

# Strong hydrogen bonding between neutral noble-gas molecules (HNgF, Ng = Ar, Kr, and Xe) and hydrogen fluoride: a theoretical study

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## Abstract

High-level electronic structure calculation has been performed on the hydrogen-bond complexes of the neutral noble-gas molecules, HArF, HKrF, and HXeF with hydrogen fluoride. Hydrogen bonding from either the hydrogen or the fluorine sides was considered. Very strongly bonding strengths (13–18 kcal/mol) were predicted for the fluorine-side complexes while those of the hydrogen-side complexes were found to be normal for polar neutral molecules. Large increases (409 and 364  $\text{cm}^{-1}$ ) of the H–Ar and H–Kr stretching frequencies were predicted for HArF $\cdots$ HF and HKrF $\cdots$ HF complexes. The complexation was found to decrease the dissociation barriers of HNgF along the bending coordinates by approximately 20 kcal/mol.

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## 1. Introduction

Since the discovery of the first noble-gas compound by Barlett in 1962, the chemistry and reactivity of noble gas have fascinated chemists [1–4]. In the last decade, the preparation of various neutral noble-gas molecules HNgY (Ng, noble gas atom; Y, electronegative atom or group) in solid noble-gas matrix has opened a fascinating new chapter in the study of noble-gas chemistry [5–7]. In particular, the recent discovery of HArF [8,9], HKrF [10], solvated HXeOH [11], noble-gas inserted hydrocarbons [12–14], and various noble-gas coordinated metal complexes [15–18] has attracted considerable new attentions to this field [19].

These interesting HNgY molecules can be viewed as containing Ng–Y ionic bonds and covalent H–Ng bonds. It has been shown that these molecules are very polar with large dipole moments (e.g.,  $\sim 7$  D for HArF) [8,20,21]. Thus these molecules are expected to form dipole or hydrogen-bond complexes with small molecules. Recently, complexation of HArF, HKrF, and

HKrCl with N<sub>2</sub>, P<sub>2</sub>, and CO, have been theoretically predicted or experimentally studied [22–26]. Significant blue-shifts of the H–Ng stretching frequencies were observed in most cases while for HArF $\cdots$ P<sub>2</sub> a large red-shift was predicted [25].

In the current research, we studied the hydrogen bonding capability of the series of molecules: HArF, HKrF and HXeF to hydrogen fluoride with quantum mechanical calculation. Hydrogen bonding through both the hydrogen and fluorine sides of the noble-gas molecules is considered. We also studied the effects of hydrogen bonding to the dissociation energy barriers of these complexes. We noticed that very recently the complexation of HF with HArF through the F side [27] and with HKrCl through the H side has also been studied theoretically by McDowell [28]. Comparison will be made to those studies.

## 2. Method

The geometry and harmonic vibrational frequencies of HNgF (Ng = Ar, Kr, and Xe) molecules, hydrogen fluoride, and the corresponding hydrogen bonding

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complexes have been calculated using MP2 theory with 6-311+G(2df,2pd) and aug-cc-pVTZ basis sets, and QCISD theory with 6-311+G(2df,2pd) basis sets. Single-point energy calculation at QCISD(T)/aug-cc-pVTZ level on QCISD/6-311+G(2df,2pd) geometry was carried out to better estimate the hydrogen bonding strengths. Since the basis sets for Xe are not available in either 6-311+G(2df,2pd) or aug-cc-pVTZ sets and the relativistic effects might be important [29], we used the valence triple-zeta basis sets B2 we developed in an earlier work [30] for Xe together with 6-311+G(2df,2pd) set, and the Stuttgart/Dresden (SDD) basis set with relativistic effective core potential for Xe [31] together with aug-cc-pVTZ basis set in calculation. Counterpoise (CP) calculation was performed to estimate the basis set superposition errors (BSSE) in the hydrogen-bonding energies. We also calculated the transition states of the dissociation channels to Ng atom and HF for both the monomers and the complexes at MP2/aug-cc-pVTZ level. Energy barriers were then estimated by QCISD(T)/aug-cc-pVTZ single-point calculation. The electronic structure calculations were performed using the GAUSSIAN 98 program [32].

