleculares separadamente,

$$\psi_i(x) = \begin{cases} \phi_j(\mathbf{r})\alpha(\omega) \\ \phi_j(\mathbf{r})\beta(\omega) \end{cases} \tag{2.23}$$

onde α e β representam, respectivamente, spin *up* e *down*. Quando nenhuma restrição é feita aos orbitais moleculares, o método é denominado Hartree-Fock não Restrito (UHF), tornando-se adequado para sistemas de camada aberta. Sistemas de camada aberta podem ser descritos também por uma função de onda do tipo restrita, onde as partes espaciais dos spins-orbitais, duplamente ocupados, sejam necessariamente as mesmas. Nestas condições, tem-se o método Hartree-Fock Restrito de Camada Aberta (ROHF). Aqui considerar-se-á o método HF restrito [39,41] para o caso em que o sistema possui camada fechada, ou seja, o sistema possui um número par de elétrons e cada orbital está ocupado por dois elétrons: um com spin α e outro com spin β. Levando-se em conta essas considerações para HF restrito, obtem-se a equação de HF, que agora será espacial, e a equação para o valor da energia média do sistema é dada por,

$$f\mathbf{r}_1\phi_p(\mathbf{r}_1) = \epsilon_p\phi_p(\mathbf{r}_1), \tag{2.24}$$

$$E = 2\sum_{p=1}^{N/2}\langle p|h|p\rangle + \sum_{p,q=1}^{N/2} 2\langle pq|pq\rangle - \langle pq|pq\rangle\,, \tag{2.25}$$

onde $f(\mathbf{r}_1)$ é o operador de Fock para camadas fechadas, definido da seguinte maneira:

$$f\mathbf{r}_1 = h(r_1) + \sum_{q=1}^{N/2} 2\mathcal{J}_q(\mathbf{r}_1) - \mathcal{K}_q(\mathbf{r}_1) \tag{2.26}$$

Na equacão acima, $\mathcal{J}_q(\mathbf{r}_1)$ e $\mathcal{K}_q(\mathbf{r}_1)$ são, respectivamente, os operadores de coulomb e de troca para camadas fechadas. Dessa forma, com a eliminação dos termos relacionados ao spin, o problema passa a ser o de resolver uma equação diferencial espacial. Uma possibilidade de solução dessa equação será expandir a parte espacial dos spin-orbitais em um conjunto formado por K funções base conhecidas $g_\nu(r)$,

$$\phi_p(\mathbf{r}) = \sum_{\nu=1}^{k} C_{\nu p} g_\nu(\mathbf{r}), \tag{2.27}$$

onde $g_\nu(r)$ são as funções base conhecidas, k é o número de funções do conjunto e $C_{\nu p}$ são os coeficientes da expansão linear dos orbitais espaciais a serem determinados. Substituindo a equação 2.27 em 2.24, encontrar-se-á a equação de Hartree-Fock-Roothaan (HFR) [39, 41, 42],

$$\mathbf{FC} = \mathbf{SC}\epsilon \tag{2.28}$$

sendo $\mathbf{S}$ a matriz de superposição e $\mathbf{F}$ a matriz de Fock , ambas, matrizes formadas pelos seguintes elementos:

$$S_{\mu\nu} = \int d\mathbf{r}_1 g_\mu^* \mathbf{r}_1 g_\nu \mathbf{r}_1 \tag{2.29}$$

$$F_{\mu\nu} = \int d\mathbf{r}_1 g_\mu^* \mathbf{r}_1 f(\mathbf{r}_1) g_\nu \mathbf{r}_1 \tag{2.30}$$

Na equação 2.28, $\mathbf{C}$ é a matriz dos coeficientes da expansão e ϵ é a matriz diagonal que contém as energias orbitais. A equação 2.28 deve ser resolvida de maneira iterativa, e pode ser utilizado o procedimento SCF (*Self Consistent Field*) [41] como algoritmo para sua solução.

2.3.2 Método Coupled Cluster

O método de *coupled cluster* (CC) [39] é uma técnica numérica usada para descrever sistemas de muitos corpos, capaz de fornecer a energia de correlação eletrônica de maneira eficiente. Foi primeiramente desenvolvido por Coster [43] e Kümmel e colaboradores [44] e tornou-se muito popular na última década [1, 3, 8]. A ideia básica no método CC é tratar um sistema de muitos elétrons, separando-o em vários aglomerados

com poucos elétrons, denominados de clusters. Em seguida, calculam-se as interações entre os elétrons de um mesmo aglomerado e depois entre diferentes aglomerados. A função de onda CC é escrita na seguinte forma

$$|\Phi\rangle = e^{T}|\Phi_0\rangle, \tag{2.31}$$

onde $|\Phi\rangle$ é a função de onda HF e T é o operador de cluster dado por:

$$T = T_1 + T_2 + ... + T_p \tag{2.32}$$

sendo

$$T_1 = \sum_{ar} t_a^r a_r^\dagger a_a, \tag{2.33}$$

$$T_2 = \frac{1}{4}\sum_{abrs} t_{ab}^{rs} a_r^\dagger a_s^\dagger a_b a_a \tag{2.34}$$

e

$$T_p = \frac{1}{(p!)^2}\sum_{ab...rs...} t_{ab}^{rs} a_r^\dagger a_s^\dagger ... a_b a_a. \tag{2.35}$$

Na notação acima, a, b,... representam orbitais ocupados no determinante HF, e r, s,... representam orbitais virtuais. Os operadores $a^\dagger$ e a atuam como operadores de criação e aniquilação, respectivamente. Os coeficientes t são números reais chamados amplitudes de cluster. O operador T_1 gera as configurações com substituições simples, T_2 gera as configurações com substituições duplas e assim sucessivamente.

Levando-se em conta a forma da eq. 2.32 o operador exponencial e^T pode ser expandido em série de Taylor

$$e^{T_1+T_2+...+T_p} = 1 + T_1 + T_2 + \frac{1}{2!}T_1^2 + T_3 + \frac{1}{3!}T_1^3 + T_1T_2 + ..., \tag{2.36}$$

onde T_1, T_2 e T_3,... são chamados termos conexos e T_1^2, T_1T_2, ... são chamados termos desconexos. Essa série é finita, pois o número de orbitais ocupados é finito, assim como o número de excitações. As amplitudes de cluster t, devem ser tais que a função de onda $|\Phi\rangle$ satisfaça a equação de Schröndiger.

$$He^{T}|\Phi_0\rangle = Ee^{T}|\Phi_0\rangle. \tag{2.37}$$

Multiplicando essa equação por e^{-T} pela esquerda, temos

$$e^{-T}He^{T}|\Phi_0\rangle = E|\Phi_0\rangle. \tag{2.38}$$

A função de onda $|\Phi\rangle$ conterá todas as substituições possíveis, desde que p seja igual ao número de spin-orbitais ocupados. Sendo o conjunto de funções de base completo, a otimização das amplitudes de clusters levará a uma solução extra, que não é viável computacionalmente. Sendo assim, é necessário truncar o operador de cluster T, levando em consideração apenas alguns operadores de cluster.

Umas das aproximações dentro do método CC, é considerar as substituições simples e duplas $T = T_1 + T_2$. Pelo teorema de Brillouin [41], apenas as substituições duplas interagem com o determinante HF. Dessa maneira, a maior contribuição das substituições simples para a energia se dá por meio do termo desconexo T_1^2. Essa aproximação é denominada CCSD (CC com determinantes com simples e duplas excitações). Para calcular a energia nesta aproximação, projeta-se a equação 2.38 no estado $|\Phi_0\rangle$:

$$E_{CCSD} = \langle\Phi_0|e^{-T_2}He_2^T|\Phi_0\rangle = \mathcal{E} + \frac{1}{4}\sum_{\substack{ab\\rs}}\langle ab||rs\rangle t_{ab}^{rs} + \frac{1}{2}\sum_{\substack{ab\\rs}}\langle ab||rs\rangle t_a^r t_b^s. \tag{2.39}$$

Essa energia não é restrita apenas à aproximação CCSD, uma vez que operadores de clusters de ordem mais alta não contribuem diretamente para a energia, pois pelas regras de Condon-Slater [41], tem-se que:

$$\langle\Phi_0|H|\Phi_{abc}^{rst}\rangle = \langle\Phi_0|H|\Phi_{abc...}^{rst...}\rangle = 0. \tag{2.40}$$

No entanto, esses operadores de ordem mais alta contribuem indiretamente para a energia, por meio das equações usadas para determinar as amplitudes de cluster t_a^r e t_{ab}^{rs}, que são necessárias para a obtenção da energia.

Para obter as amplitudes de cluster t_a^r e t_{ab}^{rs} na aproximação CCSD projeta-se a eq. 2.38 nos estados $|\Phi_a^r\rangle$ e $|\Phi_{ab}^{rs}\rangle$. Sabendo que os determinantes excitados são ortonormais entre si, temos que:

$$\langle\Phi_a^r|e^{-T}He^T\Phi_0\rangle = 0 \tag{2.41}$$

denominado equação de amplitude T_1, e

$$\langle\Phi_{ab}^{rs}|e^{-T}He^T\Phi_0\rangle = 0 \tag{2.42}$$

denominado de equação de amplitude T_2.

O procedimento para a construção das equações algébricas que resultam nas amplitudes de cluster T_1 e T_2 pode ser visto na Referência [45]. A maior dificuldade do

método CC é obter a solução das equações para as amplitudes de cluster, pois todos os coeficientes aparecem em todas as equações. Dessa maneira, essas equações devem ser resolvidas de forma autoconsistente, sendo o método de Newton-Raphson multidimensional é o mais utilizado.

Como mencionado anteriormente, incluir apenas T_1 e T_2 no operador de cluster não quer dizer que apenas as substituições simples e duplas são incluídas na função de onda, pois além destas, também são incluídas termos desconexos de substituções de terceira, quarta,... ordem. Uma aproximação mais sofisticada dentro do método CC é denominado CCSDT (CC com determinantes com simples, duplas e tripla excitações). Essa aproximação inclui substituçõs simples, duplas e triplas no operador de cluster [46]. No entanto, a inclusão desses novos termos no operador de cluster implica em um elevado custo computacional tornando-o em um método dispendioso [46]. Uma maneira mais viável de incluir as substituições triplas conexas foi proposta por Gauss e Cremer [47]. Essa forma é denominada CCSD(T), onde o termo que envolve as excitações triplas é incluído via teoria de pertubação.

2.3.3 Funções de base

O principal objetivo de cálculos *ab initio* é a obtenção de resultados de um sistema molecular a partir da resolução da equação de Schrödinger eletrônica, sem a utilização de parâmetros com ajuste de dados experimentais. Existem diversas aproximações para resolver a equação acima citada, uma das mais comuns na aplicação de métodos *ab initio* é a incorporação de um conjunto de base, que consiste na expansão de uma função desconhecida em um conjunto de funções conhecidas.

Existem dois tipos de funções de base comumente utilizado nos cálculos de estrutura eletrônica: *Slater Type Orbital* (STO) e *Gaussian Type Orbital* (GTO). Os orbitais do tipo Slater são geralmente representados como $STO-nG$, onde n representa o número de orbitais gaussianos (ϕ) usados na expansão da função de onda eletrônica do sistema, ou seja, gaussianas contraídas [48]. Matematicamente, os $STO-nG$ podem ser escritos na forma:

$$\psi_{STO-3G} = c_1\phi_1 + c_2\phi_2 + c_3\phi_3, \tag{2.43}$$

Nesta equação, temos

- $\phi_1 = (\frac{2\alpha_1}{\pi})e^{-\alpha_1 r^2}$;
- $\phi_2 = (\frac{2\alpha_2}{\pi})e^{-\alpha_2 r^2}$;
- $\phi_3 = (\frac{2\alpha_3}{\pi})e^{-\alpha_3 r^2}$;

sendo α_1, α_2, α_3,c_1, c_2 e c_3 obtidos de forma que as gaussianas contraídas sobreponham o máximo os STO. As funções de Slater descrevem os orbitais monoeletrônicos de forma precisa, porém suas integrais são de difícil resolução, tornando sua aplicabilidade restrita apenas à sistemas monoatômicos e diatômicos.

Sendo assim, para moléculas maiores, geralmente utiliza-se um conjunto de funções gaussianas (GTO). De modo geral, mesmo sendo necessário combinar várias GTO para descrever um orbital atômico com formato aproximado ao de uma STO, as integrais de dois elétrons e multicêntricas calculadas para sistemas moleculares são feitas mais rapidamente por GTO, uma vez que o produto de duas gaussianas gera uma terceira gaussiana, o que facilita consideravelmente a resolução das integrais.

Uma aproximação muito utilizada na maioria dos conjuntos de funções base é a combinação linear de gaussianas primitivas, denominada de contração de gaussianas ou contração de orbitais do tipo gaussiana (CGTO-*Contracted Gaussian Type Orbital*). Aos conjuntos de bases que utilizam apenas uma CGTO para orbitais de camada interna e várias CGTOS para descrever os orbitais de camada de valência, dá-se o nome de conjuntos de bases de *Split-valence basis set*, proposta por People [48]. Geralmente é representada por $X - YZG$, sendo X o número de gaussianas utilizadas para os elétrons mais internos (que não estão na camada de valência), Y e Z os números de gaussianas utilizados no orbitais de valência.

Embora as bases *Split-valence* sejam muito utilizadas, existem sistemas moleculares como os estudados neste trabalho que necessitam de orbitais adicionais que representem bem a difusão e dispersão, pois sistemas envolvendo gases nobres estão sempre sujeitos a dispersão. Desta forma, para uma melhor acurácia no estudo destes sistemas utilizamos as funções de base desenvolvidadas por Dunning [40].

O conjunto de base desenvolvido por Dunning é geralmente escrita na forma

$cc-pVnZ$. Nessa nomeclatura, cc é o termo de correlação consistente, p significa polarização, V significa valência e nZ = DZ, TZ, QZ, 5Z,... (*DZ=double-zeta, TZ=triple-zeta, QZ= quaduple-zeta,...*), que é o número de exitações consideradas. Neste trabalho, as funções de base utilizadas foram *aug-cc-pVTZ*, *aug-cc-pVQZ* e *aug-cc-pV5Z*, o termo *aug* significa que foram utilizadas funções difusas. Cálculos realizados utilizando as funções de base acima citadas estão sujeitos a um pequeno erro, conhecido como BSSE (do inglês "Basis set superposition error"), que será melhor explicado na próxima secção.

2.3.4 Correção para o erro de superposição de funções de base

Em geral, conjuntos de funções de base finitas são utilizados no cálculo da energia eletrônica. Essas funções de base são geralmente centradas sobre os átomos que as originam, e cada átomo pode ser representado por um conjunto de funções idênticas ou diferentes entre si. Como já mencionado antes, o objetivo deste trabalho é o estudo dos sistemas diatômicos formados pelos gases nobres. Denominando um dos átomos do sistema de A e o outro de B, a energia de interação é dada por:

$$\Delta E^{AB} = E^{AB} - (E^A + E^B), \tag{2.44}$$

onde E^{AB} é a energia do sistema, E^A e E^B são as energias de cada átomo calculadas separadamente. No entanto, a Equacão (2.44) só é consistente quando utilizamos um conjunto de bases suficientemente grande para garantir que o orbital molecular dos átomos seja descrito da mesma maneira, seja no sistema ou separadamente.

A utilização de um conjunto incompleto de funções de base leva a um erro na energia de interação, denominado BSSE. Isso ocore pelo compartilhamento das funções de base de A e B quando estão próximos, esse compartilhamento é benéfico e ajuda a suprir a defasagem do conjunto de base incompleto dos átomos. Entretanto, quanto maior for a distância entre os átomos, menor é o compartilhamento, de modo que ao se dissociarem, cada átomo passa a ser descrito apenas por seu próprio conjunto de base.

Quando os átomos estão separados, ambos possuem menor acessibilidade às funções de base, isto faz com que suas energias E^A e E^B sejam superestimadas (menos negativas) devido à pior descrição matemática de seus orbitais moleculares em relação às que possuem no sistema. Dessa maneira, a energia ΔE^{AB} descrita na Equacão (2.44) é

menor do que deveria ser se o número de funções de base acessíveis para cada átomo fosse igual durante todo o cálculo.

Existem diferentes aproximações para minimizar ou extinguir o BSSE. Uma das aproximações mais utilizadas é a *Counterpoise Correction* desenvolvido por Boys e Bernardi [52].

Para corrigir o BSSE no cálculo da energia de interação ΔE^{AB} utilizando a metodologia *Counterpoise Correction*, substitui-se os conjuntos de base dos átomos pelo conjunto de base do sistema. De forma que para calcular a energia do átomo A, o átomo B passa a ser definido como *átomo fantasma*, posicionado na mesma geometria do sistema, porém sem elétrons ou núcleos. A energia de A passa a ser dada por $E^A(AB)$, na qual a notação entre parênteses (AB) se refere ao conjunto de base do sistema. A energia de interação corrigida pelo *Counterpoise Correction* ΔE^{AB}_{CP} passa a ser dada por:

$$\Delta E^{AB}_{CP} = E^{AB} - (E^A(AB) + E^B(AB)). \tag{2.45}$$

2.3.5 Pseudopotenciais

Investigar um sistema molecular com uma quantidade muito grande de elétrons levando em consideração todas as interações entre suas partículas torna-se computacionalmente muito dispendioso e em alguns caso inviável. A teoria do pseudopotencial (PP), obtido pela primeira vez por Phillips e Kleimann [49], foi umas das primeiras aproximações para a resolução da equação de Schrodinger eletrônica. Esta aproximação consiste basicamente em aproximar o potencial correspondente à interação elétron-núcleo por um psedopotencial efetivo muito mais fraco, e substituir as funções de onda de elétrons de valência, que oscilam rapidamente na região central, por funções de pseudo-onda, que variam suavemente no região central.

Nos átomos, os elétrons mais próximos do núcleo sentem um forte potencial atrativo e possuem pouca participação nas ligações químicas. Por outro lado, os elétrons de valência estão fracamente ligados ao núcleo e por isso apresentam grande participação nas ligações químicas, determinando a maior parte das propriedades físicas de uma molécula.

O pseudopotencial é um potencial efetivo utilizado para substituir o poten-

cial real gerado pelos prótons e elétrons próximos ao núcleo (caroço). Desta forma, os estados eletrônicos do caroço são eliminados e os elétrons de valência são descritos por uma pseudofunção de onda sem nodos. Isto reduz o custo computacional simplificando os cálculos de estrutura eletrônica.

Os PPs de norma conservado são os mais utilizados. Estes devem satisfazer as seguintes condições [50]:

1. Os autovalores obtidos devem ser idênticos aos verdadeiros.

2. Para $r \geqslant r_c$, as pseudofunções devem ser iguais às funções de onda reais, onde r_c é o raio de corte.

3. A carga total na região $r \leqslant r_c$ calculada pelas pseudofunções e pelas autofunçõess originais é idêntica.

4. A derivada logarítmica da pseudofunção é equivalente à da função de onda real para $r \geqslant r_c$.

Nesse trabalho, utilizou-se o pseudopotencial de Peterson e colaboradores [51] para todos os sistemas que envolveram os átomos de xenônio e o radônio. Este pseudopotencial foi testado com cálculos CCSD(T) de afinidades eletrônicas atômicas, polarizabilidades de gases nobres, e as constantes espectroscópicas de vários sistemas diatômicos de camadas fechadas. Em todos os casos, os erros devidos à aproximação pseudopotencial foram calculados como sendo quase insignificantes.

2.3.6 Modelo Lennard-Jones aprimorado - ILJ

As moléculas estão sujeitas a duas forças distintas, no limite de menor e maior separação. Essas forças são respectivamente a força repulsiva em distâncias menores e a força atrativa a distâncias longas. O potencial de Lennard-Jones (LJ) [38], proposto em 1924 por John Lennard-Jones, é um modelo matemático simples que descreve este comportamento das moléculas. O potencial LJ é dado por:

$$V(R) = 4\varepsilon \left[\left(\frac{\sigma}{R} \right)^{12} - 2 \left(\frac{\sigma}{R} \right)^{6} \right], \tag{2.46}$$

onde ε é a profundidade do potencial e σ é a distância internuclear de equilibrio. Na equação acima o primeiro termo descreve a repulsão e o segundo termo descreve a atração.

Experiências realizadas envolvendo gases nobres têm sido usadas para verificar a confiança de uma função (potencial) de interação proposta por Pirani e colaboradores [37] que envolve apenas um parâmetro a mais que o modelo LJ, e é denominada de Improved Lennard-Jones (ILJ). O potencial ILJ elimina a maioria das deficiências de curto e longo alcance do modelo LJ, e tem a seguinte forma:

$$V(R) = \varepsilon \left[\frac{m}{n(R) - m} \left(\frac{R_m}{R} \right)^{n(R)} - \frac{n(R)}{n(R) - m} \left(\frac{R_m}{R} \right)^{m} \right], \tag{2.47}$$

onde ε e R_m representam respectivamente a profundidade do potencial e a sua localização.

Na equação 2.47, o primeiro termo descreve a repulsão ao passo que o segundo descreve a atração. O expoente do segundo termo assume os seguintes valores: m = 6 para sistemas que contenham átomos ou moléculas neutro-neutro, m = 4 para sistemas íon-neutro e m = 1 para casos íon-íon. O termo $n(R)$ é dado por:

$$n(R) = \beta + 4 \left(\frac{R}{R_m} \right)^2, \tag{2.48}$$

onde β é um fator relacionado à dureza dos dois elementos (átomos) que interagem.

2.4 Solução da Equação de Schrödinger Nuclear

Como visto na seção 2.1, a equação de Schrödinger nuclear é dada por:

$$\left[-\sum_{A=1}^{M} \frac{1}{2M_A} \nabla_A^2 + V(\mathbf{R}) \right] \chi(\mathbf{R}) = E\chi(\mathbf{R}), \tag{2.49}$$

onde $V(\mathbf{R}) = \sum_{A=1}^{M-1} \sum_{B>A}^{M} \frac{Z_A Z_B}{R_{AB}} + \epsilon(\mathbf{R})$ corresponde ao potencial efetivo à que os núcleos estão sujeitos.

Antes de resolver a equação 2.49, para os sistemas diatômicos envolvendo os gases nobres, é conveniente expressar esta equação em um referencial localizado no centro de massa da molécula. De fato, deslocando o sistema de referência do laboratório para o centro de massa do sistema, pode-se escrever a Equação 2.49 como sendo:

$$\left[-\frac{1}{2\mu} \nabla_{12}^2 + V(R_{12}) \right] \varphi_{12}(\mathbf{R}_{12}) = E_{int} \varphi_{12}(\mathbf{R}_{12}), \tag{2.50}$$

onde a função φ_{12} depende somente da distância internuclear que une os dois núcleos e E_{int} é a energia interna da molécula, ou seja, a soma da energia vibracional e rotacional da molécula diatômica.

Para explorar a simetria esférica do potencial $V(R_{12})$, um novo sistema de coordenadas com origem fixa no centro de massa da molécula é introduzido. Na figura 2.1, O' é a origem do novo sistema de coordenadas fixado no centro de massa, μ é a massa reduzida e $\mathbf{R}_{12}$ é a posição do núcleo 2 em relação ao núcleo 1. Reescrevendo a equação 2.50 em coordenadas esféricas, tem-se:

$$-\frac{1}{2\mu}\left[\frac{\partial^2}{\partial {R_{12}}^2}+\frac{2}{R_{12}}\frac{\partial}{\partial R_{12}}-\frac{\hat{L}^2}{R_{12}^2}-2\mu V(R_{12})\right]\varphi_{12}(\mathbf{R}_{12})=E_{int}\varphi_{12}(\mathbf{R}_{12}), \tag{2.51}$$

onde $\hat{L}^2$ é o operador laplaciano que é dado por:

$$\hat{L}^2=\frac{-1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)-\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}. \tag{2.52}$$

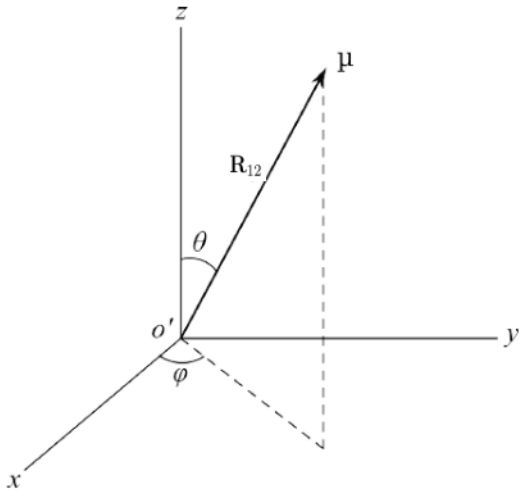

Figura 2.1: Novo sistema de coordenadas com origem fixa no centro de massa da molécula.

Como o potencial $V(R_{12})$ não depende das variáveis angulares, então o hamiltoniano pode ser separado em uma parte radial ($\mathbf{R}_{12}$) e outra angular (θ,φ). Dessa maneira a função de onda fica:

$$\varphi_{12}(\mathbf{R}_{12})=\Psi(R_{12})Y_j^{m_j}(\theta,\varphi), \tag{2.53}$$

onde $Y_j^{m_j}(\theta,\varphi)$ são os harmônicos esféricos, autofunções do operador $\hat{L}^2$ [52]. Assim a

equacão 2.51, pode ser reescrita da seguinte forma:

$$-\frac{1}{2\mu}\left[\frac{\partial^2}{\partial {R^2}_{12}}+\frac{2}{R_{12}}\frac{\partial}{\partial R_{12}}-\frac{\hat{L}^2}{{R^2}_{12}}-2\mu V(R_{12})\right]\Psi(R_{12})Y_j^{m_j}(\theta,\varphi)=E_{int}\Psi(R_{12})Y_j^{m_j}(\theta,\varphi). \tag{2.54}$$

Sabendo que $\hat{L}^2Y_j^{m_j}(\theta,\varphi)=j(j+1)Y_j^{m_j}(\theta,\varphi)$, temos:

$$-\frac{1}{2\mu}\left[\frac{d^2\Psi(R_{12})}{d{R^2}_{12}}+\frac{2}{R_{12}}\frac{d\Psi(R_{12})}{dR_{12}}-\Psi(R_{12})\frac{j(j+1)}{{R^2}_{12}}-2\mu V(R_{12})\Psi(R_{12})\right]=E_{int}\Psi(R_{12}), \tag{2.55}$$

onde j representa o número quântico rotacional da molécula diatômica.

Como a função de onda depende apenas da parte radial, propõe-se a seguinte substituição:

$$\widetilde{\Psi}(R_{12})=R_{12}\Psi(R_{12}). \tag{2.56}$$

Substituindo a equacão 2.56 na equacão 2.55, temos:

$$-\frac{1}{2\mu}\frac{d^2\widetilde{\Psi}(R_{12})}{d{R^2}_{12}}+\widetilde{V}(R_{12})\widetilde{\Psi}(R_{12})=E_{int}\widetilde{\Psi}(R_{12}), \tag{2.57}$$

onde $\widetilde{V}(R_{12})=\dfrac{j(j+1)}{2\mu{R^2}_{12}}+V(R_{12})$ é o potencial efetivo.

Para resolver a Equacão (2.57) usa-se o método variacional [41, 56], que consiste em expandir a função de onda $\widetilde{\Psi}(R_{12})$ da seguinte forma:

$$\widetilde{\Psi}(R_{12})\approx\sum_{j=1}^{n}c_j\eta_j(R_{12}), \tag{2.58}$$

onde c_j são os coeficientes da expansão a serem determinados e $\eta_j(R_{12})$ são funções de base conhecidas.

Dessa maneira a substituição de 2.58 em 2.57, transforma a equação diferencial de segunda ordem 2.57, na seguinte equação matricial:

$$\mathbf{HC}=E\mathbf{SC}, \tag{2.59}$$

onde $\mathbf{H}=\mathbf{T}+\mathbf{V}$ e $\mathbf{S}$ é a matriz de sobreposição.

Assim, os elementos de matrizes $\mathbf{T}$, $\mathbf{V}$ e $\mathbf{S}$ são dados por:

$$T_{ij}=\frac{1}{2\mu}\int_0^\infty\frac{d\eta_i^*(R_{12})}{dR_{12}}\frac{d\eta_j(R_{12})}{dR_{12}}dR_{12}, \tag{2.60}$$

$$V_{ij} = \int_0^\infty \eta_i^*(R_{12})\widetilde{V}(R_{12})\eta_j(R_{12})dR_{12} \tag{2.61}$$

e

$$S_{ij} = \int_0^\infty \eta_i^*(R_{12})\eta_j(R_{12})dR_{12}. \tag{2.62}$$

onde os elementos de matrizes T_{ij}, V_{ij} e S_{ij}, serão calculados via método DVR (do inglês "Discrete Variable Representation").

2.5 Método da Representação da Variável Discreta

Assim como a equação de Schrödinger eletrônica, a equação de Schrödinger nuclear para sistemas com muitas partículas não pode ser resolvida de forma exata, portanto é necessário introduzir aproximações que busquem a melhor solução possível. O método DVR é uma aproximação que se baseia na expansão da função de onda em um conjunto de funções de base ortonormais $\phi_i(R_{12})$; $i = 1, ..., N$ e a utilização de regras de quadraturas para calcular as integrais envolvidas [57].

Assim, os elementos de matrizes de energia potencial $\mathbf{V}_{ij}$ (calculados apenas nos pontos de quadraturas gaussianas) tornam-se diagonais e os elementos de matrizes do operador energia cinética $\mathbf{T}_{ij}$ passam ser calculados analiticamente.

Para expandir a solução $\widetilde{\Psi}(R_{12})$ utilizamos funções $\phi_i(R)$ como funções de base, onde ϕ_j é um conjunto de funções pertencentes ao espaço L^2 com a seguinte propriedade:

$$\phi_j(R_k) = \delta_{jk}(j, k = 1, 2, ..., n), \tag{2.63}$$

sendo que R_k representa os pontos de quadratura gaussiana onde as funções de base serão avaliadas.

Portanto, expandindo $\widetilde{\Psi}(R_{12})$ como uma combinação de $\phi_j(R)$, e omitindo a indexação R_{12}, temos:

$$\widetilde{\Psi}(R) \approx \sum_{j=1}^{n} c_j\phi_j(R), \tag{2.64}$$

onde c_j são os coeficientes da expansão a serem determinados e as funções $\phi_j(R)$ representam a discretização da variável R.

Usando a notação de Dirac para obter a representação da variável discreta, temos:

$$\phi_j(R) = \langle R|\phi_j\rangle. \tag{2.65}$$

Inserindo a relação de completeza $\sum_{i=1}^{n} |f_i\rangle\langle f_i| = \mathbf{1}$ na equacão 2.65, obtêm-se:

$$\phi_j(R) = \sum_{i=1}^{n}\langle R|f_i\rangle\langle f_i|\phi_j\rangle = \sum_{i=1}^{n} f_i(R)\langle f_i|\phi_j\rangle \tag{2.66}$$

onde as integrais dos elementos da matriz $\langle f_i|\phi_j\rangle$ podem ser calculadas através de quadraturas gaussianas, como segue:

$$\langle f_i|\phi_j\rangle \approx \sum_{k=1}^{n} w_k f_i^*(R_k)\phi_j(R_k), \tag{2.67}$$

onde w_k são os pesos correspondentes aos pontos R_k da quadratura.

Substituindo a equacão 2.67 na equacão 2.66, obtém-se:

$$\phi_j(R) = \sum_{i=1}^{n}\sum_{k=1}^{n} f_i(R) w_k f_i^*(R_k)\phi_j(R_k). \tag{2.68}$$

Como as funções de base $\phi_j(R_k)$ são ortogonais, a equacão 2.68 é dada por:

$$\phi_j(R) = \sum_{i=1}^{n} w_j f_i(R) f_i^*(R_k). \tag{2.69}$$

Assim, para um ponto R_j qualquer da quadratura, temos:

$$\phi_j(R_j) = w_j \sum_{i=1}^{n} f_i(R_j) f_i^*(R_j). \tag{2.70}$$

Se $w_j \sum_{i=1}^{n} f_i(R_j) f_i^*(R_j) = 1$ (funções de base normalizadas), então o peso associado a cada ponto da quadratura é dado por:

$$w_j = \frac{1}{\sum_{i=1}^{n} f_i(R_j) f_i^*(R_j)}. \tag{2.71}$$

No entanto, as funções de base $\phi_j(R)$ não estão normalizadas em todos os pontos da quadratura, portanto precisamos normalizá-las fazendo:

$$\overline{\phi}_j(R) = \lambda_j \phi_j(R), \tag{2.72}$$

onde λ_j é a costante de normalização [58] e a função $\overline{\phi}_j(R)$ deve satisfazer a seguinte condição:

$$\langle\overline{\phi}_j|\overline{\phi}_j\rangle = 1, \tag{2.73}$$

assim, substituindo a equacão 2.72 na equacão 2.73, temos:

$$\lambda_j^2\langle\phi_j|\phi_j\rangle = 1. \tag{2.74}$$

Utilizando mais uma vez as quadraturas gaussianas, temos:

$$\lambda_j^2\sum_{k=1}^{n} w_k\phi_j^*(R_k)\phi_j(R_k) = 1, \tag{2.75}$$

usando a ortogonalidade das funções primitivas $\phi_j(R_k)$ (2.63), temos:

$$\lambda_j^2 w_j = 1. \tag{2.76}$$

Portanto, a constante de normalização é:

$$\lambda_j = \frac{1}{\sqrt{w_j}}. \tag{2.77}$$

Assim, substituindo as Equações 2.77 e 2.70 em 2.72, obtemos a função de base discreta normalizada $\overline{\phi}_j(R)$:

$$\overline{\phi}_j(R_j) = \sqrt{w_j}\sum_{i=1}^{n} f_i(R_j)f_i^*(R_j). \tag{2.78}$$

Finalmente, expandindo a função de onda utilizando a representação da variável discreta normalizada $\overline{\phi}_j(R)$, temos:

$$\widetilde{\Psi}(R) \approx \sum_{j=1}^{n} c_j\overline{\phi}_j(R). \tag{2.79}$$

Substituindo 2.79 em 2.61, temos:

$$V_{ij} = \int_0^\infty \overline{\phi}_j^*(R)\widetilde{V}(R)\overline{\phi}_i(R)dR. \tag{2.80}$$

Repetindo o procedimento das quadraturas gaussianas, pode-se reescrever a equacão 2.80 como segue:

$$V_{ij} = \sum_{k=1}^{n} \overline{\phi}_j^*(R_k)\widetilde{V}(R_k)\overline{\phi}_i(R_k)w_k, \tag{2.81}$$

onde $\overline{\phi}_j(R_k) = \delta_{jk}$ (funções de base ortogonais), portanto a matriz de energia potencial $\mathbf{V}$ torna-se diagonal. Essa é uma das principais caracteristicas do DVR. R_k são os pontos da quadratura gaussiana, que são os autovalores da matriz, cujos elementos são dados por:

$$R_{ij} = \langle f_i|\hat{R}|f_j\rangle. \tag{2.82}$$

2.5.1 DVR com Pontos Igualmentes Espaçados

Para calcular os elementos de matriz do operador energia cinética, podemos utilizar as quadraturas gaussianas com pontos igualmentes espaçados [58,59], pertencentes a um intervalo [a,b], de modo que cada ponto da quadratura gaussiana seja dado por:

$$R_i = a + \frac{(b-a)}{N} i, \tag{2.83}$$

onde $i = 1, 2, ..., N-1$; considerando que a função de base seja nula nas extremidades, isso sugere que se pode utilizar as funções de onda de uma partícula numa caixa como funções de base [60]:

$$f_n(R) = \sqrt{\frac{2}{b-a}} \sin\left[\frac{n\pi(R-a)}{b-a}\right], \tag{2.84}$$

onde $n = 1, 2, ..., N-1$.

Os elementos de matriz do operador energia cinética são dados por:

$$T_{ij} = \langle R_i|\hat{T}|R_j\rangle, \tag{2.85}$$

onde $\hat{T}$ é o operador diferencial energia cinética e tem a seguinte forma:

$$\hat{T} = -\frac{1}{2\mu}\frac{d^2}{dR^2}. \tag{2.86}$$

Introduzindo a relação de fechamento em 2.85 e explicitando o operador energia cinética $\hat{T}$, obtém-se a representação da variável discreta do operador T_{ij}, que é dada por:

$$T_{ij} = -\frac{1}{2\mu}\frac{(b-a)}{N}\sum_{n}^{N-1}\frac{d^2 f_n(R_i)}{dR^2} f_n(R_j). \tag{2.87}$$

Substituindo 2.84 em 2.87, temos:

$$T_{ij} = \frac{1}{2\mu}\frac{1}{(b-a)^2}\frac{\pi^2}{2}\left[\frac{1}{\sin^2\left(\frac{\pi(i-j)}{2N}\right)} - \frac{1}{\sin^2\left(\frac{\pi(i+j)}{2N}\right)}\right], \tag{2.88}$$

e no caso em que $j = i$, temos:

$$T_{ij} = \frac{1}{2\mu}\frac{1}{(b-a)^2}\frac{\pi^2}{2}\left[\frac{(2N^2+1)}{3} - \frac{1}{\sin^2\left(\frac{\pi i}{N}\right)}\right]. \tag{2.89}$$

Portanto, o DVR diagonaliza o potencial da matriz hamiltoniana, e permite que os elementos da matriz energia cinética sejam obtidos analiticamente.

2.6 Propriedades Espectroscópicas Rovibracionais

Nesse trabalho, as constantes rovibracionais foram obtidas por dois métodos diferentes. No primeiro monta-se um sistema de cinco equações fazendo o número quântico vibracional $\upsilon = 0$, 1, 2, 3 e o número quântico rotacional j = 0 e 1 na expressão da energia rovibracional [61]:

$$\begin{aligned} E_{\upsilon,J} = &\left(\upsilon+\frac{1}{2}\right)\omega_e - \left(\upsilon+\frac{1}{2}\right)^2\omega_e x_e + \left(\upsilon+\frac{1}{2}\right)^3\omega_e\gamma_e + ...+ \\ &+\left[B_e - \alpha_e\left(\upsilon+\frac{1}{2}\right) + \gamma_e\left(\upsilon+\frac{1}{2}\right)^2 + ...\right]J(J+1) + ..., \end{aligned} \tag{2.90}$$

sendo $B_e = \frac{1}{4\pi C\mu R_e^2}$.

Em seguida, substituim-se os valores das energias rovibracionais $E_{\upsilon,J}$ obtidas através da resolução da equação de Schrödinger nuclear. Pode-se então montar um sistema de equações para as constantes espectroscópicas rovibracionais, como segue:

$$\begin{aligned} \omega_e &= \frac{1}{24}\left[14\left(E_{1,0}-E_{0,0}\right) - 93\left(E_{2,0}-E_{0,0}\right) + 23\left(E_{3,0}-E_{1,0}\right)\right] \\ \omega_e x_e &= \frac{1}{4}\left[13\left(E_{1,0}-E_{0,0}\right) - 11\left(E_{2,0}-E_{0,0}\right) + 3\left(E_{3,0}-E_{1,0}\right)\right] \\ \omega_e y_e &= \frac{1}{6}\left[3\left(E_{1,0}-E_{0,0}\right) - 3\left(E_{2,0}-E_{0,0}\right) + \left(E_{3,0}-E_{1,0}\right)\right] \\ \alpha_e &= \frac{1}{8}\left[-12\left(E_{1,1}-E_{0,1}\right) + 4\left(E_{2,1}-E_{0,1}\right) + 4\omega_e - 23\omega_e y_e\right] \\ \gamma_e &= \frac{1}{4}\left[-2\left(E_{1,1}-E_{0,1}\right) + \left(E_{2,1}-E_{0,1}\right) + 2\omega_e x_e - 9\omega_e y_e\right]. \end{aligned} \tag{2.91}$$

O segundo método utilizado para encontrar as constantes espectroscópicas foi o método de Dunham [62]. Em 1932, utilizando teoria de perturbação, Dunham encontrou uma expressão para a energia rovibracional de uma molécula diatômica em termos das derivadas do potencial na distância internuclear de equilíbrio R_e. A expansão do potencial em torno de R_e é dada por:

$$V(R) = V(R_e) + \frac{1}{2!}\left(\frac{d^2V}{dR^2}\right)_{R_e}(R - Re)^2 + \frac{1}{3!}\left(\frac{d^3V}{dR^3}\right)_{R_e}(R - R_e)^3 + \\ + \frac{1}{4!}\left(\frac{d^4V}{dR^4}\right)_{R_e}(R - R_e)^4 + ... \tag{2.92}$$

Reescrevendo a equação 2.92 de forma mais simples, tem-se:

$$V(\rho) = V(0) + \frac{1}{2}d_2\rho^2 + \frac{1}{6}d_3\rho^3 + \frac{1}{24}d_4\rho^4 + ..., \tag{2.93}$$

onde ρ=R-R_e é o deslocamento em relação à distância internuclear de equilíbrio e d_2, d_3 e d_4 são a segunda, terceira e quarta derivada, respectivamente, do potencial em ρ=0.

Como mostrado por Dunham as constantes espectroscópicas rovibracionais que multiplicam $(\upsilon+\frac{1}{2})$ em 2.90, podem ser escritas em termos das derivadas do potencial, através de uma comparação entre 2.90 e 2.93. A segunda derivada é dada pela mesma expressão de um oscilador harmônico:

$$\upsilon = \frac{1}{2\pi}\sqrt{\frac{d_2}{m}}. \tag{2.94}$$

Identificando υ como $c\omega_e$, obtêm-se:

$$\omega_e = \frac{1}{2\pi c}\sqrt{\frac{d_2}{m}}. \tag{2.95}$$

A constante α_e pode ser determinada através da derivada terceira do potencial, dada por:

$$d_3 = -3\frac{d_2}{R_e}\left(1 + \frac{\alpha_e\omega_e}{6B_e^2}\right), \tag{2.96}$$

isolando α_e, temos:

$$\alpha_e = -6B_e^2\left(\omega_e^{-1} + \frac{R_e d_3}{3\omega_e d_2}\right), \tag{2.97}$$

onde B_e é dada por:

$$B_e = \frac{1}{4\pi C\mu R_e^2}. \tag{2.98}$$

A constante $\omega_e x_e$ é obtida a partir da derivada de quarta ordem do potencial, dada por:

$$d_4 = \frac{d_2}{R_e^2}\left[15\left(1+\frac{\alpha_e\omega_e}{6B_e^2}\right)^2 - \frac{8\omega_e x_e d_2}{B_e R_e^2}\right]. \tag{2.99}$$

Portanto, isolando $\omega_e x_e$, temos:

$$\omega_e x_e = \frac{B_e R_e}{8d_2}\left[\frac{d_2}{R_e^2}\left(15\left(1+\frac{\alpha_e\omega_e}{6B_e^2}\right)^2\right) - d_4\right]. \tag{2.100}$$

A constante vibracional $\omega_e y_e$ e a constante rotacional γ_e podem ser obtidas usando as expressões das derivadas superiores de sétima ordem.

3 Resultados e Discussões

Neste capítulo serão mostrados e analisados os resultados obtidos para a contrução das curvas de energias potenciais e das propriedades dinâmica dos 21 sistemas moleculares envolvendo os gases nobres a saber He-He, He-Ne, He-Ar, He-Kr, He-Xe,He-Rn, Ne-Ne, Ne-Ar, Ne-Kr, Ne-Xe, Ne-Rn, Ar-Ar, Ar-Kr, Ar-Xe, Ar-Rn, Kr-Kr, Kr-Xe, Kr-Rn, Xe-Xe, Xe-Rn e Rn-Rn. De posse das curvas de energia potenciais de cada sistema estudado (obtidas a partir das energias eletrônicas), então passou-se para o outro objetivo desta tese que foi o cálculo das constantes espectroscópicas rovibracionais dos complexos usando tanto a forma do modelo LJ quanto a do modelo ILJ, com o objetivo de testar a qualidade dos dois modelos.

As constantes espectroscópicas rovibracionais foram então calculadas através de duas metodologias: o método DVR e o método de Dunham. A primeira, combina as soluções da equação de Schrödinger Nuclear com uma equação espectroscópica. A segunda, consiste basicamente na expansão da forma analítica em uma série de Taylor, então relaciona-se as derivadas de segunda à sétima ordem em torno da distância internuclear de equilíbrio, R_e, com as constantes rovibracionais.

3.1 Distância internuclear de equilíbrio e Energia de dissociação de cada sistema molecular

Todas as curvas de energias eletrônicas foram contruídas usando o método *coupled cluster* e com a correção BSSE implementada no pacote de programas Gaussian 09 [63]. Essas curvas foram contruidas utilizando os seguintes conjuntos de funções base: *aug-cc-pVTZ*, *aug-cc-pVQZ* e *aug-cc-pV5Z*. Foram calculadas as energias eletrônicas de cada sistema molecular, no estado fundamental, para diferentes valores de distância internucleares (mostradas no apêndice B). Na região próxima ao poço de potencial foi utilizado

um incremento de 0,01 Å para uma melhor caracterização da distância de equilíbrio de cada sistema molecular considerado. A Tabela 3.1 mostra a distância internuclear de equilibrio de cada sistema diatômico, bem como as distâncias de equilíbrio disponíveis na literatura.

Tabela 3.1: Distância de equilibrio em Å para cada sistema diatômico considerando o nível de cálculo CCSD(T) e os conjunto de funções de base $aug-cc-pVTZ$, $aug-cc-pVQZ$ e $aug-cc-pV5Z$.

Sistema	aug-cc-pvtz	aug-cc-pvqz	aug-cc-pv5z	Exp.
He-He	3,04	3,01	2,99	2,970 [16]
He-Ne	3,12	3,07	3,05	3,03 [64]
He-Ar	3,59	3,54	3,51	3,48 [36]
He-Kr	3,83	3,75	3,72	3,70 [65]
He-Xe	4,10	4,04	4,01	3,994 [36]
He-Rn	4,26	4,16	4,13	–
Ne-Ne	3,22	3,15	3,13	3,094 [36]
Ne-Ar	3,62	3,55	3,52	3,520 [36]
Ne-Kr	3,81	3,72	3,69	3,660 [36]
Ne-Xe	4,07	3,96	3,93	3,885 [36]
Ne-Rn	4,18	4,06	4,02	–
Ar-Ar	3,89	3,83	3,80	3,76 [36]
Ar-Kr	4,05	3,96	3,94	3,910 [36]
Ar-Xe	4,25	4,16	4,13	4,10 [36]
Ar-Rn	4,32	4,23	4,20	–
Kr-Kr	4,19	4,09	4,06	4,01 [36]
Kr-Xe	4,28	4,27	4,25	4,20 [36]
Kr-Rn	4,45	4,34	4,31	–
Xe-Xe	4,60	4,44	4,41	4,35 [36]
Xe-Rn	4,61	4,49	4,46	–
Rn-Rn	4,66	4,54	4.50	–

A partir da Tabela 3.1, pode-se inferir que à medida que o conjunto de funções de base torna-se mais extenso, essas distâncias se aproximam cada vez mais das distâncias experimentais. De fato, a melhor concordância com os dados experimentais é encontrada com a base *aug-cc-pV5Z*. A Tabela 3.2 mostra a energia de dissociação correspondente para cada sistema molecular. Dessa tabela, nota-se que as energias obtidas ficaram próximas, porém um pouco abaixo das experimentais. Assim como no caso das distâncias internucleares de equilíbrio, a melhor energia de dissociação de cada sistema foi obtida com o conjunto de base *aug-cc-pV5Z*.

Tabela 3.2: Energia de dissociação em meV para cada sistema diatômico considerando o nível de cálculo CCSD(T) e os conjunto de funções de base $aug-cc-pVTZ$, $aug-cc-pVQZ$ e $aug-cc-pV5Z$.

Sistema	aug-cc-pvtz	aug-cc-pvqz	aug-cc-pv5z	Exp.
He-He	0,737	0,806	0,849	0,942 [16]
He-Ne	1,279	1,522	1,655	1,83 [64]
He-Ar	1,929	2,204	2,373	2,59 [36]
He-Kr	1,911	2,254	2,429	2,67 [65]
He-Xe	1,807	2,172	2,349	2,624 [36]
He-Rn	1,756	2,138	2,323	–
Ne-Ne	2,220	2,879	3,199	3,660 [36]
Ne-Ar	3,750	4,656	5,135	5,740 [36]
Ne-Kr	3,890	5,017	5,536	6,160 [36]
Ne-Xe	3,907	5,152	5,711	6,350 [36]
Ne-Rn	3,919	5.259	5,854	–
Ar-Ar	8,835	10,295	11,239	12,370 [36]
Ar-Kr	10,093	12,119	13,165	14,330 [36]
Ar-Xe	11,369	13,770	14,993	16,090 [36]
Ar-Rn	12,065	14,758	16,100	–
Kr-Kr	11,882	14,648	15,782	17,300 [36]
Kr-Xe	13,463	17,159	18,504	19,950 [36]
Kr-Rn	14,923	18,690	20,209	–

Xe-Xe	16,618	20,878	22,501	24,200 [36]
Xe-Rn	18,290	23,220	25,019	–
Rn-Rn	20,351	26,222	28,220	–

De posse das energias eletrônicas, das distâncias internucleares de equilíbrio e das energias de dissociação, ajustou-se esses dados para a forma analítica ILJ a fim de obter o parâmetro β característco de cada sistema molecular uma vez que experimentalmente o valor estimado para todos os sistemas envolvendo gases nobres é 9. Todos os parâmetros β foram determinados usando o método de Powell [66]. O desvio quadrático médio (dqm) foi obtido via equação:

$$dqm = \sqrt{\sum_{i=1}^{N} \frac{(E(i) - V(i))^2}{N(N-1)}} \tag{3.1}$$

onde $E(i)$ são as energias eletrônicas, $V(i)$ são as energias obtidas através do ajuste da função ILJ e N é o número de energias eletrônicas ajustadas (o valor de N para cada sistema estudado está descrito no apêndice B). Todos os desvios quadráticos médios obtidos são mostrados na Tabela 3.4.

