

An application of the dynamical Lie algebraic method to potential energy surface of the stable linear asymmetric tetratomic molecules

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Potential energy surfaces play an important role in studying theoretical chemistry. In the present paper, we first use the dynamical symmetry group $G = U_1(4) \otimes U_2(4) \otimes U_3(4)$ to get the expression of the potential energy surface for the stable linear asymmetric tetratomic molecules with the stretching vibration and the dissociation energy. The method can be applied to a number of stable tetratomic molecules. As an example we use the method to calculate the potential energy surface of C_2HD .

KEY WORDS: potential energy surface, dissociation energy, tetratomic molecules

1. Introduction

It has been shown that the Lie algebraic approach is a useful method to treat the molecular problems in recent years. Some comprehensive reviews of the algebraic approach have recently been published [1–3]. Since Iachello, Levine and others have successfully treated molecular rovibrational states using Lie algebraic approach [1,2,4,9,10,21], many researchers [4–8] extend the hybrid algebraic method to treat molecular rovibrational states. On the other hand, some researchers are interested in treating time-dependent problems and statistical problems using lie algebraic method [11–14].

As an active method, the analytical potential energy surfaces of small polyatomic molecules can be obtained by using molecular algebraic Hamiltonian, since this algebraic Hamiltonian can reproduce the molecular rovibrational states well. Cooper [15] recently derived diatomic potential functions using algebraic theory. Levine and coworkers [16,17] obtained the potential-energy surfaces of the triatomic molecules using $U(2)$ algebra. Shiliang Ding and coworkers [18] obtained the potential energy surface of triatomic molecular with $U_1(4) \otimes U_2(4)$. So far, there are few workers to calculate the potential energy surface of the tetratomic molecular with the algebraic method because of its complication. In

this paper, we use algebraic Hamiltonian to calculate potential energy surface of the stable tetratomic molecules. In each bond we introduce a $U(4)$ group, so that we use $U_1(4) \otimes U_2(4) \otimes U_3(4)$ group to describe the tetratomic molecules. With the Hamiltonian classified, we get the potential energy surface and the dissociation energy of the tetratomic molecules. The coordinates introduced in taking the semiclassical limit need not be the bond distance; they must be therefore subjected to a correlated transformation. In this paper, we have chosen the simplest transformation that yields the correct results in the asymptotic limit (i.e., when one or three bonds are broken). The method we proposed could be applied to any algebraic Hamiltonian, that is to say the potential energy surface that we will propose is a generic one for stable linear asymmetric tetratomic molecules. We shall not discuss the bending motion, which is the subject of the work in progress.

In the present paper, first of all, we review the algebraic Hamiltonian of the tetratomic molecules by using group $U(4)$. Then we get the potential energy surface of the stable tetratomic molecules and the dissociation energy. Finally, the results of calculation for molecules C_2HD is presented. What's more, we can get the potential energy surface of the other stable linear asymmetric tetratomic molecules.

2. The brief review of the Hamiltonian of the linear asymmetry tetratomic molecule

2.1. The expression of the potential energy surface

For a tetratomic molecule, there are three bonds, which are related to the groups $U_1(4)$, $U_2(4)$ and $U_3(4)$, respectively. The expression of the C_2HD is in figure 6. So the symmetric group of a tetratomic molecule is

$$G = U_1(4) \otimes U_2(4) \otimes U_3(4). \quad (1a)$$

Hence, the dynamical symmetric subgroup chain can be written in local group and normal group as follows:

$$\begin{aligned} U_1(4) \otimes U_2(4) \otimes U_3(4) \supset SO_1(4) \otimes SO_2(4) \otimes SO_3(4) \supset SO_{12}(4) \otimes SO_3(4) \supset \\ SO_{123}(4) \supset SO_{123}(3) \supset SO_{123}(2), \end{aligned} \quad (1b)$$

$$\begin{aligned} U_1(4) \otimes U_2(4) \otimes U_3(4) \supset U_{12}(4) \otimes U_3(4) \supset U_{123}(4) \supset \\ SO_{123}(4) \supset SO_{123}(2) \supset SO_{123}(2). \end{aligned} \quad (1c)$$