### 3. Results and discussion

Fig. 1 shows the general structure for the fluorine- and the hydrogen-side complexes. Table 1 lists the calculated geometry parameters of HNgF, HF, and the fluorine-side complexes and Table 2 lists those for the hydrogen-side complexes. All the calculated structures

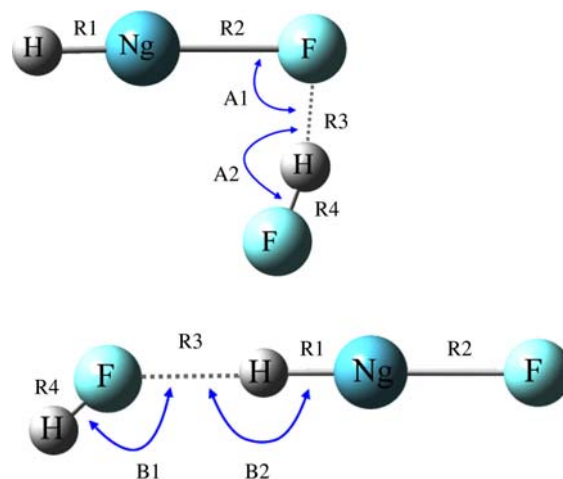


Fig. 1. The general structures of the fluorine-side (HNgF...HF) and the hydrogen-side (HF...HNgF) complexes.

are planar, and all the H–Ng–F bond angles are very close to 180° (within 1°). Table 3 shows the calculated atomic charges and dipole moments. The calculated vibrational frequencies are listed in Table 4. The changes in bond lengths, vibrational frequencies, and energies upon complexation between HNgF and HF calculated at the highest theoretical levels are summarized in Table 5 for easier comparison.

#### 3.1. HArF...HF

As shown in Table 1, the calculated hydrogen-bond strength for HArF...HF is 17–18 kcal/mol and the hy-

Table 1  
Calculated geometry parameters<sup>a</sup> and hydrogen-bond strengths (in kcal/mol) of HNgF...HF

	HNgF		HNgF...HF						$E_{\text{H-bond}}^b$
	H–Ng	Ng–F	R1	R2	R3	R4	A1	A2	
Ng=Ar									
MP2/6-311+G(2df,2pd)	1.322	1.973	1.282	2.110	1.392	0.984	87.0	163.4	–17.3
MP2/aug-cc-pVTZ	1.320	1.981	1.283	2.118	1.400	0.988	86.1	163.6	–18.4
QCISD/6-311+G(2df,2pd)	1.324	1.999	1.284	2.123	1.403	0.974	87.4	163.4	–17.2
QCISD(T)/aug-cc-pVTZ									–17.9
Ng=Kr									
MP2/6-311+G(2df,2pd)	1.467	2.038	1.436	2.148	1.446	0.967	92.8	163.9	–14.9
MP2/aug-cc-pVTZ	1.462	2.034	1.446	2.163	1.475	0.974	92.0	163.5	–15.6
QCISD/6-311+G(2df,2pd)	1.469	2.053	1.439	2.160	1.454	0.960	93.3	163.9	–15.0
QCISD(T)/aug-cc-pVTZ									–15.5
Ng=Xe									
MP2/6-311+G(2df,2pd)	1.655	2.103	1.632	2.187	1.508	0.953	102.6	165.3	–12.3
MP2/aug-cc-pVTZ	1.656	2.130	1.631	2.218	1.496	0.961	98.7	165.1	–13.8
QCISD/6-311+G(2df,2pd)	1.659	2.101	1.638	2.186	1.521	0.946	105.2	166.0	–12.2
QCISD(T)/aug-cc-pVTZ									–12.7

<sup>a</sup> Bond lengths (Å) and the bond angles (°).

<sup>a</sup> The calculated H–F distance in HF are 0.918, 0.922, and 0.915 Å at MP2/6-311+G(2df,2pd), MP2/aug-cc-pVTZ, and QCISD/6-311+G(2df,2pd) levels, respectively.