Para todos os ajustes, as curvas se ajustaram bem tanto para as regiões harmônicas como para as regiões anarmônicas do potencial, uma vez que o dqm de cada curva é muito pequeno.

Tabela 3.3: Valores do desvio quadrático médio em Hartree obtido no ajuste do parâmetro β para cada sistema diatômico.

Sistema	aug-cc-pvtz	aug-cc-pvqz	aug-cc-pv5z
He-He	8,70x10^{-8}	9,76x10^{-8}	1,18x10^{-7}
He-Ne	1,95x10^{-7}	2,15x10^{-7}	9,14x10^{-8}
He-Ar	1,74x10^{-7}	1,50x10^{-7}	2,59x10^{-7}
He-Kr	2,96x10^{-7}	1,29x10^{-7}	1,52x10^{-7}
He-Xe	1,00x10^{-6}	1,25x10^{-7}	2,77x10^{-7}
He-Rn	6,54x10^{-6}	1,58x10^{-7}	2,78x10^{-7}
Ne-Ne	2,87x10^{-7}	2,12x10^{-7}	3,58x10^{-7}
Ne-Ar	2,70x10^{-7}	4,70x10^{-7}	5,35x10^{-7}
Ne-Kr	3,26x10^{-7}	3,69x10^{-7}	5,67x10^{-7}
Ne-Xe	1,99x10^{-6}	5,39x10^{-7}	7,67x10^{-7}
Ne-Rn	1,24x10^{-7}	5,09x10^{-7}	9,21x10^{-7}
Ar-Ar	1,50x10^{-6}	1,21x10^{-6}	1,82x10^{-6}
Ar-Kr	1,36x10^{-6}	1,40x10^{-6}	2,54x10^{-6}
Ar-Xe	1,16x10^{-6}	1,86x10^{-6}	2,98x10^{-6}
Ar-Rn	1,50x10^{-6}	2,41x10^{-6}	2,93x10^{-6}
Kr-Ar	1,69x10^{-6}	2,18x10^{-6}	2,63x10^{-6}
Kr-Xe	1,68x10^{-6}	2,60x10^{-6}	4,62x10^{-6}
Kr-Rn	2,40x10^{-6}	3,99x10^{-6}	5.15x10^{-6}
Xe-Xe	1,51x10^{-5}	4,22x10^{-6}	4,90x10^{-6}
Xe-Rn	2,31x10^{-6}	4,23x10^{-6}	6,19x10^{-6}
Rn-Rn	2,77x10^{-6}	7,34x10^{-6}	5,94x10^{-6}

As figuras 3.1, 3.2 e 3.3 mostram a curva de energia potencial *ab initio* (linha azul contínua) e ajustada (linha tracejada vermelha) de cada sistema para o conjunto de base *aug-cc-pV5Z*. Através destas figuras, observa-se que cada sistema foi cuidadosamente ajustado, de modo que o β encontrado fosse o melhor possível para cada sistema molecular.

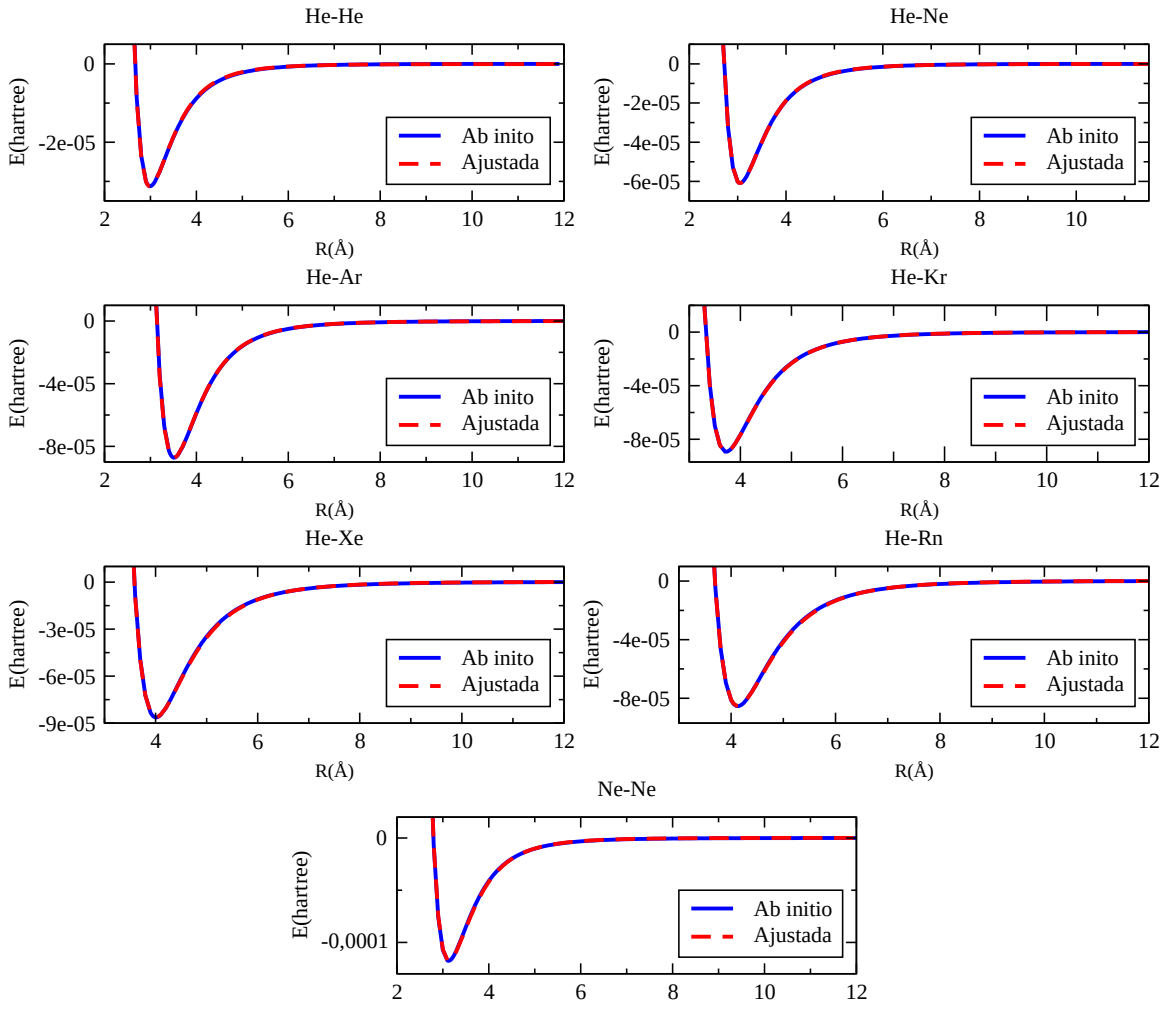

Figura 3.1: Curvas de energia potencial dos sistemas He-He, He-Ne, He-Ar, He-Kr, He-Xe, He-Rn e Ne-Ne ajustadas pela forma analítica ILJ.

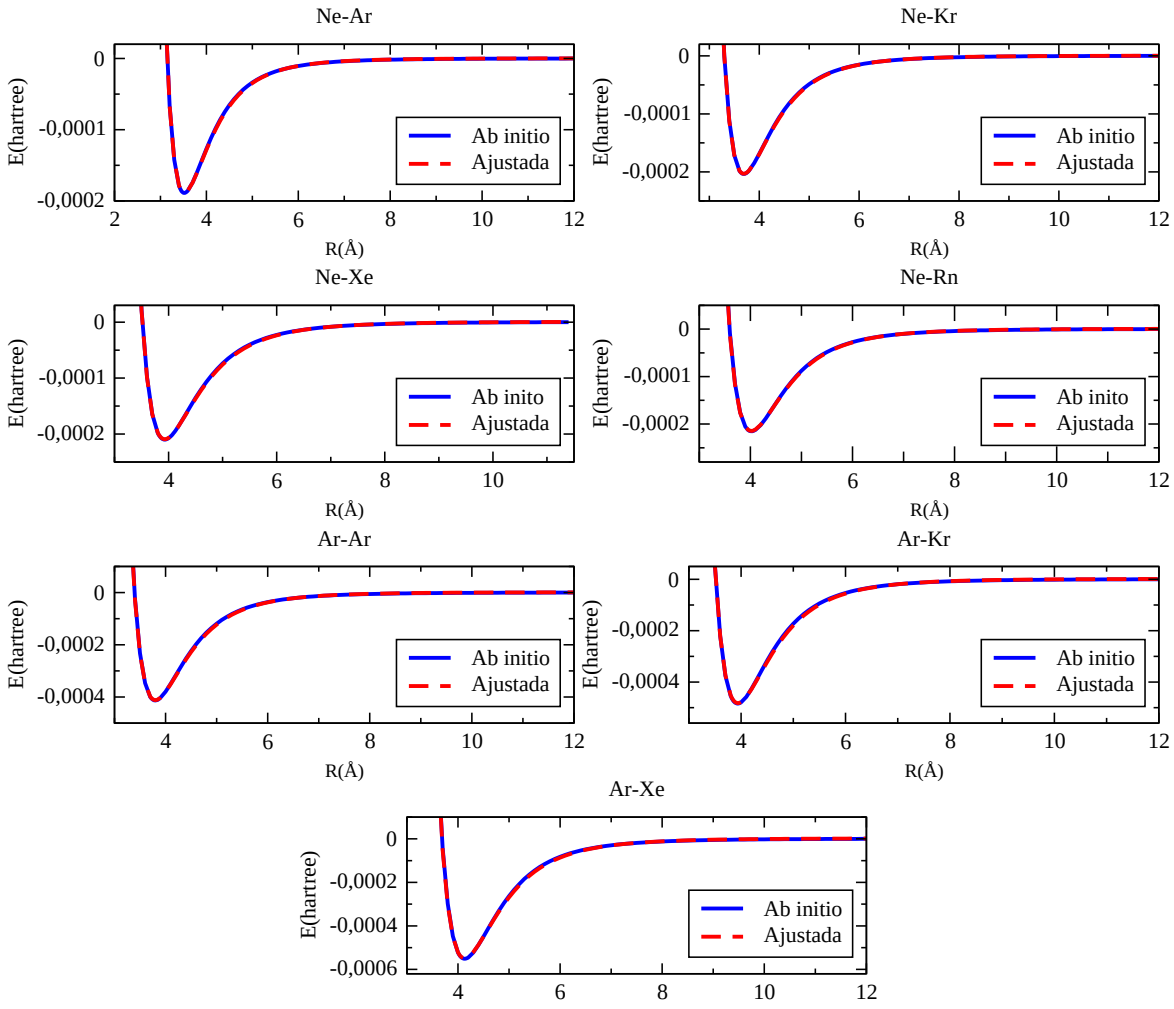

Figura 3.2: Curvas de energia potencial dos sistemas Ne-Ar, Ne-Kr, Ne-Xe, Ne-Rn, Ar-Ar, Ar-Kr e Ar-Xe ajustadas pela forma analítica ILJ.

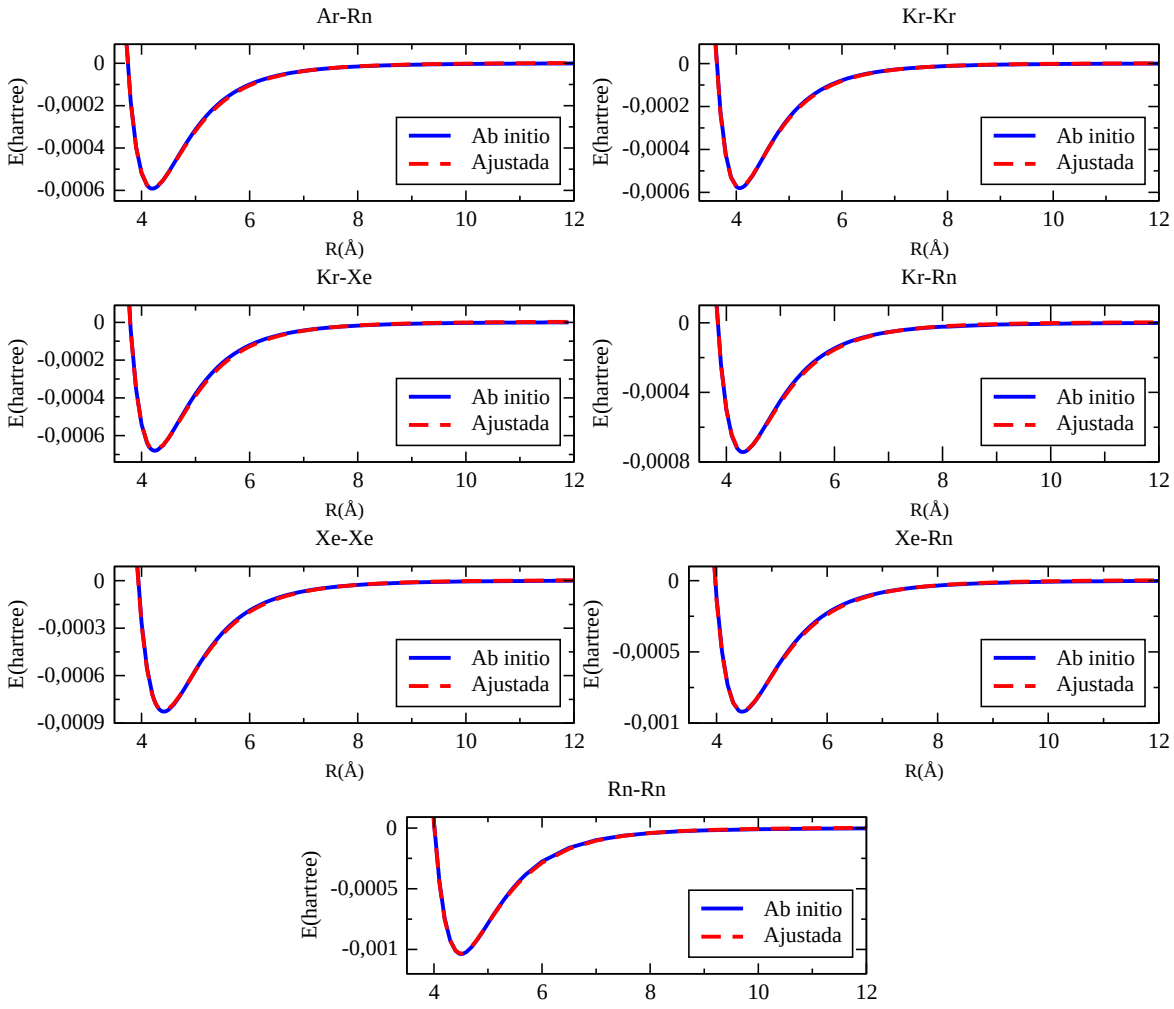

Figura 3.3: Curvas de energia potencial dos sistemas Ar-Rn, Kr-Kr, Kr-Xe, Kr-Rn, Xe-Xe, Xe-Rn e Rn-Rn ajustadas pela forma analítica ILJ.

A Tabela 3.4 mostra o parâmetro β ajustado para cada sistema molecular com os três conjuntos de funções de base. De modo geral, todos os β ficaram próximos de 9, que é aproximadamente o valor experimental. Em particular, observa-se que o conjunto de base *aug-cc-pV5Z*, gerou excelentes resultados, com todos os valores de β muito próximos de 9.

Tabela 3.4: Valores obtidos do parâmetro β para cada sistema diatômico.

Sistema	aug-cc-pvtz	aug-cc-pvqz	aug-cc-pv5z
He-He	8,87	8,67	8,74
He-Ne	9,19	9,15	8,87
He-Ar	9,46	9,15	9,31
He-Kr	9,05	9,26	9,32
He-Xe	10,41	9,58	9,40
He-Rn	9,02	9,60	9,28
Ne-Ne	9,51	9,70	9,18
Ne-Ar	9,58	9,40	9,34
Ne-Kr	9,80	9,63	9,49
Ne-Xe	9,75	9,78	9,46
Ne-Rn	9,46	9,49	9,31
Ar-Ar	9,57	9,15	9,02
Ar-Kr	9,30	9,37	9,00
Ar-Xe	9,49	9,35	9,06
Ar-Rn	9,44	9,12	8,83
Kr-Kr	9,36	9,22	9,20
Kr-Xe	9,38	9,40	8,80
Kr-Rn	9,06	8,89	8,68
Xe-Xe	7,98	9,24	9,03
Xe-Rn	9,22	9,17	8,75
Rn-Rn	9,01	8,71	8,68

3.2 Energias Rovibracionais

Com os parâmetros β ajustados, foi possível representar a curva de energia potencial ILJ para cada sistema estudado. Em seguida passou-se para o cálculo das energias rovibracionais utilizando o método DVR, usando as massas reduzidas descritas na tabela 3.5.

Tabela 3.5: Valores de massa reduzida experimental em u.a (unidades atômicas) de cada sistema molecular [67].

Sistema	Massa reduzida	Sistema	Massa reduzida
He-He	3648,1437531	Ar-Ar	36410,344938
He-Ne	6088,587421329	Ar-Kr	49312,90858526
He-Ar	6631,811472373	Ar-Xe	55823,465724
He-Kr	6963,676394771	Ar-Rn	61715,276132942
He-Xe	7080,28485261	Kr-Kr	76378,9653
He-Rn	7167,067221246	Kr-Xe	93217,86276614
Ne-Ne	18392,0183865	Kr-Rn	110896,862633094
Ne-Ar	24439,082296	Xe-Xe	119581,3872
Ne-Kr	29645,431111834	Xe-Rn	150323,14812231
Ne-Xe	31880,681102515	Rn-Rn	202340,457
Ne-Rn	33719,09275208	–	–

Em todos os sistemas foram usadas 500 quadraturas gaussianas para calcular as energias rovibracionais menores do que as energias de dissociação de cada sistema estudado. Além disso, para cada sistema foram calculadas as energias vibracionais considerando os números quânticos rotacionais J=0 e J=1. Essas escolhas rotacionais são suficientes para a determinação das constantes espectroscópicas rovibracionais via equação 2.91.

Analisando as energias vibracionais obtidas pelas formas analíticas ILJ e LJ usando o método DVR, nota-se que a energia do primeiro nível vibracional, tanto ILJ (8.48364891 cm^{-1}) como LJ (8.35558824 cm^{-1}) da complexo He-He é maior que a energia de dissociação, obtida via método *coupled cluster* (De = 6,854 cm^{-1}). Essas análises são extremamente importantes, pois nos revelam que o complexo He-He não permanece ligada em seu estado fundamental. Esse resultado corrobora os resultados e as conclusões obtidas por Ogilvie e Wang [16]. Nesse trabalho Ogilvie e Wang refutam o resultado de Aziz, Mccourt e Wong [69] que defende a existência do estado ligado do sistema diatômico He-He.

As energias rovibracionais, obtidas pela forma analítica ILJ, menores que a

energia de dissociação para cada um dos 20 sistemas moleculares restantes, são mostradas nas Tabelas 3.6, 3.7, 3.8, 3.9, 3.10, 3.11 e 3.12. Nessas tabelas, além dos níveis de energia encontrados com cada uma das bases ultilizadas, também são mostrados, quando disponíveis, os níveis de energias rovibracionais calculados via forma analítica ILJ com a distância internuclear de equilíbrio e a energia de dissociação experimentais (ver tabelas 3.2 e 3.1), além do valor 9 para o β (designados pela notação ILJ-Exp).

Pela Tabela 3.6, observa-se que todos os sistemas envolvendo o átomo de hélio são fracamente ligados, exceto para o sistema He-Rn, que possui 2 níveis de energia vibracional com o conjunto de base *aug-cc-pV5Z*. À medida que a base é melhorada, melhor é a concordância dos níveis de energias *ab initio* com os níveis de energias experimentais, sendo os níveis da base *aug-cc-pV5Z* os que estão em melhor concordância.

Para os sistemas envolvendo o radônio, não há como se fazer algum tipo de comparação, uma vez que não disponibilizamos de dados expereimentais para esses complexos.

Tabela 3.6: Níveis de energias rovibracionais em cm^{-1} para os sistemas He-Ne, He-Ar, He-Kr, He-Xe, He-Rn e Ne-Ne.

		He-Ne				He-Ar			
υ	J	3-zeta	4-zeta	5-zeta	ILJ-Exp.	3-zeta	4-zeta	5-zeta	ILJ-Exp.
0	0	9,2361	10,5896	11,2464	12,1630	11,1546	12,2118	12,9369	13,6719
0	1	9,8346	11,2422	11,9294	12,8753	13,0265	14,1911	14,9710	15,7771
		He-Kr				He-Xe			
υ	J	3-zeta	4-zeta	5-zeta	ILJ-Exp.	3-zeta	4-zeta	5-zeta	ILJ-Exp.
0	0	10,3313	11,7197	12,3803	13,0880	9,7333	10,8578	11,4179	12,1401
0	1	10,7933	12,2111	12,8842	13,6054	11,1461	12,3628	12,9628	13,7253
		He-Rn				Ne-Ne			
υ	J	3-zeta	4-zeta	5-zeta	ILJ-Exp.	3-zeta	4-zeta	5-zeta	ILJ-Exp.
0	0	9,2168	10,9187	11,5724	-	9,0419	10,7895	11,3635	12,3345

1		-	-	18,8303	-	17,3325	21,6648	23,5495	26,2731
0	1	9,5814	11,3049	11,9673	-	10,0185	11,8304	12,4285	13,4347
1		-	-	-	-	17,8776	22,2868	24,2174	26,9976

Tabela 3.7: Níveis de energias rovibracionais em cm^{-1} para os sistemas Ne-Ar, Ne-Kr, Ne-Xe e Ne-Rn.

		Ne-Ar				Ne-Kr			
υ	J	3-zeta	4-zeta	5-zeta	ILJ-Exp.	3-zeta	4-zeta	5-zeta	ILJ-Exp.
0		9,8020	11,1755	11,8589	12,4600	8,8159	10,2900	10,8828	11,4233
1	0	23,0171	26,9410	28,8965	30,8823	21,5431	25,7692	27,5184	29,2783
2		28,9695	34,9687	37,9926	41,4056	28,4843	35,0790	37,8856	40,9193
3		30,8272	-	41,2404	45,6653	31,2531	39,3876	43,0144	47,1541
0		10,4292	11,8334	12,5306	13,1352	9,2896	10,7909	11,3935	11,9444
1	1	23,5065	27,4719	29,4455	31,4444	21,9331	26,1932	27,9550	29,7292
2		29,2767	35,3345	38,3843	41,8246	28,7684	35,4082	38,2318	41,2853
3		-	-	-	45,9138	-	39,6048	43,2506	47,4160
		Ne-Xe				Ne-Rn			
υ	J	3-zeta	4-zeta	5-zeta	ILJ-Exp.	3-zeta	4-zeta	5-zeta	ILJ-Exp.
0		8,0352	9,5739	10,0818	10,6157	7,5851	9,1524	9,7428	-
1		20,1005	24,4552	26,0298	27,7115	19,2447	23,6940	25,4345	-
2	0	27,3379	34,1129	36,7494	39,6034	26,5999	33,5558	36,3674	-
3		30,8430	39,3324	42,8907	46,8063	30,3209	39,2858	43,0116	-
4		-	-	45,9606	50,4218	31,5553	41,8162	46,2123	-
0		8,1442	9,5739	10,1999	10,7370	7,6832	9,2571	9,8498	-
1		20,1927	24,4552	26,1331	27,8185	19,3288	23,7856	25,5288	-
2	1	27,4096	34,1129	36,8352	39,6937	26,6671	33,6321	36,4469	-
3		30,8952	39,3324	42,9554	46,8765	30,3674	39,3438	43,0737	-
4		-	-	46,0111	50,4738	31,5804	41,8525	46,2538	-

Tabela 3.8: Níveis de energias rovibracionais em cm^{-1} para os sistemas Ar-Ar e Ar-Kr.

		Ar-Ar				Ar-Kr			
υ	J	3-zeta	4-zeta	5-zeta	ILJ-Exp.	3-zeta	4-zeta	5-zeta	ILJ-Exp.
0		12,0939	13,1073	13,7624	14,6055	10,6922	12,0433	12,4656	13,1205
1		32,4391	35,5104	37,4622	39,9147	29,5114	33,4249	34,7628	36,6858
2		47,9211	53,0407	56,2543	60,2084	45,0315	51,3219	53,6491	56,7828
3		58,8857	65,9671	70,3798	75,7145	57,3866	65,8640	69,2284	73,5113
4	0	65,8555	74,7011	80,2060	86,7746	66,7626	77,2250	81,6410	87,0045
5		69,6955	79,8755	86,2931	93,9037	73,4222	85,6436	91,0822	97,4452
6		-	82,9059	89,6991	97,9290	77,7982	91,4473	97,8242	105,0854
7		-	-	-	-	81,2575	95,2956	102,3057	110,2819
8		-	-	-	-	-	-	105,8919	113,9767
,									
0		12,2009	13,2181	13,8751	14,7208	10,7658	12,1205	12,5437	13,1999
1		32,5365	35,6120	37,5659	40,0212	29,5801	33,4973	34,8363	36,7607
2		48,0074	53,1319	56,3480	60,3051	45,0948	51,3891	53,7176	56,8528
3		58,9594	66,0465	70,4622	75,8003	57,4439	65,9254	69,2914	73,5760
4	1	65,9147	74,7670	80,2755	86,8478	66,8133	77,2801	81,6980	87,0634
5		69,7409	79,9264	86,3479	93,9628	73,4655	85,6917	91,1326	97,4977
6		-	82,9493	89,7429	97,9746	77,8342	91,4877	97,8673	105,1309
7		-	-	-	-	81,2922	95,3304	102,3417	110,3199
8		-	-	-	-	-	-	105,9267	114,0112

Tabela 3.9: Níveis de energias rovibracionais em cm^{-1} para os sistemas Ar-Xe e Ar-Rn

		Ar-Xe				Ar-Rn			
υ	J	3-zeta	4-zeta	5-zeta	ILJ-Exp.	3-zeta	4-zeta	5-zeta	ILJ-Exp.
0		10,2945	11,5444	12,0196	12,5249	9,9349	11,1181	11,5819	-
1		28,7803	32,4660	33,9230	35,4205	27,9700	31,5000	32,9199	-

2		44,5522	50,5816	53,0512	55,5134	43,6303	49,4703	51,8762	-
3		57,7001	65,9702	69,4702	72,8660	56,9824	65,0823	68,4947	-
4		68,3395	78,7313	83,2636	87,5569	68,1101	78,4022	82,8302	-
5		76,6226	88,9942	94,5402	99,6875	77,1203	89,5138	94,9523	-
6	0	82,7506	96,9282	103,4436	109,3912	84,1518	98,5253	104,9511	-
7		86,9940	102,7518	110,1625	116,8431	89,3821	105,5766	112,9445	-
8		90,0325	106,7654	114,9415	122,2683	93,0311	110,8450	119,0848	-
9		-	109,8075	118,2729	126,0127	95,3559	114,5473	123,5632	-
10		-	-	-	129,1373	96,6417	116,9339	126,6075	-
11		-	-	-	-	97,2894	118,2805	128,4749	-
12		-	-	-	-	-	118,9624	129,4539	-
									-
0		10,3538	11,6065	12,0826	12,5890	9,9870	11,1726	11,6372	-
1		28,8363	32,5249	33,9830	35,4815	28,0195	31,5520	32,9728	-
2		44,6047	50,6371	53,1079	55,5712	43,6770	49,5196	51,9265	-
3		57,7487	66,0220	69,5234	72,9203	57,0261	65,1288	68,5424	-
4		68,3839	78,7791	83,3130	87,6075	68,1505	78,4457	82,8750	-
5		76,6624	89,0377	94,5854	99,7340	77,1572	89,5540	94,9939	-
6		82,7852	96,9670	103,4843	109,4334	84,1849	98,5620	104,9893	-
7		87,0232	102,7855	110,1983	116,8805	89,4110	105,6095	112,9791	-
8		90,0589	106,7938	114,9720	122,3006	93,0554	110,8738	119,1155	-
9		-	109,8341	118,2996	126,0403	95,3754	114,5716	123,5897	-
10		-	-	-	129,1642	96,6559	116,9534	126,6295	-
11		-	-	-	-	97,3006	118,2949	128,4920	-
12		-	-	-	-	-	118,9736	129,4662	-

Tabela 3.10: Níveis de energias rovibracionais em cm^{-1} para os sistemas Kr-Kr e Kr-Xe

		Kr-Kr				Kr-Xe			
υ	J	3-zeta	4-zeta	5-zeta	ILJ-Exp.	3-zeta	4-zeta	5-zeta	ILJ-Exp.
0		9,1293	10,3538	10,8267	11,4018	8,5823	9,8290	10,0363	10,6299

1		25,8231	29,4409	30,8383	32,5565	24,5683	28,2434	28,9294	30,6559
2		40,4868	46,4196	48,7125	51,5597	39,0192	45,0362	46,2775	49,0675
3		53,1707	61,3339	64,4918	68,4490	51,9632	60,2344	62,0998	65,8857
4		63,9363	74,2373	78,2271	83,2694	63,4332	73,8689	76,4183	81,1348
5	0	72,8616	85,1955	89,9813	96,0762	73,4684	85,9758	89,2589	94,8430
6		80,0459	94,2918	99,8327	106,9386	82,1159	96,5978	100,6527	107,0435
7		85,6159	101,6312	107,8800	115,9435	89,4332	105,7860	110,6375	117,7763
8		89,7298	107,3453	114,2466	123,2007	95,4901	113,6015	119,2593	127,0892
9		92,5824	111,5953	119,0834	128,8463	100,3710	120,1174	126,5745	135,0401
10		94,5828	114,5736	122,5696	133,0444	104,1759	125,4200	132,6519	141,6986
11		-	116,6521	124,9546	135,9892	107,0197	129,6098	137,5741	147,1474
12		-	-	126,9459	138,0743	109,0497	132,8003	141,4380	151,4826
13		-	-	-	-	110,6795	135,1205	144,3541	154,8133
14		-	-	-	-	-	136,8434	146,4630	157,2621
15		-	-	-	-	-	-	148,1640	159,0621
0		9,1741	10,4009	10,8746	11,4509	8,7029	9,9561	10,1646	10,7614
1		25,8658	29,4860	30,8842	32,6036	24,6845	28,3662	29,0536	30,7833
2		40,5274	46,4626	48,7564	51,6048	39,1307	45,1545	46,3975	49,1906
3		53,2088	61,3747	64,5334	68,4919	52,0699	60,3480	62,2153	66,0043
4		63,9719	74,2756	78,2664	83,3101	63,5347	73,9776	76,5291	81,2487
5		72,8945	85,2313	90,0181	96,1145	73,5644	86,0793	89,3648	94,9520
6		80,0758	94,3248	99,8668	106,9742	82,2061	96,6958	100,7534	107,1473
7	1	85,6426	101,6612	107,9113	115,9763	89,5171	105,8782	110,7327	117,8746
8		89,7530	107,3722	114,2747	123,2305	95,5674	113,6876	119,3487	127,1818
9		92,6020	111,6187	119,1082	128,8729	100,4413	120,1969	126,6578	135,1266
10		94,6002	114,5934	122,5909	133,0676	104,2387	125,4926	132,7286	141,7787
11		-	116,6696	124,9726	136,0089	107,0746	129,6751	137,6439	147,2206
12		-	-	126,9635	138,0918	109,0969	132,8579	141,5005	151,5486
13		-	-	-	-	110,7246	135,1701	144,4089	154,8717
14		-	-	-	-	-	136,8884	146,5104	157,3127
15		-	-	-	-	-	-	148,2092	159,1073

Tabela 3.11: Níveis de energias rovibracionais em cm^{-1} para os sistemas Kr-Rn e Xe-Xe.

		Kr-Rn				Xe-Xe			
v	J	3-zeta	4-zeta	5-zeta	ILJ-Exp.	3-zeta	4-zeta	5-zeta	ILJ-Exp.
0		7,9732	9,1053	9,4631	-	7,5319	9,9688	9,5404	10,0226
1		22,9899	26,3552	27,4367	-	21,8785	28,8653	27,7447	29,1695
2		36,7905	42,3462	44,1600	-	35,2796	46,4001	44,7998	47,1385
3		49,3915	57,0921	59,6450	-	47,7411	62,5901	60,7169	63,9406
4		60,8115	70,6090	73,9055	-	59,2697	77,4541	75,5086	79,5882
5		71,0722	82,9150	86,9570	-	69,8734	91,0138	89,1891	94,0950
6		80,1994	94,0314	98,8179	-	79,5617	103,2936	101,7742	107,4767
7		88,2236	103,9831	109,5096	-	88,3461	114,3221	113,2820	119,7507
8		95,1817	112,7997	119,0575	-	96,2407	124,1323	123,7333	130,9372
9		101,1178	120,5166	127,4922	-	103,2632	132,7630	133,1521	141,0594
10	0	106,0851	127,1760	134,8501	-	109,4353	140,2596	141,5660	150,1440
11		110,1463	132,8280	141,1751	-	114,7843	146,6748	149,0073	158,2220
12		113,3743	137,5316	146,5189	-	119,3439	152,0699	155,5132	165,3292
13		115,8515	141,3549	150,9424	-	123,1549	156,5144	161,1265	171,5066
14		117,6681	144,3746	154,5151	-	126,2665	160,0860	165,8962	176,8014
15		118,9207	146,6755	157,3151	-	128,7362	162,8697	169,8769	181,2663
16		119,7103	148,3481	159,4274	-	130,6651	164,9573	173,1292	184,9600
17		120,1433	149,4879	160,9427	-	132,4093	166,4926	175,7190	187,9465
18		-	150,1942	161,9560	-	-	167,9029	177,7368	190,2960
19		-	150,5741	162,5658	-	-	-	179,4808	192,1440
20		-	-	162,8882	-	-	-	181,4365	193,9125
0		8,0008	9,1343	9,4925	-	7,5558	9,9991	9,5665	10,0494
1		23,0166	26,3834	27,4653	-	21,9018	28,8948	27,7702	29,1958
2		36,8163	42,3735	44,1878	-	35,3023	46,4287	44,8246	47,1640
3		49,4164	57,1186	59,6719	-	47,7631	62,6178	60,7410	63,9654
4		60,8354	70,6345	73,9315	-	59,2910	77,4809	75,5320	79,6123

5		71,0951	82,9396	86,9821	-	69,8940	91,0396	89,2118	94,1184
6		80,2212	94,0549	98,8420	-	79,5815	103,3183	101,7962	107,4993
7		88,2443	104,0055	109,5327	-	88,3650	114,3457	113,3032	119,7725
8		95,2011	112,8211	119,0795	-	96,2588	124,1548	123,7537	130,9582
9		101,1359	120,5368	127,5131	-	103,2804	132,7844	133,1715	141,0796
10	1	106,1018	127,1950	134,8698	-	109,4516	140,2797	141,5845	150,1633
11		110,1616	132,8457	141,1935	-	114,7996	146,6937	149,0249	158,2404
12		113,3881	137,5479	146,5360	-	119,3581	152,0874	155,5298	165,3466
13		115,8637	141,3697	150,9581	-	123,1681	156,5304	161,1421	171,5230
14		117,6787	144,3879	154,5294	-	126,2784	160,1005	165,9107	176,8167
15		118,9295	146,6872	157,3279	-	128,7470	162,8827	169,8903	181,2805
16		119,7172	148,3581	159,4386	-	130,6749	164,9685	173,1415	184,9731
17		120,1483	149,4962	160,9522	-	132,4189	166,5026	175,7300	187,9583
18		-	150,2007	161,9637	-	-	167,9129	177,7467	190,3066
19		-	150,5789	162,5717	-	-	-	179,4904	192,1536
20		-	-	162,8927	-	-	-	181,4466	193,9223

Tabela 3.12: Níveis de energias rovibracionais em cm^{-1} para os sistemas Xe-Rn e Rn-Rn.

		Xe-Rn				Rn-Rn			
v	J	3-zeta	4-zeta	5-zeta	ILJ-Exp.	3-zeta	4-zeta	5-zeta	ILJ-Exp.
0		7,3969	8,5520	8,7993	-	6,6189	7,6320	7,9807	-
1		21,5395	24,9728	25,7357	-	19,3930	22,4229	23,4621	-
2		34,8289	40,4974	41,8015	-	31,5581	36,5910	38,3115	-
3		47,2735	55,1337	57,0027	-	43,1185	50,1399	52,5322	-
4		58,8828	68,8903	71,3460	-	54,0788	63,0732	66,1279	-
5		69,6671	81,7765	84,8387	-	64,4442	75,3949	79,1022	-
6		79,6381	93,8027	97,4889	-	74,2201	87,1091	91,4594	-
7		88,8087	104,9804	109,3054	-	83,4126	98,2207	103,2038	-
8		97,1938	115,3223	120,2983	-	92,0284	108,7345	114,3404	-
9		104,8100	124,8429	130,4791	-	100,0748	118,6563	124,8743	-

10		111,6765	133,5584	139,8604	-	107,5600	127,9922	134,8116	-
11		117,8153	141,4871	148,4570	-	114,4931	136,7489	144,1587	-
12		123,2511	148,6496	156,2856	-	120,8844	144,9341	152,9226	-
13		128,0126	155,0695	163,3651	-	126,7453	152,5562	161,1114	-
14		132,1318	160,7730	169,7174	-	132,0886	159,6245	168,7338	-
15		135,6447	165,7900	175,3673	-	136,9287	166,1497	175,7998	-
16		138,5911	170,1533	180,3427	-	141,2816	172,1434	182,3203	-
17	0	141,0141	173,8993	184,6751	-	145,1652	177,6189	188,3076	-
18		142,9598	177,0677	188,3992	-	148,5991	182,5907	193,7754	-
19		144,4769	179,7008	191,5531	-	151,6049	187,0750	198,7387	-
20		145,6161	181,8436	194,1780	-	154,2060	191,0898	203,2144	-
21		146,4294	183,5433	196,3176	-	156,4276	194,6545	207,2206	-
22		146,9704	184,8485	198,0178	-	158,2961	197,7905	210,7774	-
23		147,2976	185,8094	199,3263	-	159,8396	200,5206	213,9063	-
24		-	186,4774	200,2924	-	161,0870	202,8690	216,6305	-
25		-	186,9052	200,9665	-	162,0682	204,8615	218,9743	-
26		-	187,1683	201,4008	-	162,8141	206,5247	220,9635	-
27		-	-	201,6688	-	163,3559	207,8866	222,6249	-
28		-	-	-	-	163,7259	208,9755	223,9860	-
29		-	-	-	-	163,9658	209,8209	225,0753	-
30		-	-	-	-	-	210,9015	226,5558	-
32		-	-	-	-	-	211,1998	227,0070	-
33		-	-	-	-	-	211,4158	227,3079	-
34		-	-	-	-	-	-	227,5256	-
0		7,4159	8,5721	8,8196	-	6,6327	7,6466	7,9955	-
1		21,5581	24,9924	25,7557	-	19,4066	22,4372	23,4767	-
2		34,8470	40,5166	41,8210	-	31,5715	36,6052	38,3259	-
3		47,2912	55,1525	57,0218	-	43,1316	50,1538	52,5464	-
4		58,8999	68,9086	71,3647	-	54,0916	63,0869	66,1418	-
5		69,6838	81,7943	84,8569	-	64,4567	75,4082	79,1158	-
6		79,6542	93,8200	97,5066	-	74,2323	87,1222	91,4727	-

7		88,8243	104,9972	109,3226	-	83,4245	98,2335	103,2169	-
8		97,2088	115,3386	120,3151	-	92,0400	108,7471	114,3532	-
9		104,8245	124,8587	130,4953	-	100,0861	118,6686	124,8869	-
10		111,6904	133,5736	139,8761	-	107,5709	128,0041	134,8239	-
11		117,8285	141,5017	148,4721	-	114,5037	136,7605	144,1706	-
12		123,2637	148,6636	156,3001	-	120,8947	144,9454	152,9342	-
13		128,0244	155,0828	163,3790	-	126,7552	152,5671	161,1226	-
14		132,1429	160,7857	169,7307	-	132,0981	159,6351	168,7447	-
15		135,6551	165,8020	175,3799	-	136,9378	166,1600	175,8104	-
16		138,6007	170,1646	180,3547	-	141,2903	172,1533	182,3306	-
17	1	141,0229	173,9099	184,6863	-	145,1735	177,6284	188,3175	-
18		142,9678	177,0775	188,4097	-	148,6070	182,5998	193,7849	-
19		144,4840	179,7098	191,5629	-	151,6123	187,0838	198,7479	-
20		145,6222	181,8519	194,1870	-	154,2130	191,0981	203,2231	-
21		146,4346	183,5507	196,3258	-	156,4341	194,6625	207,2289	-
22		146,9747	184,8550	198,0251	-	158,3021	197,7980	210,7853	-
23		147,3009	185,8151	199,3328	-	159,8451	200,5276	213,9138	-
24		-	186,4821	200,2979	-	161,0919	202,8756	216,6375	-
25		-	186,9089	200,9712	-	162,0727	204,8676	218,9809	-
26		-	187,1713	201,4045	-	162,8180	206,5304	220,9696	-
27		-	-	201,6719	-	163,3593	207,8917	222,6305	-
28		-	-	-	-	163,7286	208,9801	223,9911	-
29		-	-	-	-	163,9681	209,8250	225,0799	-
30		-	-	-	-	-	210,4563	225,9261	-
31		-	-	-	-	-	210,9045	226,5594	-
32		-	-	-	-	-	211,2022	227,0100	-
33		-	-	-	-	-	211,4180	227,3103	-
34		-	-	-	-	-	-	227,5278	-

3.3 Constantes Espectroscópicas Rovibracionais

Para o cálculo das constantes espectroscópicas rovibracionais via equação 2.91, como já mencionado antes, utilizaram-se as massas reduzidas dadas na Tabela 3.5. Em todos os sistemas foram usadas 500 quadraturas gaussianas e calculadas todas as energias vibracionais menores do que as energias de dissociação de cada sistema estudado. Além disto, para cada sistema foram calculadas as energias vibracionais considerando os números quânticos rotacionais J=0 e J=1. Essas escolhas rotacionais são suficientes para a determinação das constantes espectroscópicas rovibracionais via equação 2.91. As constantes espectroscópicas determinadas usando a equação 2.91 e o método Dunham para as sistemas diatômicos homonucleares estão apresentadas na Tabela 3.13, para os sistemas diatômicos heteronucleares são mostrados na Tabela 3.14 e para os sistemas envolvendo o radônio estão disponíveis na Tabela 3.15.

Para facilitar a comparação dos valores apresentados nestas tabelas utilizamos a seguinte notação:

1. ILJ-Exp - Cálculo das constantes espectroscópicas rovibracionais (via método de Dunham) usando a forma analítica ILJ e os parâmetros R_e, D_e e β experimental igual a 9.

2. ILJ-DVR- Cálculo das constantes espectroscópicas rovibracionais (via equação 2.91) usando a forma analítica ILJ e os parâmetros R_e e D_e *ab initio* (com o nível de cálculo CCSD(T)/$aug-cc-pV5Z$) e o parâmetro β ajustado.

3. ILJ-DVR ($\beta = 9$) - Cálculo das constantes espectroscópicas rovibracionais (via equação 2.91) usando a forma analítica ILJ e os parâmetros R_e, D_e *ab initio* (com nível de cálculo CCSD(T)/$aug-cc-pV5Z$) e o parâmetro β experimental igual a 9.

4. ILJ-Dunham - Cálculo das constantes espectroscópicas rovibracionais (via método de Dunham) usando a forma analítica ILJ e os parâmetros Re e De *ab initio* (com o nível de cálculo CCSD(T)/$aug-cc-pV5Z$) e o parâmetro β ajustado.

5. ILJ-Dunham ($\beta = 9$) - Cálculo das constantes espectroscópicas rovibracionais (via método de Dunham) usando a forma analítica ILJ e os parâmetros R_e D_e *ab initio*

(com nível de cálculo CCSD(T)/$aug-cc-pV5Z$) e o parâmetro β experimental igual a 9.

6. LJ-Dunham - Cálculo das constantes espectroscópicas rovibracionais (via método de Dunham) usando a forma analítica LJ e os parâmetros R_e e D_e *ab initio* (com o nível de cálculo CCSD(T)/$aug-cc-pV5Z$).

7. LJ-DVR - Cálculo das constantes espectroscópicas rovibracionais (via equação 2.91) usando a forma analítica LJ e os parâmetros R_e e D_e *ab initio* (com o nível de cálculo CCSD(T)/$aug-cc-pV5Z$).

Tabela 3.13: Constantes espectroscópicas rovibracionais cm^{-1} obtidas para os sistemas homonucleares.

Sistema	Método	ω_e	$\omega_e x_e$	$\omega_e y_e$	α_e	γ_e
	Exp. [16]	28,5	–	–	–	–
	ILJ-Exp.	28,350	7,748	0,185	3,6x10^{-2}	4,0x10^{-3}
	Teo. [68]	25,8	–	–	–	–
Ne-Ne	Dunham-ILJ	26,381	7,727	2,1x10^{-1}	3,8x10^{-2}	5,0x10^{-3}
	Dunham-ILJ($\beta=9$)	26,200	7,581	0,191	3,8x10^{-2}	5,0x10^{-3}
	Dunham- LJ	25,172	7,847	6,22x10^{-1}	4,17x10^{-2}	4,03 x10^{-3}
	Exp. [16]	30,9	–	–	–	–
	ILJ-Exp.	30,543	2,678	3,8x10^{-2}	3,0x10^{-3}	2,0x10^{-4}
	Teo. [68]	27,9	–	–	–	–
	DVR- ILJ	28,83	2,634	4,0x10^{-2}	3,9x10^{-3}	2,59x10^{-4}
	DVR- ILJ($\beta=9$)	28,816	2,628	3,98 x10^{-2}	3,97 x10^{-3}	2,59 x10^{-4}
Ar-Ar	Dunham-ILJ	28,771	2,575	2,0x10^{-2}	4,0x10^{-3}	1,8x10^{-4}
	Dunham-ILJ($\beta=9$)	28,749	2,570	2,0x10^{-2}	4,0x10^{-3}	1,0x10^{-4}
	DVR- LJ	27,645	2,687	7,66 x10^{-2}	4,42x10^{-3}	1,60x10^{-4}
	Dunham- LJ	27,621	2,662	6,65x10^{-2}	4,45x10^{-3}	1,35 x10^{-4}
	Exp. [16]	23,6	–	–	–	–
	ILJ-Exp.	23,337	1,099	4,0x10^{-3}	9,0x10^{-4}	2,15x10^{-5}
	Teo. [68]	21,8	–	–	–	–
	DVR- ILJ	22.189	1,100	7,06x10^{-3}	9,27x10^{-4}	2,76 x10^{-5}

	DVR- ILJ($\beta = 9$)	22,020	1,077	6,38 x10^{-3}	9,21 x10^{-4}	2,72 x10^{-5}
Kr-Kr	Dunham-ILJ	22,184	1,095	5,2x10^{-4}	9,3x10^{-4}	2,2x10^{-5}
	Dunham-ILJ($\beta = 9$)	22,015	1,072	4,0x10^{-3}	9,0x10^{-4}	2.24x10^{-5}
	DVR- LJ	21,153	1,113	1,63x10^{-2}	1,01x10^{-3}	1,84x10^{-5}
	Dunham- LJ	21,151	1,110	1,51x10^{-2}	1,01 x10^{-3}	1,67x10^{-5}
	Exp. [16]	20,9	–	–	–	–
	ILJ-Exp.	20,335	0,596	0,001	0,0003	4.52x10^{-6}
	Teo. [68]	18,5	–	–	–	–
	DVR- ILJ	19.364	0,583	1,89x10^{-3}	3,09x10^{-4}	5,20x10^{-6}
	DVR- ILJ($\beta = 9$)	19,342	0,581	1,86 x10^{-3}	3,08 x10^{-4}	5,18 x10^{-6}
Xe-Xe	Dunham-ILJ	19,363	0,582	1,5x10^{-3}	3,0x10^{-4}	4,6x10^{-6}
	Dunham-ILJ($\beta = 9$)	19,341	0,580	0,001	0,0003	4,61 x10^{-5}
	DVR- LJ	18,582	0,601	5,29x10^{-3}	3,37x10^{-4}	3,64x10^{-6}
	Dunham- LJ	18,582	0,601	5,05x10^{-3}	3,38x10^{-4}	3,44x10^{-6}

As constantes espectroscópicas rovibracionais do sistema Ne-Ne (Tabela 3.13) foram obtidas somente com o método de Dunham. Isso se deve ao fato de a curva de energia potencial deste sistema não comportar o mínimo de quatro níveis de energias vibracionais (ν=0, 1, 2, e 3) necessários para se usar as equações 2.91. A mesma justificativa é dada para justificar os cálculos somente com o método de Dunham das constantes espectroscópicas rovibracionais dos sistemas He-Ne, He-Ar, He-Kr, He-Xe e He-Rn.

Na Tabela 3.13, é apresentada a frequência vibracional ω_e dos sistemas homonucleares. Como referência, optou-se por utilizar as constantes espectroscópicas experimentais relatadas por Ogilvie e Wang [16] com base em um reexame de dados espectroscópicos disponíveis, como também são apresentados os resultados obtidos por Goll, Werner e Stoll [68]. Esses autores realizaram cálculos CCSD(T) com os conjuntos de funções de base $aug-cc-pVTZ$, $aug-cc-pVQZ$ para todos os complexos formados pelos átomos de He, Ne, Ar, Kr e Xe.

Pela Tabela 3.13, pode-se observar que a frequência vibracional ω_e de cada sistema, obtida via potencial ILJ (com os parâmetros D_e, R_e e β experimentais) concorda muito bem com as medidas diretas experimentais disponíveis na literatura. Este fato reforça a confiabilidade da forma analítica ILJ.