From the knowledge of the Lie algebra [1], The Hamiltonian of a linear asymmetry tetratomic molecule can be written as:

$$\hat{H}^{\text{total}} = E_0 + A_1\hat{C}_1 + A_2\hat{C}_2 + A_3\hat{C}_3 + A_{12}\hat{C}_{12} + A_{123}\hat{C}_{123} + \lambda_{12}\hat{M}_{12} + \lambda_{23}\hat{M}_{23} + \lambda_{13}\hat{M}_{13}, \tag{2}$$

where $\hat{C}_1, \hat{C}_2, \hat{C}_3, \hat{C}_{12}, \hat{C}_{123}$ are defined as [1]; $A_1, A_2, A_3, A_{12}, A_{123}, \lambda_{12}, \lambda_{23}, \lambda_{13}$ are expansion coefficients, they can be obtained by fitting the spectroscopic data. $\hat{C}_i = \hat{D}_i^2 + \hat{J}_i^2$ ($i = 1, 2, 3$), $\hat{C}_{12} = (\hat{D}_1 + \hat{D}_2)^2 + (\hat{J}_1 + \hat{J}_2)^2$, M_{12}, M_{13}, M_{23} and $\hat{C}_{123} = (\hat{D}_1 + \hat{D}_2 + \hat{D}_3)^2 + (\hat{J}_1 + \hat{J}_2 + \hat{J}_3)^2$ are the Majorana operator. From [18], we know:

$$\begin{aligned} J_i &= N_i q_i \times p_i, D_i = N_i(2 - p_i^2 - q_i^2)^{1/2} q_i, \\ \hat{M}_{ij} &= \frac{1}{4} N_i N_j (2 - p_j^2 - q_j^2)(q_i^2 + p_i^2) + \frac{1}{4} N_i N_j (2 - p_i^2 - q_i^2)(q_j^2 + p_j^2) \\ &\quad - \frac{1}{2} N_i N_j [(2 - p_i^2 - q_i^2)(2 - p_j^2 - q_j^2)]^{1/2}, \\ &\quad (q_i \cdot q_j + p_i \cdot p_j) + \frac{1}{2} N_i N_j [(q_i \times q_j - p_i \times p_j)^2 + (q_i \times p_j + p_i \times q_j)^2] \end{aligned} \tag{3}$$

Inserting equation (3) into equation (2), and defining the kinetic energy operator p_i as zero, we can get the classical Hamiltonian of the linear asymmetric tetra-atomic molecules

$$\begin{aligned} H_{\text{cl}}(q_1, q_2, q_3, \theta_1, \theta_2; p_1 = 0, p_2 = 0, p_3 = 0) &= \hat{A}_1 \{N_1^2(2 - q_1^2)q_1^2\} + \hat{A}_2 \{N_2^2(2 - q_2^2)q_2^2\} + \hat{A}_3 \{N_3^2(2 - q_3^2)q_3^2\} \\ &\quad + \hat{A}_{12} \left\{ N_1^2(2 - q_1^2)q_1^2 + N_2^2(2 - q_2^2)q_2^2 + 2N_1N_2\sqrt{(2 - q_1^2)(2 - q_2^2)}q_1 \cdot q_2 \right\} \\ &\quad + \hat{A}_{123} \left\{ N_1^2(2 - q_1^2)q_1^2 + N_3^2(2 - q_3^2)q_3^2 + N_2^2(2 - q_2^2)q_2^2 \right. \\ &\quad \left. + 2N_1N_2\sqrt{(2 - q_1^2)(2 - q_2^2)}q_1 \cdot q_2 + 2N_1N_3\sqrt{(2 - q_1^2)(2 - q_3^2)}q_1 \cdot q_3 \right. \\ &\quad \left. + 2N_2N_3\sqrt{(2 - q_2^2)(2 - q_3^2)}q_2 \cdot q_3 \right\} + \lambda_{12} \left\{ \frac{1}{4} N_1N_2(2 - q_2^2)q_1^2 \right. \\ &\quad \left. + \frac{1}{4} N_1N_2(2 - q_1^2)q_2^2 - \frac{1}{2} N_1N_2\sqrt{(2 - q_1^2)(2 - q_2^2)}q_1 \cdot q_2 \right. \\ &\quad \left. + \frac{1}{2} N_1N_2(q_1 \times q_2)^2 \right\} + \lambda_{13} \left\{ \frac{1}{4} N_1N_3(2 - q_3^2)q_1^2 + \frac{1}{4} N_1N_3(2 - q_1^2)q_3^2 \right. \\ &\quad \left. - \frac{1}{2} N_1N_3\sqrt{(2 - q_1^2)(2 - q_3^2)}q_1 \cdot q_3 + \frac{1}{2} N_1N_3(q_1 \times q_3)^2 \right\} \\ &\quad + \lambda_{23} \left\{ \frac{1}{4} N_2N_3(2 - q_3^2)q_2^2 + \frac{1}{4} N_2N_3(2 - q_2^2)q_3^2 \right. \\ &\quad \left. - \frac{1}{2} N_2N_3\sqrt{(2 - q_2^2)(2 - q_3^2)}q_2 \cdot q_3 + \frac{1}{2} N_2N_3(q_2 \times q_3)^2 \right\}. \end{aligned} \tag{4}$$