<sup>b</sup> Relative Born–Oppenheimer energies ( $E_{\text{complex}} - E_{\text{HF}} - E_{\text{HNgF}}$ ).

Table 2  
Calculated geometry parameters and hydrogen-bond strengths (in kcal/mol) of HF...HNgF

	R1	R2	R3	R4	B1	B2	E <sub>H-bond</sub>
Ng=Ar							
MP2/6-311+G(2df,2pd)	1.305	2.027	1.847	0.922	133.0	179.2	-4.4
MP2/aug-cc-pVTZ	1.307	2.042	1.798	0.927	128.6	178.9	-5.0
QCISD/6-311+G(2df,2pd)	1.306	2.041	1.902	0.919	137.8	178.1	-4.3
QCISD(T)/aug-cc-pVTZ							-4.5
Ng=Kr							
MP2/6-311+G(2df,2pd)	1.456	2.066	2.095	0.920	152.5	179.3	-2.9
MP2/aug-cc-pVTZ	1.451	2.064	2.060	0.925	143.2	178.8	-3.1
QCISD/6-311+G(2df,2pd)	1.459	2.078	2.131	0.917	154.4	173.4	-2.9
QCISD(T)/aug-cc-pVTZ							-3.0
Ng=Xe							
MP2/6-311+G(2df,2pd)	1.649	2.115	2.743	0.919	175.9	100.6	-1.8
MP2/aug-cc-pVTZ	1.650	2.143	2.616	0.923	174.0	106.4	-2.1
QCISD/6-311+G(2df,2pd)	1.655	2.114	2.828	0.916	179.6	97.5	-1.8
QCISD(T)/aug-cc-pVTZ							-1.9

Bond lengths (Å) and the bond angles (°).

Table 3  
ChelpG charges and dipole moments calculated at QCISD/6-311+G(2df,2pd) level

Monomer	H	Ng	F	μ (D)		
HArF	0.17	0.46	-0.63	7.14		
HKrF	0.08	0.49	-0.57	6.27		
HXeF	-0.04	0.54	-0.50	4.98		
H-Ng-F...H-F						
Ng	H	Ng	F	H	F	μ (D)
Ar	0.28	0.45	-0.61	0.43	-0.54	8.97
Kr	0.17	0.49	-0.56	0.41	-0.52	8.24
Xe	0.05	0.53	-0.49	0.40	-0.49	7.35
H-F...H-Ng-F						
	H	F	H	Ng	F	μ (D)
Ar	0.46	-0.42	0.18	0.49	-0.71	10.28
Kr	0.46	-0.45	0.09	0.51	-0.62	9.09
Xe	0.44	-0.45	0.02	0.49	-0.51	5.68

drogen-bond length (R3) is approximately 1.40 Å, consistent with a very strong hydrogen bond. Due to the hydrogen bonding, the Ar-F (R2) and H-F (R4) distances increase by 0.12–0.14 and 0.06–0.07 Å, respectively, as compared to those in free molecules. Interestingly, the Ar-H (R1) distance *decreases* by 0.04 Å. Similar shortening of the H-Ng bonds have also been recently predicted in the complexes of HXeOH, HArF, HKrF, and HKrCl with small molecules [11,23–28]. The calculated hydrogen bonding energies and geometry parameters for HArF...HF here are similar to those obtained by McDowell using MP2 and QCISD theory with 6-311++G(2d,2p) basis set [27]. The only significant difference is the F...H distance where our values using a slightly larger basis set are ~0.03–0.04 Å smaller. The use of higher correlation methods (QCISD,

QCISD(T)) makes very small differences to the MP2 results in the calculated hydrogen-bond strength (<1 kcal/mol). In the remainder of this paper, unless stated otherwise, we will focus on our highest level results for geometry (QCISD/6-311+G(2df,2pd)) and energies (QCISD(T)/aug-cc-pVTZ//QCISD/6-311+G(2df,2pd)) with BSSE correction for all complexes.

