# Stable Structures of Nitrogen-Rich Sulfides: $S(N_3)_m$ ($m = 1-4$)

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Stable structures of neutral, positive, and negative nitrogen-rich sulfides $S(N_3)_m$ ($m = 1-4$) were studied. Three minima of $S(N_3)_2$, one of $S(N_3)_2^{2+}$, one of $S(N_3)_3^+$ and one of $S(N_3)_4$ were optimized. An isomerization reaction pathway of $SN_3^-$, and dissociation reaction pathways of $SN_3^-$ and $SN_3^+$ were investigated. The special properties of a sulfur atom, a large atomic radius and a loose electron density, allow the sulfur atom to link to several nitrogen atoms, and nitrogen-rich sulfides $SN_x$ (or ions) can be formed easily. The properties of high energy-density of $S(N_3)_x$ were investigated.

## Introduction

Nitrogen clusters have been the subject of several theoretical investigations as potential high energy−density materials (HEDMs). Therefore, besides theoretical interest in pure-nitrogen clusters, other nitrogen-rich compounds have also attracted interest because of their possible use as HEDMs.[1−5] The properties of nitrogen clusters $(Ar)_n(N_2)_m^+$ and benzene-$(N_2)_n$ were studied by Adams and Hiraoka.[6,7] Bartlett[8] suggested some nitrogen-rich compounds formed by N, O, and H as HEDMs. Hammerl and Klapötke[9] studied nitrogen-rich clusters $CN_x$ both experimentally and theoretically. Recently, Gagliardi and Pyykkö[10,11] designed and calculated the structures of $ScN_7$ and $N_5$−metal−$N_7$ and their dissociation pathways. We have also designed some possible reaction pathways for synthesizing the nitrogen-rich ionic compounds $HN_8^+$, $N_4H_2F^+$, and $N_7H_2^+$.[12−14] The main task is to create polynitrogen or nitrogen-rich compounds which store energy and yet are stable enough for practical applications as HEDMs.

The critical properties for applications as effective HEDM molecules are a high dissociation energy barrier and facile syntheses. Stability and synthesis methods of many pure-nitrogen compounds are challenging questions because of their meta-stable nature. Gagliardi et al.[15,16] investigated the potential energy surfaces (PES) of even-numbered nitrogen clusters and discussed the dissociation barriers. Fau et al. studied the stability of $N_5^+N_5^-$ as an isolated species and in a potential periodic structure.[17] The PES of $N_8$ isomers was investigated by Chung et al.[18] Thompson and co-worker[19] studied the dissociation barriers for odd-numbered acyclic nitrogen molecules $N_9$ and $N_{11}$. Two important investigations on $N_5^+$ [20] and $N_5^-$ [21] were studied by experiment. Some studies on the PES of nitrogen clusters have been reported in our previous works.[22−25]

The properties of nitrogen clusters are determined by the bonding between the nitrogen atoms. Nitrogen atoms have unshared pairs of electrons repelling each other, so their single bonds are much weaker than, for example, a carbon−carbon single bond. At the most fundamental level, a molecule will exist only if it has a high enough energy barrier to dissociation. Although N−N single bonds store more energy, the existence of a molecule would suggest that it must have enough double bonds to ensure adequate bond strength to keep the molecule stable. We hope to design nitrogen-rich compounds which are able to store a large amount of energy, will be stable enough, and could be synthesized easily.

The SN bond has very special properties in part because of the diffuse electron density on the sulfur atom and also to *d*-type symmetry of a part of the electron distribution, resulting in such unusual properties as rotation-independent conjugation in some compounds.[26−28] The special role of d orbitals in the representation of diffuse electron densities has also been the subject of detailed studies.[29−31] The special property of a sulfur atom with large atomic radius and loose electron density makes it a candidate to link well with nitrogen clusters. Based on the expectation, some structures of neutral, positive, and negative $SN_x$ systems were designed and optimized using HF, B3LYP, and MP2 methods, and the stability of these systems were analyzed with respect to thermodynamics and kinetics. Based on the experience obtained for structures of $SN_3$, structures of the $S(N_3)_m$ type were also designed.