If we only consider the stretching motion, we can get the potential energy surface with the classical coordinates

$$\begin{aligned}
V(q_1, q_2, q_3) = & \hat{A}_1\{N_1^2(2 - q_1^2)q_1^2\} + \hat{A}_2\{N_2^2(2 - q_2^2)q_2^2\} + \hat{A}_3\{N_3^2(2 - q_3^2)q_3^2\} \\
& + \hat{A}_{12} \left\{ N_1^2(2 - q_1^2)q_1^2 + N_2^2(2 - q_2^2)q_2^2 \right. \\
& \left. + 2N_1N_2\sqrt{(2 - q_1^2)(2 - q_2^2)}q_1q_2 \right\} \\
& + \hat{A}_{123} \left\{ N_1^2(2 - q_1^2)q_1^2 + N_3^2(2 - q_3^2)q_3^2 + N_2^2(2 - q_2^2)q_2^2 \right. \\
& + 2N_1N_2\sqrt{(2 - q_1^2)(2 - q_2^2)}q_1q_2 + 2N_1N_3\sqrt{(2 - q_1^2)(2 - q_3^2)}q_1q_3 \\
& \left. + 2N_2N_3\sqrt{(2 - q_2^2)(2 - q_3^2)}q_2q_3 \right\} + \lambda_{12} \left\{ \frac{1}{4}N_1N_2(2 - q_2^2)q_1^2 \right. \\
& \left. + \frac{1}{4}N_1N_2(2 - q_1^2)q_2^2 - \frac{1}{2}N_1N_2\sqrt{(2 - q_1^2)(2 - q_2^2)}q_1q_2 \right\} \\
& + \lambda_{13} \left\{ \frac{1}{4}N_1N_3(2 - q_3^2)q_1^2 + \frac{1}{4}N_1N_3(2 - q_1^2)q_3^2 \right. \\
& \left. - \frac{1}{2}N_1N_3\sqrt{(2 - q_1^2)(2 - q_3^2)}q_1q_3 \right\} + \lambda_{23} \left\{ \frac{1}{4}N_2N_3(2 - q_3^2)q_2^2 \right. \\
& \left. + \frac{1}{4}N_2N_3(2 - q_2^2)q_3^2 - \frac{1}{2}N_2N_3\sqrt{(2 - q_2^2)(2 - q_3^2)}q_2q_3 \right\}. \quad (5)
\end{aligned}$$

We assumed the transformation between bond coordinates and classical coordinate q_i as [18]

$$q_i^2 = e^{-\beta_i(r_i - r_{ie})} \quad (i = 1, 2, 3), \quad (6)$$

where r_i is the i th bond coordinate, r_{ie} is the equilibrium bond length, and β_i is a parameter. Substituting (6) into (5), we can get the potential energy surface in the form of the internal molecular coordinates r_1, r_2, r_3 .

2.2. The dissociation energy

It is obvious that at $\{q_1 = 0, q_2 = 0, q_3 = 0\}$, that is, $\{r_1 \rightarrow r_{1\infty}, r_2 \rightarrow r_{2\infty}, r_3 \rightarrow r_{3\infty}\}$. The solution corresponds to the case in which the three bonds are completely broken, that is to say, the molecule is dissociated. The potential energy is to zero. At $r_1 \rightarrow r_{1e}, r_2 \rightarrow r_{2e}, r_3 \rightarrow r_{3e}$, that is $q_1 = 1, q_2 = 1$ and $q_3 = 1$. It shows that the potential energy surface has the global minimum, and the well depth at the minimum of the potential is

$$D_e = -(A_1N_1^2 + A_2N_2^2 + A_3N_3^2 + A_{12}(N_1 + N_2)^2 + A_{123}(N_1 + N_2 + N_3)^2). \quad (7)$$