### 3.2. HKrF...HF

As seen in Tables 1 and 5, when Ar is replaced by Kr, the hydrogen bonding strength (15.5 kcal/mol) is lowered by 2.4 kcal/mol, and the hydrogen-bond distance (~1.45 Å) is ~0.05 Å longer. The H-Kr distance in the complex is *shorter* than that in free HKrF by 0.03 Å,

Table 4  
Calculated vibrational frequencies (in  $\text{cm}^{-1}$ ) at QCISD/6-311+G(2df,2pd) level

	HF	HNgF	HNgF...HF	HF...HNgF
Ng = Ar				
$\nu_{\text{H-F}}$	4208		2975	4153
$\nu_{\text{H-Ar}}$		2201	2610	2443
$\nu_{\text{H-Ar-F}}$		723	602	736
		723	606	747
$\nu_{\text{Ar-F}}$		465	330	431
Others			1187, 1087	233, 108
			434, 100	52, 44
Ng = Kr				
$\nu_{\text{H-F}}$	4208		3246	4180
$\nu_{\text{H-Kr}}$		2034	2398	2295
$\nu_{\text{H-Kr-F}}$		696	616	714
		696	616	714
$\nu_{\text{Kr-F}}$		438	395	415
Others			1097, 1003	112, 76
			319, 72	32, 27
Ng = Xe				
$\nu_{\text{H-F}}$	4208		3540	4195
$\nu_{\text{H-Xe}}$		1971	2148	2069
$\nu_{\text{H-Xe-F}}$		640	602	647
		640	605	651
$\nu_{\text{Xe-F}}$		447	384	435
Others			965, 910	121, 95
			308, 38	66, 18

and the lengthening in the Kr–F distance (0.11 Å) is similar to that in the Ar complex.

### 3.3. HXeF...HF

The calculated hydrogen bonding strength of HXeF...HF complex is 12.7 kcal/mol, which is 2.8 kcal/mol lower than that of the Kr complex. Nevertheless, it is still a strong hydrogen bond with a bonding distance of  $\sim 1.52$  Å. Interestingly, while the H–Ng distances are sensitive to the identities of the noble gas, the Ng–F distance showed relatively small variations ( $< 0.1$  Å) with different Ng in both the monomers and in the complexes. This is consistent with an earlier study that from HNeF to HXeF the H–Ng bond lengths increase

by 0.65 Å while the Ng–F distances increase only 0.19 Å [21].

### 3.4. HF...HArF

As shown in Table 2, the hydrogen-bond strength of HF...HArF is 4.5 kcal/mol,  $\sim 13$  kcal/mol weaker than the fluorine-side complex. The hydrogen-bond length of 1.90 Å is  $\sim 0.5$  Å longer than that in HArF...HF. The Ar–F distance increases by 0.04 Å upon complexation with HF, while the H–F distance increases by only 0.004 Å. Interestingly, in the complex the H–Ar distance is 0.02 Å shorter than in free HArF. This is uncommon since the H–X (where X is any heavy atom) bonding in the hydrogen bond donor is usually weakened due to loss of electron density.

### 3.5. HF...HKrF

The calculated hydrogen-bond strength of HF...HKrF is 3.0 kcal/mol,  $\sim 1.5$  kcal/mol weaker than that of HF...HArF. The hydrogen-bond length is  $\sim 0.23$  Å longer than in the HF...HArF. The H–Kr distances decrease by  $\sim 0.01$  Å and the Kr–F distance increases by  $\sim 0.03$  Å upon complexation. These results can be compared to a recent theoretical study of HF...HKrCl complex by McDowell [28], in which the interaction energy was found to be 3.7 kcal/mol, and the hydrogen-bond length was 1.99 Å. The H–Kr distance was predicted to decrease by  $\sim 0.03$  Å and the Kr–Cl distance increases by  $\sim 0.05$  Å upon complexation.