Pode-se observar pela Tabela 3.13 que os resultados de ω_e para o sistema Xe-Xe encontrados utilizando as formas analítica ILJ e LJ concordam mais com os dados experimentais do que os relatados por Goll, Werner e Stoll [68]. No entanto, para os demais sistemas homonucleares os resultados de Goll, Werner e Stoll são mais próximos dos experimentais do que os resultados encontrados via LJ. Porém os resultados da forma analítica ILJ são melhores do que ambos. Este fato reforça a confiabilidade desta forma analítica, uma vez que geralmente ela consegue se aproximar cerca de $1cm^{-1}$ a mais dos valores experimentais em comparação com o potencial LJ.

A Tabela 3.14 mostra todas as constantes espectroscópicas obtidas via métodos de Dunham e equação 2.91 para as duas formas analíticas, ILJ e LJ. Pode-se verificar o mesmo padrão que foi observado com os sistemas homonucleares, ou seja, os resultados de ω_e do ILJ concordam mais com os dados experimentais do que os dados téoricos relatados na literatura, e que os resultados do LJ. Esse fato pode ser entendido através das curvas de energia potencial mostradas nas Figuras 3.3, 3.3 e 3.3. Através destas figuras é possível notar que as CEP IJ são mais anarmônicas que as CEP ILJ. Essa característica faz com que os níveis de energias vibracionais da CEP ILJ sejam mais próximos um do outro do que os da CEP LJ. Essa diferença faz com que as constantes espectroscópicas ILJ sejam um pouco maiores que as LJ.

Tabela 3.14: Constantes espectroscópicas rovibracionais cm^{-1} obtidas para os sistemas heteronucleares.

Sistema	Método	ω_e	$\omega_e x_e$	$\omega_e y_e$	α_e	γ_e
	Exp. [17]	35,0	–	–	–	–
	ILJ-Exp.	35,578	25,793	1,466	2,91x10^{-1}	9,80x10^{-2}
	Teo. [68]	32,2	–	–	–	–
He-Ne	**Dunham-ILJ**	33,443	25,238	1,404	3,05x10^{-1}	1,04x10^{-1}
	Dunham-ILJ($\beta = 9$)	33,612	25,606	1,512	3,07x10^{-1}	1,05x10^{-1}
	Dunham- LJ	32,293	26,427	4,907	3,34x10^{-1}	7,90x10^{-2}
	Exp. [17]	34,8	–	–	–	–
	ILJ-Exp.	35,311	17,367	0,715	1,42x10^{-1}	3,30x10^{-2}
	Teo. [68]	32,4	–	–	–	–
He-Ar	Dunham-ILJ	33,908	17,691	0,858	1,47x10^{-1}	3,62x10^{-2}

	Dunham-ILJ($\beta = 9$)	33,510	17,112	0,728	1,46x10^{-1}	3,54x10^{-2}
	Dunham- LJ	32,196	17,693	2,365	1,59x10^{-1}	2,64x10^{-2}
	Exp. [17]	32,0	–	–	–	–
	ILJ-Exp.	32,907	14,544	0,545	1,08x10^{-1}	2,30x10^{-2}
	Teo. [68]	30,4	–	–	–	–
He-Kr	Dunham-ILJ	31,600	14,924	0,665	1,13x10^{-1}	2,54x10^{-2}
	Dunham-ILJ($\beta = 9$)	31,218	14,422	0,562	1,12x10^{-1}	2,48x10^{-2}
	Dunham- LJ	29,993	14,916	1,825	1,22x10^{-1}	1,85x10^{-2}
	Exp. [17]	29,1	–	–	–	–
	ILJ-Exp.	29,971	12,230	0,426	8,40x10^{-2}	1,60x10^{-2}
	Teo. [68]	27,2	–	–	–	–
He-Xe	Dunham-ILJ	28,675	12,691	0,548	9,00x10^{-2}	1,90x10^{-2}
	Dunham-ILJ($\beta = 9$)	28,244	12,163	0,445	8,90x10^{-2}	1,80x10^{-2}
	Dunham- LJ	27,136	12,582	1,445	9,37x10^{-2}	1,37x10^{-2}
	Exp. [17]	28,2	–	–	–	–
	ILJ-Exp.	27,072	4,475	0,065	1,30x10^{-2}	1,00x10^{-3}
	Teo. [68]	25,1	–	–	–	–
	DVR- ILJ	26,98	5,540	0,348	4,40x10^{-2}	8,66x10^{-3}
	DVR- ILJ($\beta = 9$)	26,626	5,350	0,322	4,33 x10^{-2}	8,64 x10^{-3}
Ne-Ar	Dunham-ILJ	25,938	4,640	0,830	1,39x10^{-2}	1,22x10^{-3}
	Dunham-ILJ($\beta = 9$)	25,606	4,477	0,069	1,30x10^{-2}	1,19x10^{-3}
	DVR- LJ	24,837	4,853	0,304	5,21x10 $^{-2}$	4,57x10 $^{-2}$
	Dunham- LJ	24,601	4,636	0,225	1,50x10^{-2}	8,90x10^{-4}
	Exp. [17]	26,2	–	–	–	–
	ILJ-Exp.	24,490	3,408	0,042	8,00x10^{-3}	5,00x10^{-3}
	Teo. [68]	22,6	–	–	–	–
	DVR- ILJ	23,891	3,906	0,171	2,89x10^{-2}	4,07x10^{-3}
	DVR- ILJ($\beta = 9$)	23,432	3,702	0,148	2,84 x10^{-2}	4,02 x10^{-3}
Ne-Kr	Dunham-ILJ	23,457	3,530	0,055	8,75x10^{-3}	6,45x10^{-4}
	Dunham-ILJ($\beta = 9$)	23,027	3,354	0,043	8,64x10^{-3}	6,22x10^{-4}
	DVR- LJ	22,226	3,571	0,178	3,30 x10^{-2}	2,23 x10^{-3}
	Dunham- LJ	22,124	3,473	0,141	9,43x10^{-3}	4,65 x10^{-4}

	Exp. [17]	24,3	–	–	–	–
	ILJ-Exp.	22,588	2,811	0,031	$6{,}00\text{x}10^{-3}$	$3{,}00\text{x}10^{-4}$
	Teo. [68]	20,4	–	–	–	–
	DVR- ILJ	21,799	3,101	0,108	$6{,}02\text{x}10^{-3}$	$6{,}94\ \text{x}10^{-4}$
	DVR- ILJ($\beta = 9$)	21,407	2,946	0,092	$5{,}93\ \text{x}10^{-3}$	$6{,}84\ \text{x}10^{-4}$
Ne-Xe	Dunham-ILJ	21,451	2,847	0,037	$6{,}37\text{x}10^{-3}$	$4{,}15\text{x}10^{-4}$
	Dunham-ILJ($\beta = 9$)	21,176	2,748	0,031	$6{,}31\ \text{x}10^{-3}$	$4{,}05\ \text{x}10^{-4}$
	DVR- LJ	20,410	2,908	0,127	$6{,}78\text{x}10^{-3}$	$3{,}90\text{x}10^{-4}$
	Dunham- LJ	20,345	2,846	0,103	$6{,}89\text{x}10^{-3}$	$3{,}02\text{x}10^{-4}$
	Exp. [17]	27,9	–	–	–	–
	ILJ-Exp.	27,109	1,791	0,010	$2{,}00\text{x}10^{-3}$	$6{,}89\text{x}10^{-5}$
	Teo. [68]	25,2	–	–	–	–
	DVR- ILJ	25,807	1,783	0,017	$2{,}11\text{x}10^{-3}$	$9{,}57\text{x}10^{-5}$
	DVR- ILJ($\beta = 9$)	25,807	1,783	0,017	$2{,}11\ \text{x}10^{-3}$	$9{,}57\ \text{x}10^{-5}$
Ar-Kr	Dunham-ILJ	25,786	1,764	0,010	$2{,}14\text{x}10^{-3}$	$7{,}27\text{x}10^{-5}$
	Dunham-ILJ($\beta = 9$)	25,786	1,764	0,010	$2{,}14\text{x}10^{-3}$	$7{,}27\text{x}10^{-5}$
	DVR- LJ	24,783	1,837	0,038	$2{,}33\text{x}10^{-3}$	$6{,}20\text{x}10^{-5}$
	Dunham- LJ	24,774	1,827	0,035	$2{,}34\text{x}10^{-3}$	$5{,}43\ \text{x}10^{-5}$
	Exp. [17]	27,1	–	–	–	–
	ILJ-Exp.	25,716	1,439	0,007	$1{,}00\text{x}10^{-3}$	$3{,}97\text{x}10^{-5}$
	Teo. [68]	23,7	–	–	–	–
	DVR- ILJ	24,741	1,437	0,011	$1{,}43\text{x}10^{-3}$	$5{,}21\text{x}10^{-5}$
	DVR- ILJ($\beta = 9$)	24,684	1,427	0,010	$1{,}43\ \text{x}10^{-3}$	$5{,}19\ \text{x}10^{-5}$
Ar-Xe	Dunham-ILJ	24,731	1,427	0,007	$1{,}45\text{x}10^{-3}$	$4{,}14\text{x}10^{-5}$
	Dunham-ILJ($\beta = 9$)	24,674	1,418	0,007	$1{,}44\text{x}10^{-3}$	$4{,}12\ \text{x}10^{-5}$
	DVR- LJ	23,710	1,474	0,025	$1{,}57\text{x}10^{-3}$	$3{,}44\text{x}10^{-5}$
	Dunham- LJ	23,706	1,469	0,023	$1{,}58\text{x}10^{-3}$	$3{,}08\ \text{x}10^{-5}$
	Exp. [17]	22,7	–	–	–	–
	ILJ-Exp.	21,658	0,821	$2{,}00\text{x}10^{-3}$	$5{,}00\text{x}10^{-4}$	$1{,}04\text{x}10^{-5}$
	Teo. [68]	20,1	–	–	–	–
	DVR- ILJ	20,456	0,786	$3{,}17\text{x}10^{-3}$	$1{,}96\text{x}10^{-3}$	$4{,}39\ \text{x}10^{-5}$
	DVR- ILJ($\beta = 9$)	20,615	0,803	$3{,}00\text{x}10^{-3}$	$1{,}97\ \text{x}10^{-3}$	$4{,}45\ \text{x}10^{-5}$

Kr-Xe	**Dunham-ILJ**	20,454	0,784	2,48x10^{-3}	5,51x10^{-4}	1,05x10^{-5}
	Dunham-ILJ($\beta = 9$)	20,613	0,801	2,79x10^{-3}	5,55x10^{-4}	1,06x10^{-5}
	DVR- LJ	19,805	0,831	9,60x10^{-3}	7,38x10^{-4}	1,05x10^{-5}
	Dunham- LJ	19,804	0,830	9,05x10^{-3}	6,05 x10^{-4}	7,99x10^{-6}

Tabela 3.15: Constantes espectroscópicas rovibracionais cm^{-1} obtidas para os sistemas envolvendo o radônio.

Sistema	Método	ω_e	$\omega_e x_e$	$\omega_e y_e$	α_e	γ_e
He-Rn	Dunham-ILJ	27,396	11,654	0,467	0,081	0,016
	Dunham-ILJ($\beta = 9$)	27,105	11,311	0,402	0,080	0,016
	Dunham- LJ	26,042	11,701	1,306	0,087	0,012
	DVR- ILJ	20,900	2,731	0,078	0,005	0,0005
	DVR- ILJ ($\beta = 9$)	20,656	2,638	0,069	0,005	0,0005
Ne-Rn	Dunham-ILJ	20,622	2,564	0,031	0,005	0,0003
	Dunham-ILJ($\beta = 9$)	20,380	2,482	0,026	0,005	0,0003
	DVR- LJ	19,728	2,631	0,104	0,005	0,0002
	Dunham- LJ	19,581	2,571	0,087	0,005	0,0002
	DVR- ILJ	23,762	1,223	0,007	0,001	3,57x10^{-5}
	DVR- ILJ ($\beta = 9$)	23,919	1,246	0,008	0,001	3,61 x10^{-5}
Ar-Rn	Dunham-ILJ	23,755	1,218	0,005	0,001	2,90x10^{-5}
	Dunham-ILJ($\beta = 9$)	23,912	1,240	0,005	0,001	2,94x10^{-5}
	DVR- LJ	22,977	1,288	0,020	0,001	2,43x10^{-5}
	Dunham- LJ	22,974	1,284	0,018	0,001	2.19x10^{-5}
	DVR- ILJ	19,235	0,634	0,002	0,0003	7,29x10^{-6}
	DVR- ILJ ($\beta = 9$)	19,476	0,656	0,002	0,0003	7,45 x10^{-6}
Kr-Rn	Dunham-ILJ	19,234	0,633	0,001	0,0003	6,38x10^{-6}
	Dunham-ILJ($\beta = 9$)	19,475	0,655	0,001	0,0003	6,54x10^{-6}
	DVR- LJ	18,712	0,679	0,006	0,0004	5,21x10^{-6}
	Dunham- LJ	18,711	0,678	0,006	0,0004	4,89x10^{-6}
	DVR- ILJ	17,812	0,439	0,001	0,0001	2,72x10^{-6}
	DVR- ILJ ($\beta = 9$)	17,986	0,451	0,001	0,0002	2,76 x10^{-6}

Xe-Rn	Dunham-ILJ	17,812	0,439	0,0008	0,0001	2,46x10^{-6}
	Dunham-ILJ($\beta = 9$)	17,986	0,451	0,0002	0,0002	2,50x10^{-6}
	DVR- LJ	17,280	0,467	0,003	0.0002	1,96x10^{-6}
	Dunham- LJ	17,280	0,467	0,003	0,0002	1.87x10^{-6}
	DVR- ILJ	16,116	0,318	0,0005	0,0001	1.25x10^{-6}
	DVR- ILJ ($\beta = 9$)	16.318	0,329	0,0006	0,0001	1,28 x10^{-6}
Rn-Rn	Dunham-ILJ	16,116	0,318	0,0004	0,0001	1,15x10^{-6}
	Dunham-ILJ($\beta = 9$)	16,318	0,329	0,0005	0,0001	1,18x10^{-6}
	DVR- LJ	15,678	0,341	0,001	0,0001	9,166x10^{-7}
	Dunham- LJ	15,678	0,341	0,001	0,0001	8.85x10^{-7}

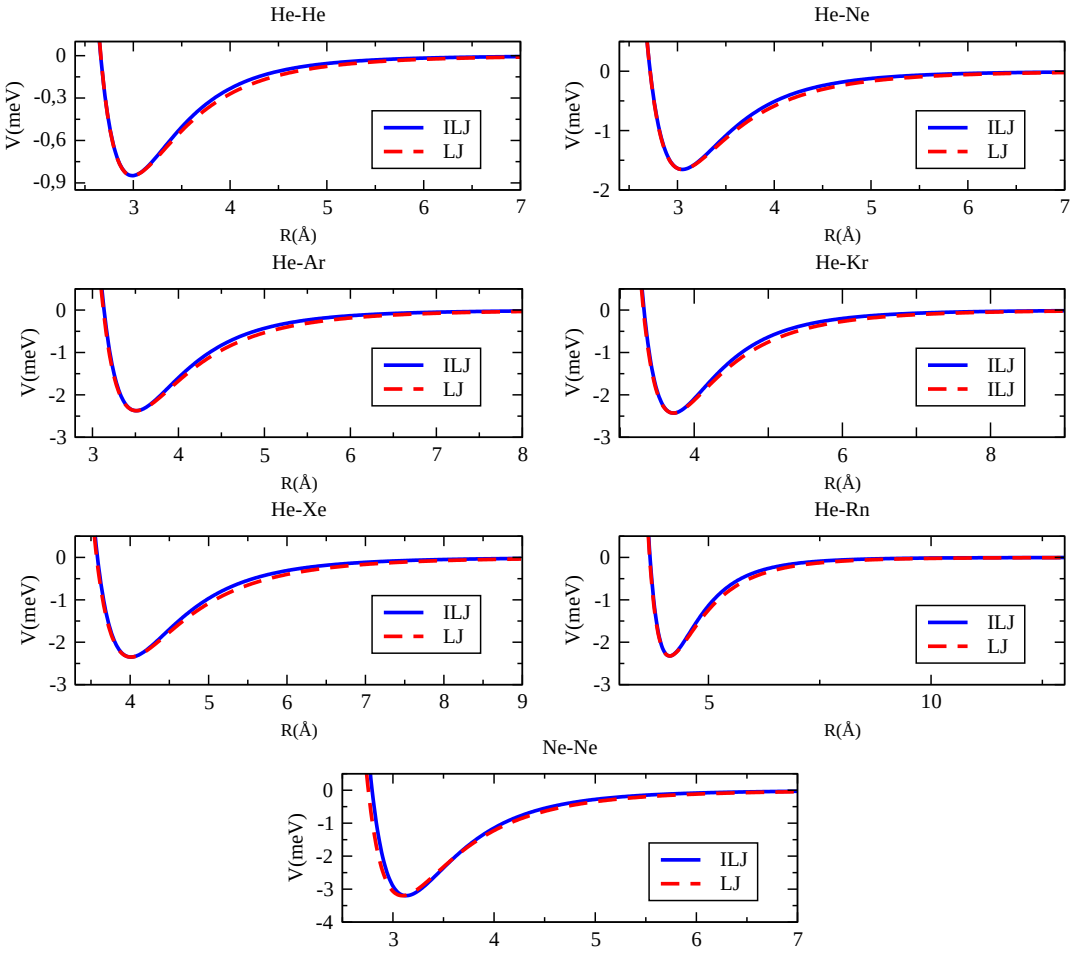

Figura 3.4: Curvas de energia potencial obtidas para os sistemas diatômicos He-He, He-Ne, He-Ar, He-Kr, He-Xe, He-Rn e Ne-Ne usando as formas analíticas LJ (R_e e D_e *ab initio*) e ILJ (R_e e D_e *ab initio* com beta ajustado).

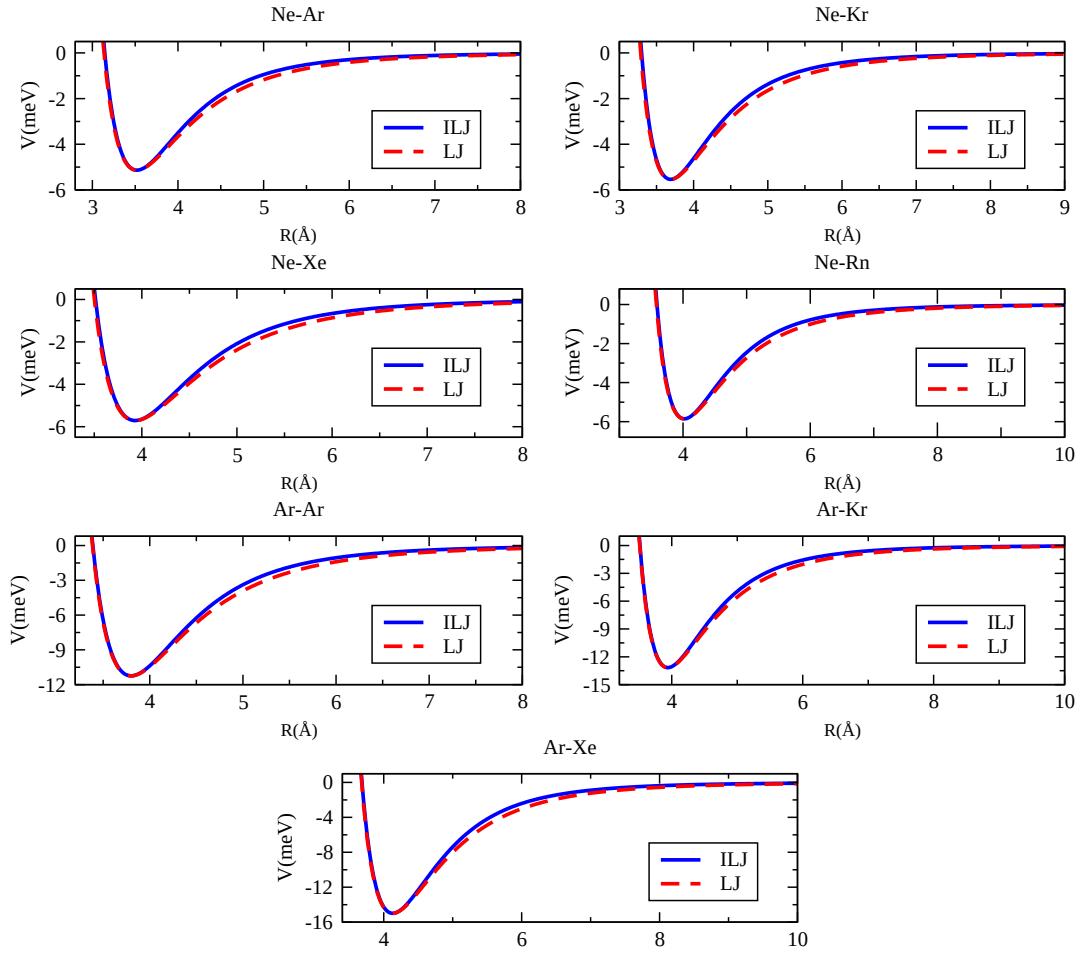

Figura 3.5: Curvas de energia potencial obtidas para os sistemas diatômicos Ne-Ar, Ne-Kr, Ne-Xe, Ne-Rn, Ar-Ar, Ar-Kr e Ar-Xe usando as formas analíticas LJ (R_e e D_e *ab initio*) e ILJ (R_e e D_e *ab initio* com beta ajustado).

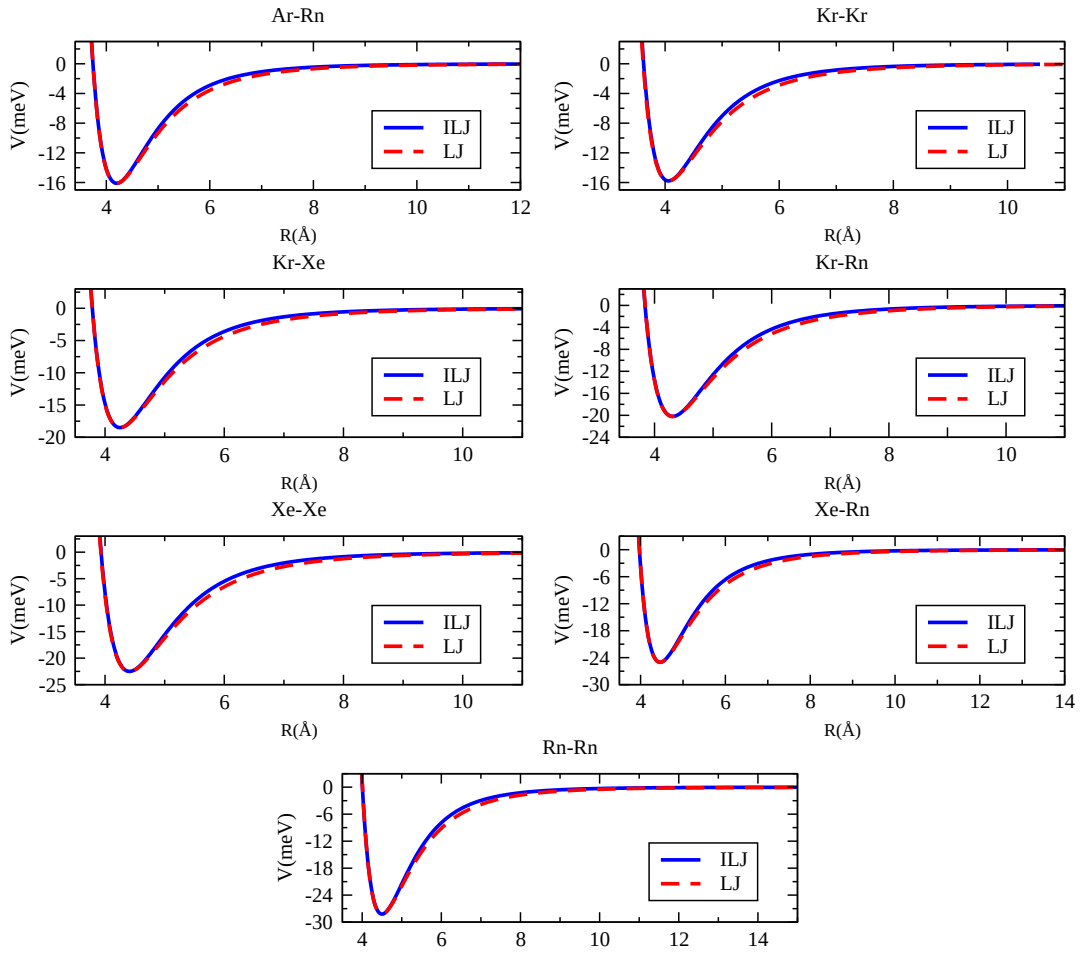

Figura 3.6: Curvas de energia potencial obtidas para os sistemas diatômicos Ar-Rn, Kr-Kr, Kr-Xe, Kr-Rn, Xe-Xe, Xe-Rn e Rn-Rn usando as formas analíticas LJ (R_e e D_e *ab initio*) e ILJ (R_e e D_e *ab initio* com beta ajustado).

3.4 Tempo de Vida

O tempo de vida para a decomposição dos complexos aqui estudados foi calculado utilizando a teoria de Slater [70, 71], que consiste em uma formulação puramente dinâmica, com uma análise vibracional completa dos complexos. A decomposição unimolecular (ou primeira ordem) do complexo deve ocorrer quando a interação da coordenada atinge a energia de dissociação. Se um complexo adquire o limiar de energia, a frequência de uma decomposição é simplesmente a frequência da própria vibração e a constante de taxa para este processo é dada por:

$$k(T) = \omega_e e^{-\frac{D_e - E_{0,0}}{RT}}, \tag{3.2}$$

sendo ω_e a freqüência de vibração de cada complexo obtida pela equação 2.91, R é a constante universal dos gases ideais e T é a temperatura absoluta. Desta forma, o tempo de vida para a decomposição é o recíproco da equação 3.2, dado por:

$$\tau(T) = \frac{1}{k(T)} = \frac{1}{\omega_e} e^{\frac{D_e - E_{0,0}}{RT}}. \tag{3.3}$$

O comportamento cinético da teoria de Slater é aplicável em regiões de pressão baixa e intermediária e, na região de pressão alta, as taxas calculadas são muito menores que os valores experimentais.

Em geral, um sistema é considerado estável, para tempos de vida maiores que 1 pico segundo (ps) [72]. De posse da energia de dissociação (D_e), da freqüência de vibração (ω_e) e do primeiro nível de energia vibracional ($E_{0,0}$), todos obtidos com o nível de cálculo CCSD(T) e o conjunto de base *aug-cc-pV5Z*, calculou-se o tempo de vida para os 21 complexos estudados (conforme Figuras 3.7, 3.8 e 3.9), exceto para o sistema He-He, para a faixa de temperatura considerada entre 200 e 500 K.

Como mencionado antes, o primeiro nível vibracional, tanto obtido usando o ILJ (8.48364891 cm^{-1}) como o LJ (8.35558824 cm^{-1}) do complexo He-He é maior que a energia de dissociação, obtida via nível de cálculo CCSD(T)/$aug-cc-pV5Z$ (De = 6,854 cm^{-1}). Desta forma, não se pode calcular o tempo de vida desse sistema.

É possível notar a partir das Figuras 3.7, 3.8 e 3.9 que o tempo de vida encontrados com a forma analítica ILJ (com R_e e D_e *ab initio*, com o β ajustado) ficaram mais próximos dos resultados ILJ-Exp (com R_e, D_e e β experimentais) do que os resultados usando a forma anlítica LJ (com R_e e D_e *ab initio*). Na Figura 3.7, observa-se que os sistemas He-Ne e He-Ar são estáveis de pelas formas analítica ILJ e LJ, no entanto, os resultados da ILJ experimental garantem que esses sistemas são instáveis. Os demais sistemas da Figura 3.7 demonstram ser todos estáveis.

Todos os sistemas mostrados nas figuras 3.8 e 3.9 são estáveis. De acordo com a equação 3.3, o tempo de vida é inversamente proporcional à frequência de vibração (ω_e). Pelas Tabelas 3.13 e 3.14, é possível notar que à medida que os sistemas ficam mais pesados menor é a ω_e. Por outro lado, o primeiro nível de energia vibracional ($E_{0,0}$) tende a diminuir para sistemas mais pesados, enquanto que a energia de dissociação (D_e)

sempre aumenta. Desta forma, percebe-se um aumento no tempo de vida desses sistemas, à medida que vão sendo formados os complexos mais pesados. Assim, como já era de se esperar, o sistema com maior tempo de vida é o Rn-Rn.

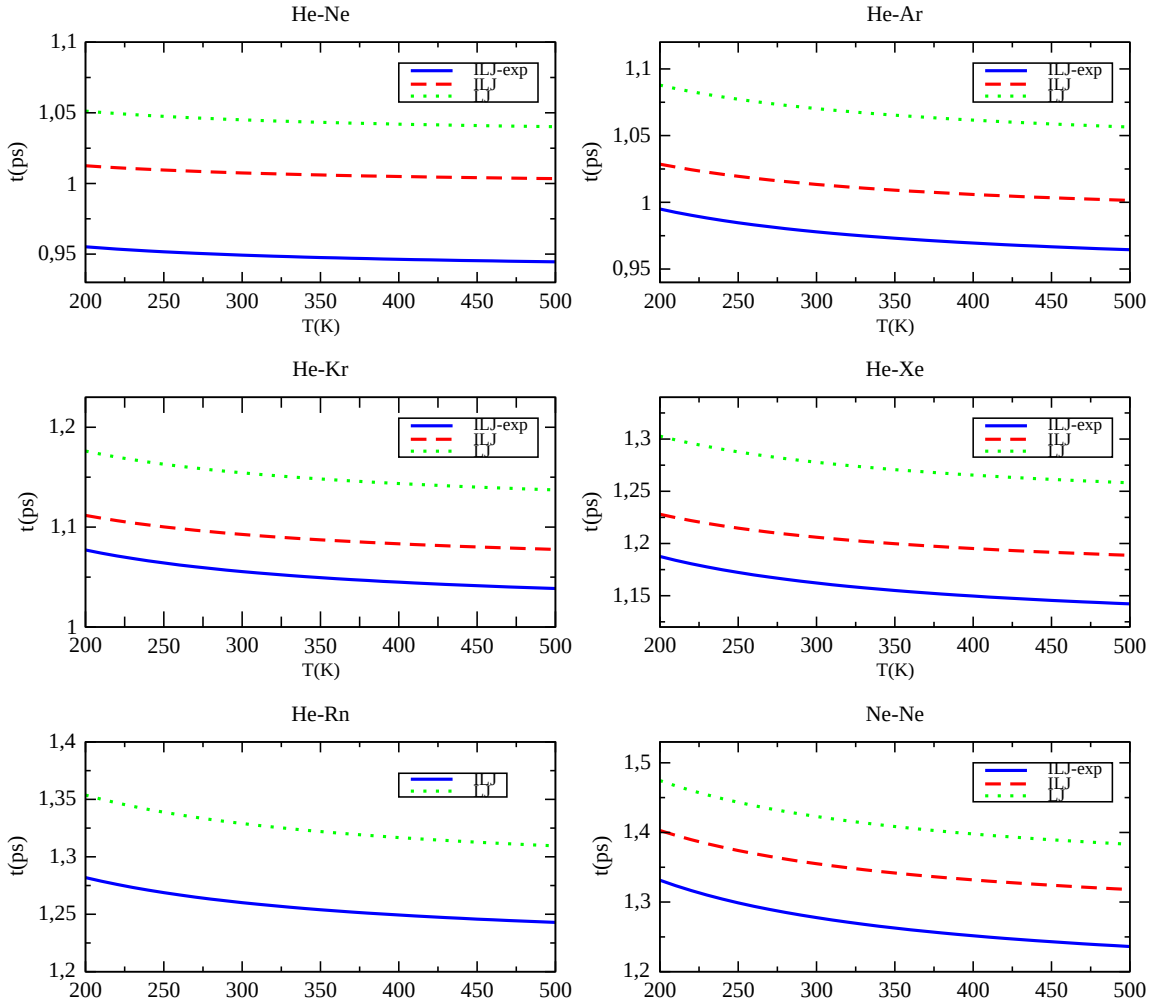

Figura 3.7: Tempo de vida dos sistemas diatômicos He-Ne, He-Ar, He-Kr, He-Xe, He-Rn e Ne-Ne usando as formas analíticas ILJ-Exp (com R_e, D_e e β experimentais), ILJ (R_e e D_e *ab initio* com beta ajustado) e LJ (R_e e D_e *ab initio*).

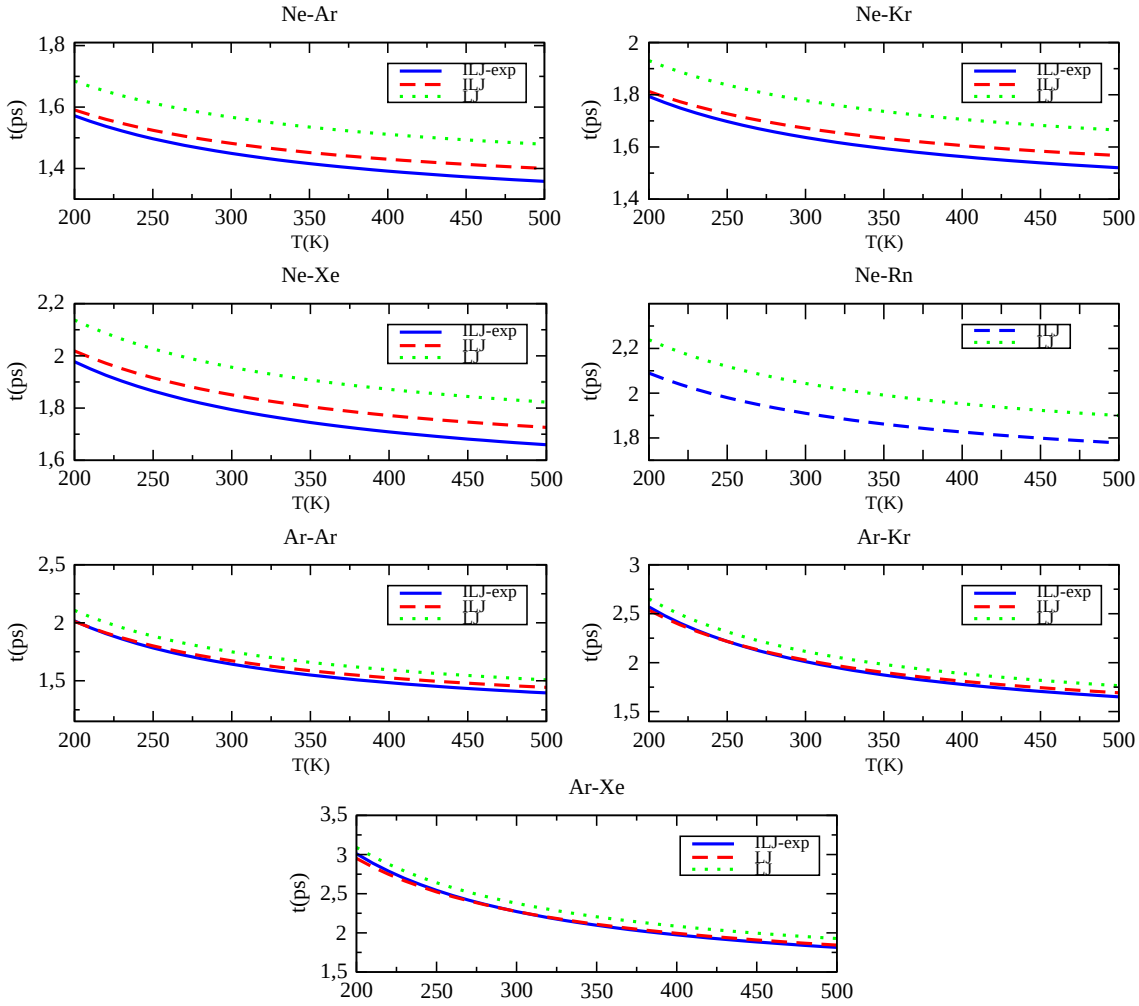

Figura 3.8: Tempo de vida dos sistemas diatômicos Ne-Ar, Ne-Kr, Ne-Xe, Ne-Rn, Ar-Ar, Ar-Kr e Ar-Xe usando as formas analíticas ILJ-Exp (com R_e, D_e e β experimentais), ILJ (R_e e D_e *ab initio* com beta ajustado) e LJ (R_e e D_e *ab initio*).

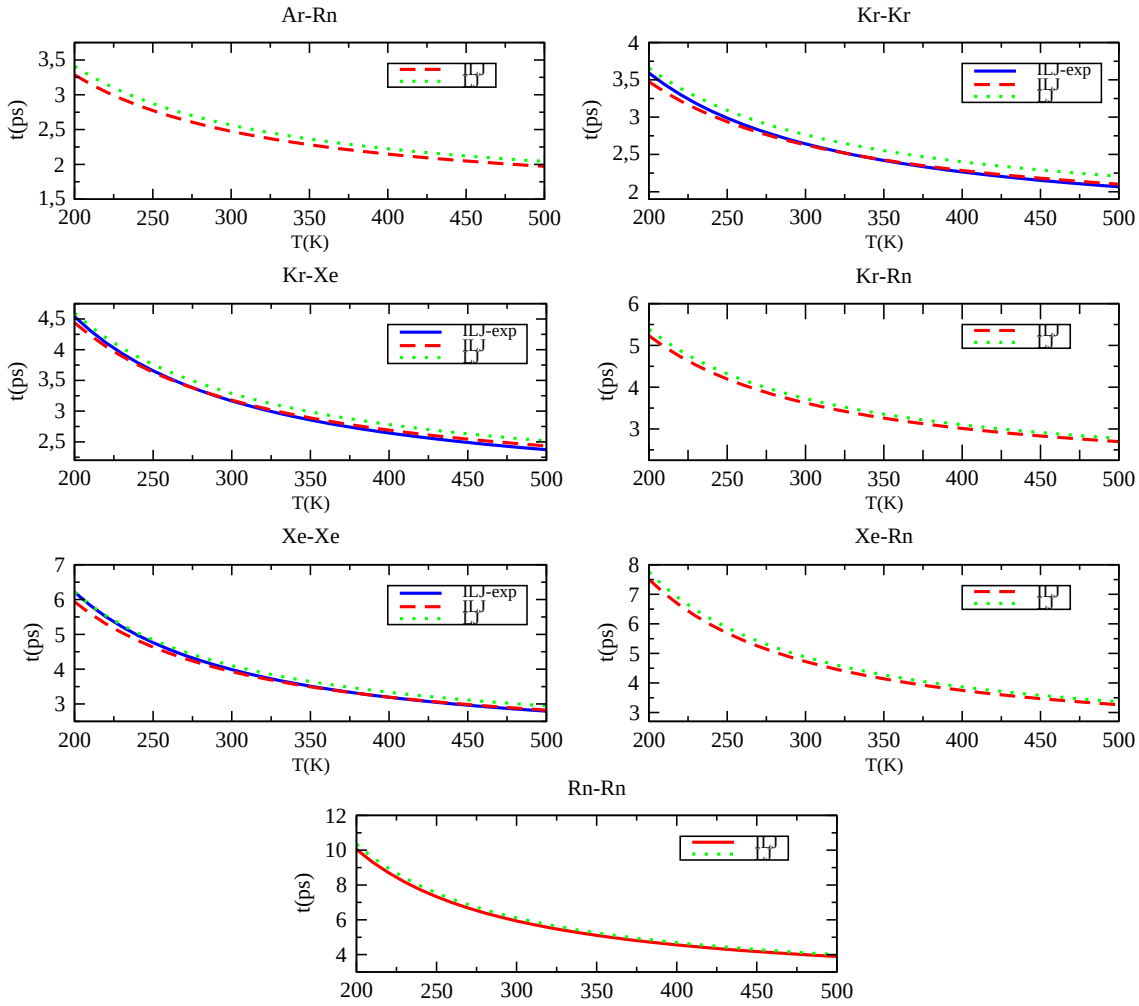

Figura 3.9: Tempo de vida dos sistemas diatômicos Ar-Rn, Kr-Kr, Kr-Xe, Kr-Rn, Xe-Xe, Xe-Rn e Rn-Rn usando as formas analíticas ILJ-Exp (com R_e, D_e e β experimentais), ILJ (R_e e D_e *ab initio* com beta ajustado) e LJ (R_e e D_e *ab initio*).

4 Conclusões e Perspectivas

Nesse trabalho foram calculadas as energias eletrônicas do estado fundamental dos sistemas He-He, He-Ne, He-Ar, He-Kr, He-Xe,He-Rn, Ne-Ne, Ne-Ar, Ne-Kr, Ne-Xe, Ne-Rn, Ar-Ar, Ar-Kr, Ar-Xe, Ar-Rn, Kr-Kr, Kr-Xe, Kr-Rn, Xe-Xe, Xe-Rn e Rn-Rn, para várias configurações internucleares que vão desde a região de forte interação até a região assintótica. Esses cálculos foram realizados via método CCSD(T) com três conjuntos de funcões de base; *aug-cc-pVTZ*, *aug-cc-pVQZ* e *aug-cc-pV5Z*. Para todos os sistemas moleculares estudados, os resultados obtidos para as energias de dissociação e distâncias de equilíbrio que mais se aproximaram dos dados experimentais foram alcançados usando a base mais extensa $aug-cc-pV5Z$ com a correção de BSSE.

De posse dessas energias eletrônicas, da distância internuclear de equilibrio e da energia de dissociação, ajustou-se cuidadosamente esses dados via método de Powell para a forma analítica ILJ a fim de obtermos o parâmetro β caracteríStco de cada sistema molecular. Foram ajustados os dados para os três conjuntos de funções de bases, e os melhores resultados foram obtidos pelo conjunto de base *aug-cc-pV5Z* com a correção BSSE, resultando em valores de β muito próximo do valor experimental que é 9.

Para determinar as constantes espectroscópicas rovibracionais utilizaram-se dois métodos diferentes: equação 2.91 e Dunham. Em particular, obtiveram-se excelentes resultados para a constante ω_e do sistema Xe-Xe, tanto com a forma analítica ILJ como a LJ. É conveniente ressaltar que estes resultados concordam melhor com os dados experimentais que os relatados por Goll, Werner e Stoll.

Para os demais sistemas homonucleares Ne-Ne, Ar-Ar e Kr-Kr, os resultados obtidos por Goll, Werner e Stoll para a constante espectroscópica w_e ficaram mais próximos dos dados experimentais do que os resultados encontrados via LJ. Porém os resultados da forma analítica ILJ (considerando tanto R_e, D_e e beta experimentais como R_e e D_e *ab initio* com β ajustado ou fixo igual a 9) são melhores do que ambos. Este fato reforça a confiabilidade desta forma analítica.

Nesse trabalho, concluiu-se também que as formas analíticas ILJ e LJ possuem comportamento muito semelhante na região harmônica da curva de energia potencial. Porém, à medida que a distância internuclear entre os átomos aumenta, essas formas analíticas descrevem os sistemas moleculares de maneira cada vez mais distinta. Dessa forma, as constantes espectroscópicas que dependem da parte anarmônica da curva tendem a divergir.

Através do cálculo do tempo de vida de cada complexo, com uma função da temperatura, foi possível observar quais os sistemas moleculares mais estáveis. Como era esperado, um aumento maior no tempo de vida desse estado aconteceu para as moléculas compostas pelos átomos de gases nobres mais pesados (sistemas mais fortemente ligados), com o diátomo Rn-Rn tendo o maior tempo de vida.

Como perspectivas futuras, pretende-se investigar as curvas de energia potential (PEC) de dímeros heteronucleares de gases nobres com o oganésio (Z=118), o último gás nobre descoberto e no qual espera-se que os fortes efeitos da relatividade sejam importantes. Para tanto, aplicar-se-á uma combinação da teoria de longo alcance de Moller-Plesset de segunda ordem com a teoria de curto alcance DFT (MP2-srDFT) dentro da etrutura do método relativístico de 4 componentes para gerar as PECs. Os espectros rovibracionais serão investigados através dos métodos de Dunham e DVR em conjunto com o potencial "Improved Lennard-Jones" (IJL), e a importância das interações de Gaunt (Breit) também serão investigadas.