And, the other stationary points of $V(r_1, r_2, r_3)$ are at, $r_1 \rightarrow r_{1\infty}, r_2 \rightarrow r_{2\infty}, r_3 = r_{3e}$ or at $r_1 \rightarrow r_{1\infty}, r_2 = r_{2\infty}, r_3 \rightarrow r_{3e}$ and $r_1 = r_{1\infty}, r_2 \rightarrow r_{2\infty}, r_3 \rightarrow r_{3\infty}$ which are the three valleys where two bonds are fully extended and another bond is at its equilibrium position. The depth of the i th valley is \hat{D}_{ei} :

$$\begin{aligned} D_{e1} &= -(A_1N_1^2 + A_{12}N_1^2 + A_{123}N_1^2 + 0.5\lambda_{12}N_1N_2 + 0.5\lambda_{13}N_1N_3), \\ D_{e2} &= -(A_2N_2^2 + A_{12}N_2^2 + A_{123}N_2^2 + 0.5\lambda_{12}N_1N_2 + 0.5\lambda_{23}N_2N_3), \\ D_{e3} &= -(A_3N_3^2 + A_{123}N_3^2 + 0.5\lambda_{23}N_3N_2 + 0.5\lambda_{13}N_1N_3). \end{aligned} \tag{8}$$

The potential energy difference between the stable tetratomic molecules and either exit valley is thus $D_e - D_{ei}$.

At this point all the parameters in the Hamiltonian are determined from the fitting of the spectrum. Hence the X_2YZ vibration spectrum can be used to determine the Hamiltonian and the potential energy surface. From equation (8), we get the dissociation energy of the X_2YZ .

3. Applications

We have deduced the potential energy surface of C_2HD by using the Hamiltonian given by equation (2). The parameters required to reproduce the potential energy surface are given in table 1. They are got by fitting the Hamiltonian. The fitting spectroscopic data and the observed spectroscopic data are listed in table 2. Table 1 also provides the dissociation energies of the tetratomic molecules as predicted by the potential (5). We know that the dissociation energy of CH [20] is 3.648 (eV) when the three bonds are at their equilibrium, here we get the dissociation energy of CH is 3.7058 (eV). The difference is caused by the influence of CD. The value of β_i is calculated using the formula [19]:

$$\beta_i = \sqrt{\frac{2\pi^2cu_{iA}}{D_{ie}}}w_{ie}. \tag{9}$$

Here w_{ie}, u_{iA}, D_{ie} has the usual meaning as in reference [19].

If we take q_2 as a constant, we can take the molecules as triatomic molecules, then we can get the dissociation energy of the triatomic molecule.

- (1) $\{q_2 = 1\}$, this is the equilibrium position, we can get the dissociation energy:

$$\begin{aligned} D_e &= -(A_1N_1^2 + A_2N_2^2 + A_3N_3^2 + A_{12}(N_1 + N_2)^2 \\ &\quad + A_{123}(N_1 + N_2 + N_3)^2) \text{ for } C_2HD \text{ is } 20.8397 \text{ eV}, \\ D_{e1} &= -(A_1N_1^2 + A_2N_2^2 + A_{12}(N_1 + N_2)^2 + A_{123}(N_1^2 + N_2^2 + N_1N_2) \\ &\quad + 0.25\lambda_{12}N_1N_2 + 0.5\lambda_{13}N_1N_3 + 0.5\lambda_{23}N_2N_3) \text{ for CH is } 8.6233 \text{ eV}, \\ D_{e3} &= -(A_{12}N_2^2 + A_2N_2^2 + A_3N_3^2 + A_{123}(N_2^2 + N_3^2 + N_2N_3) + 0.5\lambda_{12}N_1N_2 \\ &\quad + 0.5\lambda_{13}N_1N_3 + 0.25\lambda_{23}N_2N_3) \text{ or CCD is } 15.7463 \text{ eV}. \end{aligned} \tag{10}$$

Table 1
The fitting parameters and dissociation energy of C₂HD.

C ₂ HD	This paper	Ref. [20]
N_1	43	
N_2	61	
N_3	137	
A_1	-0.17982587(+2)	
A_2	-0.10075547(+2)	
A_3	-0.33740922(+1)	
A_{12}	-0.73353190(0)	
A_{123}	-0.10663047(1)	
λ_{12}	0.30309053(+1)	
λ_{13}	-0.78271471(-4)	
λ_{23}	0.45338175(-3)	
r_{1e}	1.1198(Å)	
r_{2e}	1.118(Å)	
r_{3e}	1.3117(Å)	
D_e	20.8397 (eV)	
D_{e1}	3.7058 (eV)	3.648 (eV)
D_{e2}	4.3086 (eV)	
D_{e3}	10.3325 (eV)	

All parameters are in cm⁻¹, except N_1, N_2, N_3 which is dimensionless, and r_{1e}, r_{2e}, r_{3e} are in Å.

