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Accurate calculation of electron affinity for S_3*

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The accurate equilibrium structures of S_3 and S_3^- are determined by the coupled-cluster method with single, double excitation and perturbative triple excitation (CCSD(T)) with basis sets of aug-cc-pV(n+d)Z (n = T, Q, 5, or 6), complete basis set extrapolation functions with two-parameters and three-parameters, together with considering the contributions due to the core-valence electron correlation, scalar relativistic effects, spin–orbit coupling, and zero-point vibrational corrections. Our calculations show that both the neutral S_3 and anion S_3^- have open forms with C_{2v} symmetry. On the basis of the stable geometries, the adiabatic electron affinity of S_3 is determined to be 19041(11) cm^{-1}, which is in excellent agreement with the experimental data (19059(7) cm^{-1}). The dependence of geometries and electron affinity on the computation level and physical corrections is discussed. The present computational results are helpful to the experimental molecular spectroscopy and bonding of S_3.

Keywords: S_3, molecular geometry, adiabatic electron affinity, coupled-cluster method with single, double excitation and perturbative triple excitation (CCSD(T))

PACS: 32.10.Hq, 33.15.–e, 31.15.A–, 31.15.vq **DOI:** 10.1088/1674-1056/28/1/013203

1. Introduction

Sulfur has drawn considerable interest because the sulfur element and its compounds exist widely in the earth's atmosphere and outer space.[1–3] Sulfur compounds have a large number of allotropes, many of which comprise cyclic molecules.[4,5] Among these compounds, thiozone (S_3) molecule, which is stable in the gas phase, has been observed in supersonic molecular beams, inert gases, interstellar and astronomical sources.[6] The ground electronic state of S_3 is a singlet with $^1A_1$ symmetry. Its anion, S_3^-, has an unpaired electron in π^*-orbital and the ground electronic state is a doublet with $^2B_1$ symmetry. Thiozone anion is the most important chromophore in the brilliant blue pigment of Lapis lazuli and is the dominant form of sulfur in certain high pressure and temperature conditions approximating crustal and subduction-zone geologic fluids.[7–9] It may also play an important role in the transport of sulfur and chalcophile metals in the earth.[10]

Transition from the anionic ground state $^2B_1$ to the neutral ground state $^1A_1$ has been investigated by several studies using anion photoelectron spectroscopy (PES).[3,10–12] Electron affinity of S_3 can be determined from the PES; however, there are some deviations in the measured results. By assuming that the anions were at the ground vibrational state, Nimlos *et al.*[10] found an electron affinity of 2.093 ± 0.025 eV by self-constructed negative ion photoelectron spectrometer firstly, and located the peak in the progression which was defined the vibrational origin of the ν_1 symmetric stretch of S_3^-. Later, a different onset was found for the band by the same experimental method, suggesting the possibility that the two experiments produced anions with different vibrational temperatures and that some of the low binding energy peaks came from hot bands. This was assigned to the $0 \rightarrow 0$ transition in the photoelectron spectrum of S_3, giving a possible electron affinity ranging from 2.33 eV to 2.40 eV, and should hence correspond to the adiabatic value.[3] The two previous studies disagree over which peak in this progression is the vibrational origin and the electron affinity energy is also different. Recently, the high-resolution anion photoelectron spectrum of S_3 was obtained by slow electron velocity-map imaging (SEVI),[12] which measured an adiabatic electron affinity (AEA) of 2.3630(9) eV (19059(7) cm^{-1}), resolving discrepancies in the previously reported photoelectron spectra that resulted from the presence of vibrational hot bands. However, the existing theoretical results on the adiabatic electron affinity (AEA) for S_3 cannot well support the experiments, as these values have a large range and the calculation methods are not accurate enough.[2,12,13] For example, the AEA value is calculated to be 2.377 eV for $S_3(^1A_1) \rightarrow S_3^-(^2B_1)$ by the configuration interaction method with single and double excitations including Davidson correction (CISD + Q) employing ANO basis set.[2] The calculated results of AEA using the coupled-cluster method with single, double excitation and perturbative triple excitation (CCSD(T)) and the method of multireference configuration interaction including Davidson correction

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(MRCI + Q) with different basis sets are in a relatively large range of 2.10–2.35 eV.[13] The calculated data is 2.383 eV by CCSD(T)/aug-cc-pV(Q + d)Z, which was used to support the experimental result (2.3630(9) eV).[12]