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5 Apêndices

5.1 Apêndices A: Fatores de Conversão

Massa

Unidade	u.a	u.m.a	Kg
u.a	1	5,485804 x 10^{-4}	9,109397 x 10^{-31}
u.m.a	1822,887	1	1.6605402 x 10^{-27}
Kg	1,09776746 x 10^{30}	6,0221367 x 10^{26}	1

u.a = unidade atômica

u.m.a = unidade de massa atômica

Kg = quilograma

Comprimento

Unidade	a_0	Å	M
a_0	1	0,529172249	5,2917097 x 10^{-11}
Å	1,88974384	1	10^{-10}
M	1,88974384 x 10^{10}	10^{10}	1

a_0 = raio de Bohr

Å= angstron

M = metro

Energia

Unidade	eV	J	cm^{-1}	E_h	Kcal/mol
eV	1	1,6022 x 10^{-19}	8065,48	3,6749 x 10^{-2}	23,045
J	6,2415 x 10^{18}	1	5,0340 x 10^{22}	2,2937 x 10^{17}	1,4384 x 10^{20}
cm^{-1}	1,23985 x 10^{-4}	1,9865 x 10^{-23}	1	4,5563x 10^{-6}	2,8573 x 10^{-3}
E_h	27,2116	4,3598 x 10^{-18}	2,1947 x 10^{5}	1	6,2709x 10^{2}
Kcal/mol	4,3393 x 10^{-2}	6,9524x 10^{-21}	3,4999 x 10^{2}	1,5946 x 10^{-3}	1

eV = elétron-volt

J = Joule

cm^{-1} = centímetro recíproco

E_h = hartree

Kcal/mol = quilocaloria por mol

5.2 Apêndice B: Energias Eletrônicas *ab initio* em cm^{-1}

Tabela 5.1: Sistema diatômico He-He

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-5,799377338445	2,00	-5,8033189597	2,00	-5,8046755184
2,10	-5,800093365422	2,10	-5,8040164346	2,10	-5,8053685586
2,20	-5,800544025077	2,20	-5,804452849	2,20	-5,8058013855
2,30	-5,800824282877	2,30	-5,8047224658	2,30	-5,8060680255
2,40	-5,800995984044	2,40	-5,804886413	2,40	-5,8062294864
2,50	-5,801099155215	2,50	-5,8049840425	2,50	-5,8063250417
2,60	-5,801159517820	2,60	-5,8050405004	2,60	-5,8063798134
2,70	-5,801193486065	2,70	-5,8050717326	2,70	-5,8064097098
2,80	-5,801211422623	2,80	-5,8050877661	2,80	-5,8064247135
2,90	-5,801219828761	2,90	-5,8050948472	2,90	-5,8064310192
2,91	-5,8012203162	2,91	-5,8050952267	2,91	-5,8064313328
2,92	-5,8012207526	2,92	-5,8050955586	2,92	-5,8064316007
2,93	-5,8012211412	2,93	-5,8050958465	2,93	-5,8064318268
2,94	-5,8012214846	2,94	-5,8050960926	2,94	-5,8064320131
2,95	-5,8012217853	2,95	-5,8050962995	2,95	-5,8064321619
2,96	-5,8012220458	2,96	-5,8050964694	2,96	-5,8064322756
2,97	-5,8012222685	2,97	-5,8050966046	2,97	-5,8064323563
2,98	-5,8012224554	2,98	-5,8050967071	2,98	-5,806432406
2,99	-5,8012226089	2,99	-5,805096779	**2,99**	**-5,8064324267**
3,00	-5,8012227308	3,00	-5,8050968222	3,00	-5,8064324202
3,01	-5,8012228231	**3,01**	**-5,8050968384**	3,01	-5,8064323884
3,02	-5,8012228876	3,02	-5,8050968294	3,02	-5,8064323328
3,03	-5,801222926	3,03	-5,8050967967	3,03	-5,806432255
3,04	**-5,80122294**	3,04	-5,805096742	3,04	-5,8064321566
3,05	-5,801222931	3,05	-5,8050966667	3,05	-5,806432039

3,06	-5,8012229006	3,06	-5,8050965721	3,06	-5,8064319035
3,07	-5,8012228502	3,07	-5,8050964597	3,07	-5,8064317514
3,08	-5,8012227811	3,08	-5,8050963305	3,08	-5,8064315839
3,09	-5,8012226946	3,09	-5,8050961859	3,09	-5,8064314021
3,10	-5,801222589827	3,10	-5,8050960268	3,10	-5,8064312076
3,20	-5,801220892208	3,20	-5,8050938545	3,20	-5,806428733
3,30	-5,801218501739	3,30	-5,8050911162	3,30	-5,8064257761
3,40	-5,801215913778	3,40	-5,8050882652	3,40	-5,8064227672
3,50	-5,801213393755	3,50	-5,8050855423	3,50	-5,8064199288
3,60	-5,801211069340	3,60	-5,8050830607	3,60	-5,8064173623
3,70	-5,801208999842	3,70	-5,805080863	3,70	-5,8064150996
3,80	-5,801207187098	3,80	-5,8050789506	3,80	-5,8064131368
3,90	-5,801205620110	3,90	-5,8050773043	3,90	-5,806411451
4,00	-5,801204275422	4,00	-5,8050758966	4,00	-5,806410012
4,10	-5,801203124278	4,10	-5,8050746973	4,10	-5,8064087876
4,20	-5,801202146073	4,20	-5,8050736773	4,20	-5,8064077474
4,30	-5,801201310703	4,30	-5,8050728099	4,30	-5,8064068637
4,40	-5,801200597371	4,40	-5,8050720716	4,40	-5,8064061123
4,50	-5,801199987289	4,50	-5,8050714421	4,50	-5,8064054723
4,60	-5,801199464443	4,60	-5,8050709044	4,60	-5,8064049261
4,70	-5,801199017931	4,70	-5,8050704439	4,70	-5,8064044603
4,80	-5,801198632887	4,80	-5,8050700484	4,80	-5,8064040578
4,90	-5,801198300848	4,90	-5,805069708	4,90	-5,8064037128
5,00	-5,801198013750	5,00	-5,805069414	5,00	-5,8064034152
5,10	-5,801197764314	5,10	-5,8050691595	5,10	-5,8064031577
5,20	-5,801197548465	5,20	-5,8050689385	5,20	-5,8064029343
5,30	-5,801197359904	5,30	-5,8050687461	5,30	-5,80640274
5,40	-5,801197195131	5,40	-5,8050685782	5,40	-5,8064025711
5,50	-5,801197050795	5,50	-5,8050684313	5,50	-5,8064024227
5,60	-5,801196923915	5,60	-5,8050683023	5,60	-5,806402292
5,70	-5,801196812500	5,70	-5,805068189	5,70	-5,8064021777
5,80	-5,801196714092	5,80	-5,805068089	5,80	-5,8064020773

5,90	-5,801196627085	5,90	-5,8050680007	5,90	-5,806401988
6,00	-5,801196549993	6,00	-5,8050679225	6,00	-5,8064019093
6,10	-5,801196481593	6,10	-5,8050678531	6,10	-5,8064018394
6,20	-5,801196420648	6,20	-5,8050677914	6,20	-5,8064017773
6,30	-5,801196366346	6,30	-5,8050677365	6,30	-5,806401722
6,40	-5,801196317885	6,40	-5,8050676874	6,40	-5,8064016727
6,50	-5,801196274511	6,50	-5,8050676435	6,50	-5,8064016286
6,60	-5,801196235752	6,60	-5,8050676042	6,60	-5,8064015891
6,70	-5,801196200730	6,70	-5,805067569	6,70	-5,8064015536
6,80	-5,801196169341	6,80	-5,8050675372	6,80	-5,8064015217
6,90	-5,801196141066	6,90	-5,8050675087	6,90	-5,8064014931
7,00	-5,801196115558	7,00	-5,8050674829	7,00	-5,8064014672
7,10	-5,801196092645	7,10	-5,8050674597	7,10	-5,8064014438
7,20	-5,801196071654	7,20	-5,8050674386	7,20	-5,8064014227
7,30	-5,801196052758	7,30	-5,8050674196	7,30	-5,8064014036
7,40	-5,801196035610	7,40	-5,8050674023	7,40	-5,8064013863
7,50	-5,801196020029	7,50	-5,8050673866	7,50	-5,8064013705
7,60	-5,801196005991	7,60	-5,8050673723	7,60	-5,8064013562
7,70	-5,801195992938	7,70	-5,8050673593	7,70	-5,8064013431
7,80	-5,801195981161	7,80	-5,8050673474	7,80	-5,8064013312
7,90	-5,801195970404	7,90	-5,8050673366	7,90	-5,8064013204
8,00	-5,801195960570	8,00	-5,8050673267	8,00	-5,8064013104
8,10	-5,801195951705	8,10	-5,8050673177	8,10	-5,8064013014
8,20	-5,801195943317	8,20	-5,8050673094	8,20	-5,806401293
8,30	-5,801195935751	8,30	-5,8050673017	8,30	-5,8064012854
8,40	-5,801195928802	8,40	-5,8050672948	8,40	-5,8064012784
8,50	-5,801195922414	8,50	-5,8050672883	8,50	-5,806401272
8,60	-5,801195916672	8,60	-5,8050672824	8,60	-5,806401266
8,70	-5,801195911119	8,70	-5,805067277	8,70	-5,8064012606
8,80	-5,801195906128	8,80	-5,805067272	8,80	-5,8064012556
8,90	-5,801195901521	8,90	-5,8050672673	8,90	-5,8064012509
9,00	-5,801195897265	9,00	-5,8050672631	9,00	-5,8064012467

9,10	-5,801195893330	9,10	-5,8050672591	9,10	-5,8064012427
9,20	-5,801195889689	9,20	-5,8050672555	9,20	-5,806401239
9,30	-5,801195886316	9,30	-5,8050672521	9,30	-5,8064012356
9,40	-5,801195883190	9,40	-5,8050672489	9,40	-5,8064012325
9,50	-5,801195880291	9,50	-5,805067246	9,50	-5,8064012296
9,60	-5,801195877599	9,60	-5,8050672433	9,60	-5,8064012269
9,70	-5,801195875097	9,70	-5,8050672408	9,70	-5,8064012244
9,80	-5,801195872771	9,80	-5,8050672385	9,80	-5,806401222
9,90	-5,801195870606	9,90	-5,8050672363	9,90	-5,8064012199
10,00	-5,801195868727	10,00	-5,8050672343	10,00	-5,8064012178
10,10	-5,801195866701	10,10	-5,8050672324	10,10	-5,806401216
10,20	-5,801195864957	10,20	-5,8050672306	10,20	-5,8064012142
10,30	-5,801195863324	10,30	-5,805067229	10,30	-5,8064012126
10,40	-5,801195861797	10,40	-5,8050672275	10,40	-5,806401211
10,50	-5,801195860370	10,50	-5,805067226	10,50	-5,8064012096
10,60	-5,801195859036	10,60	-5,8050672247	10,60	-5,8064012083
10,70	-5,801195857787	10,70	-5,8050672234	10,70	-5,806401207
10,80	-5,801195856618	10,80	-5,8050672223	10,80	-5,8064012058
10,90	-5,801195855523	10,90	-5,8050672212	10,90	-5,8064012047
11,00	-5,801195854496	11,00	-5,8050672202	11,00	-5,8064012037
11,10	-5,801195853533	11,10	-5,8050672192	11,10	-5,8064012027
11,20	-5,801195852629	11,20	-5,8050672183	11,20	-5,8064012018
11,30	-5,801195851780	11,30	-5,8050672174	11,30	-5,806401201
11,40	-5,801195850982	11,40	-5,8050672166	11,40	-5,8064012002
11,50	-5,801195850233	11,50	-5,8050672159	11,50	-5,8064011994
11,60	-5,801195849527	11,60	-5,8050672152	11,60	-5,8064011987
11,70	-5,801195848863	11,70	-5,8050672145	11,70	-5,8064011981
11,80	-5,801195848238	11,80	-5,8050672139	11,80	-5,8064011974
11,90	-5,801195847649	11,90	-5,8050672133	11,90	-5,8064011968
12,00	-5,801195847231				

Tabela 5.2: Sistema diatômico He-Ne

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-131,708644394265	2,00	-131,7455729475	2,00	-131,7586952802
2,10	-131,7104277075	2,10	-131,7473055782	2,10	-131,7604120412
2,20	-131,7115519415	2,20	-131,7483937939	2,20	-131,7614870695
2,30	-131,7122540593	2,30	-131,7490705522	2,30	-131,7621529526
2,40	-131,7126875606	2,40	-131,7494861673	2,40	-131,7625597473
2,50	-131,7129513242	2,50	-131,7497372058	2,50	-131,7628037912
2,60	-131,7131086864	2,60	-131,7498854056	2,60	-131,7629465689
2,70	-131,7131999955	2,70	-131,7499700188	2,70	-131,763027069
2,80	-131,7132507946	2,80	-131,7500158447	2,80	-131,7630698207
2,90	-131,7132771442	2,90	-131,7500384318	2,90	-131,7630901336
3,00	-131,7132890526	3,00	-131,7500474504	3,00	-131,7630974665
3,01	-131,7132897113	3,01	-131,7500478479	3,01	-131,7630977303
3,02	-131,7132902938	3,02	-131,7500481841	3,02	-131,7630979295
3,03	-131,7132908043	3,03	-131,750048455	3,03	-131,7630980669
3,04	-131,7132912471	3,04	-131,7500486637	3,04	-131,7630981461
3,05	-131,713291626	3,05	-131,750048814	**3,05**	**-131,7630981709**
3,06	-131,7132919452	3,06	-131,7500489097	3,06	-131,7630981447
3,07	-131,7132922075	**3,07**	**-131,750048954**	3,07	-131,7630980708
3,08	-131,7132924167	3,08	-131,7500489503	3,08	-131,7630979522
3,09	-131,7132925759	3,09	-131,7500489015	3,09	-131,763097792
3,10	-131,7132926882	3,10	-131,7500488106	3,10	-131,7630975929
3,11	-131,7132927561	3,11	-131,7500486804	3,11	-131,7630973576
3,12	**-131,7132927831**	3,12	-131,7500485136	3,12	-131,7630970886
3,13	-131,7132927714	3,13	-131,7500483125	3,13	-131,7630967884
3,14	-131,7132927236	3,14	-131,7500480795	3,14	-131,7630964591
3,15	-131,7132926419	3,15	-131,750047817	3,15	-131,7630961029
3,16	-131,7132925286	3,16	-131,750047527	3,16	-131,7630957218
3,17	-131,7132923858	3,17	-131,7500472115	3,17	-131,7630953178

3,18	-131,7132922155	3,18	-131,7500468725	3,18	-131,7630948927
3,19	-131,7132920196	3,19	-131,7500465117	3,19	-131,7630944482
3,20	-131,7132917999	3,20	-131,7500461303	3,20	-131,7630939865
3,30	-131,7132886289	3,30	-131,7500415358	3,30	-131,7630886859
3,40	-131,7132844802	3,40	-131,750036255	3,40	-131,7630828612
3,50	-131,7132800895	3,50	-131,7500309644	3,50	-131,7630771366
3,60	-131,7132758488	3,60	-131,75002601	3,60	-131,7630718362
3,70	-131,7132719496	3,70	-131,7500215462	3,70	-131,7630670915
3,80	-131,7132684652	3,80	-131,7500176157	3,80	-131,763062919
3,90	-131,7132654064	3,90	-131,750014205	3,90	-131,7630593394
4,00	-131,7132627507	4,00	-131,7500112712	4,00	-131,7630562552
4,10	-131,7132604616	4,10	-131,7500087615	4,10	-131,7630536238
4,20	-131,7132584965	4,20	-131,7500066202	4,20	-131,7630513853
4,30	-131,7132568128	4,30	-131,750004795	4,30	-131,7630494811
4,40	-131,7132553714	4,40	-131,750003239	4,40	-131,763047862
4,50	-131,7132541366	4,50	-131,7500019021	4,50	-131,7630464833
4,60	-131,7132530773	4,60	-131,7500007761	4,60	-131,7630453073
4,70	-131,7132521683	4,70	-131,7499998039	4,70	-131,7630443018
4,80	-131,7132513811	4,80	-131,749998969	4,80	-131,7630434395
4,90	-131,7132507082	4,90	-131,7499982505	4,90	-131,7630426987
5,00	-131,7132501284	5,00	-131,7499976303	5,00	-131,7630420601
5,10	-131,7132496223	5,10	-131,7499970936	5,10	-131,7630415082
5,20	-131,7132491832	5,20	-131,7499966282	5,20	-131,76304103
5,30	-131,7132488008	5,30	-131,7499962228	5,30	-131,7630406141
5,40	-131,7132484667	5,40	-131,7499958694	5,40	-131,7630402518
5,50	-131,7132481744	5,50	-131,7499955603	5,50	-131,7630399351
5,60	-131,713247918	5,60	-131,7499952893	5,60	-131,7630396578
5,70	-131,7132476919	5,70	-131,7499950512	5,70	-131,7630394143
5,80	-131,7132474931	5,80	-131,7499948413	5,80	-131,7630391997
5,90	-131,7132473172	5,90	-131,749994656	5,90	-131,7630390105
6,00	-131,7132471609	6,00	-131,7499944921	6,00	-131,763038843
6,10	-131,7132470236	6,10	-131,7499943467	6,10	-131,7630386947

6,20	-131,7132469003	6,20	-131,7499942175	6,20	-131,7630385631
6,30	-131,7132467909	6,30	-131,7499941023	6,30	-131,7630384456
6,40	-131,7132466931	6,40	-131,7499940001	6,40	-131,763038341
6,50	-131,7132466057	6,50	-131,7499939079	6,50	-131,7630382475
6,60	-131,7132465278	6,60	-131,7499938257	6,60	-131,7630381639
6,70	-131,7132464571	6,70	-131,7499937521	6,70	-131,763038089
6,80	-131,713246394	6,80	-131,7499936857	6,80	-131,7630380215
6,90	-131,713246337	6,90	-131,749993626	6,90	-131,7630379609
7,00	-131,7132462858	7,00	-131,7499935722	7,00	-131,7630379062
7,10	-131,7132462398	7,10	-131,7499935238	7,10	-131,7630378569
7,20	-131,7132461974	7,20	-131,7499934799	7,20	-131,7630378125
7,30	-131,7132461596	7,30	-131,74999344	7,30	-131,7630377719
7,40	-131,7132461251	7,40	-131,749993404	7,40	-131,7630377354
7,50	-131,7132460938	7,50	-131,7499933712	7,50	-131,7630377021
7,60	-131,7132460657	7,60	-131,7499933415	7,60	-131,7630376719
7,70	-131,7132460393	7,70	-131,7499933144	7,70	-131,7630376446
7,80	-131,7132460158	7,80	-131,7499932896	7,80	-131,7630376193
7,90	-131,7132459942	7,90	-131,749993267	7,90	-131,7630375965
8,00	-131,7132459745	8,00	-131,7499932464	8,00	-131,7630375756
8,10	-131,7132459568	8,10	-131,7499932276	8,10	-131,7630375565
8,20	-131,7132459398	8,20	-131,7499932102	8,20	-131,7630375391
8,30	-131,7132459247	8,30	-131,7499931945	8,30	-131,7630375229
8,40	-131,7132459107	8,40	-131,7499931799	8,40	-131,7630375082
8,50	-131,713245898	8,50	-131,7499931665	8,50	-131,7630374947
8,60	-131,7132458865	8,60	-131,7499931543	8,60	-131,7630374822
8,70	-131,7132458754	8,70	-131,7499931428	8,70	-131,7630374709
8,80	-131,7132458653	8,80	-131,7499931325	8,80	-131,7630374602
8,90	-131,7132458561	8,90	-131,7499931228	8,90	-131,7630374505
9,00	-131,7132458475	9,00	-131,7499931139	9,00	-131,7630374415
9,10	-131,7132458397	9,10	-131,7499931057	9,10	-131,7630374332
9,20	-131,7132458324	9,20	-131,7499930981	9,20	-131,7630374255
9,30	-131,7132458256	9,30	-131,7499930911	9,30	-131,7630374184

9,40	-131,7132458194	9,40	-131,7499930846	9,40	-131,7630374118
9,50	-131,7132458136	9,50	-131,7499930785	9,50	-131,7630374057
9,60	-131,7132458082	9,60	-131,7499930729	9,60	-131,7630374
9,70	-131,7132458032	9,70	-131,7499930677	9,70	-131,7630373947
9,80	-131,7132457985	9,80	-131,7499930628	9,80	-131,7630373898
9,90	-131,7132457942	9,90	-131,7499930583	9,90	-131,7630373853
10,00	-131,7132457905	10,00	-131,7499930542	10,00	-131,763037381
10,10	-131,7132457862	10,10	-131,7499930501	10,10	-131,7630373772
10,20	-131,7132457829	10,20	-131,7499930466	10,20	-131,7630373734
10,30	-131,7132457796	10,30	-131,7499930431	10,30	-131,76303737
10,40	-131,7132457766	10,40	-131,74999304	10,40	-131,7630373667
10,50	-131,7132457737	10,50	-131,749993037	10,50	-131,7630373637
10,60	-131,713245771	10,60	-131,7499930342	10,60	-131,7630373609
10,70	-131,7132457685	10,70	-131,7499930316	10,70	-131,7630373583
10,80	-131,7132457662	10,80	-131,7499930292	10,80	-131,7630373558
10,90	-131,713245764	10,90	-131,7499930269	10,90	-131,7630373535
11,00	-131,7132457619	11,00	-131,7499930248	11,00	-131,7630373514
11,10	-131,71324576	11,10	-131,7499930228	11,10	-131,7630373494
11,20	-131,7132457582	11,20	-131,7499930209	11,20	-131,7630373475
11,30	-131,7132457565	11,30	-131,7499930191	11,30	-131,7630373457
11,40	-131,7132457549	11,40	-131,7499930175	11,40	-131,763037344
11,50	-131,7132457534	11,50	-131,7499930159	11,50	-131,7630373424
11,60	-131,713245752	11,60	-131,7499930144	11,60	-131,763037341
11,70	-131,7132457507	11,70	-131,7499930131	11,70	-131,7630373396
11,80	-131,7132457494	11,80	-131,7499930118	11,80	-131,7630373383
11,90	-131,7132457483	11,90	-131,7499930105	11,90	-131,763037337
				12,00	-131,7630939865

Tabela 5.3: Sistema diatômico He-Ar

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)

2,00	-529,9261264565	2,00	-529,9549989866	2,00	-529,964274523
2,10	-529,933650633	2,10	-529,9623943541	2,10	-529,9716153726
2,20	-529,9388217996	2,20	-529,9674611891	2,20	-529,9766416682
2,30	-529,9423554678	2,30	-529,9709095666	2,30	-529,9800597727
2,40	-529,9447555892	2,40	-529,9732399704	2,40	-529,9823674431
2,50	-529,9463750284	2,50	-529,9748028136	2,50	-529,9839130943
2,60	-529,9474595673	2,60	-529,9758419312	2,60	-529,9849391005
2,70	-529,948179581	2,70	-529,9765259992	2,70	-529,9856130653
2,80	-529,948652604	2,80	-529,9769710072	2,80	-529,9860501844
2,90	-529,948959346	2,90	-529,9772562513	2,90	-529,9863291896
3,00	-529,9491549497	3,00	-529,9774355963	3,00	-529,9865035523
3,10	-529,9492768905	3,10	-529,9775453958	3,10	-529,9866093509
3,20	-529,9493504996	3,20	-529,9776100307	3,20	-529,9866707583
3,30	-529,9493927816	3,30	-529,9776457258	3,30	-529,9867038506
3,40	-529,9494150822	3,40	-529,9776632046	3,40	-529,9867192333
3,50	-529,949424907	3,41	-529,977664247	3,41	-529,9867200895
3,51	-529,9494254099	3,42	-529,9776651835	3,42	-529,9867208447
3,52	-529,9494258424	3,43	-529,9776660208	3,43	-529,9867215045
3,53	-529,9494262082	3,44	-529,9776667637	3,44	-529,9867220739
3,54	-529,9494265107	3,45	-529,9776674171	3,45	-529,9867225575
3,55	-529,9494267533	3,46	-529,9776679854	3,46	-529,9867229599
3,56	-529,9494269391	3,47	-529,9776684731	3,47	-529,9867232853
3,57	-529,9494270711	3,48	-529,9776688844	3,48	-529,9867235377
3,58	-529,9494271523	3,49	-529,9776692231	3,49	-529,9867237213
3,59	**-529,9494271855**	3,50	-529,9776694932	3,50	-529,9867238395
3,60	-529,9494271753	3,51	-529,9776696982	**3,51**	**-529,9867238962**
3,61	-529,9494271203	3,52	-529,9776698418	3,52	-529,9867238946
3,62	-529,9494270248	3,53	-529,9776699271	3,53	-529,9867238381
3,63	-529,9494268913	**3,54**	**-529,9776699574**	3,54	-529,9867237298
3,64	-529,949426722	3,55	-529,9776699358	3,55	-529,9867235726
3,65	-529,9494265189	3,56	-529,9776698651	3,56	-529,9867233694
3,66	-529,9494262841	3,57	-529,9776697483	3,57	-529,986723123

3,67	-529,9494260195	3,58	-529,9776695878	3,58	-529,986722836
3,68	-529,949425727	3,59	-529,9776693863	3,59	-529,9867225107
3,69	-529,9494254083	3,60	-529,977669145	3,60	-529,986722149
3,70	-529,9494250629	3,70	-529,9776650804	3,70	-529,9867170164
3,80	-529,9494206033	3,80	-529,9776591377	3,80	-529,9867102295
3,90	-529,9494150576	3,90	-529,9776524472	3,90	-529,9867028713
4,00	-529,9494091899	4,00	-529,9776456813	4,00	-529,9866955776
4,10	-529,9494034415	4,10	-529,9776392186	4,10	-529,9866886989
4,20	-529,9493980533	4,20	-529,9776332565	4,20	-529,9866824042
4,30	-529,9493931347	4,30	-529,9776278743	4,30	-529,9866767584
4,40	-529,949388723	4,40	-529,9776230871	4,40	-529,9866717601
4,50	-529,9493848109	4,50	-529,9776188707	4,50	-529,9866673735
4,60	-529,9493813671	4,60	-529,9776151814	4,60	-529,9866635453
4,70	-529,9493783516	4,70	-529,9776119653	4,70	-529,9866602231
4,80	-529,9493757178	4,80	-529,9776091693	4,80	-529,9866573312
4,90	-529,9493734217	4,90	-529,9776067409	4,90	-529,9866548294
5,00	-529,9493714203	5,00	-529,977604632	5,00	-529,9866526608
5,10	-529,9493696753	5,10	-529,9776028002	5,10	-529,9866507799
5,20	-529,9493681541	5,20	-529,9776012058	5,20	-529,9866491467
5,30	-529,9493668253	5,30	-529,9775998176	5,30	-529,9866477263
5,40	-529,9493656632	5,40	-529,9775986062	5,40	-529,9866464887
5,50	-529,9493646452	5,50	-529,977597547	5,50	-529,9866454082
5,60	-529,9493637518	5,60	-529,9775966205	5,60	-529,9866444629
5,70	-529,9493629661	5,70	-529,9775958055	5,70	-529,9866436343
5,80	-529,949362274	5,80	-529,9775950896	5,80	-529,9866429061
5,90	-529,949361663	5,90	-529,9775944585	5,90	-529,9866422649
6,00	-529,9493611225	6,00	-529,9775939011	6,00	-529,9866416989
6,10	-529,9493606439	6,10	-529,9775934085	6,10	-529,9866411982
6,20	-529,949360218	6,20	-529,97759297	6,20	-529,9866407547
6,30	-529,9493598395	6,30	-529,977592581	6,30	-529,9866403606
6,40	-529,949359502	6,40	-529,9775922346	6,40	-529,9866400099
6,50	-529,9493592007	6,50	-529,9775919256	6,50	-529,9866396971

6,60	-529,9493589319	6,60	-529,9775916501	6,60	-529,9866394176
6,70	-529,9493586894	6,70	-529,9775914019	6,70	-529,9866391676
6,80	-529,9493584724	6,80	-529,9775911799	6,80	-529,9866389433
6,90	-529,9493582773	6,90	-529,9775909804	6,90	-529,9866387419
7,00	-529,9493581015	7,00	-529,9775908009	7,00	-529,9866385606
7,10	-529,9493579438	7,10	-529,9775906398	7,10	-529,9866383972
7,20	-529,9493577996	7,20	-529,9775904929	7,20	-529,9866382498
7,30	-529,9493576699	7,30	-529,9775903607	7,30	-529,9866381165
7,40	-529,9493575524	7,40	-529,9775902409	7,40	-529,9866379959
7,50	-529,9493574458	7,50	-529,9775901323	7,50	-529,9866378864
7,60	-529,9493573499	7,60	-529,9775900344	7,60	-529,986637787
7,70	-529,9493572608	7,70	-529,9775899439	7,70	-529,9866376967
7,80	-529,9493571804	7,80	-529,9775898622	7,80	-529,9866376145
7,90	-529,9493571071	7,90	-529,9775897877	7,90	-529,9866375395
8,00	-529,9493570402	8,00	-529,9775897197	8,00	-529,9866374711
8,10	-529,94935698	8,10	-529,9775896583	8,10	-529,9866374085
8,20	-529,949356923	8,20	-529,9775896007	8,20	-529,9866373514
8,30	-529,9493568716	8,30	-529,9775895485	8,30	-529,986637299
8,40	-529,9493568245	8,40	-529,9775895007	8,40	-529,9866372509
8,50	-529,9493567812	8,50	-529,9775894568	8,50	-529,9866372068
8,60	-529,9493567424	8,60	-529,9775894173	8,60	-529,9866371662
8,70	-529,9493567048	8,70	-529,9775893794	8,70	-529,986637129
8,80	-529,9493566711	8,80	-529,9775893452	8,80	-529,9866370946
8,90	-529,9493566399	8,90	-529,9775893137	8,90	-529,986637063
9,00	-529,9493566112	9,00	-529,9775892846	9,00	-529,9866370338
9,10	-529,9493565847	9,10	-529,9775892577	9,10	-529,9866370068
9,20	-529,9493565601	9,20	-529,9775892329	9,20	-529,9866369819
9,30	-529,9493565374	9,30	-529,9775892099	9,30	-529,9866369588
9,40	-529,9493565164	9,40	-529,9775891886	9,40	-529,9866369375
9,50	-529,9493564969	9,50	-529,9775891689	9,50	-529,9866369177
9,60	-529,9493564788	9,60	-529,9775891506	9,60	-529,9866368993
9,70	-529,9493564619	9,70	-529,9775891336	9,70	-529,9866368823

9,80	-529,9493564463	9,80	-529,9775891178	9,80	-529,9866368664
9,90	-529,9493564318	9,90	-529,9775891031	9,90	-529,9866368517
10,00	-529,9493564183	10,00	-529,9775890894	10,00	-529,986636838
10,10	-529,9493564057	10,10	-529,9775890767	10,10	-529,9866368253
10,20	-529,9493563939	10,20	-529,9775890648	10,20	-529,9866368134
10,30	-529,949356383	10,30	-529,9775890538	10,30	-529,9866368023
10,40	-529,9493563727	10,40	-529,9775890435	10,40	-529,986636792
10,50	-529,9493563632	10,50	-529,9775890338	10,50	-529,9866367823
10,60	-529,9493563542	10,60	-529,9775890248	10,60	-529,9866367733
10,70	-529,9493563459	10,70	-529,9775890164	10,70	-529,9866367648
10,80	-529,9493563381	10,80	-529,9775890085	10,80	-529,9866367569
10,90	-529,9493563308	10,90	-529,9775890011	10,90	-529,9866367495
11,00	-529,9493563239	11,00	-529,9775889942	11,00	-529,9866367426
11,10	-529,9493563175	11,10	-529,9775889877	11,10	-529,9866367361
11,20	-529,9493563114	11,20	-529,9775889816	11,20	-529,98663673
11,30	-529,9493563058	11,30	-529,9775889759	11,30	-529,9866367243
11,40	-529,9493563004	11,40	-529,9775889705	11,40	-529,9866367189
11,50	-529,9493562954	11,50	-529,9775889655	11,50	-529,9866367139
11,60	-529,9493562907	11,60	-529,9775889608	11,60	-529,9866367092
11,70	-529,9493562863	11,70	-529,9775889563	11,70	-529,9866367047
11,80	-529,9493562821	11,80	-529,9775889521	11,80	-529,9866367005
11,90	-529,9493562782	11,90	-529,9775889482	11,90	-529,9866366965
12,00	-529,9493562745	12,00	-529,9775889444	12,00	-529,9866366928
12,10	-529,949356271			12,10	-529,9866366893
12,20	-529,9493562677				

Tabela 5.4: Sistema diatômico He-Kr

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-2755,1747529217	2,00	-2755,252990564	2,00	-2755,3399207161
2,10	-2755,1861167516	2,10	-2755,2641508703	2,10	-2755,3510022172

2,20	-2755,1941590495	2,20	-2755,272029362	2,20	-2755,3588165925
2,30	-2755,1998179452	2,30	-2755,2775574432	2,30	-2755,3642923663
2,40	-2755,2037772407	2,40	-2755,2814128013	2,40	-2755,3681051107
2,50	-2755,206531543	2,50	-2755,2840846404	2,50	-2755,3707425112
2,60	-2755,2084361697	2,60	-2755,2859237231	2,60	-2755,3725541391
2,70	-2755,2097448113	2,70	-2755,2871800994	2,70	-2755,3737889779
2,80	-2755,2106375764	2,80	-2755,288031074	2,80	-2755,3746233172
2,90	-2755,2112416563	2,90	-2755,2886017296	2,90	-2755,3751812617
3,00	-2755,2116464246	3,00	-2755,2889798337	3,00	-2755,3755497142
3,10	-2755,2119143839	3,10	-2755,2892266403	3,10	-2755,3757891865
3,20	-2755,212089051	3,20	-2755,2893846559	3,20	-2755,3759415908
3,30	-2755,2122005706	3,30	-2755,2894831824	3,30	-2755,3760357807
3,40	-2755,2122697332	3,40	-2755,2895422922	3,40	-2755,3760914959
3,50	-2755,2123107956	3,50	-2755,2895756333	3,50	-2755,3761221512
3,60	-2755,2123334714	3,60	-2755,2895924131	3,60	-2755,3761367852
3,70	-2755,2123443375	3,70	-2755,2895987858	3,70	-2755,376141447
3,71	-2755,2123449624	3,71	-2755,2895990169	3,71	-2755,37614152
3,72	-2755,2123455142	3,72	-2755,2895991947	**3,72**	**-2755,3761415503**
3,73	-2755,2123460002	3,73	-2755,2895993159	3,73	-2755,3761415261
3,74	-2755,2123464233	3,74	-2755,2895993841	3,74	-2755,3761414525
3,75	-2755,2123467866	**3,75**	**-2755,2895994021**	3,75	-2755,3761413316
3,76	-2755,212347093	3,76	-2755,2895993724	3,76	-2755,3761411661
3,77	-2755,2123473454	3,77	-2755,2895992978	3,77	-2755,3761409586
3,78	-2755,2123475465	3,78	-2755,2895991805	3,78	-2755,3761407113
3,79	-2755,2123476987	3,79	-2755,289599023	3,79	-2755,3761404267
3,80	-2755,2123478047	3,80	-2755,2895988275	3,80	-2755,3761401069
3,81	-2755,2123478667	3,81	-2755,2895985962	3,81	-2755,3761397539
3,82	-2755,2123478871	3,82	-2755,2895983293	3,82	-2755,3761393698
3,83	**-2755,2123478681**	3,83	-2755,2895980321	3,83	-2755,3761389565
3,84	-2755,2123478117	3,84	-2755,2895977051	3,84	-2755,3761385157
3,85	-2755,2123477199	3,85	-2755,28959735	3,85	-2755,3761380493
3,86	-2755,2123475948	3,86	-2755,2895969685	3,86	-2755,376137559

3,87	-2755,212347438	3,87	-2755,2895965622	3,87	-2755,3761370461
3,88	-2755,2123472513	3,88	-2755,2895961326	3,88	-2755,3761365125
3,89	-2755,2123470366	3,89	-2755,2895956814	3,89	-2755,3761359594
3,90	-2755,2123467953	3,90	-2755,2895952134	3,90	-2755,3761353979
4,00	-2755,2123432354	4,00	-2755,2895896561	4,00	-2755,3761289548
4,10	-2755,2123383529	4,10	-2755,2895832352	4,10	-2755,3761218264
4,20	-2755,2123329404	4,20	-2755,2895766271	4,20	-2755,37611466
4,30	-2755,2123274661	4,30	-2755,2895702169	4,30	-2755,3761078007
4,40	-2755,2123222086	4,40	-2755,2895642206	4,40	-2755,3761014482
4,50	-2755,2123173162	4,50	-2755,2895587346	4,50	-2755,3760956848
4,60	-2755,212312854	4,60	-2755,2895538121	4,60	-2755,3760905273
4,70	-2755,2123088439	4,70	-2755,2895494179	4,70	-2755,3760859586
4,80	-2755,2123052695	4,80	-2755,2895455431	4,80	-2755,3760819349
4,90	-2755,2123021055	4,90	-2755,2895421355	4,90	-2755,3760784077
5,00	-2755,2122993119	5,00	-2755,2895391485	5,00	-2755,3760753244
5,10	-2755,2122968554	5,10	-2755,2895365403	5,10	-2755,3760726327
5,20	-2755,2122946991	5,20	-2755,2895342487	5,20	-2755,3760702825
5,30	-2755,2122928049	5,30	-2755,2895322506	5,30	-2755,3760682317
5,40	-2755,2122911414	5,40	-2755,2895305067	5,40	-2755,3760664402
5,50	-2755,2122896798	5,50	-2755,2895289739	5,50	-2755,3760648736
5,60	-2755,2122883933	5,60	-2755,2895276304	5,60	-2755,3760635017
5,70	-2755,212287262	5,70	-2755,2895264503	5,70	-2755,3760622984
5,80	-2755,2122862637	5,80	-2755,289525412	5,80	-2755,3760612406
5,90	-2755,2122853817	5,90	-2755,2895244969	5,90	-2755,3760603096
6,00	-2755,2122846014	6,00	-2755,2895236888	6,00	-2755,3760594881
6,10	-2755,2122839091	6,10	-2755,2895229739	6,10	-2755,376058762
6,20	-2755,2122832953	6,20	-2755,2895223399	6,20	-2755,3760581189
6,30	-2755,212282749	6,30	-2755,2895217771	6,30	-2755,3760575482
6,40	-2755,2122822621	6,40	-2755,2895212761	6,40	-2755,3760570407
6,50	-2755,2122818273	6,50	-2755,2895208295	6,50	-2755,3760565885
6,60	-2755,2122814384	6,60	-2755,2895204306	6,60	-2755,3760561849
6,70	-2755,2122810902	6,70	-2755,2895200735	6,70	-2755,3760558239

6,80	-2755,2122807778	6,80	-2755,2895197537	6,80	-2755,3760555006
6,90	-2755,2122804969	6,90	-2755,2895194663	6,90	-2755,3760552103
7,00	-2755,212280244	7,00	-2755,2895192079	7,00	-2755,3760549494
7,10	-2755,2122800159	7,10	-2755,2895189751	7,10	-2755,3760547143
7,20	-2755,2122798099	7,20	-2755,2895187649	7,20	-2755,3760545024
7,30	-2755,2122796238	7,30	-2755,2895185752	7,30	-2755,376054311
7,40	-2755,2122794551	7,40	-2755,2895184033	7,40	-2755,3760541378
7,50	-2755,2122793021	7,50	-2755,2895182476	7,50	-2755,3760539808
7,60	-2755,2122791632	7,60	-2755,2895181062	7,60	-2755,3760538383
7,70	-2755,2122790366	7,70	-2755,2895179777	7,70	-2755,376053709
7,80	-2755,2122789217	7,80	-2755,2895178609	7,80	-2755,3760535913
7,90	-2755,2122788167	7,90	-2755,2895177543	7,90	-2755,376053484
8,00	-2755,2122787209	8,00	-2755,2895176571	8,00	-2755,3760533861
8,10	-2755,2122786334	8,10	-2755,2895175681	8,10	-2755,3760532967
8,20	-2755,2122785531	8,20	-2755,2895174868	8,20	-2755,376053215
8,30	-2755,2122784799	8,30	-2755,2895174125	8,30	-2755,3760531402
8,40	-2755,2122784125	8,40	-2755,2895173442	8,40	-2755,3760530716
8,50	-2755,2122783507	8,50	-2755,2895172816	8,50	-2755,3760530087
8,60	-2755,212278294	8,60	-2755,2895172241	8,60	-2755,3760529508
8,70	-2755,2122782415	8,70	-2755,2895171711	8,70	-2755,3760528977
8,80	-2755,2122781935	8,80	-2755,2895171225	8,80	-2755,3760528488
8,90	-2755,2122781491	8,90	-2755,2895170776	8,90	-2755,3760528037
9,00	-2755,2122781081	9,00	-2755,2895170362	9,00	-2755,3760527621
9,10	-2755,2122780703	9,10	-2755,289516998	9,10	-2755,3760527237
9,20	-2755,2122780353	9,20	-2755,2895169626	9,20	-2755,3760526883
9,30	-2755,212278003	9,30	-2755,2895169299	9,30	-2755,3760526555
9,40	-2755,212277973	9,40	-2755,2895168997	9,40	-2755,3760526251
9,50	-2755,2122779452	9,50	-2755,2895168717	9,50	-2755,376052597
9,60	-2755,2122779195	9,60	-2755,2895168456	9,60	-2755,3760525708
9,70	-2755,2122778955	9,70	-2755,2895168214	9,70	-2755,3760525466
9,80	-2755,2122778733	9,80	-2755,2895167991	9,80	-2755,3760525242
9,90	-2755,2122778526	9,90	-2755,2895167782	9,90	-2755,3760525033

10,00	-2755,2122778334	10,00	-2755,2895167589	10,00	-2755,3760524838
10,10	-2755,2122778155	10,10	-2755,2895167408	10,10	-2755,3760524657
10,20	-2755,2122777988	10,20	-2755,289516724	10,20	-2755,3760524488
10,30	-2755,2122777832	10,30	-2755,2895167083	10,30	-2755,3760524331
10,40	-2755,2122777687	10,40	-2755,2895166937	10,40	-2755,3760524185
10,50	-2755,2122777551	10,50	-2755,28951668	10,50	-2755,3760524048
10,60	-2755,2122777424	10,60	-2755,2895166672	10,60	-2755,3760523919
10,70	-2755,2122777304	10,70	-2755,2895166552	10,70	-2755,37605238
10,80	-2755,2122777195	10,80	-2755,2895166441	10,80	-2755,3760523688
10,90	-2755,212277709	10,90	-2755,2895166336	10,90	-2755,3760523583
11,00	-2755,2122776993	11,00	-2755,2895166239	11,00	-2755,3760523485
11,10	-2755,2122776902	11,10	-2755,2895166147	11,10	-2755,3760523393
11,20	-2755,2122776816	11,20	-2755,2895166061	11,20	-2755,3760523307
11,30	-2755,2122776736	11,30	-2755,289516598	11,30	-2755,3760523226
11,40	-2755,212277666	11,40	-2755,2895165904	11,40	-2755,376052315
11,50	-2755,2122776589	11,50	-2755,2895165833	11,50	-2755,3760523079
11,60	-2755,2122776523	11,60	-2755,2895165766	11,60	-2755,3760523011
		11,70	-2755,2895165702	11,70	-2755,3760522948
		11,80	-2755,2895165643	11,80	-2755,3760522889
		11,90	-2755,2895165587	11,90	-2755,3760522833
		12,00	-2755,2895165535	12,00	-2755,376052278
		12,10	-2755,2895165485		

Tabela 5.5: Sistema diatômico He-Xe

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-331,4018875254	2,00	-331,5173188458	2,00	-331,5937502896
2,10	-331,4192250455	2,10	-331,5343322241	2,10	-331,6106435185
2,20	-331,4319520797	2,20	-331,546792671	2,20	-331,6230062665
2,30	-331,4412407767	2,30	-331,5558619375	2,30	-331,6319954535
2,40	-331,4479830874	2,40	-331,5624241177	2,40	-331,6384916951

2,50	-331,4528512208	2,50	-331,5671452511	2,50	-331,6431583699
2,60	-331,4563476066	2,60	-331,5705226807	2,60	-331,6464907404
2,70	-331,4588451897	2,70	-331,5729248513	2,70	-331,6488557056
2,80	-331,4606191804	2,80	-331,574622909	2,80	-331,6505232721
2,90	-331,4618715707	2,90	-331,5758152328	2,90	-331,6516908679
3,00	-331,462749939	3,00	-331,5766462069	3,00	-331,6525020526
3,10	-331,463361454	3,10	-331,5772203778	3,10	-331,6530606312
3,20	-331,4637836035	3,20	-331,5776131609	3,20	-331,6534412584
3,30	-331,4640721202	3,30	-331,5778785918	3,30	-331,6536973289
3,40	-331,464266896	3,40	-331,5780552423	3,40	-331,6538668222
3,50	-331,4643963479	3,50	-331,5781704831	3,50	-331,6539766004
3,60	-331,464480621	3,60	-331,5782436416	3,60	-331,6540455597
3,70	-331,4645339237	3,70	-331,5782882364	3,70	-331,6540869196
3,80	-331,4645662198	3,80	-331,5783137117	3,80	-331,6541098483
3,90	-331,4645844529	3,90	-331,5783266058	3,90	-331,654120739
3,91	-331,4645857016	3,91	-331,578327392	3,91	-331,6541213505
3,92	-331,4645868638	3,92	-331,5783280989	3,92	-331,654121885
3,93	-331,464587942	3,93	-331,5783287329	3,93	-331,6541223507
3,94	-331,46458894	3,94	-331,5783292973	3,94	-331,6541227504
3,95	-331,4645898612	3,95	-331,5783297952	3,95	-331,654123087
3,96	-331,4645907089	3,96	-331,5783302296	3,96	-331,6541233636
3,97	-331,4645914862	3,97	-331,5783306036	3,97	-331,6541235833
3,98	-331,4645922136	3,98	-331,5783309199	3,98	-331,6541237487
3,99	-331,464592861	3,99	-331,5783311812	3,99	-331,6541238624
4,00	-331,4645934453	4,00	-331,5783313902	4,00	-331,6541239416
4,01	-331,4645939707	4,01	-331,5783315495	**4,01**	**-331,6541239595**
4,02	-331,4645944401	4,02	-331,5783316612	4,02	-331,6541239331
4,03	-331,4645948558	4,03	-331,5783317277	4,03	-331,6541238643
4,04	-331,4645952204	**4,04**	**-331,5783317514**	4,04	-331,654123748
4,05	-331,4645955361	4,05	-331,5783317344	4,05	-331,6541236022
4,06	-331,4645958052	4,06	-331,5783316786	4,06	-331,6541234189
4,07	-331,4645960299	4,07	-331,578331586	4,07	-331,6541232026

4,08	-331,4645962122	4,08	-331,5783314586	4,08	-331,6541229535
4,09	-331,4645963542	4,09	-331,5783312981	4,09	-331,654122674
4,10	**-331,4645964586**	4,10	-331,5783311057	4,10	-331,6541223672
4,20	-331,4645957528	4,20	-331,578327802	4,20	-331,6541180231
4,30	-331,464592835	4,30	-331,5783228352	4,30	-331,6541122103
4,40	-331,4645887048	4,40	-331,5783170857	4,40	-331,6541057821
4,50	-331,464584013	4,50	-331,5783111177	4,50	-331,6540992496
4,60	-331,4645791735	4,60	-331,5783052628	4,60	-331,654092941
4,70	-331,4645744401	4,70	-331,5782997228	4,70	-331,6540870346
4,80	-331,4645699597	4,80	-331,5782946014	4,80	-331,6540816177
4,90	-331,4645658093	4,90	-331,5782899404	4,90	-331,6540767183
5,00	-331,4645620212	5,00	-331,5782857442	5,00	-331,6540723298
5,10	-331,4645585988	5,10	-331,578281995	5,10	-331,6540684258
5,20	-331,4645555293	5,20	-331,5782786641	5,20	-331,6540649665
5,30	-331,4645527898	5,30	-331,5782757143	5,30	-331,6540619147
5,40	-331,4645503532	5,40	-331,5782731077	5,40	-331,6540592249
5,50	-331,4645481907	5,50	-331,5782708073	5,50	-331,6540568561
5,60	-331,464546274	5,60	-331,5782687779	5,60	-331,6540547706
5,70	-331,4645445764	5,70	-331,5782669875	5,70	-331,6540529341
5,80	-331,4645430723	5,80	-331,578265411	5,80	-331,6540513157
5,90	-331,4645417394	5,90	-331,5782640139	5,90	-331,654049888
6,00	-331,4645405583	6,00	-331,5782627788	6,00	-331,6540486269
6,10	-331,4645395078	6,10	-331,5782616849	6,10	-331,6540475116
6,20	-331,4645385752	6,20	-331,5782607148	6,20	-331,6540465236
6,30	-331,4645377452	6,30	-331,5782598531	6,30	-331,654045647
6,40	-331,4645370055	6,40	-331,5782590865	6,40	-331,6540448679
6,50	-331,4645363453	6,50	-331,5782584034	6,50	-331,6540441742
6,60	-331,4645357551	6,60	-331,5782577937	6,60	-331,6540435556
6,70	-331,4645352267	6,70	-331,5782572485	6,70	-331,6540430029
6,80	-331,4645347528	6,80	-331,5782567602	6,80	-331,6540425083
6,90	-331,4645343271	6,90	-331,5782563222	6,90	-331,6540420649
7,00	-331,4645339429	7,00	-331,5782559287	7,00	-331,6540416667

7,10	-331,4645335994	7,10	-331,5782555745	7,10	-331,6540413085
7,20	-331,464533288	7,20	-331,5782552552	7,20	-331,6540409858
7,30	-331,4645330067	7,30	-331,5782549669	7,30	-331,6540406946
7,40	-331,4645327522	7,40	-331,5782547063	7,40	-331,6540404314
7,50	-331,4645325215	7,50	-331,5782544703	7,50	-331,6540401932
7,60	-331,4645323122	7,60	-331,5782542563	7,60	-331,6540399773
7,70	-331,464532122	7,70	-331,578254062	7,70	-331,6540397813
7,80	-331,4645319489	7,80	-331,5782538853	7,80	-331,6540396031
7,90	-331,4645317912	7,90	-331,5782537244	7,90	-331,654039441
8,00	-331,4645316473	8,00	-331,5782535777	8,00	-331,6540392931
8,10	-331,4645315159	8,10	-331,5782534438	8,10	-331,6540391582
8,20	-331,4645313958	8,20	-331,5782533214	8,20	-331,654039035
8,30	-331,4645312858	8,30	-331,5782532095	8,30	-331,6540389222
8,40	-331,464531185	8,40	-331,578253107	8,40	-331,6540388189
8,50	-331,4645310925	8,50	-331,5782530129	8,50	-331,6540387242
8,60	-331,4645310075	8,60	-331,5782529265	8,60	-331,6540386373
8,70	-331,4645309294	8,70	-331,5782528471	8,70	-331,6540385574
8,80	-331,4645308575	8,80	-331,578252774	8,80	-331,6540384839
8,90	-331,4645307912	8,90	-331,5782527068	8,90	-331,6540384163
9,00	-331,4645307301	9,00	-331,5782526448	9,00	-331,6540383539
9,10	-331,4645306737	9,10	-331,5782525876	9,10	-331,6540382963
9,20	-331,4645306215	9,20	-331,5782525347	9,20	-331,6540382432
9,30	-331,4645305733	9,30	-331,5782524858	9,30	-331,654038194
9,40	-331,4645305286	9,40	-331,5782524406	9,40	-331,6540381486
9,50	-331,4645304873	9,50	-331,5782523987	9,50	-331,6540381065
9,60	-331,4645304489	9,60	-331,5782523599	9,60	-331,6540380674
9,70	-331,4645304133	9,70	-331,5782523239	9,70	-331,6540380313
9,80	-331,4645303803	9,80	-331,5782522905	9,80	-331,6540379977
9,90	-331,4645303496	9,90	-331,5782522594	9,90	-331,6540379664
10,00	-331,464530321	10,00	-331,5782522305	10,00	-331,6540379374
10,10	-331,4645302943	10,10	-331,5782522036	10,10	-331,6540379104
10,20	-331,4645302696	10,20	-331,5782521786	10,20	-331,6540378852

10,30	-331,4645302464	10,30	-331,5782521552	10,30	-331,6540378618
10,40	-331,4645302249	10,40	-331,5782521335	10,40	-331,6540378399
10,50	-331,4645302047	10,50	-331,5782521132	10,50	-331,6540378195
10,60	-331,4645301859	10,60	-331,5782520942	10,60	-331,6540378005
10,70	-331,4645301683	10,70	-331,5782520764	10,70	-331,6540377827
10,80	-331,4645301519	10,80	-331,5782520598	10,80	-331,654037766
10,90	-331,4645301365	10,90	-331,5782520443	10,90	-331,6540377504
11,00	-331,464530122	11,00	-331,5782520298	11,00	-331,6540377358
11,10	-331,4645301085	11,10	-331,5782520161	11,10	-331,6540377222
11,20	-331,4645300958	11,20	-331,5782520034	11,20	-331,6540377093
11,30	-331,4645300839	11,30	-331,5782519914	11,30	-331,6540376973
11,40	-331,4645300728	11,40	-331,5782519801	11,40	-331,654037686
11,50	-331,4645300623	11,50	-331,5782519696	11,50	-331,6540376754
11,60	-331,4645300524	11,60	-331,5782519596	11,60	-331,6540376654
11,70	-331,4645300431	11,70	-331,5782519503	11,70	-331,6540376561
11,80	-331,4645300344	11,80	-331,5782519415	11,80	-331,6540376473
11,90	-331,4645300261	11,90	-331,5782519332	11,90	-331,654037639
12,00	-331,4645300184	12,00	-331,5782519254	12,00	-331,6540376311

Tabela 5.6: Sistema diatômico He-Rn

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
3,00	-290,7123992045	3,00	-290,8478632322	3,00	-290,9433623324
3,10	-290,7131963628	3,10	-290,8486121173	3,10	-290,9440902255
3,20	-290,7137577573	3,20	-290,8491356538	3,20	-290,9445970548
3,30	-290,7141499776	3,30	-290,8494981805	3,30	-290,9449464576
3,40	-290,7144214339	3,40	-290,8497463281	3,40	-290,9451844069
3,50	-290,7146071653	3,50	-290,8499137425	3,50	-290,9453439816
3,60	-290,7147324221	3,60	-290,850024585	3,60	-290,9454488312
3,70	-290,7148153182	3,70	-290,8500961258	3,70	-290,9455157908
3,80	-290,7148687855	3,80	-290,8501406268	3,80	-290,9455567762