NS is known to play key roles in both combustion and atmospheric chemistry.[32] Ongstad and co-workers[33] reported photodissociation dynamics of $S_4N_4$ at 222 and 248 nm. Most studies of $S_xN_x$ are on the structures of alternating atoms of nitrogen and sulfur. Collins et al.[34] studied the electronic ground state of the dinitrogen sulfide ($N_2S$) molecule. $S_2N_3^+$, a cation with an $N_3$ unit, was studied by theory and experiment.[35] This $S_2N_3^+$ ion represents the first binary SN ring with an $N_3$ unit.

We expect that theoretical investigations on novel nitrogen-rich compounds $SN_x$ could provide useful information for further studies of their synthesis and application.

## Computational Methods

The geometries of the compounds $SN_x$ have been optimized with ab initio and density functional methods at the levels of HF/6-31G*, B3LYP/6-31G*, B3LYP/6-311+G*, and MP2/6-31G*, where B3LYP is a hybrid functional method using

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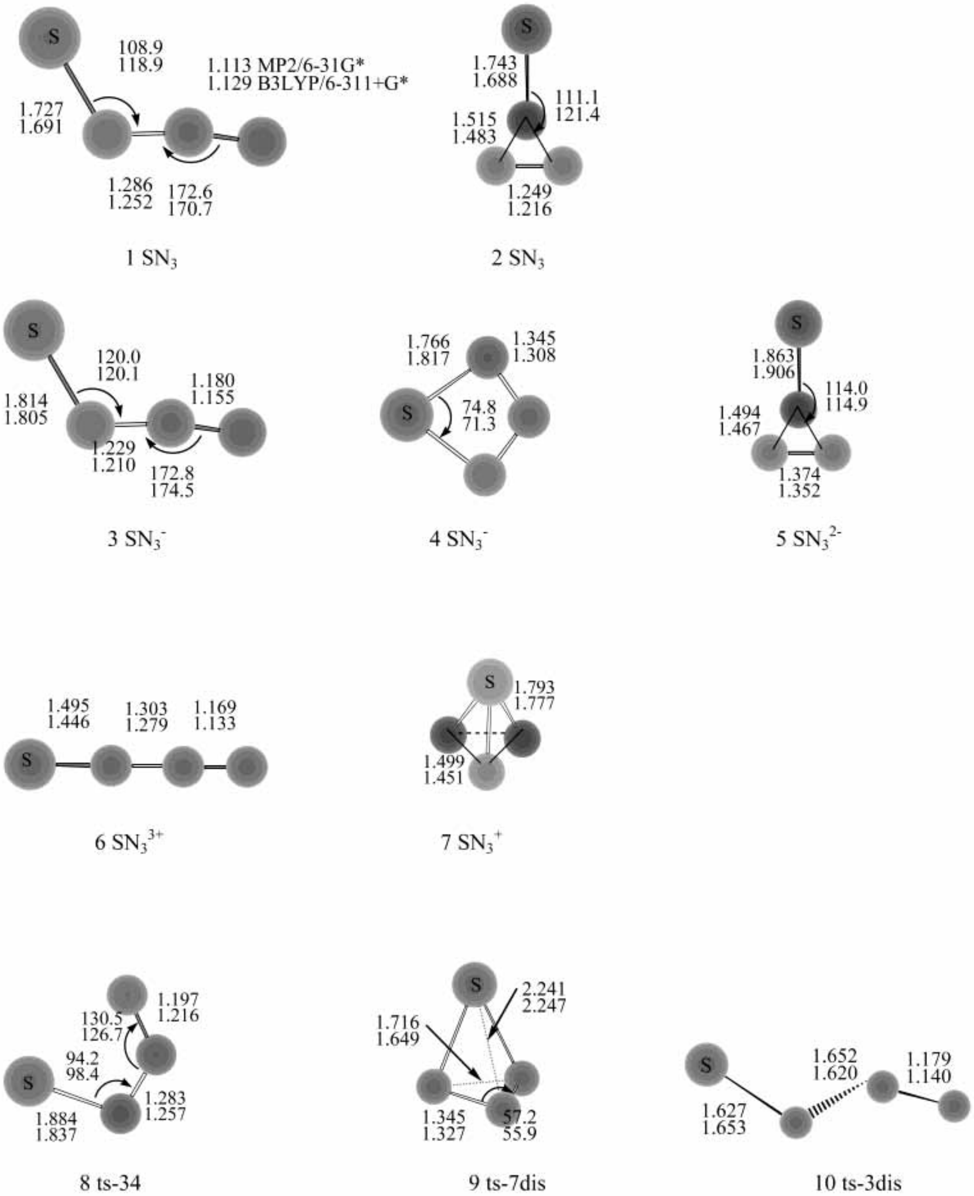