- (2) $\{q_2 = 1.2\}$, which is corresponding to that $r < r_e$, the dissociation energy is:

$$\begin{aligned}
 D_e &= -(A_1 N_1^2 + 0.8064 A_2 N_2^2 + A_3 N_3^2 + A_{12}(N_1^2 + 0.8064 N_2^2 \\
 &\quad + 1.796 N_1 N_2) + A_3 N_3^2 + A_{123}(N_1^2 + 0.8064 N_2^2 + 0.897998 N_1 N_2 \\
 &\quad + N_1 N_3 + N_3^2 + 0.897998 N_2 N_3)), \quad \text{or C}_2\text{HD is 19.79 eV,} \\
 D_{e1} &= -(A_1 N_1^2 + 0.8064 A_2 N_2^2 + A_{123}(N_1^2 + 0.8064 N_2^2 + 0.897998 N_1 N_2) \\
 &\quad + A_{12}(N_1^2 + 0.8064 N_2^2 + 1.796 N_1 N_2) + 0.275501 \lambda_{12} N_1 N_2 \\
 &\quad + 0.5 \lambda_{13} N_1 N_3 + 0.72 \lambda_{23} N_2 N_3), \quad \text{or CH is 8.44791 eV,} \\
 D_{e3} &= -(0.8064 A_{12} N_2^2 + 0.8064 A_2 N_2^2 + A_{123}(N_3^2 + 0.8064 N_2^2 \\
 &\quad + 0.897998 N_2 N_2) + A_3 N_3^2 + 0.72 \lambda_{12} N_1 N_2 + 0.5 \lambda_{13} N_1 N_3 \\
 &\quad + 0.275501 \lambda_{23} N_2 N_3), \quad \text{or CCD is 14.4871 eV.} \tag{11}
 \end{aligned}$$

- (3) $\{q_2 = 0.9\}$, which is corresponding to that $r > r_e$, we also can get the dissociation energy:

$$\begin{aligned}
 D_e &= -(A_1 N_1^2 + 0.9639 A_2 N_2^2 + A_3 N_3^2 + A_{12}(N_1^2 + 0.9639 N_2^2 \\
 &\quad + 1.96357 N_1 N_2) + A_3 N_3^2 + A_{123}(N_1^2 + 0.9639 N_2^2 + 0.981784 N_1 N_2 \\
 &\quad + N_1 N_3 + N_3^2 + 0.981784 N_2 N_3)), \quad \text{or C}_2\text{HD is 20.6442 eV,}
 \end{aligned}$$

Table 2
Comparison of observed and calculated levels for C₂HD (cm⁻¹).