3,90	-290,7149020063	3,90	-290,850166749	3,90	-290,9455801766
4,00	-290,7149214607	4,00	-290,8501805605	4,00	-290,9455918668
4,10	-290,7149316606	4,10	-290,850186314	4,01	-290,9455925629
4,20	-290,7149358255	4,11	-290,8501865677	4,02	-290,9455931847
4,21	-290,7149360011	4,12	-290,8501867714	4,03	-290,9455937376
4,22	-290,7149361384	4,13	-290,8501869287	4,04	-290,9455942247
4,23	-290,7149362408	4,14	-290,8501870418	4,05	-290,9455946467
4,24	-290,7149363099	4,15	-290,8501871129	4,06	-290,9455950127
4,25	-290,7149363473	**4,16**	**-290,850187144**	4,07	-290,9455953193
4,26	**-290,7149363545**	4,17	-290,8501871371	4,08	-290,9455955712
4,27	-290,7149363329	4,18	-290,8501870939	4,09	-290,9455957709
4,28	-290,714936284	4,19	-290,8501870163	4,10	-290,9455959208
4,29	-290,714936209	4,20	-290,850186906	4,11	-290,9455960231
4,30	-290,7149361092	4,21	-290,8501867646	4,12	-290,9455960802
4,31	-290,7149359858	4,22	-290,8501865937	**4,13**	**-290,9455960943**
4,32	-290,7149358401	4,23	-290,8501863947	4,14	-290,9455960672
4,33	-290,7149356731	4,24	-290,8501861692	4,15	-290,9455959909
4,34	-290,714935486	4,25	-290,8501859186	4,16	-290,9455958894
4,35	-290,7149352798	4,26	-290,8501856442	4,17	-290,9455957512
4,36	-290,7149350555	4,27	-290,8501853474	4,18	-290,9455955797
4,37	-290,7149348141	4,28	-290,8501850293	4,19	-290,9455953764
4,38	-290,7149345566	4,29	-290,8501846911	4,20	-290,945595143
4,39	-290,7149342837	4,30	-290,850184334	4,21	-290,9455948811
4,40	-290,7149339964	4,40	-290,8501799392	4,22	-290,945594592
4,50	-290,7149304982	4,50	-290,850174624	4,23	-290,9455942775
4,60	-290,7149263021	4,60	-290,8501689588	4,24	-290,9455939387
4,70	-290,7149218024	4,70	-290,850163314	4,25	-290,9455935772
4,80	-290,7149173009	4,80	-290,8501578939	4,30	-290,945591478
4,90	-290,7149129662	4,90	-290,8501528281	4,40	-290,9455861895
5,00	-290,7149088952	5,00	-290,8501481749	4,50	-290,9455801348
5,10	-290,7149051361	5,10	-290,8501439514	4,60	-290,9455738709
5,20	-290,7149017066	5,20	-290,8501401516	4,70	-290,9455677184

5,30	-290,7148986042	5,30	-290,8501367521	4,80	-290,9455618885
5,40	-290,7148958146	5,40	-290,8501337237	4,90	-290,945556487
5,50	-290,7148933172	5,50	-290,8501310337	5,00	-290,9455515596
5,60	-290,7148910877	5,60	-290,8501286504	5,10	-290,9455471295
5,70	-290,7148891018	5,70	-290,8501265374	5,20	-290,9455431427
5,80	-290,7148873339	5,80	-290,8501246662	5,30	-290,9455395978
5,90	-290,7148857614	5,90	-290,8501230083	5,40	-290,9455364505
6,00	-290,714884362	6,00	-290,8501215388	5,50	-290,9455336638
6,10	-290,7148831173	6,10	-290,8501202351	5,60	-290,9455311993
6,20	-290,7148820089	6,20	-290,8501190773	5,70	-290,9455290213
6,30	-290,714881021	6,30	-290,8501180478	5,80	-290,9455270967
6,40	-290,7148801395	6,40	-290,8501171311	5,90	-290,945525395
6,50	-290,714879352	6,50	-290,8501163138	6,00	-290,9455238895
6,60	-290,7148786475	6,60	-290,8501155839	6,10	-290,9455225561
6,70	-290,7148780164	6,70	-290,8501149311	6,20	-290,9455213737
6,80	-290,7148774504	6,80	-290,8501143464	6,30	-290,9455203238
6,90	-290,7148769418	6,90	-290,8501138218	6,40	-290,94551939
7,00	-290,7148764824	7,00	-290,8501133504	6,50	-290,9455185584
7,10	-290,7148760721	7,10	-290,8501129262	6,60	-290,9455178165
7,20	-290,7148756999	7,20	-290,8501125438	6,70	-290,9455171536
7,30	-290,7148753638	7,30	-290,8501121986	6,80	-290,9455165603
7,40	-290,7148750596	7,40	-290,8501118866	6,90	-290,9455160284
7,50	-290,714874784	7,50	-290,850111604	7,00	-290,9455155508
7,60	-290,7148745339	7,60	-290,8501113479	7,10	-290,9455151211
7,70	-290,7148743066	7,70	-290,8501111153	7,20	-290,9455147342
7,80	-290,7148740999	7,80	-290,8501109039	7,30	-290,9455143852
7,90	-290,7148739115	7,90	-290,8501107114	7,40	-290,9455140697
8,00	-290,7148737397	8,00	-290,8501105359	7,50	-290,9455137843
8,10	-290,7148735829	8,10	-290,8501103757	7,60	-290,9455135256
8,20	-290,7148734394	8,20	-290,8501102294	7,70	-290,9455132908
8,30	-290,7148733081	8,30	-290,8501100955	7,80	-290,9455130774
8,40	-290,7148731878	8,40	-290,8501099729	7,90	-290,9455128833

8,50	-290,7148730774	8,50	-290,8501098604	8,00	-290,9455127063
8,60	-290,714872976	8,60	-290,8501097573	8,10	-290,9455125449
8,70	-290,7148728828	8,70	-290,8501096624	8,20	-290,9455123975
8,80	-290,714872797	8,80	-290,8501095751	8,30	-290,9455122626
8,90	-290,714872718	8,90	-290,8501094947	8,40	-290,9455121391
9,00	-290,7148726451	9,00	-290,8501094206	8,50	-290,9455120258
9,10	-290,7148725778	9,10	-290,8501093522	8,60	-290,9455119219
9,20	-290,7148725157	9,20	-290,8501092891	8,70	-290,9455118265
9,30	-290,7148724582	9,30	-290,8501092308	8,80	-290,9455117386
9,40	-290,714872405	9,40	-290,8501091768	8,90	-290,9455116578
9,50	-290,7148723557	9,50	-290,8501091268	9,00	-290,9455115833
9,60	-290,71487231	9,60	-290,8501090804	9,10	-290,9455115146
9,70	-290,7148722675	9,70	-290,8501090375	9,20	-290,9455114511
9,80	-290,7148722281	9,80	-290,8501089976	9,30	-290,9455113925
9,90	-290,7148721915	9,90	-290,8501089605	9,40	-290,9455113382
10,00	-290,7148721575	10,00	-290,850108926	9,50	-290,945511288
10,10	-290,7148721258	10,10	-290,8501088939	9,60	-290,9455112414
10,20	-290,7148720962	10,20	-290,850108864	9,70	-290,9455111983
10,30	-290,7148720687	10,30	-290,8501088362	9,80	-290,9455111582
10,40	-290,714872043	10,40	-290,8501088102	9,90	-290,945511121
10,50	-290,714872019	10,50	-290,850108786	10,00	-290,9455110864
10,60	-290,7148719966	10,60	-290,8501087633	10,10	-290,9455110542
10,70	-290,7148719757	10,70	-290,8501087422	10,20	-290,9455110241
10,80	-290,7148719561	10,80	-290,8501087223	10,30	-290,9455109962
10,90	-290,7148719377	10,90	-290,8501087038	10,40	-290,9455109701
11,00	-290,7148719206	11,00	-290,8501086865	10,50	-290,9455109458
11,10	-290,7148719045	11,10	-290,8501086703	10,60	-290,9455109231
11,20	-290,7148718894	11,20	-290,850108655	10,70	-290,9455109019
11,30	-290,7148718752	11,30	-290,8501086407	10,80	-290,945510882
11,40	-290,7148718619	11,40	-290,8501086273	10,90	-290,9455108634
11,50	-290,7148718494	11,50	-290,8501086147	11,00	-290,945510846
11,60	-290,7148718376	11,60	-290,8501086028	11,10	-290,9455108298

11,70	-290,7148718266	11,70	-290,8501085917	11,20	-290,9455108144
11,80	-290,7148718162	11,80	-290,8501085812	11,30	-290,9455108001
11,90	-290,7148718064	11,90	-290,8501085714	11,40	-290,9455107867
12,00	-290,7148717972	12,00	-290,8501085621	11,50	-290,9455107741
				11,60	-290,9455107622
				11,70	-290,945510751
				11,80	-290,9455107405
				11,90	-290,9455107306
				12,00	-290,9455107213

Tabela 5.7: Sistema diatômico Ne-Ne

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-257,6118694068	2,00	-257,6820198143	2,00 -257,707008897	
2,10	-257,6170649418	2,10	-257,6870548539	2,10	-257,7119987964
2,20	-257,6203177747	2,20	-257,6901938001	2,20	-257,7150987484
2,30	-257,6223416811	2,30	-257,6921398026	2,30	-257,7170113403
2,40	-257,623589943	2,40	-257,6933366747	2,40	-257,7181803622
2,50	-257,6243505719	2,50	-257,6940645625	2,50	-257,7188858334
2,60	-257,6248066139	2,60	-257,6945001539	2,60	-257,7193040528
2,70	-257,625074242	2,70	-257,6947547138	2,70	-257,7195456632
2,80	-257,6252268065	2,80	-257,6948981519	2,80	-257,7196797777
2,90	-257,6253101936	2,90	-257,6949742693	2,90	-257,7197493572
3,00	-257,6253527268	3,00	-257,6950104078	3,00	-257,7197809377
3,10	-257,6253716235	3,10	-257,695023394	3,10	-257,719790783
3,11	-257,6253726538	3,11	-257,6950238655	3,11	-257,7197909923
3,12	-257,6253735626	3,12	-257,6950242237	3,12	-257,7197910782
3,13	-257,625374355	3,13	-257,695024468	**3,13**	**-257,719791079**
3,14	-257,625375039	3,14	-257,6950246106	3,14	-257,7197909824
3,15	-257,6253756208	**3,15**	**-257,6950246569**	3,15	-257,7197907972
3,16	-257,6253761065	3,16	-257,6950246133	3,16	-257,7197905288

3,17	-257,6253765018	3,17	-257,6950244854	3,17	-257,7197901821
3,18	-257,6253768122	3,18	-257,6950242792	3,18	-257,7197897636
3,19	-257,6253770428	3,19	-257,6950239998	3,19	-257,7197892779
3,20	-257,6253771986	3,20	-257,6950236522	3,20	-257,7197887294
3,21	-257,6253772841	3,21	-257,6950232411	3,21	-257,7197881231
3,22	**-257,6253773038**	3,22	-257,6950227712	3,22	-257,7197874628
3,23	-257,6253772618	3,23	-257,6950222466	3,23	-257,7197867526
3,24	-257,625377162	3,24	-257,6950216714	3,24	-257,7197859964
3,25	-257,6253770083	3,25	-257,6950210494	3,25	-257,7197851976
3,26	-257,625376804	3,26	-257,6950203843	3,26	-257,7197843596
3,27	-257,6253765526	3,27	-257,6950196794	3,27	-257,7197834861
3,28	-257,6253762573	3,28	-257,695018938	3,28	-257,7197825798
3,29	-257,625375921	3,29	-257,6950181632	3,29	-257,7197816437
3,30	-257,6253755459	3,30	-257,6950173573	3,30	-257,7197806775
3,40	-257,6253702307	3,40	-257,695008154	3,40	-257,7197700535
3,50	-257,6253633078	3,50	-257,6949980877	3,50	-257,7197588001
3,60	-257,6253559391	3,60	-257,6949882487	3,60	-257,7197479208
3,70	-257,6253487589	3,70	-257,6949791655	3,70	-257,719737951
3,80	-257,6253420916	3,80	-257,6949710455	3,80	-257,7197290767
3,90	-257,6253360795	3,90	-257,6949639263	3,90	-257,7197212947
4,00	-257,6253307603	4,00	-257,6949577574	4,00	-257,7197146111
4,10	-257,6253261119	4,10	-257,6949524504	4,10	-257,7197089112
4,20	-257,6253220827	4,20	-257,6949479023	4,20	-257,7197040251
4,30	-257,6253186103	4,30	-257,6949440178	4,30	-257,7196998692
4,40	-257,6253156278	4,40	-257,6949406944	4,40	-257,7196963295
4,50	-257,625313064	4,50	-257,6949378498	4,50	-257,7196933191
4,60	-257,6253108659	4,60	-257,6949354206	4,60	-257,7196907522
4,70	-257,6253089769	4,70	-257,6949333357	4,70	-257,7196885788
4,80	-257,6253073526	4,80	-257,6949315487	4,80	-257,7196866825
4,90	-257,6253059431	4,90	-257,6949300099	4,90	-257,7196850708
5,00	-257,6253047432	5,00	-257,6949286825	5,00	-257,7196836837
5,10	-257,6253036939	5,10	-257,6949275356	5,10	-257,7196824865

5,20	-257,625302783	5,20	-257,6949265398	5,20	-257,7196814493
5,30	-257,6253019907	5,30	-257,6949256742	5,30	-257,7196805492
5,40	-257,625301299	5,40	-257,6949249202	5,40	-257,7196797654
5,50	-257,625300694	5,50	-257,6949242612	5,50	-257,7196790814
5,60	-257,6253001637	5,60	-257,6949236848	5,60	-257,7196784832
5,70	-257,6252996966	5,70	-257,6949231771	5,70	-257,7196779575
5,80	-257,6252992859	5,80	-257,6949227305	5,80	-257,7196774954
5,90	-257,6252989229	5,90	-257,6949223366	5,90	-257,7196770879
6,00	-257,6252986018	6,00	-257,6949219882	6,00	-257,7196767279
6,10	-257,6252983175	6,10	-257,6949216802	6,10	-257,7196764095
6,20	-257,6252980638	6,20	-257,6949214053	6,20	-257,7196761262
6,30	-257,6252978387	6,30	-257,6949211609	6,30	-257,7196758744
6,40	-257,6252976375	6,40	-257,6949209432	6,40	-257,7196756501
6,50	-257,6252974574	6,50	-257,6949207486	6,50	-257,7196754498
6,60	-257,6252972973	6,60	-257,6949205752	6,60	-257,7196752709
6,70	-257,6252971523	6,70	-257,6949204184	6,70	-257,71967511
6,80	-257,6252970229	6,80	-257,6949202778	6,80	-257,7196749658
6,90	-257,6252969059	6,90	-257,6949201516	6,90	-257,7196748361
7,00	-257,6252968007	7,00	-257,6949200378	7,00	-257,7196747193
7,10	-257,625296706	7,10	-257,6949199358	7,10	-257,7196746142
7,20	-257,6252966193	7,20	-257,6949198424	7,20	-257,7196745186
7,30	-257,6252965417	7,30	-257,6949197581	7,30	-257,7196744324
7,40	-257,6252964709	7,40	-257,6949196819	7,40	-257,7196743543
7,50	-257,6252964068	7,50	-257,6949196126	7,50	-257,7196742834
7,60	-257,6252963488	7,60	-257,6949195505	7,60	-257,7196742193
7,70	-257,6252962951	7,70	-257,6949194927	7,70	-257,7196741604
7,80	-257,6252962469	7,80	-257,6949194402	7,80	-257,719674107
7,90	-257,6252962025	7,90	-257,6949193925	7,90	-257,7196740582
8,00	-257,6252961621	8,00	-257,694919349	8,00	-257,7196740137
8,10	-257,6252961255	8,10	-257,6949193099	8,10	-257,7196739734
8,20	-257,625296091	8,20	-257,6949192729	8,20	-257,7196739358
8,30	-257,6252960602	8,30	-257,6949192392	8,30	-257,7196739016

8,40	-257,6252960315	8,40	-257,6949192085	8,40	-257,7196738703
8,50	-257,6252960054	8,50	-257,6949191803	8,50	-257,7196738415
8,60	-257,6252959816	8,60	-257,6949191551	8,60	-257,7196738153
8,70	-257,6252959588	8,70	-257,6949191307	8,70	-257,7196737906
8,80	-257,6252959386	8,80	-257,6949191084	8,80	-257,7196737682
8,90	-257,6252959196	8,90	-257,6949190881	8,90	-257,7196737475
9,00	-257,6252959022	9,00	-257,6949190693	9,00	-257,7196737284
9,10	-257,625295886	9,10	-257,694919052	9,10	-257,7196737107
9,20	-257,6252958711	9,20	-257,6949190359	9,20	-257,7196736944
9,30	-257,6252958573	9,30	-257,6949190211	9,30	-257,7196736792
9,40	-257,6252958445	9,40	-257,6949190074	9,40	-257,7196736652
9,50	-257,6252958326	9,50	-257,6949189947	9,50	-257,7196736523
9,60	-257,6252958216	9,60	-257,6949189828	9,60	-257,7196736402
9,70	-257,6252958113	9,70	-257,6949189719	9,70	-257,7196736294
9,80	-257,6252958018	9,80	-257,6949189616	9,80	-257,7196736186
9,90	-257,625295793	9,90	-257,6949189521	9,90	-257,719673609
10,00	-257,6252957851	10,00	-257,6949189441	10,00	-257,7196735999
10,10	-257,6252957768	10,10	-257,6949189353	10,10	-257,7196735915
10,20	-257,62529577	10,20	-257,6949189273	10,20	-257,7196735837
10,30	-257,6252957631	10,30	-257,6949189201	10,30	-257,7196735764
10,40	-257,625295757	10,40	-257,6949189134	10,40	-257,7196735696
10,50	-257,6252957511	10,50	-257,6949189071	10,50	-257,7196735632
10,60	-257,6252957456	10,60	-257,6949189013	10,60	-257,7196735573
10,70	-257,6252957405	10,70	-257,6949188959	10,70	-257,7196735521
10,80	-257,6252957357	10,80	-257,6949188908	10,80	-257,7196735465
10,90	-257,6252957312	10,90	-257,694918886	10,90	-257,7196735418
11,00	-257,6252957271	11,00	-257,6949188815	11,00	-257,7196735371
11,10	-257,6252957231	11,10	-257,6949188773	11,10	-257,7196735288
11,20	-257,6252957194	11,20	-257,6949188733	11,20	-257,7196735251
11,30	-257,625295716	11,30	-257,6949188696	11,30	-257,7196735215
11,40	-257,6252957127	11,40	-257,6949188661	11,40	-257,7196735182
11,50	-257,6252957096	11,50	-257,6949188628	11,50	-257,7196735182

11,60	-257,6252957068	11,60	-257,6949188598	11,60	-257,719673515
11,70	-257,625295704	11,70	-257,6949188569	11,70	-257,7196735124
11,80	-257,6252957015	11,80	-257,6949188541	11,80	-257,7196735093
11,90	-257,6252956991	11,90	-257,6949188515	11,90	-257,7196735068
12,00	-257,6252956968	12,00	-257,6949188491	12,00	-257,7196735042
				12,10	-257,719673502

Tabela 5.8: Sistema diatômico Ne-Ar

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-655,8050327061	2,00	-655,8678603251	2,00	-655,8893126982
2,10	-655,8236249726	2,10	-655,88601833	2,10	-655,9073121981
2,20	-655,8362748133	2,20	-655,8983450195	2,20	-655,9195170341
2,30	-655,8448304895	2,30	-655,9066625598	2,30	-655,9277406831
2,40	-655,8505829819	2,40	-655,9122399805	2,40	-655,9332456317
2,50	-655,8544270942	2,50	-655,915954759	2,50	-655,9369043991
2,60	-655,8569788477	2,60	-655,918410063	2,60	-655,9393164205
2,70	-655,8586597734	2,70	-655,9200182925	2,70	-655,9408912847
2,80	-655,8597568138	2,80	-655,9210600272	2,80	-655,9419073953
2,90	-655,8604644287	2,90	-655,9217253059	2,90	-655,9425530861
3,00	-655,8609139005	3,00	-655,9221422508	3,00	-655,9429550836
3,10	-655,8611935249	3,10	-655,9223968202	3,10	-655,9431982677
3,20	-655,8613624388	3,20	-655,9225463902	3,20	-655,9433391595
3,30	-655,8614600346	3,30	-655,9226289673	3,30	-655,9434150739
3,40	-655,8615124007	3,40	-655,9226695916	3,40	-655,9434505196
3,50	-655,8615366575	3,41	-655,9226720234	3,41	-655,9434524955
3,51	-655,8615380045	3,42	-655,9226742259	3,42	-655,9434542561
3,52	-655,8615391943	3,43	-655,9226762014	3,43	-655,9434558001
3,53	-655,8615402341	3,44	-655,9226779612	3,44	-655,9434571384
3,54	-655,8615411319	3,45	-655,9226795164	3,45	-655,9434582818
3,55	-655,861541895	3,46	-655,9226808776	3,46	-655,9434592404

3,56	-655,8615425305	3,47	-655,922682055	3,47	-655,9434600242
3,57	-655,8615430453	3,48	-655,9226830583	3,48	-655,9434606425
3,58	-655,8615434459	3,49	-655,9226838967	3,49	-655,9434611041
3,59	-655,8615437385	3,50	-655,922684579	3,50	-655,9434614178
3,60	-655,8615439291	3,51	-655,9226851133	3,51	-655,9434615916
3,61	-655,8615440233	3,52	-655,9226855079	**3,52**	**-655,9434616333**
3,62	**-655,8615440254**	3,53	-655,9226857702	3,53	-655,9434615505
3,63	-655,8615439428	3,54	-655,9226859076	3,54	-655,9434613502
3,64	-655,8615437795	**3,55**	**-655,9226859355**	3,55	-655,9434610393
3,65	-655,86154354	3,56	-655,9226858437	3,56	-655,9434606242
3,66	-655,8615432308	3,57	-655,9226856472	3,57	-655,9434601112
3,67	-655,8615428523	3,58	-655,922685352	3,58	-655,9434595062
3,68	-655,8615424107	3,59	-655,922684964	3,59	-655,9434588148
3,69	-655,8615419096	3,60	-655,9226844787	3,60	-655,9434580454
3,70	-655,8615413519	3,70	-655,922675989	3,70	-655,9434468857
3,80	-655,8615334293	3,80	-655,9226632845	3,80	-655,9434319953
3,90	-655,8615229477	3,90	-655,9226489263	3,90	-655,9434158345
4,00	-655,8615115852	4,00	-655,9226344165	4,00	-655,9433998281
4,10	-655,8615003146	4,10	-655,9226205859	4,10	-655,9433847453
4,20	-655,8614896654	4,20	-655,9226078709	4,20	-655,943370986
4,30	-655,8614798975	4,30	-655,922596424	4,30	-655,9433586739
4,40	-655,8614711048	4,40	-655,9225862717	4,40	-655,9433478036
4,50	-655,8614632879	4,50	-655,922577353	4,50	-655,9433382774
4,60	-655,8614563958	4,60	-655,9225695611	4,60	-655,9433300147
4,70	-655,8614503519	4,70	-655,9225627938	4,70	-655,9433228359
4,80	-655,861445068	4,80	-655,922556916	4,80	-655,9433166295
4,90	-655,861440459	4,90	-655,9225518194	4,90	-655,943311264
5,00	-655,8614364412	5,00	-655,9225474022	5,00	-655,9433066318
5,10	-655,8614329386	5,10	-655,9225435615	5,10	-655,9433026127
5,20	-655,8614298831	5,20	-655,9225402339	5,20	-655,943299137
5,30	-655,8614272196	5,30	-655,9225373368	5,30	-655,9432961164
5,40	-655,861424892	5,40	-655,9225348124	5,40	-655,9432934905

5,50	-655,8614228552	5,50	-655,9225326081	5,50	-655,9432912019
5,60	-655,8614210713	5,60	-655,9225306765	5,60	-655,9432892014
5,70	-655,8614194956	5,70	-655,922528989	5,70	-655,9432874536
5,80	-655,8614181179	5,80	-655,922527503	5,80	-655,9432859174
5,90	-655,8614169019	5,90	-655,9225261881	5,90	-655,943284567
6,00	-655,8614158277	6,00	-655,9225250348	6,00	-655,9432833763
6,10	-655,8614148782	6,10	-655,9225240149	6,10	-655,9432823231
6,20	-655,8614140331	6,20	-655,922523115	6,20	-655,9432813934
6,30	-655,8614132822	6,30	-655,9225223104	6,30	-655,9432805664
6,40	-655,8614126131	6,40	-655,9225215949	6,40	-655,9432798315
6,50	-655,8614120161	6,50	-655,9225209568	6,50	-655,9432791766
6,60	-655,8614114826	6,60	-655,9225203824	6,60	-655,9432785911
6,70	-655,8614110039	6,70	-655,922519877	6,70	-655,9432780693
6,80	-655,8614105742	6,80	-655,9225194193	6,80	-655,9432776004
6,90	-655,8614101883	6,90	-655,9225190085	6,90	-655,9432771798
7,00	-655,8614098411	7,00	-655,9225186388	7,00	-655,9432768016
7,10	-655,8614095294	7,10	-655,9225183014	7,10	-655,9432764603
7,20	-655,8614092461	7,20	-655,9225180052	7,20	-655,9432761537
7,30	-655,8614089905	7,30	-655,9225177332	7,30	-655,9432758758
7,40	-655,8614087587	7,40	-655,9225174871	7,40	-655,9432756245
7,50	-655,8614085485	7,50	-655,9225172639	7,50	-655,9432753967
7,60	-655,861408358	7,60	-655,922517057	7,60	-655,9432751894
7,70	-655,8614081837	7,70	-655,9225168773	7,70	-655,9432750023
7,80	-655,8614080257	7,80	-655,9225167093	7,80	-655,9432748311
7,90	-655,8614078813	7,90	-655,9225165564	7,90	-655,9432746754
8,00	-655,8614077497	8,00	-655,9225164169	8,00	-655,9432745332
8,10	-655,8614076297	8,10	-655,9225162851	8,10	-655,9432744028
8,20	-655,8614075194	8,20	-655,9225161728	8,20	-655,9432742848
8,30	-655,8614074181	8,30	-655,9225160658	8,30	-655,9432741758
8,40	-655,8614073253	8,40	-655,9225159678	8,40	-655,9432740762
8,50	-655,8614072402	8,50	-655,9225158778	8,50	-655,9432739846
8,60	-655,8614071624	8,60	-655,9225157908	8,60	-655,9432739

8,70	-655,8614070595	8,70	-655,9225157192	8,70	-655,9432738235
8,80	-655,8614069934	8,80	-655,922515649	8,80	-655,9432737521
8,90	-655,8614069321	8,90	-655,9225155844	8,90	-655,9432736865
9,00	-655,8614068757	9,00	-655,9225155248	9,00	-655,943273626
9,10	-655,8614068236	9,10	-655,9225154698	9,10	-655,9432735702
9,20	-655,8614067754	9,20	-655,9225154189	9,20	-655,9432735185
9,30	-655,8614067308	9,30	-655,9225153719	9,30	-655,9432734708
9,40	-655,8614066894	9,40	-655,9225153283	9,40	-655,9432734266
9,50	-655,8614066511	9,50	-655,9225152879	9,50	-655,9432733851
9,60	-655,8614066156	9,60	-655,9225152505	9,60	-655,9432733478
9,70	-655,8614065826	9,70	-655,9225152158	9,70	-655,9432733124
9,80	-655,8614065519	9,80	-655,9225151834	9,80	-655,9432732796
9,90	-655,8614065234	9,90	-655,9225151534	9,90	-655,9432732492
10,00	-655,8614064968	10,00	-655,9225151254	10,00	-655,9432732209
10,10	-655,8614064721	10,10	-655,9225150993	10,10	-655,9432731945
10,20	-655,8614064491	10,20	-655,9225150751	10,20	-655,9432731699
10,30	-655,8614064276	10,30	-655,9225150525	10,30	-655,943273147
10,40	-655,8614064075	10,40	-655,9225150314	10,40	-655,9432731256
10,50	-655,8614063888	10,50	-655,9225150116	10,50	-655,9432731051
10,60	-655,8614063713	10,60	-655,9225149932	10,60	-655,9432730872
10,70	-655,8614063549	10,70	-655,9225149761	10,70	-655,9432730696
10,80	-655,8614063395	10,80	-655,9225149599	10,80	-655,9432730533
10,90	-655,8614063252	10,90	-655,9225149448	10,90	-655,943273038
11,00	-655,8614063117	11,00	-655,9225149306	11,00	-655,9432730237
11,10	-655,8614062991	11,10	-655,9225149174	11,10	-655,9432730103
11,20	-655,8614062873	11,20	-655,9225149049	11,20	-655,9432729977
11,30	-655,8614062762	11,30	-655,9225148933	11,30	-655,9432729859
11,40	-655,8614062658	11,40	-655,9225148823	11,40	-655,9432729748
11,50	-655,8614062559	11,50	-655,922514872	11,50	-655,9432729644
11,60	-655,8614062467	11,60	-655,9225148623	11,60	-655,9432729548
11,70	-655,8614062381	11,70	-655,9225148533	11,70	-655,9432729454
11,80	-655,8614062299	11,80	-655,9225148447	11,80	-655,9432729368

11,90	-655,8614062222	11,90	-655,9225148366	11,90	-655,9432729286
12,00	-655,861406215	12,00	-655,922514829	12,00	-655,9432729209
12,10	-655,8614062081	12,10	-655,9225148218	12,10	-655,9432729136

Tabela 5.9: Sistema diatômico Ne-Kr

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-2881,0390193816	2,00	-2881,1517177885	2,00	-2881,2509783567
2,10	-2881,0653292905	2,10	-2881,1774068488	2,10	-2881,2764879683
2,20	-2881,0838167166	2,20	-2881,1954059443	2,20	-2881,2943352951
2,30	-2881,0967187344	2,30	-2881,2079379901	2,30	-2881,3067359739
2,40	-2881,105664658	2,40	-2881,2166121631	2,40	-2881,3152963688
2,50	-2881,1118283706	2,50	-2881,2225797018	2,50	-2881,3211674734
2,60	-2881,1160480379	2,60	-2881,2266579845	2,60	-2881,3251665618
2,70	-2881,1189175733	2,70	-2881,2294241875	2,70	-2881,3278700612
2,80	-2881,1208549061	2,80	-2881,231284207	2,80	-2881,3296817552
2,90	-2881,1221522529	2,90	-2881,2325220649	2,90	-2881,3308831791
3,00	-2881,1230127623	3,00	-2881,2333355543	3,00	-2881,3316696055
3,10	-2881,1235768829	3,10	-2881,2338616641	3,10	-2881,3321757326
3,20	-2881,1239411978	3,20	-2881,2341947679	3,20	-2881,3324941352
3,30	-2881,124171772	3,30	-2881,234399498	3,30	-2881,3326879689
3,40	-2881,1243135571	3,40	-2881,2345198837	3,40	-2881,3328001877
3,50	-2881,1243969975	3,50	-2881,234585677	3,50	-2881,3328597552
3,60	-2881,124442588	3,60	-2881,2346168396	3,60	-2881,3328860488
3,70	-2881,1244640551	3,61	-2881,2346186077	3,61	-2881,3328874055
3,71	-2881,1244652563	3,62	-2881,2346201745	3,62	-2881,3328885296
3,72	-2881,1244663187	3,63	-2881,2346215514	3,63	-2881,3328895216
3,73	-2881,1244672474	3,64	-2881,2346227477	3,64	-2881,3328902947
3,74	-2881,1244680492	3,65	-2881,2346237727	3,65	-2881,3328909279
3,75	-2881,1244687304	3,66	-2881,2346246349	3,66	-2881,3328914069
3,76	-2881,1244692969	3,67	-2881,2346253426	3,67	-2881,3328917394

3,77	-2881,1244697545	3,68	-2881,234625904	3,68	-2881,3328919332
3,78	-2881,1244701088	3,69	-2881,2346263266	**3,69**	**-2881,3328919956**
3,79	-2881,1244703651	3,70	-2881,2346266177	3,70	-2881,3328919335
3,80	-2881,1244705283	3,71	-2881,2346267844	3,71	-2881,3328917539
3,81	**-2881,1244706034**	**3,72**	**-2881,2346268333**	3,72	-2881,3328914632
3,82	-2881,1244705951	3,73	-2881,2346267709	3,73	-2881,332891068
3,83	-2881,1244705077	3,74	-2881,2346266032	3,74	-2881,3328905737
3,84	-2881,1244703455	3,75	-2881,2346263361	3,75	-2881,3328899862
3,85	-2881,1244701127	3,76	-2881,2346259753	3,76	-2881,3328893111
3,86	-2881,124469813	3,77	-2881,2346255245	3,77	-2881,3328885534
3,87	-2881,1244694505	3,78	-2881,2346249924	3,78	-2881,3328877182
3,88	-2881,1244690307	3,79	-2881,2346243819	3,79	-2881,33288681
3,89	-2881,1244685524	3,80	-2881,2346236958	3,80	-2881,3328858552
3,90	-2881,1244680204	3,90	-2881,2346136859	3,90	-2881,3328731955
4,00	-2881,1244604357	4,00	-2881,2346001444	4,00	-2881,3328574246
4,10	-2881,1244502854	4,10	-2881,2345852553	4,10	-2881,3328406531
4,20	-2881,1244391246	4,20	-2881,23457034	4,20	-2881,3328241782
4,30	-2881,1244279053	4,30	-2881,2345561327	4,30	-2881,3328086325
4,40	-2881,1244171697	4,40	-2881,234543016	4,40	-2881,3327944197
4,50	-2881,1244072087	4,50	-2881,2345311483	4,50	-2881,3327816301
4,60	-2881,1243981472	4,60	-2881,234520554	4,60	-2881,3327702689
4,70	-2881,1243900185	4,70	-2881,2345111842	4,70	-2881,3327602811
4,80	-2881,1243827899	4,80	-2881,2345029456	4,80	-2881,3327515271
4,90	-2881,1243764009	4,90	-2881,2344957305	4,90	-2881,3327438832
5,00	-2881,1243707771	5,00	-2881,2344894268	5,00	-2881,3327372364
5,10	-2881,1243658377	5,10	-2881,2344839248	5,10	-2881,332731461
5,20	-2881,1243615081	5,20	-2881,2344791288	5,20	-2881,3327264377
5,30	-2881,1243577117	5,30	-2881,2344749386	5,30	-2881,3327220619
5,40	-2881,1243543827	5,40	-2881,2344712846	5,40	-2881,3327182504
5,50	-2881,1243514609	5,50	-2881,2344680903	5,50	-2881,3327149258
5,60	-2881,1243488956	5,60	-2881,2344652947	5,60	-2881,3327120186
5,70	-2881,12434664	5,70	-2881,234462842	5,70	-2881,3327094778

5,80	-2881,1243446538	5,80	-2881,2344606888	5,80	-2881,3327072468
5,90	-2881,1243428937	5,90	-2881,2344587932	5,90	-2881,332705286
6,00	-2881,1243413473	6,00	-2881,2344571215	6,00	-2881,3327035589
6,10	-2881,1243399821	6,10	-2881,2344556424	6,10	-2881,3327020323
6,20	-2881,1243387622	6,20	-2881,2344543299	6,20	-2881,332700686
6,30	-2881,1243376837	6,30	-2881,2344531771	6,30	-2881,3326994902
6,40	-2881,1243367221	6,40	-2881,2344521448	6,40	-2881,3326984283
6,50	-2881,1243358654	6,50	-2881,2344512255	6,50	-2881,3326974831
6,60	-2881,1243351008	6,60	-2881,234450401	6,60	-2881,3326966381
6,70	-2881,1243344149	6,70	-2881,2344496713	6,70	-2881,3326958876
6,80	-2881,1243338001	6,80	-2881,2344490139	6,80	-2881,3326952128
6,90	-2881,1243332477	6,90	-2881,234448424	6,90	-2881,3326946082
7,00	-2881,1243327509	7,00	-2881,2344478938	7,00	-2881,332694065
7,10	-2881,1243323032	7,10	-2881,2344474123	7,10	-2881,3326935738
7,20	-2881,1243318983	7,20	-2881,2344469857	7,20	-2881,332693136
7,30	-2881,1243315333	7,30	-2881,2344465966	7,30	-2881,3326927374
7,40	-2881,1243312025	7,40	-2881,2344462447	7,40	-2881,3326923777
7,50	-2881,1243309029	7,50	-2881,2344459258	7,50	-2881,3326920518
7,60	-2881,1243306314	7,60	-2881,2344456324	7,60	-2881,3326917541
7,70	-2881,1243303838	7,70	-2881,2344453735	7,70	-2881,3326914886
7,80	-2881,124330159	7,80	-2881,2344451344	7,80	-2881,3326912436
7,90	-2881,1243299537	7,90	-2881,2344449164	7,90	-2881,3326910215
8,00	-2881,1243297664	8,00	-2881,2344447176	8,00	-2881,3326908187
8,10	-2881,1243295953	8,10	-2881,2344445321	8,10	-2881,3326906314
8,20	-2881,1243294385	8,20	-2881,23444437	8,20	-2881,3326904651
8,30	-2881,1243292954	8,30	-2881,2344442181	8,30	-2881,3326903094
8,40	-2881,1243291639	8,40	-2881,2344440787	8,40	-2881,3326901677
8,50	-2881,1243290432	8,50	-2881,2344439509	8,50	-2881,3326900375
8,60	-2881,1243289323	8,60	-2881,2344438295	8,60	-2881,3326899158
8,70	-2881,12432883	8,70	-2881,2344437254	8,70	-2881,3326898088
8,80	-2881,1243287364	8,80	-2881,2344436261	8,80	-2881,3326897069
8,90	-2881,1243286497	8,90	-2881,2344435345	8,90	-2881,3326896139

9,00	-2881,1243285699	9,00	-2881,23444345	9,00	-2881,332689528
9,10	-2881,1243284961	9,10	-2881,234443372	9,10	-2881,3326894465
9,20	-2881,1243284279	9,20	-2881,2344433	9,20	-2881,3326893759
9,30	-2881,1243283648	9,30	-2881,2344432333	9,30	-2881,3326893077
9,40	-2881,1243283064	9,40	-2881,2344431716	9,40	-2881,3326892451
9,50	-2881,1243282522	9,50	-2881,2344431145	9,50	-2881,332689187
9,60	-2881,124328202	9,60	-2881,2344430615	9,60	-2881,332689131
9,70	-2881,1243281552	9,70	-2881,2344430123	9,70	-2881,3326890835
9,80	-2881,1243281121	9,80	-2881,2344429666	9,80	-2881,3326890368
9,90	-2881,1243280718	9,90	-2881,2344429241	9,90	-2881,3326889938
10,00	-2881,1243280343	10,00	-2881,2344428846	10,00	-2881,3326889537
10,10	-2881,1243279994	10,10	-2881,2344428478	10,10	-2881,3326889141
10,20	-2881,1243279669	10,20	-2881,2344428135	10,20	-2881,3326888817
10,30	-2881,1243279365	10,30	-2881,2344427816	10,30	-2881,3326888492
10,40	-2881,1243279082	10,40	-2881,2344427518	10,40	-2881,332688819
10,50	-2881,1243278818	10,50	-2881,234442724	10,50	-2881,3326887907
10,60	-2881,1243278571	10,60	-2881,2344426979	10,60	-2881,3326887622
10,70	-2881,1243278339	10,70	-2881,2344426736	10,70	-2881,3326887399
10,80	-2881,1243278124	10,80	-2881,2344426509	10,80	-2881,3326887167
10,90	-2881,1243277921	10,90	-2881,2344426296	10,90	-2881,3326886951
11,00	-2881,1243277732	11,00	-2881,2344426097	11,00	-2881,3326886749
11,10	-2881,1243277554	11,10	-2881,234442591	11,10	-2881,3326886538
11,20	-2881,1243277387	11,20	-2881,2344425734	11,20	-2881,3326886384
11,30	-2881,1243277231	11,30	-2881,234442557	11,30	-2881,3326886215
11,40	-2881,1243277084	11,40	-2881,2344425415	11,40	-2881,3326886059
11,50	-2881,1243276946	11,50	-2881,234442527	11,50	-2881,3326885912
11,60	-2881,1243276816	11,60	-2881,2344425134	11,60	-2881,3326885752
11,70	-2881,1243276693	11,70	-2881,2344425006	11,70	-2881,3326885646
11,80	-2881,1243276579	11,80	-2881,2344424885	11,80	-2881,3326885522
11,90	-2881,1243276471	11,90	-2881,2344424771	11,90	-2881,3326885407
12,00	-2881,1243276369	12,00	-2881,2344424664	12,00	-2881,3326885298
12,10	-2881,1243276272	12,10	-2881,2344424563		

Tabela 5.10: Sistema diatômico Ne-Xe

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-457,2461775818	2,00	-457,396904701537	2,00	-457,4859568291
2,10	-457,2828466619	2,10	-457,432631339873	2,10	-457,5214126407
2,20	-457,3096568463	2,20	-457,458710962634	2,20	-457,547273351
2,30	-457,3291210001	2,30	-457,477606707224	2,30	-457,5659850732
2,40	-457,3431586633	2,40	-457,491205384211	2,40	-457,579425607
2,50	-457,3532181999	2,50	-457,500930503093	2,50	-457,5890140808
2,60	-457,3603817596	2,60	-457,507842653791	2,60	-457,5958090874
2,70	-457,3654511816	2,70	-457,512724351486	2,70	-457,6005920185
2,80	-457,3690159591	2,80	-457,516148613921	2,80	-457,6039347877
2,90	-457,3715061682	2,90	-457,518532511270	2,90	-457,6062529827
3,00	-457,3732333391	3,00	-457,520177995968	3,00	-457,6078466428
3,10	-457,3744217957	3,10	-457,521302559712	3,10	-457,6089311102
3,20	-457,3752320715	3,20	-457,522062053104	3,20	-457,6096599728
3,30	-457,3757785003	3,30	-457,522567468464	3,30	-457,6101423303
3,40	-457,3761420597	3,40	-457,522897447813	3,40	-457,6104551186
3,50	-457,3763797741	3,50	-457,523107385976	3,50	-457,6106522829
3,60	-457,376531569	3,60	-457,523236058666	3,60	-457,6107714505
3,70	-457,3766252269	3,70	-457,523310449812	3,70	-457,610838685
3,80	-457,3766799759	3,80	-457,523349191615	3,80	-457,6108719215
3,90	-457,3767090451	3,90	-457,523365035250	3,81	-457,6108738899
3,91	-457,376710917	3,91	-457,5233657178	3,82	-457,6108756487
3,92	-457,3767126317	3,92	-457,5233662681	3,83	-457,6108772139
3,93	-457,3767141964	3,93	-457,5233666922	3,84	-457,6108785914
3,94	-457,376715618	3,94	-457,5233669954	3,85	-457,6108797881
3,95	-457,3767169026	3,95	-457,5233671839	3,86	-457,6108808255
3,96	-457,3767180567	**3,96**	**-457,5233672635**	3,87	-457,6108816955
3,97	-457,3767190859	3,97	-457,5233672397	3,88	-457,6108824128
3,98	-457,3767199961	3,98	-457,5233671179	3,90	-457,6108834103

3,99	-457,3767207926	3,99	-457,523366903	3,91	-457,6108837145
4,00	-457,3767214807	4,00	-457,5233666	3,92	-457,610883888
4,01	-457,3767220656	4,01	-457,5233662145	**3,93**	**-457,610883943**
4,02	-457,376722552	4,02	-457,5233657489	3,94	-457,6108838843
4,03	-457,3767229449	4,03	-457,5233652086	3,95	-457,6108837137
4,04	-457,3767232482	4,04	-457,5233645986	3,96	-457,6108834475
4,05	-457,3767234663	4,05	-457,5233639224	3,97	-457,610883082
4,06	-457,3767236037	4,06	-457,5233631836	3,98	-457,6108826258
4,07	**-457,3767236642**	4,07	-457,5233623858	3,99	-457,6108820826
4,08	-457,3767236515	4,08	-457,5233615326	4,00	-457,6108814551
4,09	-457,3767235694	4,09	-457,5233606273	4,01	-457,6108807547
4,10	-457,3767234192	4,10	-457,523359673323	4,02	-457,6108799786
4,20	-457,3767189933	4,20	-457,523348053248	4,03	-457,6108791338
4,30	-457,3767109405	4,30	-457,523334194888	4,04	-457,6108782243
4,40	-457,3767010757	4,40	-457,523319643688	4,05	-457,610877252
4,50	-457,3766905075	4,50	-457,523305320433	4,06	-457,6108762092
4,60	-457,3766799633	4,60	-457,523291763354	4,07	-457,6108751421
4,70	-457,3766698656	4,70	-457,523279247274	4,08	-457,6108739946
4,80	-457,3766604499	4,80	-457,523267884238	4,09	-457,6108728144
4,90	-457,3766518223	4,90	-457,523257684118	4,10	-457,6108715899
5,00	-457,3766440133	5,00	-457,523248600868	4,11	-457,6108703236
5,10	-457,376637006	5,10	-457,523240555141	4,12	-457,6108690202
5,20	-457,3766307563	5,20	-457,523233454847	4,13	-457,6108676799
5,30	-457,3766252054	5,30	-457,523227203209	4,14	-457,6108663072
5,40	-457,3766202888	5,40	-457,523221706113	4,15	-457,6108649137
5,50	-457,3766159411	5,50	-457,523216874496	4,16	-457,6108634686
5,60	-457,3766121003	5,60	-457,523212626051	4,17	-457,6108620112
5,70	-457,3766087081	5,70	-457,523208889952	4,18	-457,6108605271
5,80	-457,3766057112	5,80	-457,523205601205	4,19	-457,6108590231
5,90	-457,3766030629	5,90	-457,523202702899	4,20	-457,6108575171
6,00	-457,3766007184	6,00	-457,523200144887	4,30	-457,6108415613
6,10	-457,37659864	6,10	-457,523197883699	4,40	-457,6108251906

6,20	-457,3765967976	6,20	-457,523195881898	4,50	-457,6108093208
6,30	-457,3765951607	6,30	-457,523194106459	4,60	-457,6107944493
6,40	-457,3765937044	6,40	-457,523192528991	4,70	-457,6107808262
6,50	-457,3765924066	6,50	-457,523191125153	4,80	-457,6107685357
6,60	-457,3765912473	6,60	-457,523189873437	4,90	-457,6107575664
6,70	-457,3765902122	6,70	-457,523188755344	5,00	-457,6107478466
6,80	-457,3765892833	6,80	-457,523187749772	5,10	-457,6107392774
6,90	-457,3765884519	6,90	-457,523186853890	5,20	-457,6107317492
7,00	-457,3765877044	7,00	-457,523186053537	5,30	-457,6107251453
7,10	-457,3765870315	7,10	-457,523185329016	5,40	-457,610719358
7,20	-457,3765864248	7,20	-457,523184676388	5,50	-457,6107142862
7,30	-457,3765858769	7,30	-457,523184087544	5,60	-457,6107098348
7,40	-457,3765853812	7,40	-457,523183555499	5,70	-457,6107059386
7,50	-457,3765849325	7,50	-457,523183073944	5,80	-457,610702512
7,60	-457,3765845255	7,60	-457,523182637442	5,90	-457,6106994968
7,70	-457,3765841559	7,70	-457,523182241224	6,00	-457,6106968397
7,80	-457,3765838196	7,80	-457,523181881079	6,10	-457,6106944954
7,90	-457,3765835134	7,90	-457,523181553272	6,20	-457,610692422
8,00	-457,3765832341	8,00	-457,523181254523	6,30	-457,6106905855
8,10	-457,3765829791	8,10	-457,523180981967	6,40	-457,6106889556
8,20	-457,3765827461	8,20	-457,523180732824	6,50	-457,6106875067
8,30	-457,3765825326	8,30	-457,523180504978	6,60	-457,610686216
8,40	-457,3765823372	8,40	-457,523180296298	6,70	-457,610685064
8,50	-457,3765821577	8,50	-457,523180104970	6,80	-457,6106840341
8,60	-457,376581993	8,60	-457,523179929356	6,90	-457,6106831113
8,70	-457,3765818415	8,70	-457,523179767982	7,00	-457,6106822838
8,80	-457,3765817022	8,80	-457,523179619554	7,10	-457,6106815407
8,90	-457,3765815738	8,90	-457,523179482874	7,20	-457,6106808711
9,00	-457,3765814554	9,00	-457,523179356902	7,30	-457,6106802674
9,10	-457,3765813461	9,10	-457,523179240733	7,40	-457,610679722
9,20	-457,3765812451	9,20	-457,523179133348	7,50	-457,6106792283
9,30	-457,3765811517	9,30	-457,523179034126	7,60	-457,610678782

9,40	-457,3765810653	9,40	-457,523178942302	7,70	-457,6106783766
9,50	-457,3765809852	9,50	-457,523178857314	7,80	-457,6106780082
9,60	-457,3765809109	9,60	-457,523178778514	7,90	-457,6106776731
9,70	-457,376580842	9,70	-457,523178705444	8,00	-457,6106773672
9,80	-457,376580778	9,80	-457,523178637584	8,10	-457,6106770893
9,90	-457,3765807186	9,90	-457,523178574551	8,20	-457,6106768348
10,00	-457,3765806633	10,00	-457,523178515926	8,30	-457,6106766021
10,10	-457,3765806118	10,10	-457,523178461457	8,40	-457,610676389
10,20	-457,3765805638	10,20	-457,523178410600	8,50	-457,6106761932
10,30	-457,3765805191	10,30	-457,523178363255	8,60	-457,6106760146
10,40	-457,3765804774	10,40	-457,523178319073	8,70	-457,6106758498
10,50	-457,3765804384	10,50	-457,523178277868	8,80	-457,6106756984
10,60	-457,3765804021	10,60	-457,523178239378	8,90	-457,610675559
10,70	-457,376580368	10,70	-457,523178203406	9,00	-457,6106754305
10,80	-457,3765803362	10,80	-457,523178169781	9,10	-457,6106753121
10,90	-457,3765803064	10,90	-457,523178138291	9,20	-457,6106752025
11,00	-457,3765802786	11,00	-457,523178108816	9,30	-457,6106751014
11,10	-457,3765802524	11,10	-457,523178081300	9,40	-457,6106750078
11,20	-457,3765802279	11,20	-457,523178055305	9,50	-457,6106749206
11,30	-457,3765802049	11,30	-457,523178031012	9,60	-457,610674841
11,40	-457,3765801833	11,40	-457,523178008187	9,70	-457,6106747664
11,50	-457,376580163	11,50	-457,523177986781	9,80	-457,6106746973
11,60	-457,3765801439	11,60	-457,523177966651	9,90	-457,6106746325
11,70	-457,376580126	11,70	-457,523177947719	10,00	-457,6106745728
11,80	-457,3765801092	11,80	-457,523177929904	10,10	-457,610674518
11,90	-457,3765800933	11,90	-457,523177913145	10,20	-457,6106744662
12,00	-457,3765800783	12,00	-457,523177897354	10,30	-457,610674418
				10,40	-457,6106743731
				10,50	-457,6106743306
				10,60	-457,6106742922
				10,70	-457,6106742555
				10,80	-457,6106742213