**Figure 1.** Parameters of geometrical structures $SN_3$ and transition state structures of isomerization and dissociation reactions.

Becke's three-parameter nonlocal exchange functional[36] with the nonlocal correlation of Lee, Yang, and Parr,[37] and MP2 stands for the second-order M$\phi$ller−Plesset (many-body) perturbation theory.[38] The designation 6-31G* refers to a standard split-valence double-$\zeta$ polarization basis set, whereas 6-311+G* is a standard split-valence triple-$\zeta$ polarization basis set augmented with diffuse functions.[39] The calculation results show that geometries are insensitive to the basis set. To characterize the nature of the stationary points and determine the zero-point vibrational energy (ZPVE) corrections, harmonic vibrational frequencies were also calculated at the above-mentioned levels of the theory. Stationary points were identified as either local minima or transition structures. To confirm that a given transition structure connects reactants and products, minimum energy path calculations[40−44] were performed at the above levels with a coordinate stepsize of 0.1 $(amu)^{1/2}$ bohr. All calculations were carried out with the Gaussian 98 program package.[45]

## Results and Discussion

**1. Stability and Geometrical Structures of Species $SN_3$.** Seven isomers of $SN_3$ (molecules and ions) were optimized and were found to be stable structures (Figure 1 and Table 1). Structures **1** ($SN_3$, $^2A''$) and **3** ($SN_3^-$, $^1A'$) have similar geometries. Structure **1** $SN_3$ is more stable than **2** $SN_3$ ($^2A'$). Structure **4** for $SN_3^-$ ($^1A_1$) is a four-membered ring. Species **5** $SN_3^{2-}$ ($^2A''$) connects a three-membered ring with single bond. Structure **6** $SN_3^{3+}$ ($^1A'$) is linear with $C_{\infty v}$ symmetry. Structure **7** ($SN_3^+$, closed shell ground state) is cage-shaped ($C_3$ symmetry) with high energy density because it contains more single bonds. It will give off much more energy when it dissociates into noncage structures. Therefore, the dissociation reaction pathway of structure **7** was studied at the HF/6-31G, B3LYP/6-31G*, MP2/6-31G*, and B3LYP/6-311+G* levels. The species **9** (**ts-7dis)** is a transition structure of this dissociation process. The results of IRC analysis indicated that structure **7** dissociates into $SN^+$ and $N_2$. The dissociation barrier heights of structure **7** were predicted to be 25.2, 36.0, 35.0, and 48.2 kcal/mol at the above-mentioned four levels of theory, respectively, and the dissociation reaction gives off energies of 148.9, 103.1, 113.4, and 112.8 kcal/mol (see Table 2). So the moderate dissociation barrier and the energy release imply that structure