More research attention should be given to neutral and anionic S_3 compared to its lighter homologue ozone O_3. Theoretical computation on the electronic structures of S_3 and S_3^- is still a challenge due to the fact that the S–S bond length is quite sensitive to the level of theory and the size of the basis sets employed. As aforementioned, the previous computed values of the AEA of S_3 still spread over a relatively large range and some physical corrections, including the core-valence electrons correlations and relativistic effects, are absent in the previous computations. In this work, we report elaborate quantum chemical calculations employing CCSD(T)[14,15] based on Hartree–Fock (HF) orbitals using the series augmented correlation-consistent basis sets with extrapolation technique as well as considering various correction effects on the structures and energies of S_3 and S_3^-. Our study provides an accurate determination on the geometries and energies of S_3 and S_3^-, together with the adiabatic electron affinity for S_3, which are beneficial to the experimental spectral analysis.

2. Computational methods

The systematic electronic structure calculations of S_3 and S_3^- were performed by employing the MOLPRO package.[16] S_3 is a closed shell system with a ground state of $^1A_1$. Attaching an electron to S_3, forming anion S_3^-, will lead to an open-shell system with a ground state of $^2B_1$. The structures and energies of S_3 were obtained by the CCSD(T) method based on HF orbital, while the structures and energies of S_3^- were calculated by the unrestricted and restricted CCSD(T) (U/RCCSD(T)) based on restricted open shell HF (ROHF) orbital. The correction energies from the spin–orbit coupling of the above systems were calculated by full valence complete active space self-consistent field (CASSCF) method.

The basis sets used throughout the present work for sulfur corresponded to the series of the augmented correlation-consistent basis sets of Dunning and co-workers.[17] The additional tight d functions included in these sets have been shown to be very important for obtaining accurate structures and energies of the sulfur-containing species, denoted by aug-cc-pV(n+d)Z, with n = T, Q, 5, or 6.[18,19] The geometries were fully optimized with the CCSD(T) method at the aug-cc-pV(n+d)Z (n = T, Q, 5) level. Additionally, we also carried out systematic calculations of energies with the same theory method at the aug-cc-pV(n+d)Z (n = T, Q, 5, 6) level and excluding the correlation-consistent polarized core-valence sets cc-pwCVTZ.[20] These sets are well suited for our purposes, constituting hierarchical sequences of basis sets that allow us to approach the basis-set limits in a controlled and systematic manner. However, even the largest correlation-consistent sets do not give results that are converged to the basis-set limit, in particular for the correlated methods. To establish these limits, additional calculations are required.

Basis-set extrapolation (BSE) techniques are well established in high-accuracy energy calculations and are essential to reduce remaining errors due to basis set deficiencies. The extrapolation of energies towards the basis-set limit requires not only a systematic suite of basis sets such as the correlation-consistent sets but also a simple model according to which the extrapolation can be carried out.

For obtaining the more precise data, the systematic convergence of the correlation consistent basis sets towards the compete basis set (CBS) limit was exploited by extrapolation of the total energies using the following extrapolation functions:[21–23] two-parameters complete basis set (CBS2) extrapolation function

$$E_n = E_{\mathrm{CBS}} + B/n^3, \quad (n = 4,5 \text{ or } n = 5,6); \tag{1}$$

three-parameters complete basis set (CBS3) extrapolation function

$$E_n = E_{\mathrm{CBS}} + B\,\mathrm{e}^{-(n-1)} + C\,\mathrm{e}^{-(n-1)^2}, \quad (n = 3,4,5 \text{ or } n = 4,5,6). \tag{2}$$

Since the most suitable extrapolation scheme varies with the molecules and basis sets used, no formula invariably gives the best estimation of the CBS limit.[23–25] In this study, the best CBS limit was obtained by the average of these two results of Eqs. (1) and (2) and the spread yielded a conservative estimate of the uncertainty in the extrapolation.

Additional corrections were then added to these CBS limits, namely, contributions due to core-valence electron correlation (ΔCV), scalar relativistic effects (ΔSR), spin–orbit coupling (ΔSOC), and zero-point vibrational corrections (ΔZPE). In these corrections, ΔCV was calculated by HF-CCSD(T)/aug-cc-pwCVTZ for S_3 and ROHF-UCCSD(T)/aug-cc-pwCVTZ for S_3^-, ΔSR was calculated by HF-CCSD(T)/aug-cc-pV(Q + d)Z for S_3 and ROHF-UCCSD(T)/aug-cc-pV(Q + d)Z for S_3^-. ΔSOC was obtained by CASSCF/aug-cc-pVTZ which considered the roots of singlet states with 2A1+2B1+2B2+2A2 and triplet states with A1+B1+B2+A2 for S_3, together with the roots of doublet states with 2A1+2B1+2B2+2A2 and quartet states with A1+B1+B2+A2 for S_3^-. ΔZPE was calculated by HF-CCSD(T)/aug-cc-pV(T + d)Z for S_3 and ROHF-UCCSD(T)/aug-cc-pV(T + d)Z for S_3^-.