		10,90	-457,6106741893
		11,00	-457,6106741593
		11,10	-457,6106741314
		11,20	-457,6106741049
		11,30	-457,6106740803
		11,40	-457,6106740571

Tabela 5.11: Sistema diatômico Ne-Rn

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
3,00	-416.622429940344	3,00	-416.790985401336	3,00	-416.898324521009
3,10	-416.623937341787	3,10	-416.792409098111	3,10	-416.899697678453
3,20	-416.624984457871	3,20	-416.793390285622	3,20	-416.900639273958
3,30	-416.625705307912	3,30	-416.794058560924	3,30	-416.901276909201
3,40	-416.626196149914	3,40	-416.794507028258	3,40	-416.901701967860
3,50	-416.626525886637	3,50	-416.794802220106	3,50	-416.901979425528
3,60	-416.626743577500	3,60	-416.794991509749	3,60	-416.902155352472
3,70	-416.626883961111	3,70	-416.795108345736	3,70	-416.902262152302
3,80	-416.626971490749	3,80	-416.795176259133	3,80	-416.902322495125
3,90	-416.627023274321	3,90	-416.795211694038	3,90	-416.902362120629
4,00	-416.627051206767	4,00	-416.795226018894	**3,91**	**-416.902362201649**
4,10	-416.627063504137	4,01	-416.795226607245	3,92	-416.902362042328
4,11	-416.627064110285	4,02	-416.795227077844	3,93	-416.902361807677
4,12	-416.627064620450	4,03	-416.795227430447	3,94	-416.902361478038
4,13	-416.627065040746	4,04	-416.795227670363	3,95	-416.902361054736
4,14	-416.627065375447	4,05	-416.795227802530	3,96	-416.902360549541
4,15	-416.627065628504	**4,06**	**-416.795227832541**	3,97	-416.902359294071
4,16	-416.627065803745	4,07	-416.795227765269	4,00	-416.902361921995
4,17	-416.627065904839	4,08	-416.795227605523	4,10	-416.902359297505
4,18	**-416.627065935346**	4,09	-416.795227358188	4,20	-416.902349285746
4,19	-416.627065898678	4,10	-416.795227027427	4,30	-416.902335251981

4,20	-416.627065798058	4,11	-416.795226618255	4,40	-416.902319380347
4,21	-416.627065636708	4,12	-416.795226134464	4,50	-416.902303073083
4,22	-416.627065417622	4,13	-416.795225579975	4,60	-416.902287199557
4,23	-416.627065143667	4,14	-416.795224958637	4,70	-416.902272249448
4,24	-416.627064817690	4,15	-416.795224274191	4,80	-416.902258487856
4,25	-416.627064442359	4,16	-416.795223530022	4,90	-416.902246008988
4,26	-416.627064020257	4,17	-416.795222729462	5,00	-416.902234809144
4,27	-416.627063553812	4,18	-416.795221876194	5,10	-416.902224846998
4,28	-416.627063045439	4,19	-416.795220973019	5,20	-416.902216021826
4,29	-416.627062497353	4,20	-416.795220022991	5,30	-416.902208236453
4,30	-416.627061911788	4,30	-416.795208520631	5,40	-416.902201400221
4,40	-416.627054415111	4,40	-416.795194816731	5,50	-416.902195371992
4,50	-416.627045018673	4,50	-416.795180381546	5,60	-416.902190072000
4,60	-416.627034827656	4,60	-416.795166123046	5,70	-416.902185411607
4,70	-416.627024545508	4,70	-416.795152557044	5,80	-416.902181310208
4,80	-416.627014603770	4,80	-416.795139969484	5,90	-416.902177697391
4,90	-416.627005271066	4,90	-416.795128482476	6,00	-416.902174510885
5,00	-416.626996632069	5,00	-416.795118127335	6,10	-416.902171696352
5,10	-416.626988756575	5,10	-416.795108854385	6,20	-416.902169206561
5,20	-416.626981643330	5,20	-416.795100602837	6,30	-416.902167000314
5,30	-416.626975261874	5,30	-416.795093288272	6,40	-416.902165042103
5,40	-416.626969563794	5,40	-416.795086820806	6,50	-416.902163300959
5,50	-416.626964492425	5,50	-416.795081111698	6,60	-416.902161750019
5,60	-416.626959988440	5,60	-416.795076072958	6,70	-416.902160366097
5,70	-416.626955994090	5,70	-416.795071629994	6,80	-416.902159128987
5,80	-416.626952452048	5,80	-416.795067709946	6,90	-416.902158021168
5,90	-416.626949311573	5,90	-416.795064248801	7,00	-416.902157027444
6,00	-416.626946526203	6,00	-416.795061189876	7,10	-416.902156134451
6,10	-416.626944054637	6,10	-416.795058483344	7,20	-416.902155330800
6,20	-416.626941859018	6,20	-416.795056085303	7,30	-416.902154606387
6,30	-416.626939906377	6,30	-416.795053957425	7,40	-416.902153952176
6,40	-416.626938167523	6,40	-416.795052066760	7,50	-416.902153360598

6,50	-416.626936617006	6,50	-416.795050383315	7,60	-416.902152824787
6,60	-416.626935231408	6,60	-416.795048882161	7,70	-416.902152338786
6,70	-416.626933994036	6,70	-416.795047541283	7,80	-416.902151897355
6,80	-416.626932883553	6,80	-416.795046341538	7,90	-416.902151495846
6,90	-416.626931889440	6,90	-416.795045266234	8,00	-416.902151130173
7,00	-416.626930995706	7,00	-416.795044300865	8,10	-416.902150796647
7,10	-416.626930191261	7,10	-416.795043432726	8,20	-416.902150492097
7,20	-416.626929465875	7,20	-416.795042650761	8,30	-416.902150213657
7,30	-416.626928810964	7,30	-416.795041945345	8,40	-416.902149958792
7,40	-416.626928218981	7,40	-416.795041307891	8,50	-416.902149725223
7,50	-416.626927682823	7,50	-416.795040731067	8,60	-416.902149510925
7,60	-416.626927196575	7,60	-416.795040208287	8,70	-416.902149314081
7,70	-416.626926755013	7,70	-416.795039733849	8,80	-416.902149133101
7,80	-416.626926353463	7,80	-416.795039302670	8,90	-416.902148966514
7,90	-416.626925987762	7,90	-416.795038910273	9,00	-416.902148813035
8,00	-416.626925654322	8,00	-416.795038552665	9,10	-416.902148671423
8,10	-416.626925349929	8,10	-416.795038226397	9,20	-416.902148540729
8,20	-416.626925071678	8,20	-416.795037928361	9,30	-416.902148420031
8,30	-416.626924817019	8,30	-416.795037655756	9,40	-416.902148308296
8,40	-416.626924583691	8,40	-416.795037406104	9,50	-416.902148204907
8,50	-416.626924369664	8,50	-416.795037177257	9,60	-416.902148109117
8,60	-416.626924173056	8,60	-416.795036967230	9,70	-416.902148020280
8,70	-416.626923992397	8,70	-416.795036774290	9,80	-416.902147937842
8,80	-416.626923826149	8,80	-416.795036596792	9,90	-416.902147861251
8,90	-416.626923673014	8,90	-416.795036433410	10,00	-416.902147790042
9,00	-416.626923531819	9,00	-416.795036282821	10,10	-416.902147723828
9,10	-416.626923401495	9,10	-416.795036144384	10,20	-416.902147662157
9,20	-416.626923281087	9,20	-416.795036015727	10,30	-416.902147604698
9,30	-416.626923169747	9,30	-416.795035897103	10,40	-416.902147551128
9,40	-416.626923066721	9,40	-416.795035787414	10,50	-416.902147501134
9,50	-416.626922971258	9,50	-416.795035685851	10,60	-416.902147454458
9,60	-416.626922882774	9,60	-416.795035591748	10,70	-416.902147410839

9,70	-416.626922800677	9,70	-416.795035504437	10,80	-416.902147370070
9,80	-416.626922724425	9,80	-416.795035423435	10,90	-416.902147331914
9,90	-416.626922653563	9,90	-416.795035348169	11,00	-416.902147296196
10,00	-416.626922587661	10,00	-416.795035278180	11,10	-416.902147263128
10,10	-416.626922526313	10,10	-416.795035213067	11,20	-416.902147231232
10,20	-416.626922469177	10,20	-416.795035152412	11,30	-416.902147201990
10,30	-416.626922415910	10,30	-416.795035095899	11,40	-416.902147174300
10,40	-416.626922366210	10,40	-416.795035043210	11,50	-416.902147148394
10,50	-416.626922319833	10,50	-416.795034994013	11,60	-416.902147124008
10,60	-416.626922276499	10,60	-416.795034948091	11,70	-416.902147101109
10,70	-416.626922236003	10,70	-416.795034905147	11,80	-416.902147079549
10,80	-416.626922198108	10,80	-416.795034865004	11,90	-416.902147059273
10,90	-416.626922162664	10,90	-416.795034827457	12,00	-416.902147040181
11,00	-416.626922129451	11,00	-416.795034792295		
11,10	-416.626922098326	11,10	-416.795034759325		
11,20	-416.626922069140	11,20	-416.795034728428		
11,30	-416.626922041759	11,30	-416.795034699453		
11,40	-416.626922016035	11,40	-416.795034672265		
11,50	-416.626921991899	11,50	-416.795034646714		
11,60	-416.626921969199	11,60	-416.795034622702		
11,70	-416.626921947859	11,70	-416.795034600131		
11,80	-416.626921927767	11,80	-416.795034578873		
11,90	-416.626921908856	11,90	-416.795034558892		
12,00	-416.626921891056	12,00	-416.795034540078		

Tabela 5.12: Sistema diatômico Ar-Ar

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-1053,922949208440	2,00	-1053,9804084831	2,00	-1053,9999826646
2,10	-1053,972923224970	2,10	-1054,0292399093	2,10	-1054,0480243478
2,20	-1054,009237636520	2,20	-1054,0647494735	2,20	-1054,0829746299

2,30	-1054,035425725830	2,30	-1054,0903504252	2,30	-1054,1081774334
2,40	-1054,054185512320	2,40	-1054,1086634202	2,40	-1054,126206277
2,50	-1054,067541152130	2,50	-1054,1216655978	2,50	-1054,1390052753
2,60	-1054,076991633100	2,60	-1054,1308283726	2,60	-1054,1480223875
2,70	-1054,083636483490	2,70	-1054,1372352047	2,70	-1054,154324348
2,80	-1054,088276409610	2,80	-1054,1416770268	2,80	-1054,1586902836
2,90	-1054,091491112620	2,90	-1054,1447271533	2,90	-1054,1616851501
3,00	-1054,093698159180	3,00	-1054,1467984544	3,00	-1054,1637159229
3,10	-1054,095196911490	3,10	-1054,148186423	3,10	-1054,165073846
3,20	-1054,096200979620	3,20	-1054,1491012735	3,20	-1054,1659660057
3,30	-1054,096862054880	3,30	-1054,1496914921	3,30	-1054,1665386747
3,40	-1054,097287278810	3,40	-1054,1500612795	3,40	-1054,1668944814
3,50	-1054,097551935360	3,50	-1054,1502832027	3,50	-1054,1671049556
3,60	-1054,097708587800	3,60	-1054,1504073603	3,60	-1054,1672195244
3,70	-1054,097793694070	3,70	-1054,150468086	3,70	-1054,1672720781
3,80	-1054,097832357830	3,71	-1054,1504716398	3,71	-1054,1672748862
3,81	-1054,0978343828	3,72	-1054,15047481	3,72	-1054,1672773182
3,82	-1054,0978361324	3,73	-1054,1504776326	3,73	-1054,1672794097
3,83	-1054,0978376208	3,74	-1054,1504800982	3,74	-1054,1672811688
3,84	-1054,0978388594	3,75	-1054,1504822444	3,75	-1054,1672826294
3,85	-1054,0978398607	3,76	-1054,1504840793	3,76	-1054,1672837728
3,86	-1054,0978406361	3,77	-1054,1504856184	3,77	-1054,1672846308
3,87	-1054,0978411967	3,78	-1054,1504868759	3,78	-1054,1672852178
3,88	-1054,097841553	3,79	-1054,1504878657	3,79	-1054,1672855469
3,89	**-1054,0978417157**	3,80	-1054,1504886009	**3,80**	**-1054,1672856315**
3,90	-1054,0978416943	3,81	-1054,1504890942	3,81	-1054,1672854852
3,91	-1054,0978414984	3,82	-1054,150489358	3,82	-1054,1672851177
3,92	-1054,0978411371	**3,83**	**-1054,1504894041**	3,83	-1054,1672845449
3,93	-1054,097840619	3,84	-1054,1504892433	3,84	-1054,1672837748
3,94	-1054,0978399525	3,85	-1054,1504888864	3,85	-1054,1672828177
3,95	-1054,0978391457	3,86	-1054,1504883444	3,86	-1054,1672816845
3,96	-1054,0978382063	3,87	-1054,1504876266	3,87	-1054,1672803845

3,97	-1054,0978371417	3,88	-1054,1504867431	3,88	-1054,167278928
3,98	-1054,0978359589	3,89	-1054,1504857022	3,89	-1054,1672773243
3,99	-1054,0978346647	3,90	-1054,1504845163	3,90	-1054,1672755758
4,00	-1054,097833266930	4,00	-1054,1504661447	4,00	-1054,1672521408
4,10	-1054,097814762200	4,10	-1054,1504402124	4,10	-1054,1672219453
4,20	-1054,097791206900	4,20	-1054,1504110453	4,20	-1054,1671891966
4,30	-1054,097765798850	4,30	-1054,1503812861	4,30	-1054,167156476
4,40	-1054,097740499940	4,40	-1054,1503525257	4,40	-1054,1671252801
4,50	-1054,097716442560	4,50	-1054,1503256529	4,50	-1054,1670964107
4,60	-1054,097694218810	4,60	-1054,1503010829	4,60	-1054,1670702165
4,70	-1054,097674070930	4,70	-1054,1502789746	4,70	-1054,1670467738
4,80	-1054,097656038080	4,80	-1054,1502592681	4,80	-1054,1670259856
4,90	-1054,097640030580	4,90	-1054,1502418384	4,90	-1054,1670076727
5,00	-1054,097625898420	5,00	-1054,1502264988	5,00	-1054,16699161
5,10	-1054,097613464400	5,10	-1054,1502130425	5,10	-1054,166977559
5,20	-1054,097602543790	5,20	-1054,150201263	5,20	-1054,1669652871
5,30	-1054,097592961720	5,30	-1054,1501909598	5,30	-1054,1669545761
5,40	-1054,097584554380	5,40	-1054,1501819492	5,40	-1054,166945241
5,50	-1054,097577169500	5,50	-1054,1501740656	5,50	-1054,1669370754
5,60	-1054,097570686380	5,60	-1054,1501671608	5,60	-1054,1669299236
5,70	-1054,097564982630	5,70	-1054,1501611065	5,70	-1054,1669236751
5,80	-1054,097559959210	5,80	-1054,1501557886	5,80	-1054,1669182074
5,90	-1054,097555527720	5,90	-1054,1501511096	5,90	-1054,1669133936
6,00	-1054,097551611910	6,00	-1054,1501469852	6,00	-1054,166909157
6,10	-1054,097548146470	6,10	-1054,1501433421	6,10	-1054,1669054111
6,20	-1054,097545072580	6,20	-1054,1501401192	6,20	-1054,1669021091
6,30	-1054,097542342100	6,30	-1054,1501372609	6,30	-1054,1668991948
6,40	-1054,097539912470	6,40	-1054,1501347217	6,40	-1054,1668965925
6,50	-1054,097537746470	6,50	-1054,1501324615	6,50	-1054,1668942861
6,60	-1054,097535812700	6,60	-1054,1501304453	6,60	-1054,166892231
6,70	-1054,097534081480	6,70	-1054,1501286447	6,70	-1054,1668903895
6,80	-1054,097532530400	6,80	-1054,1501270322	6,80	-1054,166888756

6,90	-1054,097531138060	6,90	-1054,1501255864	6,90	-1054,1668872854
7,00	-1054,097529887760	7,00	-1054,1501242917	7,00	-1054,1668859656
7,10	-1054,097528759090	7,10	-1054,1501231186	7,10	-1054,1668847787
7,20	-1054,097527741210	7,20	-1054,1501220635	7,20	-1054,1668837096
7,30	-1054,097526822150	7,30	-1054,1501211148	7,30	-1054,1668827451
7,40	-1054,097525990490	7,40	-1054,150120255	7,40	-1054,1668818735
7,50	-1054,097525236880	7,50	-1054,1501194764	7,50	-1054,1668810847
7,60	-1054,097524553630	7,60	-1054,1501187701	7,60	-1054,1668803696
7,70	-1054,097523931790	7,70	-1054,1501181293	7,70	-1054,1668797206
7,80	-1054,097523365980	7,80	-1054,1501175463	7,80	-1054,1668791307
7,90	-1054,097522850670	7,90	-1054,1501170154	7,90	-1054,1668785937
8,00	-1054,097522380560	8,00	-1054,1501165314	8,00	-1054,1668781043
8,10	-1054,097521951780	8,10	-1054,150116089	8,10	-1054,1668776576
8,20	-1054,097521558400	8,20	-1054,1501156856	8,20	-1054,1668772506
8,30	-1054,097521198900	8,30	-1054,1501153159	8,30	-1054,1668768762
8,40	-1054,097520869180	8,40	-1054,1501149773	8,40	-1054,1668765343
8,50	-1054,097520566670	8,50	-1054,1501146666	8,50	-1054,1668762208
8,60	-1054,097520289430	8,60	-1054,150114381	8,60	-1054,1668759329
8,70	-1054,097520033210	8,70	-1054,1501141192	8,70	-1054,1668756686
8,80	-1054,097519797950	8,80	-1054,1501138779	8,80	-1054,1668754253
8,90	-1054,097519581130	8,90	-1054,1501136557	8,90	-1054,1668752013
9,00	-1054,097519381150	9,00	-1054,1501134508	9,00	-1054,1668749948
9,10	-1054,097519196500	9,10	-1054,1501132617	9,10	-1054,1668748042
9,20	-1054,097519025870	9,20	-1054,150113087	9,20	-1054,1668746283
9,30	-1054,097518868030	9,30	-1054,1501129255	9,30	-1054,1668744656
9,40	-1054,097518721900	9,40	-1054,150112776	9,40	-1054,1668743151
9,50	-1054,097518586510	9,50	-1054,1501126375	9,50	-1054,1668741758
9,60	-1054,097518460940	9,60	-1054,1501125092	9,60	-1054,1668740465
9,70	-1054,097518344400	9,70	-1054,1501123901	9,70	-1054,1668739268
9,80	-1054,097518236140	9,80	-1054,1501122794	9,80	-1054,1668738156
9,90	-1054,097518135500	9,90	-1054,1501121767	9,90	-1054,1668737122
10,00	-1054,097518041880	10,00	-1054,1501120811	10,00	-1054,1668736161

10,10	-1054,097517954700	10,10	-1054,1501119921	10,10	-1054,1668735266
10,20	-1054,097517873470	10,20	-1054,1501119092	10,20	-1054,1668734434
10,30	-1054,097517797740	10,30	-1054,1501118319	10,30	-1054,1668733657
10,40	-1054,097517727080	10,40	-1054,1501117599	10,40	-1054,1668732933
10,50	-1054,097517661100	10,50	-1054,1501116926	10,50	-1054,1668732258
10,60	-1054,097517599450	10,60	-1054,1501116298	10,60	-1054,1668731626
10,70	-1054,097517541810	10,70	-1054,150111571	10,70	-1054,1668731037
10,80	-1054,097517487880	10,80	-1054,1501115161	10,80	-1054,1668730485
10,90	-1054,097517437390	10,90	-1054,1501114646	10,90	-1054,1668729969
11,00	-1054,097517390100	11,00	-1054,1501114165	11,00	-1054,1668729486
11,10	-1054,097517345770	11,10	-1054,1501113713	11,10	-1054,1668729032
11,20	-1054,097517304190	11,20	-1054,150111329	11,20	-1054,1668728608
11,30	-1054,097517265170	11,30	-1054,1501112893	11,30	-1054,166872821
11,40	-1054,097517228530	11,40	-1054,150111252	11,40	-1054,1668727836
11,50	-1054,097517194100	11,50	-1054,150111217	11,50	-1054,1668727484
11,60	-1054,097517161740	11,60	-1054,1501111841	11,60	-1054,1668727154
11,70	-1054,097517131300	11,70	-1054,1501111531	11,70	-1054,1668726844
11,80	-1054,097517102650	11,80	-1054,150111124	11,80	-1054,1668726552
11,90	-1054,097517075680	11,90	-1054,1501110965	11,90	-1054,1668726277
12,00	-1054,097517050270	12,00	-1054,1501110707	12,00	-1054,1668726018
12,10	-1054,097517026320	12,10	-1054,1501110464		

Tabela 5.13: Sistema diatômico Ar-Kr

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-3279,1154637702	2,00	-3279,2238529755	2,00	-3279,3215353276
2,10	-3279,1816760415	2,10	-3279,2886160507	2,10	-3279,3854992551
2,20	-3279,2309048089	2,20	-3279,336728815	2,20	-3279,4330050035
2,30	-3279,2672302846	2,30	-3279,3721960538	2,30	-3279,4680075078
2,40	-3279,2938485009	2,40	-3279,3981511563	2,40	-3279,4936052115
2,50	-3279,3132278281	2,50	-3279,4170130427	2,50	-3279,5121915824

2,60	-3279,327250142	2,60	-3279,4306263075	2,60	-3279,5255921657
2,70	-3279,3373345751	2,70	-3279,4403829323	2,70	-3279,5351846351
2,80	-3279,3445416518	2,80	-3279,4473238702	2,80	-3279,5419992303
2,90	-3279,3496579865	2,90	-3279,452221847	2,90	-3279,5468004976
3,00	-3279,3532633299	3,00	-3279,4556467315	3,00	-3279,5501519068
3,10	-3279,3557825726	3,10	-3279,4580163331	3,10	-3279,552466003
3,20	-3279,3575255038	3,20	-3279,4596352998	3,20	-3279,5540431977
3,30	-3279,3587168788	3,30	-3279,4607243705	3,30	-3279,5551007971
3,40	-3279,3595189657	3,40	-3279,4614426171	3,40	-3279,5557951815
3,50	-3279,3600483488	3,50	-3279,461903902	3,50	-3279,556238189
3,60	-3279,3603883655	3,60	-3279,4621891577	3,60	-3279,5565091567
3,70	-3279,3605982646	3,70	-3279,4623555304	3,70	-3279,5566640994
3,80	-3279,3607199193	3,80	-3279,4624429301	3,80	-3279,5567421371
3,90	-3279,3607827134	3,90	-3279,4624790387	3,81	-3279,5567468386
4,00	-3279,3608071051	3,91	-3279,4624806257	3,82	-3279,5567510735
4,01	-3279,3608080183	3,92	-3279,4624819022	3,83	-3279,5567548594
4,02	-3279,3608087044	3,93	-3279,4624828901	3,84	-3279,5567582172
4,03	-3279,3608091733	3,94	-3279,462483603	3,85	-3279,556761166
4,04	-3279,3608094354	3,95	-3279,4624840543	3,86	-3279,5567637272
4,05	**-3279,3608095008**	**3,96**	**-3279,4624842569**	3,87	-3279,5567659146
4,06	-3279,360809379	3,97	-3279,4624842231	3,88	-3279,5567677478
4,07	-3279,3608090793	3,98	-3279,4624839649	3,89	-3279,5567692445
4,08	-3279,3608086106	3,99	-3279,4624834902	3,90	-3279,556770419
4,09	-3279,3608079815	4,00	-3279,4624828168	3,91	-3279,5567712839
4,10	-3279,3608072003	4,01	-3279,4624819516	3,92	-3279,5567718584
4,11	-3279,3608062747	4,02	-3279,4624809047	3,93	-3279,5567721556
4,12	-3279,3608052126	4,03	-3279,462479686	**3,94**	**-3279,5567721884**
4,13	-3279,3608040212	4,04	-3279,4624783047	3,95	-3279,5567719712
4,14	-3279,3608027074	4,05	-3279,4624767697	3,96	-3279,5567715169
4,15	-3279,3608012781	4,06	-3279,4624750894	3,97	-3279,5567708346
4,16	-3279,3607997397	4,07	-3279,4624732722	3,98	-3279,5567699391
4,17	-3279,3607980983	4,08	-3279,4624713261	3,99	-3279,5567688404

4,18	-3279,3607963601	4,09	-3279,462469258	4,00	-3279,5567675468
4,19	-3279,3607945306	4,10	-3279,4624670644	4,10	-3279,556746123
4,20	-3279,3607926138	4,20	-3279,4624403459	4,20	-3279,5567145533
4,30	-3279,3607698049	4,30	-3279,4624082323	4,30	-3279,5566782976
4,40	-3279,3607430385	4,40	-3279,4623742872	4,40	-3279,5566408338
4,50	-3279,3607150431	4,50	-3279,4623407047	4,50	-3279,5566043166
4,60	-3279,3606875092	4,60	-3279,4623087729	4,60	-3279,5565699154
4,70	-3279,3606614378	4,70	-3279,4622791936	4,70	-3279,5565383103
4,80	-3279,3606373221	4,80	-3279,462252252	4,80	-3279,5565096759
4,90	-3279,3606154245	4,90	-3279,4622280169	4,90	-3279,5564840544
5,00	-3279,3605957495	5,00	-3279,4622064036	5,00	-3279,5564613131
5,10	-3279,3605782076	5,10	-3279,4621872363	5,10	-3279,5564412221
5,20	-3279,3605626556	5,20	-3279,4621703268	5,20	-3279,5564235541
5,30	-3279,3605489089	5,30	-3279,4621554344	5,30	-3279,5564080392
5,40	-3279,3605367832	5,40	-3279,4621423444	5,40	-3279,556394438
5,50	-3279,3605260977	5,50	-3279,4621308476	5,50	-3279,5563825194
5,60	-3279,3605166813	5,60	-3279,4621207469	5,60	-3279,5563720779
5,70	-3279,3605083843	5,70	-3279,4621118819	5,70	-3279,5563629152
5,80	-3279,3605010658	5,80	-3279,462104083	5,80	-3279,5563548778
5,90	-3279,3604946016	5,90	-3279,4620972177	5,90	-3279,5563478176
6,00	-3279,360488886	6,00	-3279,4620911659	6,00	-3279,5563416007
6,10	-3279,3604838229	6,10	-3279,4620858165	6,10	-3279,556336117
6,20	-3279,3604793336	6,20	-3279,4620810962	6,20	-3279,5563312764
6,30	-3279,3604753469	6,30	-3279,462076909	6,30	-3279,5563269913
6,40	-3279,3604717995	6,40	-3279,462073186	6,40	-3279,5563231909
6,50	-3279,3604686378	6,50	-3279,4620698812	6,50	-3279,556319818
6,60	-3279,3604658153	6,60	-3279,4620669332	6,60	-3279,556316812
6,70	-3279,3604632904	6,70	-3279,4620643067	6,70	-3279,556314135
6,80	-3279,3604610289	6,80	-3279,4620619563	6,80	-3279,5563117404
6,90	-3279,3604589996	6,90	-3279,46205985	6,90	-3279,5563095963
7,00	-3279,3604571757	7,00	-3279,4620579595	7,00	-3279,5563076764
7,10	-3279,3604555338	7,10	-3279,4620562541	7,10	-3279,5563059482

7,20	-3279,3604540534	7,20	-3279,4620547294	7,20	-3279,5563043959
7,30	-3279,3604527168	7,30	-3279,4620533492	7,30	-3279,5563029948
7,40	-3279,360451508	7,40	-3279,4620521042	7,40	-3279,5563017289
7,50	-3279,3604504132	7,50	-3279,4620509754	7,50	-3279,5563005866
7,60	-3279,3604494197	7,60	-3279,4620499427	7,60	-3279,5562995493
7,70	-3279,3604485181	7,70	-3279,4620490238	7,70	-3279,556298611
7,80	-3279,3604476978	7,80	-3279,4620481802	7,80	-3279,5562977573
7,90	-3279,3604469508	7,90	-3279,4620474125	7,90	-3279,5562969797
8,00	-3279,3604462697	8,00	-3279,4620467131	8,00	-3279,556296274
8,10	-3279,3604456476	8,10	-3279,4620460654	8,10	-3279,5562956277
8,20	-3279,3604450795	8,20	-3279,4620454918	8,20	-3279,5562950401
8,30	-3279,3604445593	8,30	-3279,4620449584	8,30	-3279,5562945014
8,40	-3279,3604440826	8,40	-3279,46204447	8,40	-3279,5562940073
8,50	-3279,3604436454	8,50	-3279,4620440223	8,50	-3279,5562935568
8,60	-3279,3604432437	8,60	-3279,4620436019	8,60	-3279,556293141
8,70	-3279,3604428749	8,70	-3279,4620432339	8,70	-3279,5562927616
8,80	-3279,3604425354	8,80	-3279,4620428866	8,80	-3279,5562924114
8,90	-3279,3604422225	8,90	-3279,4620425668	8,90	-3279,5562920879
9,00	-3279,360441934	9,00	-3279,4620422722	9,00	-3279,5562917924
9,10	-3279,3604416678	9,10	-3279,4620419908	9,10	-3279,5562915184
9,20	-3279,3604414219	9,20	-3279,4620417493	9,20	-3279,5562912643
9,30	-3279,3604411944	9,30	-3279,4620415171	9,30	-3279,5562910321
9,40	-3279,360440984	9,40	-3279,4620413025	9,40	-3279,5562908158
9,50	-3279,360440789	9,50	-3279,4620411037	9,50	-3279,5562906146
9,60	-3279,3604406082	9,60	-3279,46204091	9,60	-3279,5562904306
9,70	-3279,3604404405	9,70	-3279,4620407486	9,70	-3279,5562902585
9,80	-3279,3604402847	9,80	-3279,46204059	9,80	-3279,5562900978
9,90	-3279,36044014	9,90	-3279,4620404425	9,90	-3279,556289951
10,00	-3279,3604400053	10,00	-3279,4620403055	10,00	-3279,556289813
10,10	-3279,3604398801	10,10	-3279,4620401685	10,10	-3279,5562896837
10,20	-3279,3604397633	10,20	-3279,4620400593	10,20	-3279,5562895657
10,30	-3279,3604396544	10,30	-3279,4620399486	10,30	-3279,5562894544

10,40	-3279,3604395528	10,40	-3279,4620398454	10,40	-3279,5562893495
10,50	-3279,360439458	10,50	-3279,4620397491	10,50	-3279,5562892541
10,60	-3279,3604393695	10,60	-3279,4620396497	10,60	-3279,5562891637
10,70	-3279,3604392867	10,70	-3279,462039575	10,70	-3279,556289078
10,80	-3279,3604392092	10,80	-3279,4620394964	10,80	-3279,5562890004
10,90	-3279,3604391368	10,90	-3279,4620394229	10,90	-3279,5562889265
11,00	-3279,3604390686	11,00	-3279,462039354	11,00	-3279,5562888561
11,10	-3279,3604390051	11,10	-3279,46203928	11,10	-3279,5562887927
11,20	-3279,3604389456	11,20	-3279,4620392288	11,20	-3279,5562887319
11,30	-3279,3604388896	11,30	-3279,4620391722	11,30	-3279,5562886737
11,40	-3279,360438837	11,40	-3279,4620391189	11,40	-3279,5562886215
11,50	-3279,3604387876	11,50	-3279,4620390689	11,50	-3279,5562885713
11,60	-3279,3604387412	11,60	-3279,4620390124	11,60	-3279,5562885229
11,70	-3279,3604386976	11,70	-3279,4620389774	11,70	-3279,5562884798
11,80	-3279,3604386565	11,80	-3279,462038936	11,80	-3279,5562884381
11,90	-3279,3604386178	11,90	-3279,4620388968	11,90	-3279,5562883976
12,00	-3279,3604385814	12,00	-3279,4620388599	12,00	-3279,5562883618

Tabela 5.14: Sistema diatômico Ar-Xe

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-855,2623458316	2,00	-855,410949888	2,00	-855,4996815005
2,10	-855,3504305548	2,10	-855,4969198633	2,10	-855,5845016184
2,20	-855,4174287417	2,20	-855,5622915676	2,20	-855,6489801693
2,30	-855,4681445827	2,30	-855,6117334969	2,30	-855,6977293467
2,40	-855,506337062	2,40	-855,6489102281	2,40	-855,7343679739
2,50	-855,5349448795	2,50	-855,6766963141	2,50	-855,7617360995
2,60	-855,5562570771	2,60	-855,6973366542	2,60	-855,7820520803
2,70	-855,5720468366	2,70	-855,712573334	2,70	-855,7970367271
2,80	-855,5836790447	2,80	-855,7237488497	2,80	-855,8080153558
2,90	-855,5921976833	2,90	-855,7318905085	2,90	-855,8160019233

3,00	-855,5983964748	3,00	-855,737779147	3,00	-855,8217673039
3,10	-855,6028756589	3,10	-855,7420043844	3,10	-855,8258940049
3,20	-855,606086898	3,20	-855,7450088234	3,20	-855,8288196288
3,30	-855,6083684454	3,30	-855,7471228326	3,30	-855,8308707821
3,40	-855,6099724157	3,40	-855,7485917053	3,40	-855,8322898087
3,50	-855,6110857867	3,50	-855,749596587	3,50	-855,8332554368
3,60	-855,6118465078	3,60	-855,7502705039	3,60	-855,8338985339
3,70	-855,6123557911	3,70	-855,7507105597	3,70	-855,8343144565
3,80	-855,6126874619	3,80	-855,7509871891	3,80	-855,8345721264
3,90	-855,6128950326	3,90	-855,751151112	3,90	-855,8347210889
4,00	-855,6130170317	4,00	-855,7512385721	4,00	-855,8347965852
4,10	-855,6130809891	4,10	-855,7512752303	4,01	-855,8348011393
4,11	-855,6130849989	4,11	-855,7512768504	4,02	-855,8348052172
4,12	-855,6130886452	4,12	-855,7512781595	4,03	-855,8348088696
4,13	-855,6130919421	4,13	-855,7512791735	4,04	-855,8348120895
4,14	-855,6130949041	4,14	-855,7512799059	4,05	-855,8348149221
4,15	-855,6130975457	4,15	-855,7512803728	4,06	-855,8348173478
4,16	-855,6130998804	**4,16**	**-855,7512805804**	4,07	-855,8348194329
4,17	-855,6131019217	4,17	-855,7512805439	4,08	-855,834821145
4,18	-855,6131036822	4,18	-855,7512802749	4,09	-855,8348225378
4,19	-855,6131051743	4,19	-855,7512797842	4,10	-855,8348236
4,20	-855,6131064098	4,20	-855,7512790825	4,11	-855,8348243524
4,21	-855,6131074002	4,21	-855,7512781811	4,12	-855,834824818
4,22	-855,6131081566	4,22	-855,7512770896	**4,13**	**-855,8348250047**
4,23	-855,6131086895	4,23	-855,7512758172	4,14	-855,8348249265
4,24	-855,6131090092	4,24	-855,7512743729	4,15	-855,8348245974
4,25	**-855,6131091257**	4,25	-855,7512727668	4,16	-855,834824026
4,26	-855,6131090483	4,26	-855,7512710061	4,17	-855,8348232237
4,27	-855,6131087863	4,27	-855,7512690997	4,18	-855,834822204
4,28	-855,6131083486	4,28	-855,7512670555	4,19	-855,8348209755
4,29	-855,6131077436	4,29	-855,7512648808	4,20	-855,8348195526
4,30	-855,6131069809	4,30	-855,7512625782	4,30	-855,834796518

4,40	-855,6130921842	4,40	-855,7512342443	4,40	-855,8347627239
4,50	-855,6130685106	4,50	-855,7511997894	4,50	-855,8347236706
4,60	-855,6130403024	4,60	-855,7511629829	4,60	-855,8346829304
4,70	-855,6130104261	4,70	-855,7511261736	4,70	-855,8346428272
4,80	-855,6129806927	4,80	-855,7510908408	4,80	-855,8346046911
4,90	-855,6129522199	4,90	-855,751057801	4,90	-855,8345692933
5,00	-855,6129255915	5,00	-855,7510274577	5,00	-855,8345369545
5,10	-855,612901123	5,10	-855,7509999372	5,10	-855,8345077697
5,20	-855,6128789056	5,20	-855,7509752045	5,20	-855,8344816363
5,30	-855,6128589006	5,30	-855,7509531206	5,30	-855,834458398
5,40	-855,6128409958	5,40	-855,750933492	5,40	-855,8344378023
5,50	-855,6128250354	5,50	-855,7509160982	5,50	-855,8344196184
5,60	-855,6128108474	5,60	-855,7509007178	5,60	-855,8344035793
5,70	-855,6127982558	5,70	-855,7508871307	5,70	-855,8343894528
5,80	-855,6127870926	5,80	-855,7508751344	5,80	-855,8343770088
5,90	-855,6127771953	5,90	-855,7508645409	5,90	-855,8343660469
6,00	-855,6127684196	6,00	-855,7508551816	6,00	-855,834356379
6,10	-855,612760634	6,10	-855,7508469048	6,10	-855,8343478463
6,20	-855,6127537206	6,20	-855,7508395784	6,20	-855,8343403051
6,30	-855,6127475757	6,30	-855,750833079	6,30	-855,8343336313
6,40	-855,6127421067	6,40	-855,7508273143	6,40	-855,8343277131
6,50	-855,6127372326	6,50	-855,7508221888	6,50	-855,8343224595
6,60	-855,6127328825	6,60	-855,7508176245	6,60	-855,8343177855
6,70	-855,6127289951	6,70	-855,7508135525	6,70	-855,8343136216
6,80	-855,612725515	6,80	-855,7508099144	6,80	-855,8343099043
6,90	-855,6127223935	6,90	-855,7508066581	6,90	-855,8343065816
7,00	-855,612719592	7,00	-855,7508037384	7,00	-855,8343036038
7,10	-855,6127170722	7,10	-855,7508011159	7,10	-855,8343009336
7,20	-855,6127148028	7,20	-855,7507987573	7,20	-855,8342985318
7,30	-855,6127127556	7,30	-855,7507966318	7,30	-855,8342963713
7,40	-855,6127109053	7,40	-855,7507947135	7,40	-855,8342944214
7,50	-855,612709232	7,50	-855,7507929798	7,50	-855,8342926619

7,60	-855,6127077157	7,60	-855,7507914103	7,60	-855,8342910681
7,70	-855,6127063397	7,70	-855,7507899874	7,70	-855,8342896263
7,80	-855,6127050894	7,80	-855,7507886954	7,80	-855,8342883162
7,90	-855,6127039501	7,90	-855,7507875209	7,90	-855,8342871275
8,00	-855,6127029142	8,00	-855,7507864517	8,00	-855,8342860441
8,10	-855,6127019687	8,10	-855,7507854783	8,10	-855,8342850587
8,20	-855,6127011054	8,20	-855,7507845885	8,20	-855,8342841579
8,30	-855,6127003157	8,30	-855,7507837747	8,30	-855,8342833368
8,40	-855,6126995927	8,40	-855,7507830306	8,40	-855,834282584
8,50	-855,61269893	8,50	-855,750782349	8,50	-855,8342818965
8,60	-855,6126983221	8,60	-855,7507817239	8,60	-855,8342812643
8,70	-855,6126977633	8,70	-855,7507811499	8,70	-855,8342806858
8,80	-855,6126972494	8,80	-855,7507806224	8,80	-855,8342801524
8,90	-855,6126967764	8,90	-855,750780137	8,90	-855,8342796636
9,00	-855,6126963404	9,00	-855,7507796899	9,00	-855,8342792117
9,10	-855,6126959382	9,10	-855,7507792776	9,10	-855,8342787969
9,20	-855,6126955669	9,20	-855,7507788973	9,20	-855,8342784124
9,30	-855,6126952237	9,30	-855,7507785459	9,30	-855,8342780589
9,40	-855,6126949062	9,40	-855,750778221	9,40	-855,8342777305
9,50	-855,6126946122	9,50	-855,7507779203	9,50	-855,8342774284
9,60	-855,6126943398	9,60	-855,7507776417	9,60	-855,8342771466
9,70	-855,6126940871	9,70	-855,7507773835	9,70	-855,8342768874
9,80	-855,6126938525	9,80	-855,750777144	9,80	-855,834276645
9,90	-855,6126936346	9,90	-855,7507769215	9,90	-855,8342764217
10,00	-855,612693432	10,00	-855,7507767147	10,00	-855,8342762125
10,10	-855,6126932435	10,10	-855,7507765224	10,10	-855,8342760197
10,20	-855,6126930679	10,20	-855,7507763434	10,20	-855,8342758384
10,30	-855,6126929043	10,30	-855,7507761766	10,30	-855,8342756714
10,40	-855,6126927517	10,40	-855,7507760212	10,40	-855,8342755139
10,50	-855,6126926093	10,50	-855,7507758762	10,50	-855,8342753688
10,60	-855,6126924764	10,60	-855,7507757408	10,60	-855,8342752316
10,70	-855,6126923521	10,70	-855,7507756144	10,70	-855,8342751053

10,80	-855,6126922359	10,80	-855,7507754961	10,80	-855,8342749853
10,90	-855,6126921271	10,90	-855,7507753855	10,90	-855,834274875
11,00	-855,6126920253	11,00	-855,750775282	11,00	-855,8342747699
11,10	-855,6126919299	11,10	-855,750775185	11,10	-855,8342746732
11,20	-855,6126918404	11,20	-855,7507750942	11,20	-855,8342745809
11,30	-855,6126917565	11,30	-855,7507750089	11,30	-855,8342744962
11,40	-855,6126916778	11,40	-855,750774929	11,40	-855,8342744148
11,50	-855,6126916038	11,50	-855,7507748539	11,50	-855,8342743402
11,60	-855,6126915343	11,60	-855,7507747833	11,60	-855,8342742684
11,70	-855,6126914689	11,70	-855,750774717	11,70	-855,8342742027
11,80	-855,6126914074	11,80	-855,7507746546	11,80	-855,8342741391
11,90	-855,6126913495	11,90	-855,7507745959	11,90	-855,8342740811
12,00	-855,612691295	12,00	-855,7507745407	12,00	-855,8342740246

Tabela 5.15: Sistema diatômico Ar-Rn

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
3,00	-814,8452260218	3,00	-815,0064580283	3,00	-815,11018989
3,10	-814,8506065245	3,10	-815,0115177209	3,10	-815,1151313929
3,20	-814,8545083338	3,20	-815,0151576115	3,20	-815,1186756303
3,30	-814,8573154531	3,30	-815,0177529721	3,30	-815,1211931205
3,40	-814,8593163634	3,40	-815,0195839958	3,40	-815,1229608124
3,50	-814,8607269839	3,50	-815,0208591084	3,50	-815,1241846821
3,60	-814,861708217	3,60	-815,0217325994	3,60	-815,1250170847
3,70	-814,8623793706	3,70	-815,0223182715	3,70	-815,1255700526
3,80	-814,8628284318	3,80	-815,0226995864	3,80	-815,1259254733
3,90	-814,8631199219	3,90	-815,0229374108	3,90	-815,1261428451
4,00	-814,8633008633	4,00	-815,0230758437	4,00	-815,1262651111
4,10	-814,8634053098	4,10	-815,0231465892	4,10	-815,1263230352
4,20	-814,8634577392	4,11	-815,0231508757	4,15	-815,1263349714
4,21	-814,8634608388	4,12	-815,0231547354	4,16	-815,1263362809

4,22	-814,8634636152	4,13	-815,0231581862	4,17	-815,1263372731
4,23	-814,8634660778	4,14	-815,0231612448	4,18	-815,1263379577
4,24	-814,8634682401	4,15	-815,023163928	4,19	-815,1263383488
4,25	-814,8634701148	4,16	-815,0231662516	**4,20**	**-815,1263384649**
4,26	-814,8634717144	4,17	-815,0231682315	4,21	-815,1263383056
4,27	-814,8634730508	4,18	-815,0231698821	4,22	-815,1263378939
4,28	-814,8634741355	4,19	-815,0231712183	4,23	-815,1263372386
4,29	-814,8634749795	4,20	-815,0231722539	4,24	-815,1263363509
4,30	-814,8634755936	4,21	-815,0231730017	4,25	-815,1263352432
4,31	-814,8634759881	4,22	-815,0231734751	4,26	-815,1263339255
4,32	**-814,8634761729**	**4,23**	**-815,0231736865**	4,27	-815,126332408
4,33	-814,8634761577	4,24	-815,023173648	4,30	-815,1263267564
4,34	-814,8634759517	4,25	-815,023173371	4,40	-815,1262985666
4,35	-814,8634755638	4,26	-815,0231728667	4,50	-815,1262611914
4,36	-814,8634750026	4,27	-815,0231721458	4,60	-815,126219529
4,37	-814,8634742765	4,28	-815,0231712187	4,70	-815,1261767953
4,38	-814,8634733935	4,29	-815,0231700955	4,80	-815,1261350306
4,39	-814,8634723611	4,30	-815,0231687859	4,90	-815,1260954545
4,40	-814,863471187	4,40	-815,0231473052	5,00	-815,1260587421
4,50	-814,8634530925	4,50	-815,0231154618	5,10	-815,1260251894
4,60	-814,8634271853	4,60	-815,0230784143	5,20	-815,1259948618
4,70	-814,8633974241	4,70	-815,0230395662	5,30	-815,1259676564
4,80	-814,8633664053	4,80	-815,0230010922	5,40	-815,1259433975
4,90	-814,8633357737	4,90	-815,0229643173	5,50	-815,1259218517
5,00	-814,8633065238	5,00	-815,0229299901	5,60	-815,1259027724
5,10	-814,8632792072	5,10	-815,0228984688	5,70	-815,1258859049
5,20	-814,8632540842	5,20	-815,0228698643	5,80	-815,1258710033
5,30	-814,8632312277	5,30	-815,0228441181	5,90	-815,125857874
5,40	-814,8632106167	5,40	-815,0228210891	6,00	-815,1258462634
5,50	-814,8631920904	5,50	-815,0228005777	6,10	-815,1258360052
5,60	-814,86317552	5,60	-815,0227823692	6,20	-815,1258269331
5,70	-814,8631607376	5,70	-815,0227662238	6,30	-815,1258189004

5,80	-814,8631475736	5,80	-815,022751929	6,40	-815,1258117778
5,90	-814,8631358616	5,90	-815,0227392783	6,50	-815,1258054525
6,00	-814,8631254459	6,00	-815,0227280815	6,60	-815,1257998266
6,10	-814,8631161832	6,10	-815,0227181666	6,70	-815,1257948142
6,20	-814,863107942	6,20	-815,0227093803	6,80	-815,1257903406
6,30	-814,8631006056	6,30	-815,022701586	6,90	-815,1257863412
6,40	-814,863094069	6,40	-815,0226946629	7,00	-815,1257827593
6,50	-814,8630882385	6,50	-815,0226885054	7,10	-815,1257795456
6,60	-814,863083032	6,60	-815,0226830206	7,20	-815,1257766584
6,70	-814,8630783763	6,70	-815,0226781275	7,30	-815,1257740595
6,80	-814,8630742053	6,80	-815,0226737552	7,40	-815,1257717163
6,90	-814,8630704674	6,90	-815,0226698419	7,50	-815,1257696004
7,00	-814,8630671104	7,00	-815,0226663338	7,60	-815,1257676868
7,10	-814,8630640919	7,10	-815,0226631837	7,70	-815,1257659535
7,20	-814,8630613731	7,20	-815,0226603505	7,80	-815,1257643811
7,30	-814,8630589204	7,30	-815,0226577981	7,90	-815,1257629528
7,40	-814,8630567048	7,40	-815,0226554952	8,00	-815,1257616535
7,50	-814,8630547001	7,50	-815,0226534143	8,10	-815,1257604699
7,60	-814,8630528842	7,60	-815,0226515309	8,20	-815,1257593903
7,70	-814,8630512366	7,70	-815,0226498238	8,30	-815,1257584044
7,80	-814,8630497392	7,80	-815,0226482744	8,40	-815,1257575028
7,90	-814,8630483755	7,90	-815,0226468689	8,50	-815,1257566774
8,00	-814,8630471358	8,00	-815,0226455855	8,60	-815,1257559209
8,10	-814,8630460046	8,10	-815,0226444169	8,70	-815,1257552266
8,20	-814,8630449718	8,20	-815,0226433507	8,80	-815,1257545889
8,30	-814,8630440272	8,30	-815,0226423764	8,90	-815,1257540023
8,40	-814,8630431625	8,40	-815,0226414851	9,00	-815,1257534624
8,50	-814,8630423706	8,50	-815,0226406686	9,10	-815,1257529646
8,60	-814,8630416432	8,60	-815,02263992	9,20	-815,1257525057
8,70	-814,8630409752	8,70	-815,0226392327	9,30	-815,1257520819
8,80	-814,8630403609	8,80	-815,0226386012	9,40	-815,1257516901
8,90	-814,8630397955	8,90	-815,0226380201	9,50	-815,1257513277