**TABLE 1: Total Energies (Hartree) and ZPVE (kcal/mol) of $S(N_3)_m$ ($m = 1-4$) at the HF, DFT, and MP2 Levels with 6-31G* and 6-311+G* Basis Sets**

| | 6-31G* | | | 6-311+G* |
|---|---|---|---|---|
| $SN_x$ | HF | B3LYP | MP2 | B3LYP |
| **1** $SN_3$ ($C_s$) | −560.73930/8.4 | −562.32826/7.7 | −561.33269/10.6 | −562.40197/7.6 |
| **2** $SN_3$ ($C_s$) | −560.66493/7.8 | −562.25083/6.1 | −561.26410/6.3 | −562.32103/6.1 |
| **3** $SN_3^-$ ($C_s$) | −560.77654/8.7 | −562.40295/7.7 | −561.40692/7.8 | −562.49263/7.6 |
| **4** $SN_3^-$ ($C_{2v}$) | −560.72871/8.6 | −562.36177/7.3 | −561.36570/7.5 | −562.45223/7.3 |
| **5** $SN_3^{2-}$ ($C_s$) | −560.49859/6.7 | −562.13302/5.4 | −561.10962/6.5 | −562.26482/5.4 |
| **6** $SN_3^{3+}$ ($C_{\infty v}$) | −558.93308/9.7 | −560.45939/8.3 | −559.54576/7.2 | −560.53111/8.2 |
| **7** $SN_3^+$ ($C_3$) | −560.27480/8.0 | −561.88801/6.9 | −560.94044/6.4 | −561.94906/6.9 |
| **8** ts-43 ($C_s$) | −560.70212/7.4 | −562.34329/6.7 | −561.32780/6.8 | −562.43392/6.6 |
| **9** ts-7dis ($C_1$) | −560.23172/6.2 | −561.82803/5.3 | −560.86124/4.9 | −561.89110/5.2 |
| **10** ts-3dis ($C_1$) | −560.72651/5.8 | −562.35442/5.1 | −561.34430/5.9 | −562.44744/5.2 |
| **11** $S(N_3)_2$ ($C_{2v}$) | −723.86239/16.1 | −726.39021/13.4 | −724.98906/12.6 | −726.50081/13.3 |
| **12** $S(N_3)_2$ ($C_{2v}$) | −723.79604/19.6 | −726.35063/15.3 | −724.95482/13.4 | −726.45403/15.2 |
| **13** $S(N_3)_2$ ($D_{3d}$) | −723.53213/17.7 | −726.12248/14.3 | −723.47151/13.0 | −726.22382/14.3 |
| **14** $S(N_3)_2^{2+}$ ($C_{2v}$) | −723.17565/18.7 | −725.65660/16.3 | −723.13703/15.4 | −725.76950/16.1 |
| **15** $S(N_3)_3^+$ ($C_3$) | −886.96014/27.6 | −890.38108/24.6 | −888.57181/24.8 | −890.53998/24.5 |
| **16** $S(N_3)_4$ ($C_1$) | −1050.40300/36.7 | −1054.81516/32.5 | −1052.59023/32.8 | −1055.02664/32.1 |