3. Results and discussion

3.1. The equilibrium structures of S_3 and S_3^-

The neutral S_3 has three isomers with C_{2v} (the open form, $^1A_1$), D_{3h} (the cyclic form, $^1A_1'$), and $D_{\infty h}$ (the linear form,

$^1\Sigma_g$) symmetries, respectively.[4,26–31] Similar to S_3, the anionic species S_3^- also has three isomers, the symmetries are C_{2v} (the open form, $^2B_1$), C_{2v} (the cyclic form, $^2B_2$), and $D_{\infty h}$ (the linear form, $^2\Pi_u$), respectively. The most stable structures of S_3 and S_3^- are both the open forms with the symmetry of C_{2v}, which are investigated in the present study to determine the AEA value.

The equilibrium structures including the bond lengths R(S–S) and bond angles ∠(S–S–S) of $S_3(^1A_1)$ and $S_3^-(^2B_1)$ are calculated by HF-CCSD(T) and RHF-UCCSD(T), respectively, using different basis sets, such as aug-cc-pV(n+d)Z (n = T, Q, 5), as well as CBS2 and CBS3 in which n = 4, 5 in Eq. (1) and n = 3, 4, 5 in Eq. (2). The ΔCV and ΔSR are also considered in the calculations. The calculations with the aug-cc-pV(n+d)Z (n = T, Q, 5) basis sets have additionally included the fully symmetry equivalence orbitals for the S atom. The results are presented in Table 1. The experiment results reported in the literature are also listed in this table for comparison.

Table 1. The calculated equilibrium structures of S_3 and S_3^- by CCSD(T). The numbers in the parentheses represent the uncertainty of the last digit.

	$S_3(^1A_1)$		$S_3^-(^2B_1)$	
	R(S–S)/Å	∠(S–S–S)/(°)	R(S–S)/Å	∠(S–S–S)/(°)
aug-cc-pV(T+d)Z	1.9300	117.38	2.0045	114.96
aug-cc-pV(Q+d)Z	1.9195	117.50	1.9934	114.97
aug-cc-pV(5+d)Z	1.9162	117.49	1.9900	114.93
CBS2	1.9127	117.48	1.9864	114.89
CBS3	1.9143	117.48	1.9880	114.91
ΔCV	–0.0047	0.04	–0.0044	0.00
ΔSR	0.0004	0.00	0.0007	–0.01
CBS2+ΔCV+ΔSR	1.9084	117.52	1.9827	114.88
CBS3+ΔCV+ΔSR	1.9100	117.52	1.9843	114.90
Exp.[12,32]	1.914(2)	117.33(5)	1.98(1)	114(1)

As one can see from Table 1, with the basis set size increased successively from aug-cc-pV(T+d)Z to aug-cc-pV(5+d)Z, the calculated R(S–S) values of S_3 are decreasing gradually from 1.9300 Å to 1.9162 Å, while the ∠(S–S–S) values are in the range from 117.38° to 117.50°. The extent of amendment for the R(S–S) values is 0.0016 Å, and the ∠(S–S–S) values have no change between CBS2 and CBS3. Comparing the results of two extrapolation schemes, it is found that the values (R(S–S) = 1.9143 Å, ∠(S–S–S) = 117.48°) obtained by CBS3 are more consistent with the experiment data (R(S–S) = 1.914(2) Å, ∠(S–S–S) = 117.33(5)°).[32] The bond length is reduced by 0.0047 Å with ΔCV, while it is increased by 0.0004 Å with ΔSR. It is worth noting that scalar relativity has almost no effect on the equilibrium geometries of either species, which also occurs in molecules with nonisotopic three atoms.[33] The final equilibrium geometries calculated by CBS2+ΔCV+ΔSR (R(S–S) = 1.9084 Å, ∠(S–S–S) = 117.52°) and CBS3+ΔCV+ΔSR (R(S–S) = 1.9100 Å, ∠(S–S–S) = 117.52°) are within 0.01 Å and 0.2° of the experimental R(S–S) and ∠(S–S–S) values,[32] respectively. The results also reproduce the *ab initio* study of Peterson *et al.*[34]