9,00	-814,8630392746	9,00	-815,022637485	9,60	-815,1257509921
9,10	-814,863038794	9,10	-815,0226369917	9,70	-815,1257506811
9,20	-814,8630383504	9,20	-815,0226365365	9,80	-815,1257503926
9,30	-814,8630379404	9,30	-815,0226361161	9,90	-815,1257501249
9,40	-814,8630375612	9,40	-815,0226357273	10,00	-815,125749876
9,50	-814,8630372101	9,50	-815,0226353676	10,10	-815,1257496446
9,60	-814,8630368849	9,60	-815,0226350345	10,20	-815,1257494294
9,70	-814,8630365832	9,70	-815,0226347257	10,30	-815,1257492289
9,80	-814,8630363031	9,80	-815,0226344392	10,40	-815,125749042
9,90	-814,863036043	9,90	-815,0226341732	10,50	-815,1257488677
10,00	-814,8630358012	10,00	-815,0226339259	10,60	-815,1257487051
10,10	-814,8630355761	10,10	-815,022633696	10,70	-815,1257485532
10,20	-814,8630353666	10,20	-815,0226334821	10,80	-815,1257484112
10,30	-814,8630351714	10,30	-815,0226332827	10,90	-815,1257482784
10,40	-814,8630349894	10,40	-815,0226330969	11,00	-815,1257481541
10,50	-814,8630348195	10,50	-815,0226329236	11,10	-815,1257480377
10,60	-814,8630346608	10,60	-815,0226327618	11,20	-815,1257479287
10,70	-814,8630345126	10,70	-815,0226326107	11,30	-815,1257478265
10,80	-814,8630343739	10,80	-815,0226324695	11,40	-815,1257477305
10,90	-814,8630342442	10,90	-815,0226323374	11,50	-815,1257476405
11,00	-814,8630341228	11,00	-815,0226322137	11,60	-815,1257475559
11,10	-814,863034009	11,10	-815,0226320979	11,70	-815,1257474765
11,20	-814,8630339023	11,20	-815,0226319893	11,80	-815,1257474017
11,30	-814,8630338023	11,30	-815,0226318875	11,90	-815,1257473313
11,40	-814,8630337083	11,40	-815,022631792	12,00	-815,1257472651
11,50	-814,8630336201	11,50	-815,0226317023	12,10	-815,1257472027
11,60	-814,8630335372	11,60	-815,0226316181	12,20	-815,125747144
11,70	-814,8630334593	11,70	-815,0226315389	12,30	-815,1257470886
11,80	-814,863033386	11,80	-815,0226314644	12,40	-815,1257470363
11,90	-814,863033317	11,90	-815,0226313944	12,50	-815,125746987
12,00	-814,863033252	12,00	-815,0226313284	12,60	-815,1257469404
12,10	-814,8630331908			12,70	-815,1257468963

12,20	-814,863033133			12,80	-815,1257468548
12,30	-814,8630330786			12,90	-815,1257468154
12,40	-814,8630330272			13,00	-815,1257467782
12,50	-814,8630329787				
12,60	-814,8630329329				
12,70	-814,8630328896				
12,80	-814,8630328487				
12,90	-814,86303281				
13,00	-814,8630327733				

Tabela 5.16: Sistema diatômico Kr-Kr

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-5504,2846029782	2,00	-5504,4440702382	2,00	-5504,6195340845
2,10	-5504,3718353946	2,10	-5504,5296392164	2,10	-5504,7044647968
2,20	-5504,4377343483	2,20	-5504,5941305477	2,20	-5504,7684310635
2,30	-5504,4872292363	2,30	-5504,6424714547	2,30	-5504,8163251641
2,40	-5504,5241769414	2,40	-5504,6784995767	2,40	-5504,8519662515
2,50	-5504,5515902556	2,50	-5504,7051933261	2,50	-5504,8783259556
2,60	-5504,5718079519	2,60	-5504,7248512572	2,60	-5504,8977005505
2,70	-5504,5866310077	2,70	-5504,7392368412	2,70	-5504,9118506376
2,80	-5504,5974348569	2,80	-5504,7496945842	2,80	-5504,9221163906
2,90	-5504,6052617708	2,90	-5504,7572430423	2,90	-5504,9295110442
3,00	-5504,6108959866	3,00	-5504,7626490143	3,00	-5504,9347958715
3,10	-5504,614923829	3,10	-5504,7664864317	3,10	-5504,9385394342
3,20	-5504,6177810466	3,20	-5504,769182616	3,20	-5504,9411639815
3,30	-5504,6197897101	3,30	-5504,7710539795	3,30	-5504,9429812902
3,40	-5504,62118666	3,40	-5504,7723336403	3,40	-5504,9442204973
3,50	-5504,6221452029	3,50	-5504,7731923413	3,50	-5504,9450489993
3,60	-5504,6227915872	3,60	-5504,7737543838	3,60	-5504,9455884197
3,70	-5504,6232173728	3,70	-5504,7741096986	3,70	-5504,9459265837

3,80	-5504,6234886683	3,80	-5504,7743228187	3,80	-5504,9461264718
3,90	-5504,6236529801	3,90	-5504,7744397277	3,90	-5504,9462329298
4,00	-5504,6237442449	4,00	-5504,7744928618	4,00	-5504,9462775718
4,10	-5504,6237865505	4,01	-5504,7744956124	4,01	-5504,9462795595
4,11	-5504,6237887908	4,02	-5504,7744979762	4,02	-5504,946281157
4,12	-5504,6237907291	4,03	-5504,7744999654	4,03	-5504,9462824089
4,13	-5504,623792379	4,04	-5504,7745016032	4,04	-5504,9462833185
4,14	-5504,6237937529	4,05	-5504,7745029033	4,05	-5504,9462839053
4,15	-5504,623794863	4,06	-5504,7745038826	**4,06**	**-5504,946284185**
4,16	-5504,6237957211	4,07	-5504,7745045561	4,07	-5504,9462841736
4,17	-5504,6237963387	4,08	-5504,774504938	4,08	-5504,9462838814
4,18	-5504,6237967268	**4,09**	**-5504,7745050426**	4,09	-5504,9462833167
4,19	**-5504,6237968958**	4,10	-5504,7745048831	4,10	-5504,9462824914
4,20	-5504,6237968564	4,11	-5504,7745044723	4,11	-5504,9462814317
4,21	-5504,623796618	4,12	-5504,7745038229	4,12	-5504,9462801413
4,22	-5504,6237961904	4,13	-5504,7745029469	4,13	-5504,9462786413
4,23	-5504,6237955826	4,14	-5504,7745018553	4,14	-5504,946276947
4,24	-5504,6237948033	4,15	-5504,7745005598	4,15	-5504,9462750504
4,25	-5504,6237938611	4,16	-5504,7744990705	4,16	-5504,9462729572
4,26	-5504,6237927642	4,17	-5504,7744973982	4,17	-5504,9462706977
4,27	-5504,6237915205	4,18	-5504,7744955519	4,18	-5504,9462682406
4,28	-5504,6237901373	4,19	-5504,7744935413	4,19	-5504,9462656873
4,29	-5504,6237886221	4,20	-5504,7744913717	4,20	-5504,9462629802
4,30	-5504,6237869816	4,30	-5504,7744629296	4,30	-5504,9462293428
4,40	-5504,6237650613	4,40	-5504,7744266319	4,40	-5504,9461885362
4,50	-5504,6237366065	4,50	-5504,7743870748	4,50	-5504,9461450645
4,60	-5504,6237052844	4,60	-5504,7743471736	4,60	-5504,9461017796
4,70	-5504,6236734567	4,70	-5504,774308689	4,70	-5504,9460604471
4,80	-5504,6236425999	4,80	-5504,7742726221	4,80	-5504,9460219592
4,90	-5504,6236135536	4,90	-5504,7742394632	4,90	-5504,945986785
5,00	-5504,6235867729	5,00	-5504,7742094044	5,00	-5504,9459550168
5,10	-5504,6235624259	5,10	-5504,7741824092	5,10	-5504,9459266088

5,20	-5504,6235405131	5,20	-5504,774158321	5,20	-5504,9459013828
5,30	-5504,623520931	5,30	-5504,774136947	5,30	-5504,9458790666
5,40	-5504,6235035121	5,40	-5504,7741180304	5,40	-5504,9458593519
5,50	-5504,6234880675	5,50	-5504,7741013298	5,50	-5504,9458420194
5,60	-5504,6234743981	5,60	-5504,7740866109	5,60	-5504,9458267636
5,70	-5504,6234623113	5,70	-5504,7740736263	5,70	-5504,9458133575
5,80	-5504,6234516251	5,80	-5504,7740621884	5,80	-5504,945801562
5,90	-5504,6234421731	5,90	-5504,7740521036	5,90	-5504,945791186
6,00	-5504,6234338064	6,00	-5504,7740432045	6,00	-5504,9457820374
6,10	-5504,6234263923	6,10	-5504,7740353501	6,10	-5504,9457739722
6,20	-5504,623419814	6,20	-5504,77402839	6,20	-5504,9457668484
6,30	-5504,623413972	6,30	-5504,7740222311	6,30	-5504,9457605457
6,40	-5504,623408768	6,40	-5504,7740167669	6,40	-5504,9457549609
6,50	-5504,6234041324	6,50	-5504,7740119111	6,50	-5504,9457500027
6,60	-5504,6233999943	6,60	-5504,7740075957	6,60	-5504,9457455929
6,70	-5504,6233962941	6,70	-5504,7740037329	6,70	-5504,9457416723
6,80	-5504,6233929806	6,80	-5504,7740002772	6,80	-5504,9457381573
6,90	-5504,6233900081	6,90	-5504,7739972061	6,90	-5504,9457350211
7,00	-5504,6233873374	7,00	-5504,7739944318	7,00	-5504,9457322116
7,10	-5504,6233849339	7,10	-5504,7739919667	7,10	-5504,9457296898
7,20	-5504,6233827677	7,20	-5504,773989725	7,20	-5504,9457274205
7,30	-5504,6233808129	7,30	-5504,7739877044	7,30	-5504,9457253811
7,40	-5504,6233790454	7,40	-5504,7739858884	7,40	-5504,9457235389
7,50	-5504,6233774454	7,50	-5504,7739842458	7,50	-5504,9457218744
7,60	-5504,6233759947	7,60	-5504,7739827705	7,60	-5504,9457203681
7,70	-5504,6233746777	7,70	-5504,7739814233	7,70	-5504,9457190027
7,80	-5504,6233734795	7,80	-5504,7739801872	7,80	-5504,9457177635
7,90	-5504,6233723903	7,90	-5504,7739790737	7,90	-5504,9457166369
8,00	-5504,6233713976	8,00	-5504,7739780587	8,00	-5504,9457156116
8,10	-5504,6233704921	8,10	-5504,773977142	8,10	-5504,9457146768
8,20	-5504,6233696641	8,20	-5504,7739762881	8,20	-5504,9457138216
8,30	-5504,623368907	8,30	-5504,7739755158	8,30	-5504,9457130446

8,40	-5504,6233682134	8,40	-5504,7739748088	8,40	-5504,9457123314
8,50	-5504,6233675775	8,50	-5504,773974161	8,50	-5504,945711678
8,60	-5504,6233669938	8,60	-5504,7739735764	8,60	-5504,9457110789
8,70	-5504,6233664574	8,70	-5504,7739730209	8,70	-5504,9457105288
8,80	-5504,6233659645	8,80	-5504,7739725193	8,80	-5504,9457100234
8,90	-5504,6233655102	8,90	-5504,7739720575	8,90	-5504,9457095584
9,00	-5504,6233650917	9,00	-5504,7739716321	9,00	-5504,9457091299
9,10	-5504,6233647055	9,10	-5504,7739712397	9,10	-5504,945708735
9,20	-5504,6233643489	9,20	-5504,7739708776	9,20	-5504,9457083705
9,30	-5504,6233640194	9,30	-5504,773970543	9,30	-5504,9457080338
9,40	-5504,6233637144	9,40	-5504,7739702336	9,40	-5504,9457077225
9,50	-5504,6233634319	9,50	-5504,7739699471	9,50	-5504,9457074342
9,60	-5504,6233631704	9,60	-5504,7739696817	9,60	-5504,9457071675
9,70	-5504,6233629276	9,70	-5504,7739694357	9,70	-5504,94570692
9,80	-5504,6233627023	9,80	-5504,7739692073	9,80	-5504,9457066906
9,90	-5504,6233624929	9,90	-5504,7739689952	9,90	-5504,9457064773
10,00	-5504,6233622981	10,00	-5504,7739687983	10,00	-5504,9457062794
10,10	-5504,6233621168	10,10	-5504,7739686146	10,10	-5504,945706095
10,20	-5504,6233619484	10,20	-5504,7739684439	10,20	-5504,9457059236
10,30	-5504,623361791	10,30	-5504,7739682848	10,30	-5504,9457057637
10,40	-5504,6233616444	10,40	-5504,7739681365	10,40	-5504,9457056149
10,50	-5504,6233615075	10,50	-5504,7739679981	10,50	-5504,945705476
10,60	-5504,6233613797	10,60	-5504,7739678688	10,60	-5504,9457053462
10,70	-5504,6233612602	10,70	-5504,7739677481	10,70	-5504,9457052249
10,80	-5504,6233611484	10,80	-5504,7739676352	10,80	-5504,9457051117
10,90	-5504,6233610437	10,90	-5504,7739675296	10,90	-5504,9457050056
11,00	-5504,6233609458	11,00	-5504,7739674411	11,00	-5504,9457049066
11,10	-5504,623360854	11,10	-5504,7739673378	11,10	-5504,9457048136
11,20	-5504,623360768	11,20	-5504,7739672514	11,20	-5504,9457047266
11,30	-5504,6233606872	11,30	-5504,7739671699	11,30	-5504,9457046448
11,40	-5504,6233606114	11,40	-5504,7739670935	11,40	-5504,9457045683
11,50	-5504,6233605402	11,50	-5504,7739670217	11,50	-5504,9457044961

11,60	-5504,6233604733	11,60	-5504,7739669543	11,60	-5504,9457044288
11,70	-5504,6233604104	11,70	-5504,7739668909	11,70	-5504,9457043651
11,80	-5504,6233603512	11,80	-5504,7739668313	11,80	-5504,9457043054
11,90	-5504,6233602955	11,90	-5504,7739667752	11,90	-5504,945704249
12,00	-5504,623360243	12,00	-5504,7739667223	12,00	-5504,9457041961

Tabela 5.17: Sistema diatômico Kr-Xe

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-3080,3944092352	2,00	-3080,5949040907	2,00	-3080,7616208454
2,10	-3080,5115988373	2,10	-3080,7096493081	2,10	-3080,8753350332
2,20	-3080,6012710473	2,20	-3080,7973353992	2,20	-3080,9622014701
2,30	-3080,6697626826	2,30	-3080,8642031765	2,30	-3081,0283999836
2,40	-3080,7219274051	2,40	-3080,9150358465	2,40	-3081,0786747842
2,50	-3080,7615094586	2,50	-3080,9535263236	2,50	-3081,1166944638
2,60	-3080,7914134836	2,60	-3080,9825391789	2,60	-3081,1453087033
2,70	-3080,8138980044	2,70	-3081,0042988087	2,70	-3081,1667323589
2,80	-3080,8307180423	2,80	-3081,0205299755	2,80	-3081,1826828334
2,90	-3080,8432334255	2,90	-3081,0325661657	2,90	-3081,1944869024
3,00	-3080,8524933057	3,00	-3081,0414345257	3,00	-3081,2031651942
3,10	-3080,859303241	3,10	-3081,0479228579	3,10	-3081,209499363
3,20	-3080,8642785886	3,20	-3081,052632573	3,20	-3081,2140851869
3,30	-3080,8678871127	3,30	-3081,0560206774	3,30	-3081,2173746464
3,40	-3080,8704826442	3,40	-3081,058432621	3,40	-3081,2197087417
3,50	-3080,8723315423	3,50	-3081,0601282961	3,50	-3081,2213435894
3,60	-3080,8736333578	3,60	-3081,0613022109	3,60	-3081,2224703316
3,70	-3080,8745368721	3,70	-3081,0620991422	3,70	-3081,2232309224
3,80	-3080,8751524766	3,80	-3081,0626262282	3,80	-3081,2237300634
3,90	-3080,8755616689	3,90	-3081,0629622584	3,90	-3081,2240446008
4,00	-3080,8758242983	4,00	-3081,0631647616	4,00	-3081,2242304555
4,10	-3080,8759840622	4,10	-3081,0632754206	4,10	-3081,224328084

4,20	-3080,8760726639	4,20	-3081,0633241954	4,11	-3081,2243341929
4,21	-3080,8760785511	4,21	-3081,0633265571	4,12	-3081,2243397379
4,22	-3080,8760839801	4,22	-3081,0633285267	4,13	-3081,2243447468
4,23	-3080,8760889679	4,23	-3081,0633301301	4,14	-3081,2243492347
4,24	-3080,8760935322	4,24	-3081,0633313822	4,15	-3081,2243532284
4,25	-3080,8760976896	4,25	-3081,0633322965	4,16	-3081,2243567468
4,26	-3080,8761014569	4,26	-3081,0633328971	4,17	-3081,2243598108
4,27	-3080,8761048496	**4,27**	**-3081,0633331884**	4,18	-3081,2243624382
4,28	**-3080,876107883**	4,28	-3081,0633331879	4,19	-3081,2243646492
4,29	-3080,8761105721	4,29	-3081,0633329093	4,20	-3081,2243664609
4,30	-3080,876112931	4,30	-3081,0633323624	4,21	-3081,2243678933
4,31	-3080,8761149736	4,31	-3081,0633315673	4,22	-3081,2243689591
4,32	-3080,876116713	4,32	-3081,0633305298	4,23	-3081,2243696769
4,33	-3080,8761181625	4,33	-3081,0633292628	4,24	-3081,2243700625
4,34	-3080,8761193339	4,34	-3081,0633277783	**4,25**	**-3081,2243701312**
4,35	-3080,8761202394	4,35	-3081,063326084	4,26	-3081,224369891
4,36	-3080,8761208907	4,36	-3081,0633241987	4,29	-3081,2243674916
4,37	-3080,8761212987	4,37	-3081,0633221237	4,30	-3081,2243661708
4,38	-3080,8761214745	4,38	-3081,0633198717	4,40	-3081,2243417035
4,39	-3080,8761214285	4,39	-3081,0633174519	4,50	-3081,2243030493
4,40	-3080,8761211716	4,40	-3081,0633148654	4,60	-3081,2242570381
4,50	-3080,8761089127	4,50	-3081,0632820823	4,70	-3081,2242081973
4,60	-3080,8760842085	4,60	-3081,0632410669	4,80	-3081,2241594716
4,70	-3080,8760526046	4,70	-3081,0631965236	4,90	-3081,2241126697
4,80	-3080,8760178433	4,80	-3081,0631515143	5,00	-3081,2240688515
4,90	-3080,8759823855	4,90	-3081,0631079069	5,10	-3081,2240285533
5,00	-3080,8759477951	5,00	-3081,0630668274	5,20	-3081,2239919265
5,10	-3080,8759150347	5,10	-3081,0630288558	5,30	-3081,2239589496
5,20	-3080,875884581	5,20	-3081,0629942261	5,40	-3081,2239294748
5,30	-3080,8758566754	5,30	-3081,0629629359	5,50	-3081,2239032329
5,40	-3080,8758313611	5,40	-3081,062934863	5,60	-3081,2238799681
5,50	-3080,8758085611	5,50	-3081,0629098003	5,70	-3081,2238593653

5,60	-3080,8757881306	5,60	-3081,0628875027	5,80	-3081,2238411625
5,70	-3080,8757698883	5,70	-3081,0628677141	5,90	-3081,2238250772
5,80	-3080,8757536385	5,80	-3081,0628501759	6,00	-3081,2238108723
5,90	-3080,8757391844	5,90	-3081,0628346442	6,10	-3081,2237983108
6,00	-3080,8757263358	6,00	-3081,0628208944	6,20	-3081,223787207
6,10	-3080,8757149153	6,10	-3081,0628087167	6,30	-3081,2237773662
6,20	-3080,8757047616	6,20	-3081,062797927	6,40	-3081,2237686498
6,30	-3080,8756957277	6,30	-3081,062788357	6,50	-3081,2237609029
6,40	-3080,8756876827	6,40	-3081,0627798606	6,60	-3081,2237540212
6,50	-3080,875680512	6,50	-3081,0627723072	6,70	-3081,2237478853
6,60	-3080,8756741094	6,60	-3081,0627655826	6,80	-3081,2237424175
6,70	-3080,8756683861	6,70	-3081,0627595877	6,90	-3081,2237375259
6,80	-3080,8756632628	6,80	-3081,0627542286	7,00	-3081,2237331529
6,90	-3080,8756586708	6,90	-3081,062749446	7,10	-3081,2237292276
7,00	-3080,8756545482	7,00	-3081,0627451566	7,20	-3081,2237257071
7,10	-3080,8756508412	7,10	-3081,0627413071	7,30	-3081,2237225359
7,20	-3080,8756475007	7,20	-3081,0627378475	7,40	-3081,2237196835
7,30	-3080,8756444911	7,30	-3081,0627347325	7,50	-3081,223717105
7,40	-3080,8756417729	7,40	-3081,0627319195	7,60	-3081,223714779
7,50	-3080,8756393144	7,50	-3081,0627293832	7,70	-3081,2237126717
7,60	-3080,8756370877	7,60	-3081,0627270838	7,80	-3081,2237107612
7,70	-3080,8756350681	7,70	-3081,0627250064	7,90	-3081,223709025
7,80	-3080,8756332332	7,80	-3081,0627231209	8,00	-3081,2237074499
7,90	-3080,8756315652	7,90	-3081,062721408	8,10	-3081,2237060123
8,00	-3080,8756300463	8,00	-3081,0627198495	8,20	-3081,2237047051
8,10	-3080,8756286612	8,10	-3081,0627184286	8,30	-3081,2237035085
8,20	-3080,8756273946	8,20	-3081,0627171347	8,40	-3081,2237024177
8,30	-3080,8756262393	8,30	-3081,0627159551	8,50	-3081,2237014164
8,40	-3080,8756251819	8,40	-3081,0627148724	8,60	-3081,2237005016
8,50	-3080,8756242132	8,50	-3081,0627138814	8,70	-3081,2236996595
8,60	-3080,8756233246	8,60	-3081,0627129729	8,80	-3081,2236988889
8,70	-3080,8756225086	8,70	-3081,0627121396	8,90	-3081,2236981775

8,80	-3080,8756217585	8,80	-3081,0627113737	9,00	-3081,2236975255
8,90	-3080,8756210682	8,90	-3081,0627106694	9,10	-3081,2236969234
9,00	-3080,8756204326	9,00	-3081,0627100209	9,20	-3081,2236963679
9,10	-3080,8756198462	9,10	-3081,0627094231	9,30	-3081,2236958551
9,20	-3080,8756193049	9,20	-3081,062708872	9,40	-3081,2236953812
9,30	-3080,8756188049	9,30	-3081,0627083628	9,50	-3081,2236949415
9,40	-3080,8756183425	9,40	-3081,0627078923	9,60	-3081,223694537
9,50	-3080,8756179145	9,50	-3081,0627074569	9,70	-3081,2236941595
9,60	-3080,875617518	9,60	-3081,0627070534	9,80	-3081,2236938121
9,70	-3080,8756171503	9,70	-3081,0627066803	9,90	-3081,2236934869
9,80	-3080,8756168091	9,80	-3081,0627063336	10,00	-3081,2236931875
9,90	-3080,8756164923	9,90	-3081,062706012	10,10	-3081,2236929064
10,00	-3080,8756161978	10,00	-3081,0627057131	10,20	-3081,2236926476
10,10	-3080,8756159237	10,10	-3081,0627054304	10,30	-3081,2236924039
10,20	-3080,8756156687	10,20	-3081,0627051764	10,40	-3081,2236921794
10,30	-3080,875615431	10,30	-3081,0627049357	10,50	-3081,2236919675
10,40	-3080,8756152094	10,40	-3081,0627047112	10,60	-3081,2236917723
10,50	-3080,8756150027	10,50	-3081,0627045019	10,70	-3081,2236915874
10,60	-3080,8756148096	10,60	-3081,0627043065	10,80	-3081,2236914173
10,70	-3080,8756146293	10,70	-3081,0627041239	10,90	-3081,2236912555
10,80	-3080,8756144606	10,80	-3081,0627039535	11,00	-3081,2236911068
10,90	-3080,8756143028	10,90	-3081,062703794	11,10	-3081,2236909649
11,00	-3080,8756141551	11,00	-3081,0627036398	11,20	-3081,2236908346
11,10	-3080,8756140167	11,10	-3081,0627035048	11,30	-3081,2236907098
11,20	-3080,875613887	11,20	-3081,0627033739	11,40	-3081,2236905954
11,30	-3080,8756137653	11,30	-3081,0627032511	11,50	-3081,2236904854
11,40	-3080,8756136511	11,40	-3081,0627031359	11,60	-3081,2236903846
11,50	-3080,8756135438	11,50	-3081,0627030277	11,70	-3081,2236902874
11,60	-3080,8756134431	11,60	-3081,0627029261	11,80	-3081,2236901985
11,70	-3080,8756133484	11,70	-3081,0627028306	11,90	-3081,2236901124
11,80	-3080,8756132593	11,80	-3081,0627027408	12,00	-3081,2243674916
11,90	-3080,8756131754	11,90	-3081,0627026563	12,10	-3081,2243661708

12,00	-3080,8756130964	12,00	-3081,0627025768	

Tabela 5.18: Sistema diatômico Kr-Rn

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
3,00	-3040,0977616912	3,00	-3040,3086813717	3,00	-3040,4901953906
3,10	-3040,1058269196	3,10	-3040,3163389654	3,10	-3040,497673169
3,20	-3040,111772261	3,20	-3040,3219466897	3,20	-3040,5031351622
3,30	-3040,1161266914	3,30	-3040,3260217002	3,30	-3040,507092527
3,40	-3040,11929233	3,40	-3040,3289562908	3,40	-3040,5099325001
3,50	-3040,1215738523	3,50	-3040,3310469554	3,50	-3040,5119474014
3,60	-3040,1232013189	3,60	-3040,3325168851	3,60	-3040,5133570065
3,70	-3040,1243477582	3,70	-3040,3335333825	3,70	-3040,5143257757
3,80	-3040,1251427446	3,80	-3040,3342213298	3,80	-3040,5149762112
3,90	-3040,1256828639	3,90	-3040,3346734108	3,90	-3040,515398989
4,00	-3040,1260397486	4,00	-3040,3349580521	4,00	-3040,5156608117
4,10	-3040,1262662339	4,10	-3040,3351254211	4,10	-3040,5158104384
4,20	-3040,1264010614	4,20	-3040,3352120437	4,20	-3040,5158831608
4,30	-3040,1264724486	4,21	-3040,3352173565	4,25	-3040,5158989333
4,31	-3040,126476936	4,22	-3040,3352221476	4,26	-3040,5159007876
4,32	-3040,126481018	4,23	-3040,3352264434	4,27	-3040,51590224
4,33	-3040,126484707	4,24	-3040,335230264	4,28	-3040,5159033145
4,34	-3040,126488019	4,25	-3040,3352336292	4,29	-3040,5159040287
4,35	-3040,1264909693	4,26	-3040,3352365574	4,30	-3040,5159043974
4,36	-3040,1264935724	4,27	-3040,3352390674	**4,31**	**-3040,5159044372**
4,37	-3040,1264958425	4,28	-3040,3352411765	4,32	-3040,5159041623
4,38	-3040,1264977933	4,29	-3040,3352429019	4,33	-3040,515903586
4,39	-3040,126499438	4,30	-3040,3352442599	4,34	-3040,5159027215
4,40	-3040,1265007897	4,31	-3040,3352452665	4,35	-3040,5159015844
4,41	-3040,1265018606	4,32	-3040,3352459372	4,36	-3040,5159001794
4,42	-3040,1265026626	4,33	-3040,3352462863	4,40	-3040,5158922198

4,43	-3040,1265032072	**4,34**	**-3040,3352463286**	4,50	-3040,5158593474
4,44	-3040,1265035057	4,35	-3040,3352460778	4,60	-3040,5158146115
4,45	**-3040,1265035687**	4,36	-3040,3352455466	4,70	-3040,5157640539
4,46	-3040,1265034069	4,37	-3040,3352447492	4,80	-3040,5157116922
4,47	-3040,1265030302	4,38	-3040,3352436971	4,90	-3040,5156601002
4,48	-3040,1265024484	4,39	-3040,3352424025	5,00	-3040,5156108809
4,49	-3040,1265016706	4,40	-3040,3352408768	5,10	-3040,5155649562
4,50	-3040,126500706	4,50	-3040,3352151716	5,20	-3040,5155227549
4,60	-3040,1264825636	4,60	-3040,3351763958	5,30	-3040,5154844128
4,70	-3040,1264536142	4,70	-3040,3351308529	5,40	-3040,5154498625
4,80	-3040,1264188688	4,80	-3040,335082759	5,50	-3040,5154189243
4,90	-3040,1263816963	4,90	-3040,3350348449	5,60	-3040,5153913387
5,00	-3040,1263443174	5,00	-3040,3349888064	5,70	-3040,5153668243
5,10	-3040,1263081393	5,10	-3040,3349456163	5,80	-3040,5153450734
5,20	-3040,1262739918	5,20	-3040,3349057728	5,90	-3040,5153257947
5,30	-3040,1262423171	5,30	-3040,3348694541	6,00	-3040,5153087595
5,40	-3040,1262132998	5,40	-3040,3348366377	6,10	-3040,5152936466
5,50	-3040,126186952	5,50	-3040,3348071701	6,20	-3040,5152802981
5,60	-3040,1261632046	5,60	-3040,3347808228	6,30	-3040,51526845
5,70	-3040,1261418613	5,70	-3040,3347573465	6,40	-3040,5152579412
5,80	-3040,1261227576	5,80	-3040,3347364732	6,50	-3040,5152486076
5,90	-3040,126105696	5,90	-3040,3347179401	6,60	-3040,5152403075
6,00	-3040,1260904781	6,00	-3040,3347014975	6,70	-3040,5152329173
6,10	-3040,1260769147	6,10	-3040,3346869121	6,80	-3040,5152263245
6,20	-3040,1260648272	6,20	-3040,3346739711	6,90	-3040,5152204339
6,30	-3040,1260540537	6,30	-3040,3346624828	7,00	-3040,5152151603
6,40	-3040,1260444455	6,40	-3040,3346522755	7,10	-3040,5152104379
6,50	-3040,1260358697	6,50	-3040,3346431966	7,20	-3040,5152061943
6,60	-3040,1260282093	6,60	-3040,3346351118	7,30	-3040,5152023802
6,70	-3040,1260213566	6,70	-3040,3346279024	7,40	-3040,5151989447
6,80	-3040,1260152197	6,80	-3040,3346214642	7,50	-3040,5151958453
6,90	-3040,1260097168	6,90	-3040,3346157058	7,60	-3040,5151930447

7,00	-3040,1260047756	7,00	-3040,3346105475	7,70	-3040,5151905119
7,10	-3040,1260003298	7,10	-3040,3346059123	7,80	-3040,5151882151
7,20	-3040,1259963295	7,20	-3040,3346017535	7,90	-3040,5151861302
7,30	-3040,1259927223	7,30	-3040,3345980104	8,00	-3040,5151842349
7,40	-3040,1259894646	7,40	-3040,3345946439	8,10	-3040,5151842319
7,50	-3040,1259865185	7,50	-3040,3345915962	8,20	-3040,5151825092
7,60	-3040,1259838506	7,60	-3040,3345888402	8,30	-3040,5151809371
7,70	-3040,1259814306	7,70	-3040,3345863441	8,40	-3040,5151795021
7,80	-3040,1259792338	7,80	-3040,33458408	8,50	-3040,5151781905
7,90	-3040,1259772361	7,90	-3040,3345820233	8,60	-3040,5151769904
8,00	-3040,1259754171	8,00	-3040,3345801526	8,70	-3040,515175891
8,10	-3040,125973758	8,10	-3040,3345784487	8,80	-3040,5151748826
8,20	-3040,1259722445	8,20	-3040,3345768946	9,00	-3040,5151723199
8,30	-3040,1259708588	8,30	-3040,3345754753	9,10	-3040,5151716005
8,40	-3040,1259695935	8,40	-3040,3345741777	9,20	-3040,5151709353
8,50	-3040,1259684342	8,50	-3040,3345729898	10,00	-3040,5151671273
8,60	-3040,125967371	8,60	-3040,3345719009	10,10	-3040,5151667945
8,70	-3040,1259663947	8,70	-3040,3345709018	10,20	-3040,5151664836
8,80	-3040,1259654973	8,80	-3040,3345699842	11,00	-3040,5151646415
8,90	-3040,1259646717	8,90	-3040,3345691402	11,10	-3040,5151644753
9,00	-3040,1259639116	9,00	-3040,3345683634	12,00	-3040,5151633606
9,10	-3040,1259632101	9,10	-3040,3345676474	13,00	-3040,5151626613
9,20	-3040,1259625628	9,20	-3040,3345669871	14,00	-3040,5151622587
9,30	-3040,1259619649	9,30	-3040,3345663774	15,00	-3040,5151620176
9,40	-3040,125961412	9,40	-3040,3345658139	16,00	-3040,5151618678
9,50	-3040,1259609003	9,50	-3040,3345652927	17,00	-3040,5151617719
9,60	-3040,1259604263	9,60	-3040,3345648101		
9,70	-3040,1259599868	9,70	-3040,3345643629		
9,80	-3040,125959579	9,80	-3040,3345639481		
9,90	-3040,1259592003	9,90	-3040,3345635631		
10,00	-3040,1259588483	10,00	-3040,3345632054		
10,10	-3040,1259585209	10,10	-3040,3345628728		

10,20	-3040,1259582161	10,20	-3040,3345625634
10,30	-3040,1259579321	10,30	-3040,3345622752
10,40	-3040,1259576674	10,40	-3040,3345620068
10,50	-3040,1259574204	10,50	-3040,3345617563
10,60	-3040,1259571899	10,60	-3040,3345615226
10,70	-3040,1259569744	10,70	-3040,3345613043
10,80	-3040,125956773	10,80	-3040,3345611003
10,90	-3040,1259565846	10,90	-3040,3345609097
11,00	-3040,1259564082	11,00	-3040,3345607311
11,10	-3040,1259562429	11,10	-3040,3345605639
11,20	-3040,125956088	11,20	-3040,3345604073
11,30	-3040,1259559427	11,30	-3040,3345602605
11,40	-3040,1259558064	11,40	-3040,3345601227
11,50	-3040,1259556784	11,50	-3040,3345599934
11,60	-3040,1259555581	11,60	-3040,334559872
11,70	-3040,125955445	11,70	-3040,3345597578
11,80	-3040,1259553386	11,80	-3040,3345596505
11,90	-3040,1259552385	11,90	-3040,3345595495
12,00	-3040,1259551442	12,00	-3040,3345594545

Tabela 5.19: Sistema diatômico Xe-Xe

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
2,00	-656,4377222823	2,00	-656,6813064271	2,00	-656,8403897785
2,10	-656,6012420745	2,10	-656,8413473362	2,10	-656,9987828223
2,20	-656,7261425482	2,20	-656,9634721721	2,20	-657,1196303505
2,30	-656,8219462649	2,30	-657,0569767842	2,30	-657,2121197374
2,40	-656,895568138	2,40	-657,128659507	2,40	-657,2829808967
2,50	-656,9521408783	2,50	-657,1835900536	2,50	-657,3372343345
2,60	-656,9955476965	2,60	-657,2256105331	2,60	-657,3786871949
2,70	-657,0287659254	2,70	-657,2576670186	2,70	-657,4102625116

2,80	-657,0540984332	2,80	-657,2820354487	2,80	-657,4342212375
2,90	-657,0733363676	2,90	-657,3004811949	2,90	-657,4523184523
3,00	-657,0878768614	3,00	-657,3143756251	3,00	-657,4659177639
3,10	-657,0988098899	3,10	-657,324783894	3,10	-657,4760780033
3,20	-657,1069841502	3,20	-657,3325320575	3,20	-657,4836195476
3,30	-657,113058263	3,30	-657,3382592924	3,30	-657,4891763638
3,40	-657,1175412446	3,40	-657,3424586527	3,40	-657,4932365821
3,50	-657,1208247449	3,50	-657,3455091022	3,50	-657,496174674
3,60	-657,1232087472	3,60	-657,3477007123	3,60	-657,4982764986
3,70	-657,1249219589	3,70	-657,3492544849	3,70	-657,4997593032
3,80	-657,1261379674	3,80	-657,3503379984	3,80	-657,5007872577
3,90	-657,1269878579	3,90	-657,3510776312	3,90	-657,5014837582
4,00	-657,1275701548	4,00	-657,3515681514	4,00	-657,5019409668
4,10	-657,1279585222	4,10	-657,3518802221	4,10	-657,502227418
4,20	-657,1282077376	4,20	-657,3520660943	4,20	-657,5023935455
4,30	-657,1283582833	4,21	-657,3520793168	4,21	-657,5024050613
4,31	-657,1283691324	4,22	-657,3520917167	4,22	-657,5024157726
4,32	-657,1283793239	4,23	-657,3521032988	4,23	-657,5024257407
4,33	-657,1283888815	4,27	-657,352114107	4,24	-657,5024349644
4,34	-657,128397828	4,28	-657,3521501404	4,25	-657,5024434675
4,35	-657,1284061876	4,29	-657,3521574941	4,26	-657,5024513131
4,36	-657,1284139788	4,30	-657,352164219	4,27	-657,502458492
4,37	-657,1284212244	4,31	-657,3521703635	4,28	-657,5024650411
4,38	-657,1284279445	4,32	-657,3521759384	4,29	-657,5024709849
4,39	-657,1284341591	4,33	-657,3521809633	4,30	-657,5024763449
4,40	-657,1284398875	4,34	-657,3521854548	4,31	-657,5024811512
4,41	-657,128445148	4,35	-657,3521894517	4,32	-657,5024854237
4,42	-657,1284499585	4,36	-657,3521929745	4,33	-657,5024891756
4,43	-657,1284543364	4,37	-657,3521960303	4,34	-657,5024924254
4,44	-657,1284582986	4,38	-657,3521986377	4,35	-657,502495223
4,45	-657,1284618612	4,39	-657,3522008101	4,36	-657,5024975502
4,46	-657,12846504	4,40	-657,3522025905	4,37	-657,5024994338

4,47	-657,1284678502	4,41	-657,3522039669	4,38	-657,5025009195
4,48	-657,1284703064	4,42	-657,3522049813	4,39	-657,5025019978
4,49	-657,128472423	4,43	-657,3522056348	4,40	-657,5025026836
4,50	-657,1284742108	**4,44**	**-657,3522059417**	**4,41**	**-657,5025030199**
4,60	**-657,1284769155**	4,45	-657,3522059215	4,42	-657,5025029876
4,70	-657,1284592011	4,46	-657,3522055796	4,43	-657,5025026391
4,80	-657,1284289895	4,47	-657,3522049517	4,44	-657,502501957
4,90	-657,1283918031	4,48	-657,3522040265	4,45	-657,5025009712
5,00	-657,1283514237	4,49	-657,3522028349	4,46	-657,5024996828
5,10	-657,1283103777	4,50	-657,352201377	4,47	-657,5024981359
5,20	-657,1282703008	4,60	-657,3521750087	4,48	-657,5024963092
5,30	-657,1282322304	4,70	-657,3521336127	4,49	-657,5024942194
5,40	-657,1281966659	4,80	-657,3520841661	4,50	-657,5024918994
5,50	-657,1281639088	4,90	-657,3520314376	4,60	-657,5024577491
5,60	-657,1281340282	5,00	-657,3519785612	4,70	-657,5024098805
5,70	-657,1281069642	5,10	-657,3519274377	4,80	-657,5023550008
5,80	-657,1280825782	5,20	-657,3518792603	4,90	-657,502297604
5,90	-657,128060687	5,30	-657,351834646	5,00	-657,5022406452
6,00	-657,1280410876	5,40	-657,351793843	5,10	-657,5021859902
6,10	-657,1280235635	5,50	-657,3517568584	5,20	-657,5021347249
6,20	-657,12800792	5,60	-657,351723556	5,30	-657,502087449
6,30	-657,127993957	5,70	-657,3516937081	5,40	-657,502044295
6,40	-657,1279814938	5,80	-657,3516670444	5,50	-657,5020052874
6,50	-657,127970365	5,90	-657,3516432832	5,60	-657,5019702511
6,60	-657,1279604214	6,00	-657,3516221369	5,70	-657,5019389313
6,70	-657,1279515295	6,10	-657,3516033329	5,80	-657,5019110326
6,80	-657,127943574	6,20	-657,3515866196	5,90	-657,5018862348
6,90	-657,1279364374	6,30	-657,351571759	6,00	-657,501864231
7,00	-657,1279300343	6,40	-657,3515585417	6,10	-657,5018447168
7,10	-657,1279242808	6,50	-657,3515467778	6,20	-657,501827413
7,20	-657,1279191038	6,60	-657,3515362974	6,30	-657,5018120652
7,30	-657,1279144393	6,70	-657,3515269491	6,40	-657,5017984394

7,40	-657,1279102329	6,80	-657,3515186008	6,50	-657,5017863309
7,50	-657,12790643	6,90	-657,3515111363	6,60	-657,5017755593
7,60	-657,1279029891	7,00	-657,351504451	6,70	-657,5017659634
7,70	-657,1278998583	7,10	-657,3514984565	6,80	-657,5017574028
7,80	-657,1278970329	7,20	-657,3514930715	6,90	-657,5017497533
7,90	-657,1278944657	7,30	-657,3514882275	7,00	-657,5017429104
8,00	-657,127892129	7,40	-657,3514838636	7,10	-657,5017367777
8,10	-657,1278899995	7,50	-657,3514799251	7,20	-657,5017312739
8,20	-657,1278880571	7,60	-657,3514763668	7,30	-657,5017263267
8,30	-657,1278862832	7,70	-657,3514731465	7,40	-657,501721873
8,40	-657,1278846607	7,80	-657,3514702273	7,50	-657,5017178578
8,50	-657,1278831752	7,90	-657,3514675774	7,60	-657,5017142318
8,60	-657,1278818134	8,00	-657,3514651689	7,70	-657,501710954
8,70	-657,1278805639	8,10	-657,3514629763	7,80	-657,5017079852
8,80	-657,1278794142	8,20	-657,3514609785	7,90	-657,5017052933
8,90	-657,1278783588	8,30	-657,3514591542	8,00	-657,5017028489
9,00	-657,1278773868	8,40	-657,3514574884	8,10	-657,5017006257
9,10	-657,1278764916	8,50	-657,3514559593	8,20	-657,5016986024
9,20	-657,127875665	8,60	-657,3514545673	8,30	-657,5016967566
9,30	-657,1278749017	8,70	-657,3514532832	8,40	-657,5016950726
9,40	-657,127874196	8,80	-657,3514521081	8,50	-657,5016935324
9,50	-657,1278735432	8,90	-657,3514510278	8,60	-657,5016921228
9,60	-657,1278729386	9,00	-657,3514500354	8,70	-657,5016908308
9,70	-657,1278723782	9,10	-657,3514491243	8,80	-657,5016896451
9,80	-657,1278718584	9,20	-657,3514482754	8,90	-657,5016885561
9,90	-657,1278713756	9,30	-657,3514474965	9,00	-657,5016875538
10,00	-657,1278709272	9,40	-657,3514467766	9,10	-657,5016866308
10,10	-657,12787051	9,50	-657,3514461109	9,20	-657,5016857808
10,20	-657,1278701219	9,60	-657,3514454949	9,30	-657,5016849957
10,30	-657,1278697604	9,70	-657,3514449242	9,40	-657,5016842708
10,40	-657,1278694233	9,80	-657,3514443945	9,50	-657,5016835997
10,50	-657,127869109	9,90	-657,3514439041	9,60	-657,50168298

10,60	-657,1278688156	10,00	-657,3514434476	9,70	-657,5016824053
10,70	-657,1278685415	10,10	-657,3514430244	9,80	-657,5016818719
10,80	-657,1278682853	10,20	-657,3514426303	9,90	-657,5016813784
10,90	-657,1278680456	10,30	-657,3514422626	10,00	-657,5016809194
11,00	-657,1278678214	10,40	-657,3514419209	10,10	-657,5016804928
11,10	-657,1278676113	10,50	-657,3514416023	12,00	-657,5016761228
11,20	-657,1278674145	10,60	-657,3514413056		
11,30	-657,1278672298	10,70	-657,351441028		
11,40	-657,1278670566	10,80	-657,3514407687		
11,50	-657,127866894	10,90	-657,3514405262		
11,60	-657,1278667412	11,00	-657,3514402994		
11,70	-657,1278665976	11,10	-657,3514400872		
11,80	-657,1278664625	11,20	-657,3514398883		
11,90	-657,1278663355	11,30	-657,3514397019		
12,00	-657,1278662158	11,40	-657,3514395265		
		11,50	-657,351439363		
		11,60	-657,3514392084		
		11,70	-657,3514390637		
		11,80	-657,3514389281		
		11,90	-657,3514388002		
		12,00	-657,3514386796		

Tabela 5.20: Sistema diatômico Xe-Rn

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
3,00	-616,3031567508	3,00	-616,5791677932	3,50	-616,7073668405
3,10	-616,3159180659	3,10	-616,591289218	3,60	-616,709910828
3,20	-616,3255169148	3,20	-616,6003651381	3,70	-616,7117257921
3,30	-616,3326980129	3,30	-616,6071195665	3,80	-616,7130006884
3,40	-616,3380377621	3,40	-616,6121109928	3,90	-616,7138784735
3,50	-616,3419810099	3,50	-616,6157693017	4,00	-616,7144668488

3,60	-616,3448699309	3,60	-616,6184245007	4,10	-616,7148464289
3,70	-616,3469668073	3,70	-616,6203291015	4,20	-616,7150772089
3,80	-616,3484719501	3,80	-616,6216755935	4,30	-616,7152033834
3,90	-616,3495376872	3,90	-616,6226100883	4,40	-616,7152574715
4,00	-616,3502793765	4,00	-616,623242956	4,42	-616,7152618266
4,10	-616,3507839546	4,10	-616,6236571314	4,43	-616,7152633321
4,20	-616,3511166001	4,20	-616,6239145895	4,44	-616,7152644173
4,30	-616,3513258987	4,30	-616,6240613257	4,45	-616,7152650981
4,40	-616,3514478406	4,40	-616,6241312278	**4,46**	**-616,7152653886**
4,50	-616,3515088969	4,41	-616,6241350172	4,47	-616,7152653079
4,51	-616,3515124473	4,42	-616,6241382962	4,48	-616,7152648719
4,52	-616,3515156036	4,43	-616,6241411095	4,49	-616,7152640935
4,53	-616,3515183805	4,44	-616,6241434674	4,50	-616,7152629894
4,54	-616,3515207927	4,45	-616,6241453875	4,51	-616,7152615731
4,55	-616,3515228546	4,46	-616,6241468889	4,52	-616,7152598601
4,56	-616,3515245802	4,47	-616,6241479887	4,53	-616,7152578646
4,57	-616,3515259828	4,48	-616,6241487038	4,54	-616,7152555956
4,58	-616,3515270761	**4,49**	**-616,6241490499**	4,55	-616,7152530739
4,59	-616,3515278725	4,50	-616,6241490431	4,56	-616,7152502994
4,60	-616,3515283841	4,51	-616,6241486991	4,57	-616,7152472914
4,61	**-616,3515286232**	4,52	-616,6241480315	4,60	-616,7152369756
4,62	-616,3515286011	4,53	-616,6241470545	4,70	-616,7151914871
4,63	-616,3515283287	4,54	-616,6241457833	4,80	-616,7151350485
4,64	-616,3515278171	4,55	-616,624144231	4,90	-616,7150735227
4,65	-616,3515270767	4,56	-616,6241424095	5,00	-616,7150108296
4,66	-616,3515261172	4,57	-616,6241403321	5,10	-616,7149495357
4,67	-616,3515249486	4,58	-616,6241380102	5,20	-616,7148912414
4,68	-616,3515235801	4,59	-616,6241354542	5,30	-616,7148368478
4,69	-616,3515220207	4,60	-616,6241326783	5,40	-616,7147867836
4,70	-616,3515202795	4,70	-616,6240949196	5,50	-616,7147411915
4,80	-616,3514945947	4,80	-616,6240447892	5,60	-616,7146999772
4,90	-616,3514583758	4,90	-616,6239885065	5,70	-616,7146629377

5,00	-616,3514165616	5,00	-616,6239302707	5,80	-616,7146298019
5,10	-616,3513725168	5,10	-616,6238728551	5,90	-616,714600241
5,20	-616,3513284824	5,20	-616,6238179239	6,00	-616,7145739353
5,30	-616,3512858967	5,30	-616,6237664887	6,10	-616,7145505443
5,40	-616,3512456312	5,40	-616,6237190398	6,20	-616,714529769
5,50	-616,3512081638	5,50	-616,6236757383	6,30	-616,7145113172
5,60	-616,3511737025	5,60	-616,6236365319	6,40	-616,714494917
5,70	-616,3511422753	5,70	-616,6236012353	6,50	-616,7144803614
5,80	-616,3511138171	5,80	-616,62356959	6,60	-616,714467391
5,90	-616,3510881285	5,90	-616,6235413023	6,70	-616,714455841
6,00	-616,3510650347	6,00	-616,6235160675	6,80	-616,7144455237
6,10	-616,3510443215	6,10	-616,6234935787	6,90	-616,7144363122
6,20	-616,3510257734	6,20	-616,6234735458	7,00	-616,7144280707
6,30	-616,3510091794	6,30	-616,6234557174	7,10	-616,7144206869
6,40	-616,3509943383	6,40	-616,6234398422	7,20	-616,7144140619
6,50	-616,3509810657	6,50	-616,6234257	7,30	-616,7144081079
6,60	-616,3509691906	6,60	-616,6234130919	7,40	-616,7144027494
6,70	-616,3509585617	6,70	-616,6234018416	7,50	-616,7143979207
6,80	-616,3509490395	6,80	-616,6233917914	7,60	-616,7143935622
6,90	-616,3509405003	6,90	-616,6233828132	7,70	-616,7143896223
7,00	-616,350932834	7,00	-616,6233747631	7,80	-616,7143860551
7,10	-616,3509259443	7,10	-616,6233675439	7,90	-616,7143828215
7,20	-616,3509197451	7,20	-616,62336106	8,00	-616,7143798859
7,30	-616,3509141574	7,30	-616,6233552282	8,10	-616,7143772169
7,40	-616,3509091171	7,40	-616,6233499751	8,20	-616,7143747873
7,50	-616,3509045629	7,50	-616,6233452363	8,60	-616,71436701
7,60	-616,3509004415	7,60	-616,6233409547	9,00	-616,7143615316
7,70	-616,3508967056	7,70	-616,6233370807	9,40	-616,7143575997
7,80	-616,3508933184	7,80	-616,6233335704	9,80	-616,7143547308
7,90	-616,3508902411	7,90	-616,6233303849	10,20	-616,714352607
8,00	-616,3508874321	8,00	-616,62332749	10,60	-616,7143510142
8,10	-616,3508848852	8,10	-616,6233248556	11,00	-616,7143498055