v_1, v_2, v_3	v_4^l, v_5^l	Exp.	Cal.	Δ	δ
0 0 0	2 ⁰ 0 ⁰	1033.93	1031.23	-2.70	-0.261
0 0 0	1 ⁻¹ 1 ¹	1198.33	1191.66	-6.67	-0.557
0 0 0	0 ⁰ 2 ⁰	1342.23	1341.13	-1.10	-0.082
0 1 0	0 ⁰ 0 ⁰	1853.78	1852.49	-1.29	-0.069
1 0 0	0 ⁰ 0 ⁰	3335.61	3329.82	-5.79	-0.174
0 1 0	1 ⁻¹ 1 ¹	3046.98	3035.59	-11.39	-0.374
0 0 1	2 ⁰ 0 ⁰	3587.01	3594.43	7.42	0.207
0 0 1	1 ¹ 1 ⁻¹	3766.18	3760.98	-5.20	-0.138
0 0 1	0 ⁰ 2 ⁰	3920.22	3915.13	-5.09	-0.130
1 0 0	2 ⁰ 0 ⁰	4361.99	4352.47	-9.52	-0.218
0 1 1	0 ⁰ 0 ⁰	4415.84	4415.72	-0.12	-0.003
1 0 0	1 ¹ 1 ⁻¹	4511.49	4515.14	3.65	0.081
1 0 0	1 ⁻¹ 1 ¹	4513.66	4522.89	9.23	0.205
1 0 0	0 ⁰ 2 ⁰	4643.17	4665.97	22.80	0.491
2 0 0	0 ⁰ 0 ⁰	6569.41	6554.41	-15.00	-0.228
0 1 1	2 ⁰ 0 ⁰	5414.06	5429.79	15.73	0.290
0 0 2	2 ⁰ 0 ⁰	6094.96	6102.83	7.87	0.129
0 2 1	0 ⁰ 0 ⁰	6237.23	6239.11	1.84	0.030
0 0 2	1 ⁻¹ 1 ¹	6284.59	6275.47	-9.12	-0.145
1 1 0	0 ⁰ 2 ⁰	6483.82	6501.33	17.51	0.270
0 1 2	0 ⁰ 0 ⁰	6932.20	6924.14	-8.06	-0.116
0 3 1	0 ⁰ 0 ⁰	8048.00	8041.94	-6.06	-0.075
1 1 1	2 ⁰ 0 ⁰	8728.80	8721.42	-7.38	-0.085
0 2 2	0 ⁰ 0 ⁰	8731.04	8734.55	3.51	0.040
0 0 0	1 ¹ 0 ⁰	519.37	525.34	5.97	1.149
0 0 0	0 ⁰ 1 ¹	678.80	680.61	1.81	0.266
0 0 0	2 ² 1 ⁻¹	1723.45	1713.24	-10.21	-0.593
0 0 0	1 ⁻¹ 2 ²	1862.86	1862.52	-0.34	-0.018
0 0 0	0 ⁰ 3 ¹	2011.22	1998.20	-13.02	-0.647
0 1 0	1 ¹ 0 ⁰	2369.93	2373.34	3.41	0.144
0 1 0	0 ⁰ 1 ¹	2528.95	2528.73	-0.22	-0.009
0 0 1	1 ¹ 0 ⁰	3087.60	3092.39	4.79	0.155
0 0 1	0 ⁰ 1 ¹	3259.55	3254.18	-5.37	-0.165
1 0 0	0 ⁰ 1 ¹	3996.74	4008.30	11.56	0.289
0 1 1	1 ¹ 0 ⁰	4916.80	4931.86	15.06	0.306
0 1 1	0 ⁰ 1 ¹	5088.09	5093.77	5.68	0.112
0 0 2	1 ¹ 0 ⁰ 4	5611.21	5604.63	-6.58	-0.117
1 1 0	1 ¹ 0 ⁰	5694.04	5690.54	-3.50	-0.061

$\Delta = \text{fit} - \text{obs}$; $\delta = \text{fit} - \text{obs} \times 100 / \text{obs}$.

$$D_{e1} = -(A_1 N_1^2 + 0.9639 A_2 N_2^2 + A_{123}(N_1^2 + 0.9639 N_2^2 + 0.981784 N_1 N_2) + A_{12}(N_1^2 + 0.9639 N_2^2 + 1.96357 N_1 N_2) + 0.254554 \lambda_{12} N_1 N_2 + 0.5 \lambda_{13} N_1 N_3 + 0.405 \lambda_{23} N_2 N_3), \quad \text{or CH is } 8.44791 \text{ eV,}$$

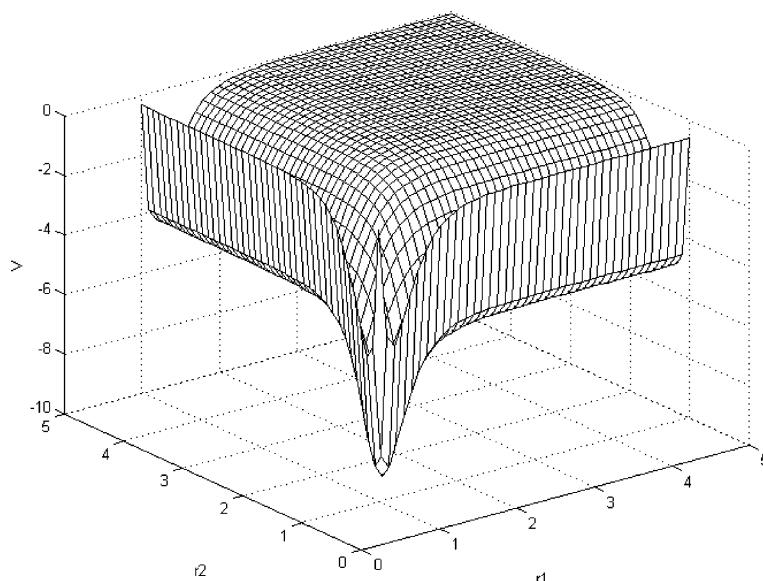


Figure 1. The potential energy surface (eV) of stable C₂HD with $r_1(\text{Å})$ and $r_2(\text{Å})$ ($r_3 \rightarrow \infty$).