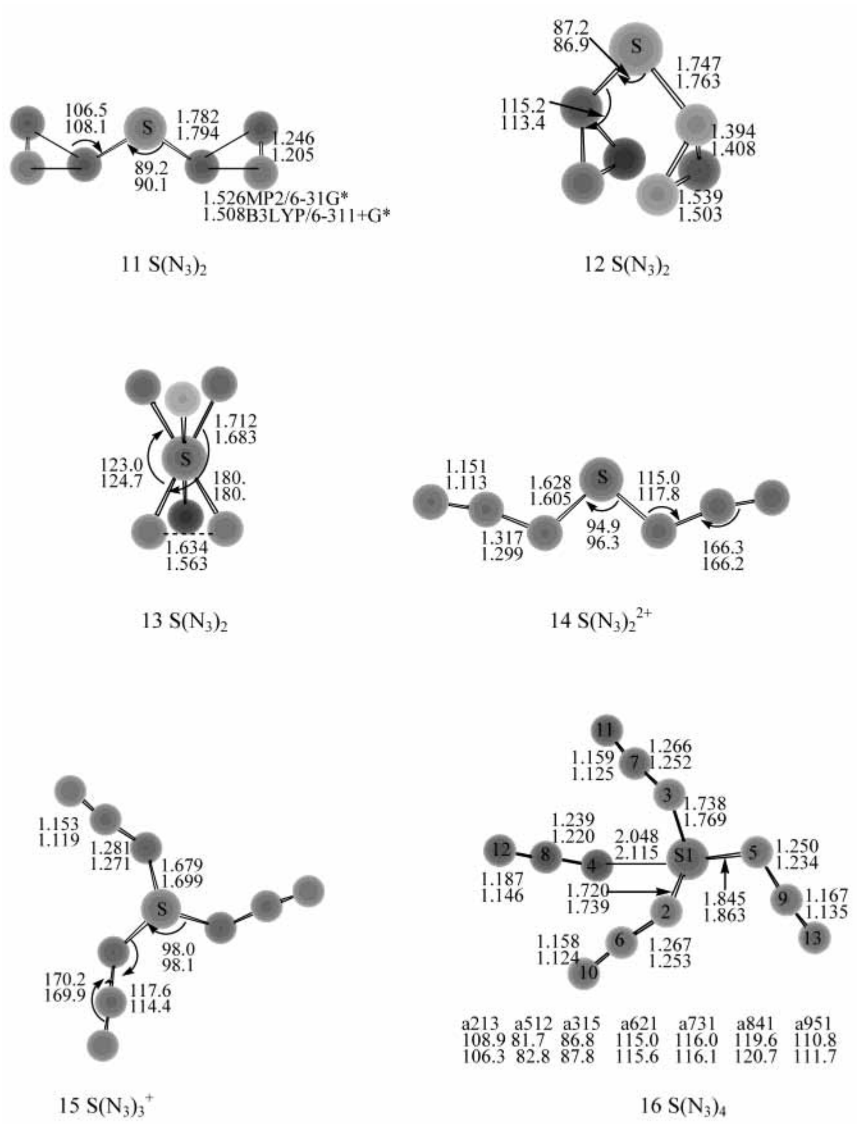

**Figure 2.** Parameters of geometrical structure of $S(N_3)_m$ ($m = 2-4$).

**7** is stable enough to be a good candidate to be used as HEDM when it combines with appropriate negative ions.

Structure **8** ($SN_3^-$, **ts-43**) was found to be a transition structure for the isomerization reaction from structure **4**−**3**, that is, from a ring-shaped structure to a chain one. The barrier heights are 15.5, 11.0, 10.5, and 23.0 kcal/mol, and the released energies are 45.6, 24.8, 24.1, and 24.6 kcal/mol at the HF/6-31G*, B3LYP/6-31G*, B3LYP/6-311+G*, and MP2/6-31G* levels, respectively. The barrier from structure **4** to **3** is not high enough. Therefore, **4** is not stable and converts into **3** easily. The

**TABLE 2: Potential Energy Surfaces of the Isomerization Reaction between 4 and 3, Dissociation Reactions of Species 3 and 7 at the HF/6-31G*, B3LYP/6-31G*, MP2/6-31G*, and B3LYP/6-311+G* Levels**

| | 6-31G* | | | 6-311+G* |
|---|---|---|---|---|
| species | HF | B3LYP | MP2 | B3LYP |
| **4** | 0.0 | 0.0 | 0.0 | 0.0 |
| **8** (ts-34) | 15.5 | 11.0 | 23.0 | 10.5 |
| **3** | −45.6 | −24.8 | −24.6 | −24.1 |
| **10** (ts-3dis) | −17.4 | 3.9 | 12.8 | 1.9 |
| $SN^- + N_2$ | | −4.8 | −5.7 | −9.8 |
| **7** | 0.0 | 0.0 | 0.0 | 0.0 |
| **9** (ts-7dis) | 25.5 | 36.0 | 48.2 | 35.0 |
| $SN^+ + N_2$ | −148.9 | −103.1 | −112.8 | −113.4 |