For anionic species S_3^-, the bond length R(S–S) and bond angle ∠(S–S–S) have been measured by SEVI experiment.[12] The aug-cc-pV(n+d)Z (n = T, Q, 5) results (1.9900–2.0045 Å) seem to overestimate the bond distance. The same as S_3, the extent of amendment for the R(S–S) values of S_3^- is also 0.0016 Å, but the ∠(S–S–S) values have changed by 0.02° between CBS2 (R(S–S) = 1.9827 Å, ∠(S–S–S) = 114.88°) and CBS3 (R(S–S) = 1.9843 Å, ∠(S–S–S) = 114.90°). The results of two extrapolation schemes are within the experimental error bar (R(S–S) = 1.98(1) Å, ∠(S–S–S) = 114(1)°).[12] The corrected R(S–S) values with CBS2+ΔCV+ΔSR and CBS3+ΔCV+ΔSR are close (1.9827 Å vs. 1.9843 Å), which are consistent to the values from the experiment measurements.[12] The scalar relativistic has almost no effect on the bond length. The bond angles are more or less the same with all the theory calculation methods herein, and they are close to the experiment data. Remarkably, both the core-valence correlation and the scalar relativistic have little effect on the bond angle. The obtained equilibrium parameters of the two CBS+ΔCV+ΔSR schemes are within the experimental error bar and better than the previous data at MRCI+Q/ANO6532[13] and CCSD(T)/aug-cc-pV(Q+d)Z levels.[12] Additionally, the S_3^- has a bond angle close to S_3, explaining the absence of a bending mode progression in the photoelectron spectra of S_3^-, which is similar to that in O_3^-.[35]

3.2. The adiabatic electron affinity of S_3

Accurate theoretical prediction of electron affinity is a difficult task in quantum chemical computations because the correlation energy of the anion with an additional electron is substantially larger than that of the neutral though weakly bound,[36,37] and an appropriate description of the

extra electron requires one-particle basis sets augmented by diffuse functions as well as functions of high angular momentum.[38] Since the stable structures of the neutral and charged molecules are generally different, the AEA is evaluated from the energy difference between the optimized neutral structure and anionic system at the neutral geometry. The total energies of S_3 are calculated by CCSD(T)/aug-cc-pV(n+d)Z (n = T, Q, 5, 6), and the ones of S_3^- are calculated by UCCSD(T) and RCCSD(T), respectively, with the same basis sets of S_3, based on the geometric structures of CBS3+ΔCV+ΔSR from Table 1. The results are listed in Table 2. To investigate the effect of the basis sets, we also calculate the total energies of S_3 and S_3^- at Q5-CBS2, 56-CBS2, TQ5-CBS3, and Q56-CBS3 levels, which are the CBS2 when n = 4, 5 and n = 5, 6 in Eq. (1), and the CBS3 when n = 3, 4, 5 and n = 4, 5, 6 in Eq. (2), respectively, the results of which are also given in Table 2. The corresponding AEAs are calculated by the above methods and the results are listed in Table 3. Furthermore, the correction energies (ΔCV, ΔSR, ΔSOC, ΔZPE) are also given in the table. In order to make the computed results more visible and clear, the AEAs of S_3 are shown in Fig. 1, which are calculated by UCCSD(T) and RCCSD(T) methods with different basis sets of aug-cc-pV(n+d)Z (n = T, Q, 5, 6), Q5-CBS2, 56-CBS2, TQ5-CBS3, and Q56-CBS3 respectively. Combined with Table 3, the calculated AEAs range from 18629 cm^{-1} to 19201 cm^{-1} considering the total energy correction (ΔCV+ΔSR+ΔSOC+ΔZPE) of −209 cm^{-1}, in which the ΔCV, ΔSR, and ΔSOC have negative values of −33 cm^{-1}, −105 cm^{-1}, and −164 cm^{-1}, respectively, only the ΔZPE has a positive value of 93 cm^{-1}. Obviously, the influence of the correction effect from ΔSOC is the biggest among them because it has the largest absolute value, which are in good agreement with the experimental data (19059(7) cm^{-1}). The best estimated data are 19175(11) cm^{-1} and 19041(11) cm^{-1}, respectively, which are obtained by the average of these four results include Q5-CBS2, 56-CBS2, TQ5-CBS3, and Q56-CBS3, as well considering the total energy correction (ΔCV+ΔSR+ΔSOC+ΔZPE). When the theoretical calculation error is calculated, the average value of Q5-CBS2 and 56-CBS2 is the upper limit and the average value of TQ5-CBS3 and Q56-CBS3 is the lower limit. In fact, the obtained best data is 19041(11) cm^{-1} by RCCSD(T), the error is only 10^{-3} eV compared with the experimental value 19059(7) cm^{-1}, which is the best result of the calculation by far.