8,20	-616,350882562	8,20	-616,6233224554	11,40	-616,7143488781
8,30	-616,3508804405	8,30	-616,6233202652	11,80	-616,7143481592
8,40	-616,3508784996	8,40	-616,6233182643	12,20	-616,714347597
8,50	-616,3508767228	8,50	-616,6233164341	12,60	-616,7143471533
8,60	-616,3508750944	8,60	-616,6233147578	13,00	-616,7143468004
8,70	-616,3508735985	8,70	-616,6233132209	13,40	-616,7143465175
8,80	-616,3508722259	8,80	-616,6233118102	13,80	-616,7143462894
8,90	-616,3508709629	8,90	-616,6233105137	14,20	-616,714346104
9,00	-616,3508698007	9,00	-616,623309321	14,60	-616,7143459524
9,10	-616,3508687295	9,10	-616,6233082226		
9,20	-616,3508677419	9,20	-616,6233072098		
9,30	-616,3508668292	9,30	-616,6233062754		
9,40	-616,3508659856	9,40	-616,6233054123		
9,50	-616,3508652052	9,50	-616,6233046143		
9,60	-616,3508644825	9,60	-616,6233038758		
9,70	-616,3508638127	9,70	-616,6233031918		
9,80	-616,3508631914	9,80	-616,6233025577		
9,90	-616,3508626145	9,90	-616,6233019693		
10,00	-616,3508620786	10,00	-616,6233014229		
10,10	-616,3508615802	10,10	-616,6233009151		
10,20	-616,3508611163	10,20	-616,6233004429		
10,30	-616,3508606844	10,30	-616,6233000033		
10,40	-616,3508602817	10,40	-616,6232995938		
10,50	-616,3508599062	10,50	-616,623299212		
10,60	-616,3508595557	10,60	-616,6232988559		
10,70	-616,3508592283	10,70	-616,6232985235		
10,80	-616,3508589223	10,80	-616,6232982128		
10,90	-616,3508586361	10,90	-616,6232979225		
11,00	-616,3508583682	11,00	-616,6232976509		
11,10	-616,3508581174	11,10	-616,6232958557		
11,20	-616,3508578823	11,20	-616,623296009		
11,30	-616,3508576619	11,30	-616,6232961718		

11,40	-616,3508574551	11,40	-616,6232963452	
11,50	-616,3508572609	11,50	-616,6232965296	
11,60	-616,3508570785	11,60	-616,623296726	
11,70	-616,3508569071	11,70	-616,6232969353	
11,80	-616,3508567459	11,80	-616,6232971585	
11,90	-616,3508565942	11,90	-616,6232973967	
12,00	-616,3508564514	12,00	-616,6232957116	

Tabela 5.21: Sistema diatômico Rn-Rn

aug−cc−pvtz		aug−cc−pvqz		aug−cc−pv5z	
R(Å)	E(H)	R(Å)	E(H)	R(Å)	E(H)
3,00	-575,5718254499	3,00	-575,8428684423	3,50	-576,0759220961
3,10	-575,5867201691	3,10	-575,8569679118	3,60	-576,0789778568
3,20	-575,5979807061	3,20	-575,8675744832	3,70	-576,0811783182
3,30	-575,6064530522	3,30	-575,875511631	3,80	-576,0827405056
3,40	-575,6127926989	3,40	-575,8814144681	3,90	-576,0838298415
3,50	-575,617506763	3,50	-575,8857722961	4,00	-576,084571674
3,60	-575,6209866918	3,60	-575,8889615042	4,10	-576,0850606169
3,70	-575,6235338088	3,70	-575,8912709406	4,20	-576,0853675138
3,80	-575,6253793635	3,80	-575,8929216941	4,30	-576,0855451309
3,90	-575,6267002224	3,90	-575,8940824193	4,40	-576,0856323049
4,00	-575,6276311415	4,00	-575,8948812892	4,47	-576,0856550983
4,10	-575,6282743643	4,10	-575,8954152286	4,48	-576,0856563471
4,20	-575,6287070953	4,20	-575,8957572166	4,49	-576,0856571546
4,30	-575,6289873176	4,30	-575,8959618499	**4,50**	**-576,0856575333**
4,40	-575,6291583257	4,40	-575,8960697547	4,51	-576,0856575003
4,50	-575,6292522246	4,50	-575,8961108808	4,52	-576,085657068
4,60	-575,62929264	4,51	-575,8961122259	4,53	-576,0856562729
4,61	-575,6292944509	4,52	-575,8961131477	4,54	-576,0856551216
4,62	-575,6292959146	4,53	-575,8961136581	4,60	-576,085641515
4,63	-575,6292970506	**4,54**	**-575,8961137764**	4,70	-576,0855992083

4,64	-575,6292978694	4,55	-575,8961135209	4,80	-576,0855411812
4,65	-575,6292983838	4,56	-575,8961129054	4,90	-576,0854749037
4,66	**-575,6292986071**	4,57	-575,8961119491	5,00	-576,0854055553
4,67	-575,6292985511	4,58	-575,8961106638	5,10	-576,0853364501
4,68	-575,6292982274	4,59	-575,8961090595	5,20	-576,0852698229
4,69	-575,6292976471	4,60	-575,8961071534	5,30	-576,0852070044
4,70	-575,6292968216	4,70	-575,8960744499	5,40	-576,0851486876
4,71	-575,6292957614	4,80	-575,8960240948	5,50	-576,0850951795
4,72	-575,6292944766	4,90	-575,8959640809	5,60	-576,0850465278
4,73	-575,6292929771	5,00	-575,8958998912	5,70	-576,0850025753
4,74	-575,6292912724	5,10	-575,8958352261	6,00	-576,0848961216
4,75	-575,629289372	5,20	-575,8957724639	6,50	-576,0847831996
4,76	-575,6292872846	5,30	-575,8957130379	7,00	-576,0847199513
4,77	-575,6292850169	5,40	-575,8956577592	7,50	-576,084683499
4,78	-575,6292825844	5,50	-575,8956069844	8,00	-576,0846617197
4,79	-575,6292799875	5,60	-575,8955607698	8,50	-576,0846482317
4,80	-575,6292772368	5,70	-575,8955190262	9,00	-576,0846395965
4,90	-575,629242797	5,80	-575,8954814414	10,00	-576,0846300529
5,00	-575,6291997945	5,90	-575,8954477464	11,00	-576,0846255103
5,10	-575,6291525969	6,00	-575,8954176123	12,00	-576,0846231783
5,20	-575,6291041716	6,10	-575,8953907087	13,00	-576,0846219089
5,30	-575,6290564886	6,20	-575,8953667116	14,00	-576,0846211799
5,40	-575,629010791	6,30	-575,8953453185	15,00	-576,0846207443
5,50	-575,6289678183	6,40	-575,8953262462	16,00	-576,0846204741
5,60	-575,6289279568	6,50	-575,895309241		
5,70	-575,6288913476	6,60	-575,8952940697		
5,80	-575,6288579769	6,70	-575,895280525		
5,90	-575,6288277708	6,80	-575,8952684208		
6,00	-575,6288004631	6,90	-575,8952575994		
6,10	-575,6287758841	7,00	-575,8952479016		
6,20	-575,6287538072	7,10	-575,8952392043		
6,30	-575,6287340057	7,50	-575,8952123361		

6,40	-575,6287162599	7,59	-575,8951944623
6,50	-575,6287003624	8,30	-575,8951822959
6,60	-575,6286861199	8,70	-575,8951738341
6,70	-575,6286733579	9,10	-575,8951678338
6,80	-575,6286619167	9,50	-575,8951635049
6,90	-575,6286516501	11,00	-575,895155157
7,00	-575,6286424319	12,00	-575,8951528338
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7,60	-575,6286034825		
7,70	-575,6285989948		
7,80	-575,6285949268		
7,90	-575,6285912321		
8,00	-575,628587872		
8,10	-575,6285848122		
8,20	-575,6285820097		
8,30	-575,628579464		
8,40	-575,6285771389		
8,50	-575,6285750088		
8,60	-575,6285730581		
8,70	-575,6285712665		
8,80	-575,6285696183		
8,90	-575,6285681052		
9,00	-575,6285667124		
9,10	-575,6285654286		
9,20	-575,6285642435		
9,30	-575,6285631494		
9,40	-575,6285621378		
9,50	-575,628561202		

9,60	-575,6285603355		
9,70	-575,6285595323		
9,80	-575,6285587872		
9,90	-575,6285580956		
10,00	-575,6285574529		
10,10	-575,6285568552		
10,20	-575,628556299		
10,30	-575,6285557811		
10,40	-575,6285552983		
10,50	-575,6285548481		
10,60	-575,6285544277		
10,70	-575,6285540353		
10,80	-575,6285536684		
10,90	-575,6285533253		
11,00	-575,6285530035		
11,10	-575,6285527038		
11,20	-575,6285524215		
11,30	-575,6285521574		
11,40	-575,6285519095		
11,50	-575,6285516769		
11,60	-575,6285514583		
11,70	-575,6285512528		
11,80	-575,6285510597		
11,90	-575,628550878		
12,00	-575,6285507068		

5.3 Apêndice C: Trabalho Apresentado

Dynamics and spectroscopy f the Ng-CCl_4, O_2 -CCl_4 , D_2O-CCl_4 and ND_3 -CCl_4 Systems.

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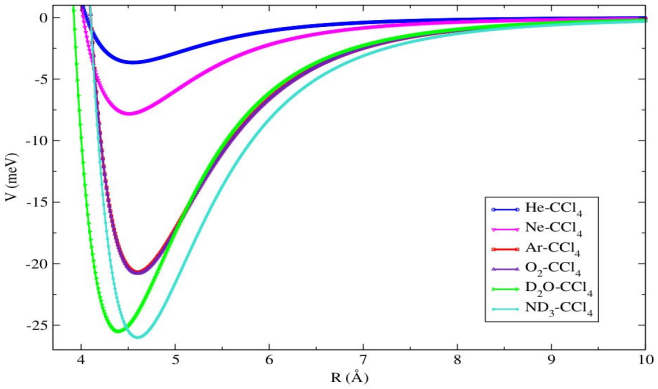
Keywords: CCl_4 , DVR, Dunham's Method, rovibrational energies, spectroscopic constants.

INTRODUCTION

The investigation of dispersion events between carbon tetrachloride molecules (CCl_4) and other atomic and molecular species have been motivated for several reasons[1] . In a short way, it is observed that the interaction between CCl_4 and another atom/molecule is characterized by a van der Waals component, since that the polarizability value of CCl 4 (α = 10, 5 Å^3) is expected to be much more elevated then a one of a heavy atom, for example (α = 4,04 Å^3 for xenon). In this work we calculated the rovibrational energies and spectroscopic constants of carbon tetrachloride with a few atoms and molecules systems (He -CCl_4 , Ne -CCl_4 , Ar-CCl_4, O_2 -CCl_4, D_2O-CCl_4 and ND_2 -CCl_4).

RESULTS AND DISCUSSION

Using the Improved Lennard-Jones model (ILJ)[1], we obtain a energy curves for each considered complexes, see figure to the side . The spectroscopic constants calculations follows two different approaches, as shown on table below. Starting with DVR methodology, we should first notice that the calculation were not performed for He-CCl_4 system. This is a consequence of the small number of vibrational bound excited states present on this system. A simple way to outline these difficulties of the DVR methodology is to apply the Dunham method. Through this procedure, all the spectroscopic constants can be obtained in an approximation as precise as one wants.



CONCLUSIONS

In this work, we presented the rovibrational energies and the spectroscopic constants for the systems formed between carbon tetrachloride and others atoms and molecules. Our calculations were based on potential energy curves obtained through molecular beam scattering experiments. The vibrational energy level distribution followed the pattern qualitatively expected from the nature of each system. By using both the DVR and the Dunham's methodology we obtained spectroscopic constant in excellent agreement.

ACKNOWLEDGMENTS

The authors are grateful for the support given from the CAPES, CNPQ and IFMA.

[1] L.F. Roncaratti, Quntum efects in molecular scattering experements: Characterization of the interaction in weakly bound complexes. Universita Degli di Perugia, 2009.

5.4 Apêndice D: Artigo Publicado

J Mol Model (2017) 23:87
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ORIGINAL PAPER

The interaction of CCl_4 with Ng (Ng = He, Ne, Ar), O_2, D_2O and ND_3: rovibrational energies, spectroscopic constants and theoretical calculations

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Abstract This investigation generated rovibrational energies and spectroscopic constants for systems of CCl_4 with Ng (Ng = He, Ne, Ar), O_2, D_2O and ND_3 from scattering experimental data, and the results presented are of interest for microwave spectroscopy studies of small halogenated molecules. The rovibrational spectra were obtained through two different approaches (Dunham and DVR) within the improved Lennard Jones (ILJ) model. Spectra were also generated within ordinary Lennard Jones and deviations suggest that the ILJ model should be preferred due to interactions beyond dispersion forces presented in these systems. Data from the literature and additional high level quantum mechanical calculations presented in this work show that these systems should not be considered as van der Waals complexes due to halogen bonding (HB) interactions, and this is especially true for the CCl_4–D_2O and CCl_4–ND_3 complexes. The charge displacement from the latter systems are one order of magnitude higher than the values from literature for CCl_4 and He, Ne, Ar and O_2 systems, and show significant deviations between DFT and Hartree-Fock values not previously reported in the literature.

Keywords Halogen bond · Rovibrational spectra · Improved Lennard-Jones · Ab initio · Charge displacement function

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Introduction

Halogen bonding (HB), the attractive interaction between an electrophilic region on a halogen and a nucleophilic region of a molecule [1] , is of relevance for a broad number of applications [2–4], such as crystal engineering [5, 6] , liquid crystals [7, 8] , nanomaterials [9] , polymer chemistry [10] , medicinal chemistry [11] and biochemistry [12, 13] . These are macromolecular systems where the correct characterization of intermolecular interactions is essential for formulation of accurate models able to describe their aggregation, dynamic and static properties [14–18] .

Nevertheless, it is difficult to separate weak intermolecular interactions from other effects in condensed phases like solid-state linkages or solvent effects in experiments for better HB characterization [19, 20] . Therefore, it is common to investigate HB interactions through rovibrational spectra [21–24] since gas-phase studies allow measurements that are analogous to condensed phase systems for separated species, although these studies frequently give unexpected results, as in the case of the value of centrifugal distortion constant of complexes [25] of H_2S-ICF_3 and H_2O-ICF_3, or in the case [23] of CF_3Cl and H_2O, where the authors could identify only a symmetric rotor spectrum when the predicted structures suggested asymmetric rotors.

In addition to spectroscopic experiments, HB interactions can be investigated from a theoretical standpoint through good electronic structure methods able to well characterize electron correlation, especially dispersion forces, in conjunction with good quality basis sets in order to obtain reliable results [26, 27] . In this contribution, we focus on interactions and rovibrational spectra between carbon tetrachloride (CCl_4) and some noble gases (He, Ne, Ar), oxygen molecule (O_2), deuterated water (D_2O) and ammonia (ND_3). Justification for the choice of CCl_4 with the mentioned systems is fivefold: (1)

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the CCl_4 has high (tetrahedral) symmetry without a permanent dipole moment, and has been investigated continuously for more than 80 years with outstanding interest due to a lack of understanding of its intermolecular structure [28] ; (2) CCl_4 can serve as a simple model to understand HB interactions on more complex systems, like freons [24]; (3) the interaction between CCl_4 and the systems of this study (He, Ne, Ar, O_2, D_2O and ND_3) is expected to possess a pronounced van der Waals component due to the CCl_4′ high values for polarizability and dispersion energy [29, 30] , and also because these complexes are suitable for scattering and microwave experiments; (4) CCl_4 is a common organic solvent used regularly on organic synthesis, purification, and in processes related to radioactive materials [31] ; and (5) CCl_4, although hydrophobic solvent, actually attracts water [32, 33] and should also attract D_2O and ND_3, and it presents an additional opportunity to study the rotational properties without the complicating effects of hydrogen bonds [34] .

The aim of this contribution was to perform high level quantum chemical calculations in order to characterize the HB interaction between CCl_4 and D_2O/ND_3 complexes, and also to generate the rovibrational spectra for some complexes —CCl_4 with He, Ne, Ar, O_2, D_2O and ND_3—from available scattering data [35, 36] through the improved Lennard Jones (ILJ) model [15]. This characterization is also of interest due to ILJ portability to other (macromolecular) systems [37, 38] by means of molecular dynamics simulations.

The paper is organized as follows: Methods outlines the main features of the theoretical methods used regarding the generation of the potential energy curves and of the rovibrational spectra. The Results and discussion emphasizes the results, and the necessity to obtain reliable data using the ILJ model for the systems investigated in this work, and also includes a discussion, with a Conclusions section to follow.

Methods

All calculations were performed with the QChem program [39] , version 4.0.1. The geometry optimizations of the interacting systems involving the complexes were performed at DFT level with the augmented correlation consistent polarized valence basis set aug-cc-pVTZ [40] . The functional used was the LC-VV10 [41]—a functional with semilocal exchange with long-range corrected hybrid exchange that performs exceptionally well for all types of weak bonding within the S66 test set [41], as well for interactions between small molecules [42, 43] . This functional used two parameters [41]: C = 0.0089, which was fitted to give accurate asymptotic dispersion C_6 coefficients; and b = 6.3, which controls the short-range damping of nonlocal correlation.

In order to investigate the charge transfer (CT) contribution in the complexes, we carried out geometry optimization on the vertex configuration. The only variable constrained was the distance between CCl_4 and the noble gases (He, Ne, Ar) or the small molecules D_2O and ND_3. Afterwards, the electron density changes due to interactions between CCl_4, D_2O and ND_3 were investigated by means of the charge displacement (CD) function, defined as follows:

$$\Delta Q(z) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{z} \Delta\varsigma(z,y,z')dz' \quad (1)$$

where $\Delta\varsigma$ is the electron density of the complex minus that of the isolated fragments [44] .This approach has been used successfully in diverse contexts, as, for example, charge fluxes in weak intermolecular systems [45–47], and to estimate the constituents of a metal–ligand interactions [48]. On the other hand, it is necessary to obtain an accurate potential energy curve (PEC) in order to generate a reliable rovibrational spectra for these systems. The ILJ model [15] gives an accurate description of the systems investigated on this work [35], so the PECs were obtained from the following equation:

$$V_{ILJ} = \varepsilon\left[\frac{m}{n(r)-m}\left(\frac{r_0}{r}\right)^{n(r)} - \frac{n(r)}{n(r)-m}\left(\frac{r_0}{r}\right)^{m}\right]. \quad (2)$$

In Eq. (2) ε, r_0 and m are pair-specific parameters, while r is the distance between the species. The first term into the bracket represents the repulsion contribution, while the second term represents the effective dispersion attraction. The n(r) exponent is formulated as:

$$n(r) = \beta + 4.0\left(\frac{r}{r_0}\right)^2 \quad (3)$$

In Eq. (3) the "hardness" β modulates the repulsion and controls the strength of the attraction, and can be varied within a limited range of values. In this work, we used β = 9.0 since it is the value used to fit the procedure on experimental data [35].

The introduction of β permits that the ILJ model can take into account of induction, CT and atom clustering effects, as well incorporates the contributions of more collective effects and corrects most of the ordinary Lennard-Jones' problems in the asymptotic region [49] . Another general advantage of the ILJ model is its portability by allowing the same values of ε and r_0 for different diatomics if the same interaction centers are considered [37].

In turn, the rovibrational spectroscopic constants were then evaluated by two different approaches. The first is the Dunham's method [50] , which assumes that the potential of a diatomic molecule can be expanded in terms of Taylor series as derivatives of V(R) with respect to R and centered at R_e,

$$V(R) = V(R_e) + \frac{1}{2!}\left(\frac{d^2V}{dR^2}\right)_{Re}(R-R_e)^2 + \frac{1}{3!}\left(\frac{d^3V}{dR^3}\right)_{Re}(R-R_e)^3 + \ldots (4)$$

In order to the Dunham method be functional, it is necessary to obtain the coefficients in a power series at $\xi = 0$· $\left(\xi = {}^{(R-R_e)}/_{R_e}\right)$ in a potential of the form

$$V = hca_0\xi^2\left(1 + a_1\xi + a_2\xi^2 + a_3\xi^3 + \ldots\right) \tag{5}$$

where $a_0 = {}^{\omega_e^2}/_{4B_e}$ and $B_e = {}^{h}/_{8\pi^2\mu R_e^2 c}$ Now comparing Eq. (4) to Eq. (5), one finds that ${}^{f_2}/_2 = {}^{hca_0}/_{R_e^2}$ This means that

$$f_2 = 4\pi^2 c^2 \mu \omega_e^2 \tag{6}$$

If one continues the process, then the values of $a_1, a_2, \ldots, a_6$ can be found as follows:

$$\begin{aligned}
a_1 &= \frac{R_e f_3}{12\pi^2 c^2 \omega_e^2 \mu}, \\
a_2 &= \frac{R_e^2 f_4}{48\pi^2 c^2 \omega_e^2 \mu}, \\
a_3 &= \frac{R_e^3 f_5}{240\pi^2 c^2 \omega_e^2 \mu}, \\
a_4 &= \frac{R_e^4 f_6}{1440\pi^2 c^2 \omega_e^2 \mu}, \\
a_5 &= \frac{R_e^5 f_7}{10080\pi^2 c^2 \omega_e^2 \mu} \quad \text{and} \\
a_6 &= \frac{R_e^6 f_8}{80640\pi^2 c^2 \omega_e^2 \mu}
\end{aligned} \tag{7}$$

The second is the discrete variable representation (DVR) [51] in which the electronic energies enter the matrix Schrödinger nuclear equation as potentials that are obtained from basis functions chosen as the eigenfunctions of a particle in a box in equally spaced points of the Gaussian quadrature [52] . The $E(\upsilon,J)$ in the DVR approach, where υ and J are the vibrational and rotational quantum numbers, obey the relation

$$\begin{aligned}
E(\upsilon, J) = {} & \omega_e\left(\upsilon + \frac{1}{2}\right) - \omega_e x_e\left(\upsilon + \frac{1}{2}\right)^2 + \omega_e y_e\left(\upsilon + \frac{1}{2}\right)^3 + \ldots \\
& + \left[B_e - \alpha_e\left(\upsilon + \frac{1}{2}\right) + \gamma_e\left(\upsilon + \frac{1}{2}\right)^2 + \ldots\right] J(J+1) + \ldots
\end{aligned} \tag{8}$$

, where $B_e = {}^{h}/_{8\pi^2 c I_e}$ is the rotational constant, $I_e$is the moment of inertia, and c is the velocity of light. Then, one can substitute $E(\upsilon,J)$ into the following system of equations [52] to obtain the rovibrational spectroscopic constants:

$$\begin{aligned}
\omega_e &= \frac{1}{24}\left[14\left(E_{1,0} - E_{0,0}\right) - 93\left(E_{2,0} - E_{0,0}\right) + 23\left(E_{3,0} - E_{1,0}\right)\right] \\
\omega_e x_e &= \frac{1}{4}\left[13\left(E_{1,0} - E_{0,0}\right) - 11\left(E_{2,0} - E_{0,0}\right) + 3\left(E_{3,0} - E_{1,0}\right)\right] \\
\omega_e y_e &= \frac{1}{6}\left[3\left(E_{1,0} - E_{0,0}\right) - 3\left(E_{2,0} - E_{0,0}\right) + 3\left(E_{3,0} - E_{1,0}\right)\right] \\
\alpha_e &= \frac{1}{8}\left[-12\left(E_{1,1} - E_{0,1}\right) + 4\left(E_{2,1} - E_{0,1}\right) + 4\omega_e - 23\omega_e y_e\right] \\
\gamma_e &= \frac{1}{4}\left[-2\left(E_{1,1} - E_{0,1}\right) + \left(E_{2,1} - E_{0,1}\right) + 2\omega_e x_e - 9\omega_e y_e\right]
\end{aligned} \tag{9}$$

Finally, 500 gaussian quadratures for the DVR step were adopted for all systems.

Results and discussion

Systematic investigation on the benchmark system CCl_4–Ar showed that coupled cluster single and double substitutions (CCSD), quadratic configuration interaction (QCISD) and Hartree-Fock with the aug-cc-pvtz basis set have similar results for charge displacement analysis [47]. Therefore, we decided to perform the constrained optimization and frequency calculations in order to obtain the electronic density at LC-VV10/aug-cc-pvtz level. As pointed out earlier, only the distance between CCl_4 and D_2O (ND_3) was fixed, and, for all structures, there was no observed imaginary frequencies.

The CD function shows the charge changes due to interaction between CCl_4 and D_2O (ND_3) in the vertex configuration. This function gives the net electronic charge that has been displaced from right (D_2O or ND_3) to left (CCl_4) across a perpendicular plane at each point in the axis joining the two interacting fragments. This CD approach was even applied to some complexes from this study (CCl_4–O_2 [47], CCl_4–Ar [47], CCl_4–Ne [53, 54] and CCl_4–He [53, 54]), and for this reason only their general results from the literature will be commented.

The results for the CD analysis for CCl_4–D_2O and CCl_4–ND_3 are both shown in Fig. 1. The main panels display the CD curves at both LC-VV10 and Hartree-Fock levels on the same horizontal scale, while the insets show the isosurfaces of the electronic density difference. Since ΔQ is always positive, CT happens from D_2O and ND_3 towards CCl_4.

Figure 1 also shows that CCl_4 boldly polarized the electronic density of both D_2O and ND_3 fragments. The charge polarization is similar for both complexes. The chlorine atoms act as electrophiles—net charge flows to CCl_4—while D_2O and ND_3 act as electron donors (since the curve is always positive). The

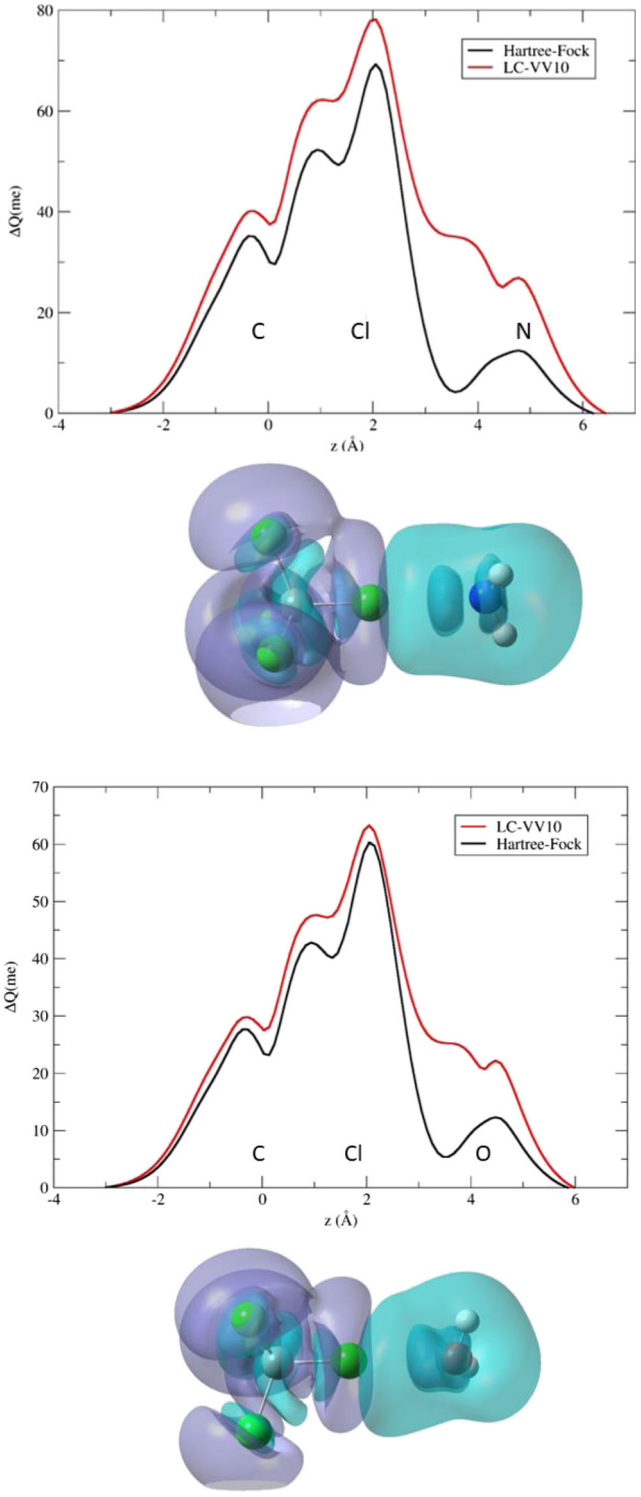

Fig. 1 Charge displacement (CD) curves for the vertex configuration of CCl_4–ND_3 (top) and CCl_4–D_2O (bottom). *Insets* 3D isodensity plots of the electron density charge due to intermolecular interaction. The isodensities are for $\Delta\rho = \pm 0.05$ me/bohr^3. The *dots* correspond to the positions of the nuclei on the *z*-axis, which is the axis joining C–Cl and N (O) of ND_3 (D_2O)

ΔQ presents a maximum close to the position of chlorine atom located at the vertex position, and the respective vales for ND_3 and D_2O obtained at LC-VV10 level are close to 77me and 62me, respectively. These values are one order of magnitude higher than the values for CCl_4–He, CCl_4–Ne, CCl_4–Ar and CCl_4–O_2 from the literature, and can be understood as a manifestation of halogen bonding. In addition, these higher values are probably responsible for the large deviations between the CD curves obtained at DFT (LC-VV10) and Hartree-Fock levels: for systems with lower CT reported in the literature, like CCl_4–Ar and CCl_4–O_2, the deviations between Hartree-Fock and correlated results were small and could be treated as similar for practical purposes. So this seems true only at small CD values, so caution is needed when one investigates CD at the HF level, especially when considerable CT occurs, as in halogen bonding of CCl_4–D_2O and CCl_4–ND_3.

Table 1 Improved Lennard-Jones (ILJ) potential parameters ε, R_e, and reduced mass μ for each system

System	ε (meV)	R_e(Å)	μ (a.u.)
He–CCl_4	3.65	4.55	7111.247054
Ne–CCl_4	7.80	4.51	32,518.194553
Ar–CCl_4	20.7	4.60	57,807.912323
O_2–CCl_4	20.8	4.60	48,284.647592
D_2O–CCl_4	25.5	4.40	32,301.751007
ND_3–CCl_4	26.0	4.60	32,332.857708

As pointed out by Capelleti et al. [45], a value for the CT can be estimated, and the common point of choice has been where the electron densities become equal (the isodensity boundary). The laplacian of the electron density suggests values of approximately 3.2 Å and 3.1 Å for ND_3 and D_2O at the LC-VV10 level. At these points, the CT values at the LC-VV10 level for ND_3 and D_2O are 35.8 me and 28.3 me, respectively. Compared to the Hartree-Fock values of 7.4 me and 13.2 me for ND_3 and D_2O, this also reinforces the idea that both electron correlation and dispersion forces should be treated in order to

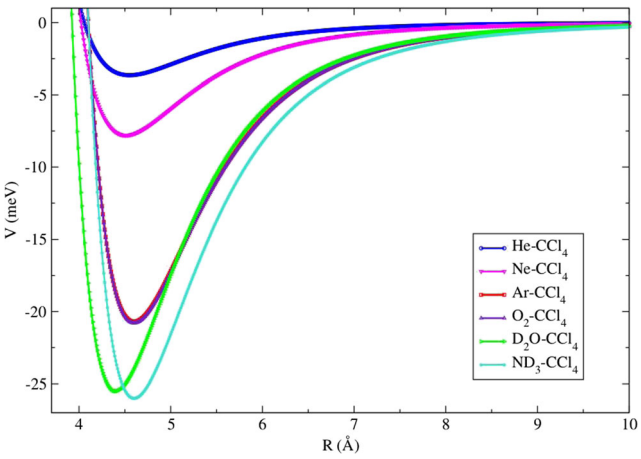

Fig. 2 Potential energy curves (PEC) for all systems investigated in this work

Table 2 Rovibrational energies $E_{(\upsilon,J)}$ (in cm^{-1}) obtained using ILJ and Lennard-Jones (LJ; in parentheses) for each system

υ	J	He–CCl_4	Ne–CCl_4	Ar–CCl_4	O_2–CCl_4	D_2O–CCl_4	ND_3–CCl_4
0		13.4506061 (12.9034003)	10.1824798 (9.7750956)	12.5217998 (12.0253574)	13.70731 (13.1634306)	19.3294528 (18.56137)	18.6872718 (17.9451305)
1		27.2977698 (26.3551248)	27.5177147 (26.2481277)	35.9084123 (34.3595487)	39.1397266 (37.4398854)	54.7546416 (52.3482942)	53.1042755 (50.7811481)
2		–	40.9761417 (39.0343369)	57.1304448 (54.5353614)	61.9859001 (59.1466669)	85.970829 (81.9805747)	83.6680086 (79.8036984)
3		–	50.7733553 (48.5285163)	76.2213999 (72.6413842)	82.2909238 (78.400266)	113.068 (107.680461)	110.454596 (105.204246)
4		–	57.2496922 (55.1584234)	93.2207194 (88.7692651)	100.108953 (95.3215966)	136.158467 (129.680067)	133.557582 (127.182264)
5		–	60.9363028 (59.3892369)	108.175725 (103.013892)	115.506458 (110.036278)	155.38615 (148.222095)	153.094784 (145.945785)
6		–	(61.8463383)	121.144112 (115.473577)	128.566437 (122.674924)	170.938595 (163.560562)	169.217209 (161.711976)
7		–	–	132.197026 (126.250244)	139.39355 (133.373435)	183.060652 (175.961522)	182.119542 (174.707693)
8	0	–	–	141.422569 (135.449615)	148.119641 (142.273284)	192.066044 (185.703731)	192.050222 (185.170024)
9		–	–	148.929277 (143.181389)	154.908346 (149.521776)	198.340545 (193.079211)	199.316997 (193.346756)
10		–	–	154.848654 (149.559405)	159.956741 (155.272281)	202.367086 (198.395278)	204.287465 (199.496869)
11		–	–	159.335583 (154.70178)	163.494402 (159.68445)	205.292532 (202.095119)	207.597368 (203.914069)
12		–	–	162.566747 (158.731027)	165.900332 (162.933869)	– (205.418419)	– (207.330278)
13		–	–	164.803414 (161.777392)	– (165.423611)	–	–
14		–	–	166.784875 (164.087996)	–	–	–
0		13.8120568 (13.2617271)	10.2718206 (9.86413911)	12.5711855 (12.0746674)	13.7663406 (13.2223625)	19.4256074 (18.6573396)	18.7752672 (18.0329654)
1		27.5191904 (26.5816779)	27.5993561 (26.3290634)	35.9560278 (34.4069536)	39.1964339 (37.4963209)	54.8463792 (52.4395309)	53.1884604 (50.8648954)
2		–	41.0491134 (39.1065718)	57.176204 (54.5808025)	62.0401594 (59.2005212)	86.0578701 (82.0668916)	83.7481565 (79.8832058)
3		–	50.8364203 (48.5913833)	76.2652062 (72.6847992)	82.3425936 (78.4514494)	113.150021 (107.761658)	110.530447 (105.279351)
4		–	57.301347 (55.2111769)	93.2624646 (88.8105884)	100.157873 (95.3700137)	136.235095 (129.75593)	133.628838 (127.252793)
5		–	60.9750947 (59.431085)	108.215287 (103.053054)	115.552447 (110.081828)	155.456955 (148.292395)	153.161106 (146.011554)
6		–	– (61.8792934)	121.181357 (115.510505)	128.609291 (122.717499)	171.003097 (163.625054)	169.278212 (161.772787)
7		–	–	132.231804 (126.284861)	139.433045 (133.412923)	183.11832 (176.019946)	182.174807 (174.763339)
8	1	–	–	141.454717 (135.48184)	148.155534 (142.309565)	192.116316 (185.755814)	192.099296 (185.220284)
9		–	–	148.958621 (143.211137)	154.94038 (149.554725)	198.382842 (193.124664)	199.359411 (193.391399)
10		–	–	154.875013 (149.586588)	159.984652 (155.301768)	202.401445 (198.433834)	204.322809 (199.535658)
11		–	–	159.358772 (154.726306)	163.517954 (159.71034)	205.324632 (202.128082)	207.627785 (203.947094)
12		–	–	162.586588 (158.752802)	165.92064 (162.956156)	– (205.451513)	– (207.360995)
13		–	–	164.820457 (161.796361)	– (165.444032)	–	–
14		–	–	166.801914 (164.105038)	–	–	–

obtain reliable results for CT, as well a reliable CD curve. Moreover, the HF CD curves for both D_2O and ND_3 show a minimum between 3 Å and 4 Å close to their isodensity point, and these minima are absent at the LC-VV10 level. These minima may be a deviation introduced by many-electron self interaction error [55], a drawback that can be minimized through using range-separated exchange correlation functionals [56], and by neglecting electron correlation as well.

The IJL parameters are presented in Table 1. The PECs and the rovibrational constants can be generated with these values of ε, R_e and reduced mass, and Eqs. (2) and (3). The dissociation energy trend is CCl_4–He < CCl_4–Ne < CCl_4–Ar ≈ CCl_4–O_2 < CCl_4–D_2O < CCl_4–ND_3 and, except for D_2O, it seems almost correlated with the α polarizability of the electron donor species (experimental [35–57] values in parenthesis): CCl_4–He (0.2 Å^3) < CCl_4–Ne (0.4 Å^3) < CCl_4–D_2O (1.47 Å^3) < CCl_4–Ar (1.64 Å^3) ≈ CCl_4–O_2 (1.60 Å^3) < CCl_4–ND_3 (2.16 Å^3). The higher dissociation value for CCl_4–D_2O can be understood as a consequence of an additional attractive force at intermediate range, the HB, that causes this deepening of the potential well. In turn, the reduced mass (rounded to three decimals) varies from 7111.247 a.u. for CCl_4–He up to 57807.912 a.u. for CCl_4–Ar. The reduced mass values for CCl_4–Ne, CCl_4–D_2O and CCl4–ND3 are not far from 32,400 a.u., while the respective value for CCl_4–O_2 is close to 48285 a.u.

The PECs of all systems are presented in Fig. 2. They were generated varying the distances from 7.0 bohr (≈3.70 Å) up to 20 bohr (≈10.58 Å), except for CCl_4–D_2O, where the distance was varied from 6.6 bohr (≈3.49 Å) up to 19.6 bohr (≈10.37 Å).

The rovibrational energies $E_{(\upsilon,J)}$ obtained from ILJ and ordinary LJ models are presented in Table 2. First, one can observe that, for all systems, the vibrational energies are close to rovibrational energies. This is observed because rotational energies are proportional to the inverse of the value of the reduced mass—the greater the reduced mass, the smaller the rotational energy. So, the rotational energies decrease as one follows the trend CCl_4–He < CCl_4–Ne < CCl_4–D_2O < CCl_4–ND_3 < CCl_4–O_2 < CCl_4–Ar. As an example, the ILJ values $E_{(0,0)}$ and $E_{(0,1)}$ values for CCl_4–Ar are 12.5217998 cm^{-1} and 12.5711855 cm^{-1}, a difference of 0.0494 cm^{-1}, while the respective values for CCl_4–He are 13.4506061 cm^{-1} and 13.8120568 cm^{-1}, a difference of 0.3615 cm^{-1}. Second, the systems have usually different numbers of $E_{(\upsilon,J)}$: CCl_4–He has just two levels at J = 0 while CCl_4–Ar has 14 levels, and this aspect can also be seen pictorially in Fig. 3.

On important aspect also presented in Table 2 is that the values obtained for $E_{(\upsilon,J)}$ obtained from ILJ and ordinary LJ models differ, and it is now convenient to make some considerations. The parameters used to generate the reliable PECs were obtained from scattering experiments using the ILJ model, which fits better with the experimental data [15]. So, due to absence of specific ordinary LJ parameters, we used the ILJ ones also to generate the LJ potential. This procedure was used before to infer

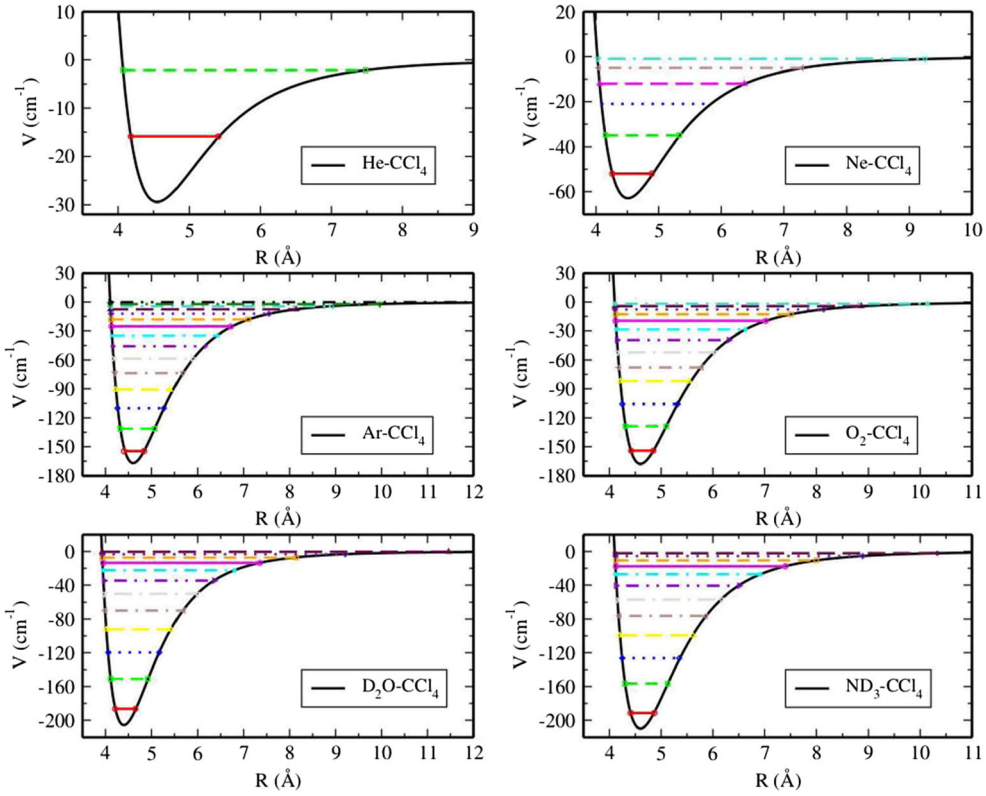

Fig. 3 Potential ILJ energy curves for He–CCl_4, N_e–CCl_4, Ar–CCl_4, O_2–CCl_4, D_2O–CCl_4 and ND_3–CCl_4 systems and their vibrational states

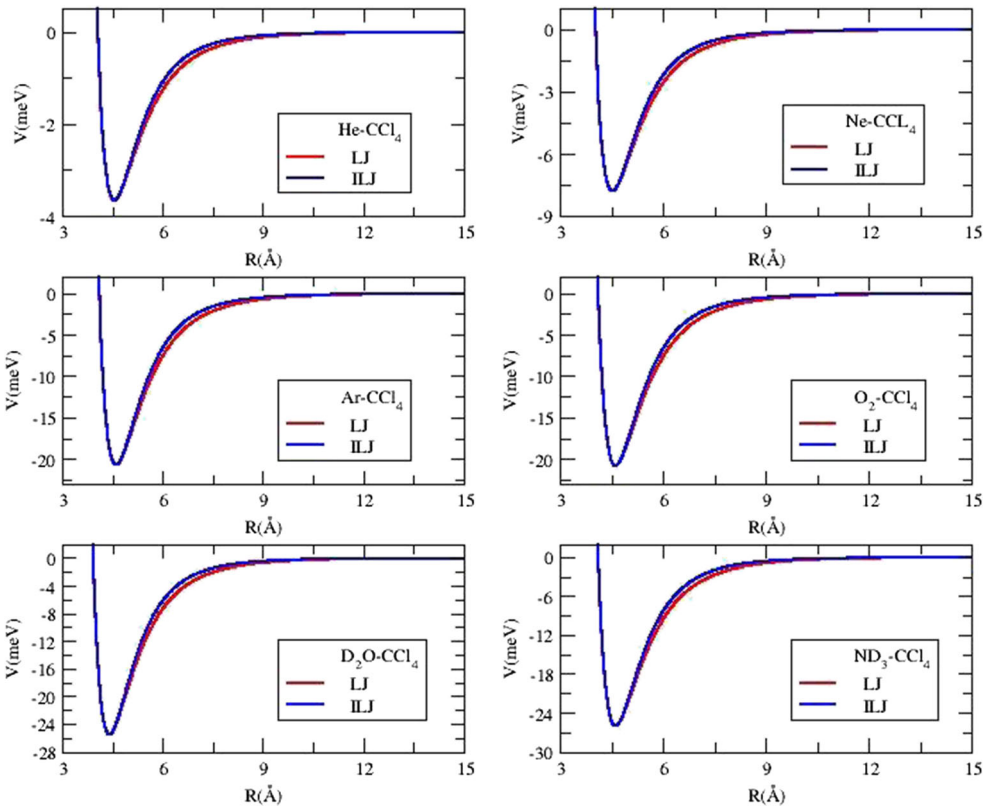

Fig. 4 PECs for each system obtained through ILJ (*blue line*) and LJ (*red line*) models

limitations of the LJ model such as the asymptotic dipole–dipole C_6 constant [15], where the ILJ gives values in agreement within 10% and LJ gives C_6 larger by a factor of two—it is known that LJ is inadequate to describe long-range interactions.

Although the same values for ε and R_e were used, deviations were observed in the spectra. The deviations were small, but were higher at intermediate levels, usually $\upsilon = 4$ or $\upsilon = 5$. This may have important consequences when one choses a potential for molecular dynamics simulation, since small changes in force field may lead to different results in molecular simulations, as in the case of small deviations in LJ potential for water leads to different self-diffusion coefficients [58] . The higher deviations for PECS obtained from ILJ and LJ models occur between 5 Å and 10 Å, as seen in Fig. 4, it is sensible to expect deviations in molecular dynamics simutations when one changes the potential from ILJ to LJ.

The spectroscopic constants obtained through the Dunham and DVR methods are presented in Table 3.

Table 3 Spectroscopic constants (in cm^{-1}) for each complex obtained through discrete variable representation (DVR) and Dunham methodologies using the ILJ and LJ (in parentheses)

System	Method	ω_e	$\omega_e x_e$	$\omega_e \gamma_e$	α_e	γ_e
He-CCl_4	DVR	–	–	–	–	–
	Dunham	30.96 (29.74)	9.28 (9.61)	0.24 (0.78)	0.04 (0.05)	−0.007 (−0.005)
Ne-CCl_4	DVR	21.41 (20.53)	2.10 (2.13)	0.03 (0.06)	0.003 (0.003)	−0.0002 (−0.0001)
	Dunham	21.35 (20.51)	2.04 (2.11)	0.01 (0.05)	0.003 (0.003)	−0.0001 (−0.0001)
Ar-CCl_4	DVR	25.58 (24.57)	1.10 (1.14)	0.005 (0.01)	0.0008 (0.0009)	−2.15E−05 (−1.47E−05)
	Dunham	25.57 (24.57)	1.10 (1.14)	0.004 (0.01)	0.0008 (0.0009)	−1.81E−05 (−1.35E−05)
O_2-CCl_4	DVR	28.06 (26.95)	1.32 (1.37)	0.007 (0.019)	0.001 (0.001)	−3.11E−05 (−2.11E−05)
	Dunham	28.05 (26.95)	1.32 (1.36)	0.005 (0.018)	0.001 (0.001)	−2.58E−05 (−1.93E−05)
D_2O-CCl_4	DVR	39.72 (38.15)	2.17 (2.24)	0.01 (0.03)	0.002 (0.002)	−6.99E−05 (−4.67E−05)
	Dunham	39.70 (38.14)	2.15 (2.23)	0.01 (0.03)	0.002 (0.002)	−5.62E−05 (−4.20E−05)
ND_3-CCl_4	DVR	38.34 (36.83)	1.98 (2.05)	0.01 (.031)	0.001 (0.001)	−5.66E−05 (−3.80E−05)
	Dunham	38.33 (36.82)	1.97 (2.04)	0.009 (0.029)	0.001 (0.001)	−4.61E−05 (−3.44E−05)

The accordance within both methods at ILJ model suggests that the PECs are reliable. Regarding the results obtained with LJ, it can be observed that higher deviations occur for anharmonic constant $\omega_e y_e$ in accordance with conclusions taken from Fig. 4 and Table 2.

Conclusions

The CT component plays an effective role in CCl_4–ND_3 and CCl_4–D_2O complexes since they present HB. The higher CD shown by CCl_4–ND_3 and CCl_4–D_2O complexes requires that the density should be obtained with a good treatment of electron correlation. In our study, the functional LC-VV10 seems to be a good choice since it can treat dispersion forces and electron correlation at both optimization and frequency calculations at a fraction of cost of a coupled cluster, CASPT2 or CISDQ calculation.

The rovibrational and spectroscopic spectra constants show deviations for ILJ and LJ even with constant ε and R_e, and this can be understood as a limitation of LJ potential. Since attraction is determined by interactions beyond dispersion forces, such as an HB system, the ILJ model is preferred over ordinary LJ.

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