**TABLE 3: Relative Energies (Hartree) of Neutral Nitrogen-Rich Clusters $S(N_3)_m$ at the B3LYP/6-31G* and B3LYP/6-311+G* Levels**

| | B3LYP | |
|---|---|---|
| $SN_x$ | 6-31G* | 6-311+G* |
| **1** $SN_3$ ($C_s$) | 96.2 | 100.1 |
| $1/8(S_8 + 12N_2)$ | 0.0 | 0.0 |
| **11** $S(N_3)_2$ ($C_{2v}$) | 237.9 | 252.0 |
| $1/8(S_8 + 24N_2)$ | 0.0 | 0.0 |
| **16** $S(N_3)_4$ ($C_1$) | 339.1 | 356.5 |
| $1/8(S_8 + 48N_2)$ | 0.0 | 0.0 |

dissociation reaction pathway of **3** was also studied. Structure **10** is a transition state structure of the dissociation reaction of species **3**. The barriers are 28.2, 28.7, 26.0, and 37.4 kcal/mol at the levels of HF/6-31G*, B3LYP/6-31G*, B3LYP/6-311+G*, and MP2/6-31G*, respectively. The endothermicities are 20.0, 14.3, and 18.9 kcal/mol at the B3LYP/6-31G*, B3LYP/6-311+G*, and MP2/6-31G* levels, respectively. The result of the HF method on a thermodynamics calculation is fundamentally different from the above three levels. We consider the results at B3LYP and MP2 levels more reliable because electron correlation effects appear significant and are included at these levels.

Thermodynamic stability of $SN_x$ has also been calculated by comparing the total energy of species with respect to that of $N_2 + S_8$. The result is presented in Table 3. The relative energy of species **1** ($SN_3$) is 96.2 and 100.1 kcal/mol higher than $(3/2)N_2 + (1/8)S_8$ at the levels of B3LYP/6-31G* and B3LYP/6-311+G*. Therefore, if stable species $SN_3$ can be obtained, $SN_3$ may be possible to be used as HEDM because of such high energy it contains.

**2. Stability and Geometrical Structures of $S(N_3)_m$ ($m = 2-4$).** Four structures of $S(N_3)_2$ (three neutral molecules, and one positive ion), one of $S(N_3)_3^+$, and one of $S(N_3)_4$ (see Table 1 and Figure 2) were optimized to be minima at the HF/6-31G*, B3LYP/6-31G*, MP2/6-31G*, and B3LYP/6-311+G* levels, respectively. The system of $S(N_3)_m$ were designed based on the structures of $SN_3$. Species **11** ($S(N_3)_2$) and **12** ($S(N_3)_2$) were formed by a sulfur atom and two triangles of $N_3$. Structure **13** ($S(N_3)_2$), a sandwich structure with $D_{3d}$ symmetry, has higher energy than the other two neutral $S(N_3)_2$ structures (**11** and **12**) because more N−N single bonds are present in structure **13**. Initially, a structure with $D_{3h}$ symmetry was designed, but the optimized result showed that the $D_{3h}$ structure is not a stable structure having one imaginary frequency.

The most interesting aspect is that structures **14** ($S(N_3)_2^{2+}$), **15** ($S(N_3)_3^+$), and **16** ($S(N_3)_4$) all were derived from $SN_3^{3+}$. From the charge distribution, most of the positive charge is concentrated on the sulfur atom. We can consider that the compounds are formed by $S^{4+}$ and linear $(N_3^-)_m$ structures ($m = 2-4$). The result suggests how a large molecule may be synthesized from small reactants. The structures **14**, **15**, and **16** are $S(N_3)_2^{2+}$, $S(N_3)_3^+$, and $S(N_3)_4$ with $C_{2v}$, $C_3$, and $C_1$ symmetries, respectively. Comparing the S−N bonds in structures **14**, **15**, and **16**, the order of bond lengths is **14** < **15** < **16**. Especially, for structure **16**, the four S−N bonds are different, and one of them is very long 2.115 Å at the B3LYP/6-311+G* level. This implies that the $N_3^-$ ion connects to the sulfur atom loosely. Therefore, structure **16** can be regarded as a complex that easily dissociates. The other bonds in structure **16** are similar to that in structure **14** or **15**.