Table 2. The calculated total energies of S_3 and S_3^-.

	S_3/Hartree	S_3^- (UCCSD(T)) /Hartree	S_3^- (RCCSD(T)) /Hartree
aug-cc-pV(T+d)Z	−1193.215729	−1193.302122	−1193.301565
aug-cc-pV(Q+d)Z	−1193.262472	−1193.350301	−1193.349706
aug-cc-pV(5+d)Z	−1193.277666	−1193.365794	−1193.365191
aug-cc-pV(6+d)Z	−1193.283890	−1193.372088	−1193.371482
Q5-CBS2	−1193.293608	−1193.382049	−1193.381437
56-CBS2	−1193.292440	−1193.380733	−1193.380124
TQ5-CBS3	−1193.286487	−1193.374786	−1193.374178
Q56-CBS3	−1193.287514	−1193.375751	−1193.375144

Table 3. The adiabatic electron affinity of S_3 by CCSD(T) with different basis sets. The numbers in the parentheses represent the uncertainty of the last digit(s).

	Adiabatic electron affinity/cm^{-1}		
	UCCSD(T)		RCCSD(T)
aug-cc-pV(T+d)Z	18960		18838
aug-cc-pV(Q+d)Z	19276		19145
aug-cc-pV(5+d)Z	19341		19209
aug-cc-pV(6+d)Z	19357		19224
Q5-CBS2	19410		19276
56-CBS2	19378		19244
TQ5-CBS3	19379		19245
Q56-CBS3	19365		19232
ΔCV		−33	
ΔSR		−105	
ΔSOC		−164	
ΔZPE		93	
Best estimated value	19175(11)		19041(11)
Expt.[12]		19059(7)	

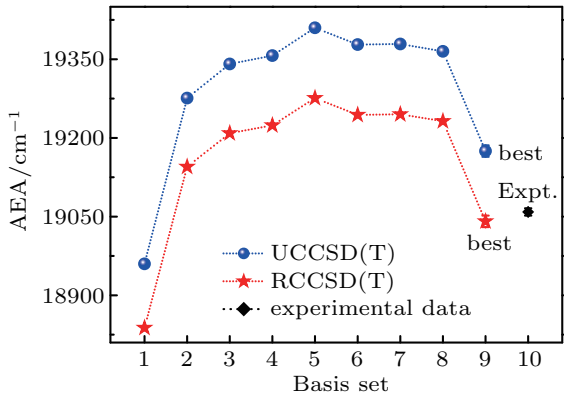


Fig. 1. The obtained adiabatic electron affinity of S_3 by different theoretical calculations and experiment. The different basis sets are given on the x axis: 1 = aug-cc-pV(T+d)Z, 2 = aug-cc-pV(Q+d)Z, 3 = aug-cc-pV(5+d)Z, 4 = aug-cc-pV(6+d)Z, 5 = Q5-CBS2, 6 = 56-CBS2, 7 = TQ5-CBS3, 8 = Q56-CBS3, 9 = the basis set with the best data.

4. Conclusion

The stable structures of S_3 and S_3^- have been given by CCSD(T) method with extrapolation function and considering various correction effects. From the calculation results, they are neither linear nor circular, but have the open forms with the symmetry of C_{2v}. Additionally, the scalar relativity has almost no effect on the equilibrium geometries of S_3 and S_3^- in the computation. The structural parameters are consistent with the experimental data, which are better than the other theoretical values.

On the basis of the stable structure, the adiabatic electron affinity of S_3 has been obtained. It is found that the best predicted AEA is 19041(11) cm^{-1}, which is obtained by the RCCSD(T) method with the basis set of average of four extrapolations for Q5-CBS2, 56-CBS2, TQ5-CBS3, and Q56-CBS3 together with considering the total energy correction, and it is in good agreement with the experimental data (19059(7) cm^{-1}). Furthermore, the effectiveness of the latest experimental method[12] can be verified, as the equilibrium geometries of S_3^- and the AEA of S_3 obtained from the experiment agree with our elaborate quantum chemical calculated results.