$$\begin{aligned}
 D_{e3} = & -(0.9639A_{12}N_2^2 + 0.9639A_2N_2^2 + A_{123}(N_3^2 + 0.9639N_2^2 \\
 & + 0.981784N_2N_2) + A_3N_3^2 + 0.405\lambda_{12}N_1N_2 + 0.5\lambda_{13}N_1N_3 \\
 & + 0.254554\lambda_{23}N_2N_3) \quad \text{or CCD is } 15.6464 \text{ eV.} \quad (12)
 \end{aligned}$$

From above we can see that the total dissociation energy has the largest value when the molecule at equilibrium bonds. When we take q_2 as a constant, we can see that the dissociation energy of CH is larger than that of equation (8) and D_{e3} is littler than equation (8). Then we can see q_2 has an influence on the dissociation energy of bond one and bond three.

From figures 1–3, we can see the change of the potential energy surface with the two coordinates when one bond at equilibrium station. From the figures, we can see that the potential energy is at its minimum when the three coordinates at equilibrium. Comparing figure 1, with figures 4 and 5, we can see the potential energy surface has the minimum value when the molecule at equilibrium, that is to say the molecule is stable when it is at equilibrium and the potential energies have the same value when they have same distance to the equilibrium station. From above we can see that the potential energy has the style of Morse-potential.

4. Concluding remarks

An analytical representation of the potential energy surface for tetratomic, X₂YZ, molecules in terms of AB, BB and CD bond distances has been derived

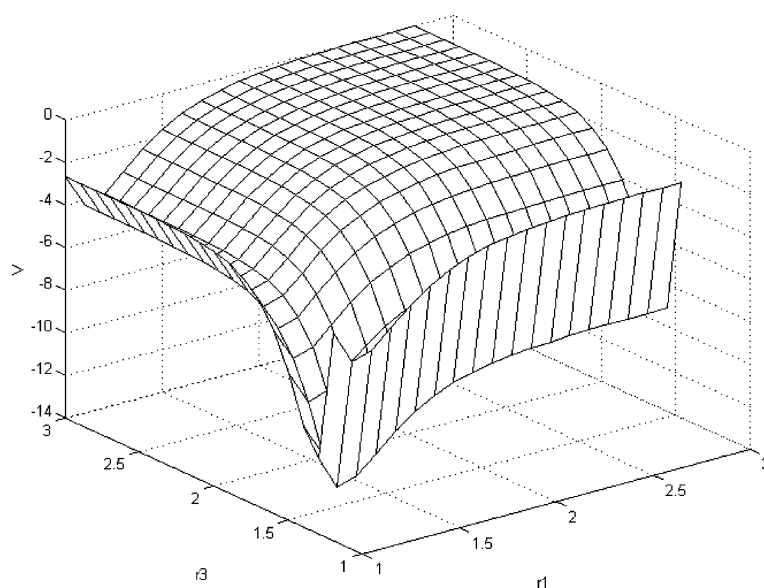


Figure 2. The potential energy surface (eV) of stable C_2HD with r_1 (Å) and r_3 (Å) ($r_2 \rightarrow \infty$).

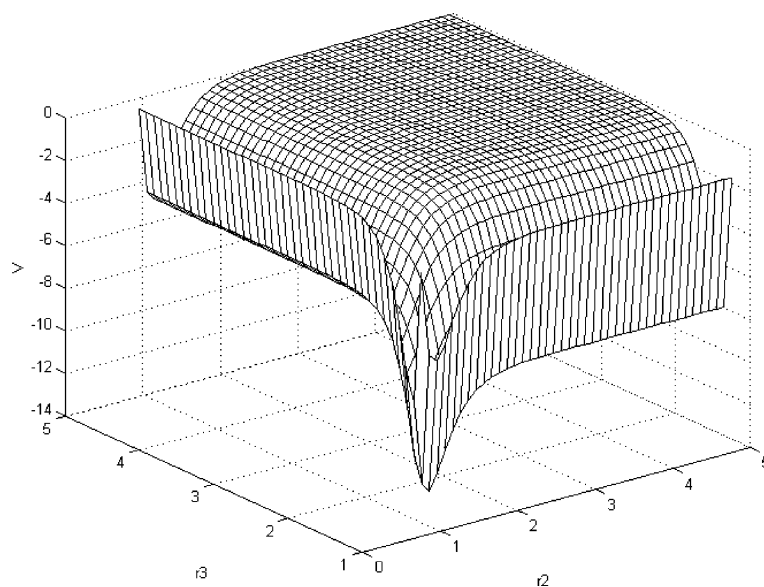


Figure 3. The potential energy surface (eV) of stable C_2HD with r_3 (Å) and r_2 (Å) ($r_1 \rightarrow \infty$).