The relative energy of species **11** $S(N_3)_2$ and **16** $S(N_3)_4$ were obtained by comparing the total energy with that of species $N_2 + S_8$. Species **11** is higher 237.9 and 252.0 kcal/mol than $1/8(S_8 + 24N_2)$ by the B3LYP method using 6-31G* and 6-311+G* basis sets. Similar for species **16**, it is 339.1 and 356.5 kcal/mol higher than $6N_2 + (1/8)S_8$. Therefore, if stable species $SN_x$ can be obtained, $S(N_3)_m$ may be possible to be used as HEDM because it contains such high energy.

## Summary

Stable structures of nitrogen-rich sulfides $S(N_3)_m$ were obtained utilizing the methods of HF, B3LYP, and MP2 with 6-31G* and 6-311+G* basis sets. The structure $SN_3^-$ **3** is the most stable among the $SN_3^-$ species. $S(N_3)_m$ structures were determined to be minimum points by analysis of vibrational frequencies. The dissociation reaction of **7** ($SN_3^+$) and the isomerization reaction from ring-shaped **4** ($SN_3^-$) to chain-shaped **3** ($SN_3^-$) indicate that $SN_x$ clusters have the properties of high-energy density materials (HEDMs). The ionic nitrogen-rich clusters may be used as a HEDM when they combine with appropriate counterions.

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## References and Notes

(1) Hammerl, A.; Klapötke, T. M. *Inorg. Chem.* **2002**, *41*, 906.
(2) Hammerl, A.; Klapötke, T. M.; Nöth, H.; Warchhold, M. *Inorg. Chem.* **2001**, *40*, 3570.
(3) Glukhovtsev, M. N.; Jiao, H.; Schleyer, P. v. R. *Inorg. Chem.* **1996**, *35*, 7124.
(4) Chavez, D. E.; Hiskey, M. A.; Gilardi, R. D. *Angew. Chem.* **2000**, *112*, 1861.
(5) Fraenk, W.; Haberader, T.; Hammerl, A.; Klapötke, T. M.; Krumm, B.; Mayer, P.; Nöth, H.; Warchhold, M. *Inorg. Chem.* **2001**, *40*, 1334.
(6) Hiraoka, K.; Fujimaki, S.; Nasu, M.; Minamitsu, A. *J. Chem. Phys.* **1997**, *107*, 2550.
(7) Adams, J. E. *J. Chem. Phys.* **1998**, *109*, 6296.
(8) Bartlett, R. *Chem., & Indust.* **2000**, *21*, 140.
(9) Hammerl, A.; Klapötke, T. M. *Inorg. Chem.* **2002**, *41*, 906.
(10) Gagliardi, L.; Pyykkö, P. *J. Am. Chem. Soc.* **2001**, *123*, 9700.
(11) Gagliardi, L.; Pyykkö, P. *J. Phys. Chem. A* **2002**, *106*, 4690.
(12) Wang, L. J.; Li, Q. S.; Warburton, P.; Mezey, P. G. *J. Phys. Chem. A* **2002**, *106*, 1872.
(13) Wang, L. J.; Mezey, P. G. *Chem. Phys. Lett.* **2002**, *363*, 87.
(14) Wang, L. J.; Mezey, P. G. *J. Phys. Chem. A* **2002**, *106*, 10391.
(15) Gagliardi, L.; Evangelisti, S.; Roos, B. O.; Widmark, P.-O. *Theochem.* **1998**, *428*, 1.
(16) Gagliardi, L.; Evangelisti, S.; Bernhardsson, A.; Lindh, R.; Roos, B. O. *Int. J. Quantum Chem.* **2000**, *77*, 311.
(17) Fau, S.; Wilson, K. J.; Bartlett, R. J. *J. Phys. Chem. A* **2002**, *106*, 4639.
(18) Chung, G.; Schmidt, M. W.; Gordon, M. S. *J. Phys. Chem. A* **2000**, *104*, 5647.
(19) Thompson, M. D.; Bledson, T. M.; Strout, D. L. *J. Phys. Chem. A* **2002**, *106*, 6880.
(20) Christe, K. O.; Wilson, W. W.; Sheehy, J. A.; Boatz, J. A. *Angew. Chem., Int. Ed. Engl.* **1999**, *38*, 13.