References

[1] Miliordos E and Xantheas S S 2014 *J. Am. Chem. Soc.* **136** 2808
[2] Steudel R and Steudel Y 2007 *Eur. J. Inorg. Chem.* **2007** 4385
[3] Hunsicker S, Jones R O and Gantefor G 1995 *J. Chem. Phys.* **102** 5917
[4] McCarthy M C, Thorwirth S, Gottlieb C A and Thaddeus P 2004 *J. Am. Chem. Soc.* **126** 4096
[5] Jin Y Y, Maroulis G, Kuang X Y, Ding L P, Lu C, Wang J J, Lv J, Zhang C Z and Ju M 2015 *Phys. Chem. Chem. Phys.* **17** 13590
[6] Greenwood N N and Earnshaw A 1984 *Chemistry of the Elements* (London: Pergamon) pp. 12–15
[7] Pokrovski G S and Dubrovinsky L S 2011 *Science* **331** 1052
[8] Manning C E 2011 *Science* **331** 1018
[9] Hark R R and Clark R J H 2010 *AIP Conf. Proc.* **1267** 315
[10] Nimlos M R and Ellison G B 1986 *J. Phys. Chem.* **90** 2574
[11] Handschuh H, Gantefor G and Eberhardt W 1995 *Rev. Sci. Instrum.* **66** 3838
[12] Kim J B, Hock C, Yacovitch T I and Neumark D M 2013 *J. Phys. Chem. A* **117** 8126
[13] Koch W, Natterer J and Heinemann C 1995 *J. Chem. Phys.* **102** 6159
[14] Knowles P J, Hampel C and Werner H J 2000 *J. Chem. Phys.* **112** 3106
[15] Zeng H and Zhao J 2012 *Chin. Phys. B* **21** 078202
[16] Werner H J, *et al.* 2010 *MOLPRO version* 2010.1 *A package of ab initio programs* (http://www.molpro.net)
[17] Woon D E and Dunning Jr T H 1993 *J. Chem. Phys.* **98** 1358
[18] Wilson A K and Dunning Jr T H 2003 *J. Chem. Phys.* **119** 11712
[19] Liu Q X, Liang M, Miao Q, Zhang J J, Sun E P and Ren T Q 2018 *Chin. Phys. Lett.* **35** 013101
[20] Peterson K A and Dunning Jr T H 2002 *J. Chem. Phys.* **117** 10548
[21] Peterson K A, Woon D E and Dunning Jr T H 1994 *J. Chem. Phys.* **100** 7410
[22] Helgaker T, Klopper W, Koch H and Noga J 1997 *J. Chem. Phys.* **106** 9639
[23] Feller D, Peterson K A and Crawford T D 2006 *J. Chem. Phys.* **124** 054107
[24] Dixon D A, Jong W A D, Peterson K A and McMahon T B 2005 *J. Phys. Chem. A* **109** 4073
[25] Feller D and Peterson K A 2007 *J. Chem. Phys.* **126** 114105
[26] Jones R O 1986 *J. Chem. Phys.* **84** 318
[27] Rice J E, Amos R D, Handy N C, Lee T J and Schaefer H F 1986 *J. Chem. Phys.* **85** 963
[28] Baird N C 1984 *J. Comput. Chem.* **5** 35
[29] Jug K and Iffert R 1989 *J. Mol. Struct. (Theochem)* **186** 347
[30] Hohl D, Jones R O, Car R and Parrinello M 1988 *J. Chem. Phys.* **89** 6823
[31] Zakrzewski V G and Niessen W V 1994 *Theor. Chim. Acta* **88** 75
[32] Thorwirth S, McCarthy M C, Gottlieb C A, Thaddeus P, Gupta H and Stanton J F 2005 *J. Chem. Phys.* **123** 054326
[33] Pan Y, Luo Z H, Chang Y C, Lau K C and Ng C Y 2017 *J. Phys. Chem. A* **121** 669
[34] Peterson K A, Lyons J R and Francisco J S 2006 *J. Chem. Phys.* **125** 084314
[35] Basch H 1989 *Chem. Phys. Lett.* **157** 129
[36] Kendall R A, Dunning T H and Harrison R J 1992 *J. Chem. Phys.* **96** 6796
[37] Han H L, Zhang X Z and Shi T Y 2007 *Chin. Phys. Lett.* **24** 3392
[38] Noro T, Yoshimine M, Sekiya M and Sasaki F 1991 *Phys. Rev. Lett.* **66** 1157