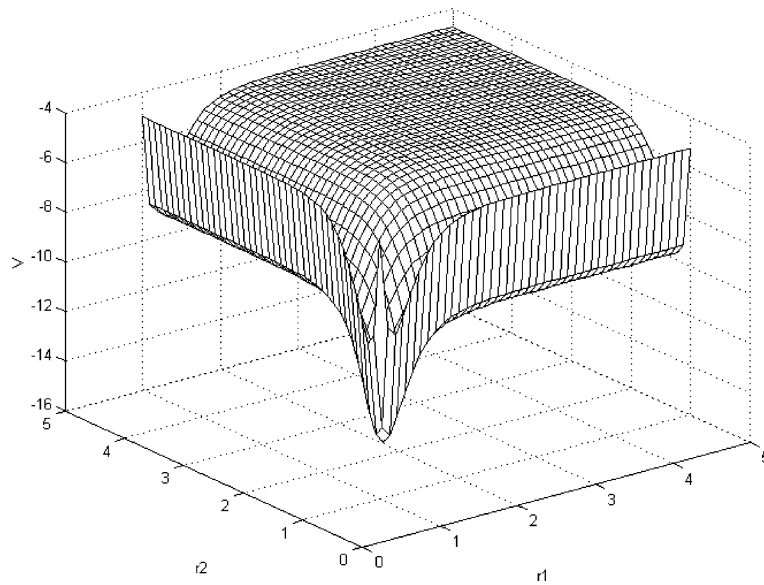


Figure 4. The potential energy surface (eV) of stable C₂HD with $r_1(\text{Å})$ and $r_2(\text{Å})$ ($q_3 = 0.6$).

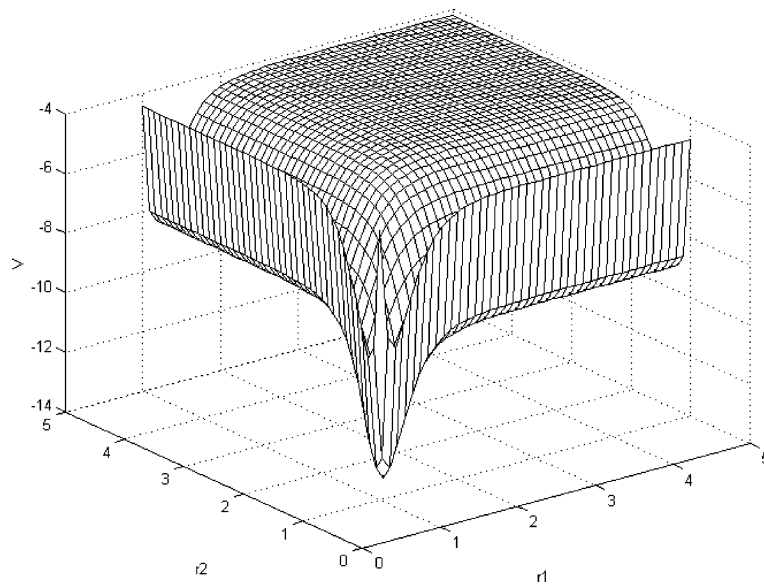


Figure 5. The potential energy surface (eV) of stable C₂HD with r_1 and r_2 ($q_3 = 1.3$).

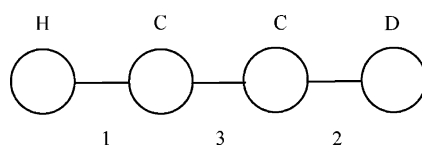


Figure 6. The expression of HCCD.

and applied. From equations (10)–(12), we can see that the bond two has an influence on the total dissociation energy and the bond dissociation energy. Work is also in progress on an extension of the approach to potential energy surfaces containing a saddle point rather than a well in their midst.

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