(21) Vij, A.; Pavlovich, J. G.; Wilsom, W. W.; Vij, V.; Christe, K. O. *Angew. Chem., Int. Ed.* **2002**, *41*, 3051.

(22) Xu, W. G.; Li, G. L.; Wang, L. J.; Li, S.; Li, Q. S. *Chem. Phys. Lett.* **1999**, *314*, 300.

(23) Li, Q. S.; Wang, L. J. *J. Phys. Chem. A* **2001**, *105*, 1979.

(24) Wang, L. J.; Li, S.; Li, Q. S. *Comput. Chem.* **2001**, *22*, 1334.

(25) Wang, L. J.; Warburton, P.; Mezey, P. G. *J. Phys. Chem. A* **2002**, *106*, 2748.

(26) Mezey, P.; Kucsman, A. *J. Chem. Soc., Faraday 2* **1972**, *68*, 2060.

(27) Mezey, P.; Kalman, A.; Kucsman, A. *Int. J. Sulfur Chem.* **1972**, *A2*, 187.

(28) Mezey, P.; Flakus, H. *J. Mol. Struct. Theochem.* **1989**, *186*, 117.

(29) Mezey, P.; Kapur, A. *Can. J. Chem.* **1980**, *58*, 559.

(30) Mezey, P.; Hass, E. C. *J. Chem Phys.* **1982**, *77*, 870.

(31) Mezey, P.; Hass, E. C. *J. Comput. Chem.* **1983**, *4*, 482.

(32) Hassanzadeh, P.; Andrews, L. *J. Am. Chem. Soc.* **1992**, *114*, 83.

(33) Ongstad, A. P.; Lawconnell, R. I.; Henshaw, T. L. *J. Chem. Phys.* **1992**, *97*, 1053.

(34) Collins, C. L.; Yamaguchi, Y.; Schaefer, H. F. III. *J. Chem. Phys.* **1993**, *98*, 4777.

(35) Herler, S.; Mayer, P.; Nth, H.; Schulz, A.; Suter, M.; Vogt, M. *Angew. Chem., Int. Ed.* **2001**, *40*, 3173.

(36) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.

(37) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

(38) Moller, C.; Plesset, M. S. *Phys. Rev.* **1934**, *46*, 618.

(39) Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley & Sons: New York, 1986.

(40) Melissas, V. S.; Truhlar, D. G.; Garrett, B. C. *J. Chem. Phys.* **1992**, *96*, 5758.

(41) Truhlar, D. G.; Garrett, B. C. *Acc. Chem. Res.* **1980**, *13*, 440.

(42) Fukui, K. *Acc. Chem. Res.* **1981**, *14*, 363.

(43) Gonzalez, C.; Schlegel, H. B. *J. Chem. Phys.* **1989**, *90*, 2154.

(44) Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.* **1990**, *94*, 5523.

(45) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A., Jr.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B. G.; Chen, W.; Wong, M. W.; Andres, J. L.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. *Gaussian 98*, revision A.5; Gaussian, Inc.: Pittsburgh, PA, 1998.