### 3.6. HF...HXeF

The hydrogen-bond strength of HF...HXeF complex is calculated to be only 1.9 kcal/mol with a long hydrogen-bond length of 2.83 Å. The structure of this complex is significantly different from the other two hydrogen-side complexes. In particular, the F...H–Xe angle (B2) is only  $98^\circ$  while in HF...HArF and HF...HKrF the angles are very close to  $180^\circ$ . On the other hand, the H–F...H angle (B1) is now very close to  $180^\circ$ .

Table 5  
Changes<sup>a</sup> in bond lengths (Å), vibrational frequencies ( $\text{cm}^{-1}$ ), and energies (kcal/mol) upon complexation

Ng	$\Delta R(\text{H-Ng})$	$\Delta R(\text{Ng-F})$	$\Delta R(\text{H-F})$	$R(\text{F}\cdots\text{H})$	$\Delta \nu_{\text{H-Ng}}$	$\Delta \nu_{\text{Ng-F}}$	$\Delta \nu_{\text{H-F}}$	$E_{\text{H-bond}}$
H–Ng–F...H–F								
Ar	–0.040	0.124	0.059	1.403	409	–135	–1233	–17.9
Kr	–0.030	0.107	0.045	1.454	364	–43	–962	–15.5
Xe	–0.021	0.085	0.031	1.521	213	–63	–668	–12.7
H–F...H–Ng–F								
Ar	–0.019	0.042	0.004	1.902	242	–34	–55	–4.5
Kr	–0.010	0.025	0.002	2.131	261	–23	–28	–3.0
Xe	–0.004	0.013	0.001	2.828	98	–12	–13	–1.9

<sup>a</sup>  $\Delta R = R(\text{complex}) - R(\text{free molecule})$ ,  $\Delta \nu = \nu(\text{complex}) - \nu(\text{free molecule})$ .

### 3.7. Charge distribution

As seen in Table 3, the charge separations in HNgF are localized on the Ng–F bonds, and the hydrogen atoms possess only negligible atomic charges. It is also clearly seen that the hydrogen-bond strengths correlate strongly with the charge separations and the dipole moments of the monomers. Table 3 also shows that the hydrogen atoms in HNgF gain more positive charges in the fluorine-side complexes while the fluorine atoms in HNgF gain more negative charges in the hydrogen-side complexes. Perhaps part of the strengthening of the H–Ng bonds is due to the somewhat stronger ionic interactions between the (HNg)<sup>+</sup> and F<sup>−</sup> in HNgF. This view has also been proposed in recent study of several HNgY complexes [11,23–28].

### 3.8. Vibrational frequencies

As shown in Tables 4 and 5, the H–F stretching frequency decreases from 4208 cm<sup>−1</sup> in free HF to 2975 cm<sup>−1</sup> in HArF···H–F, consistent with a very strong hydrogen bonding. The calculated H–Ar stretching frequency of HArF···HF showed an amazingly increase of 409 cm<sup>−1</sup> as compared to that in the HArF monomer. This is consistent with the value (442 cm<sup>−1</sup>) obtained by McDowell [27]. The H–Ng stretching frequency of H–KrF···HF and H–XeF···HF also showed noticeable increase of 364 and 213 cm<sup>−1</sup>, respectively. These frequency shifts correlate with the shortening of the H–Ng bonds upon complexation. The calculated H–Ar stretching frequency in the hydrogen-side complex HF···HArF also showed a large increase of 242 cm<sup>−1</sup>. Significant increases in the H–Ng stretching frequencies were also predicted for the other two hydrogen-side complexes. In a recent study [11], blue-shifts of ~100 and ~160 cm<sup>−1</sup> have been experimentally observed for the H–Xe stretching frequencies for HXeOH–(H<sub>2</sub>O) and HXeOH–(H<sub>2</sub>O)<sub>2</sub>, respectively. These are compared to the blue-shifts of 213 and 98 cm<sup>−1</sup> predicted for HXeF···HF and HF···HXeF, respectively, in the current study. In another study on the complexes of HArF, HKrF, and HKrCl with N<sub>2</sub> [23], blue-shifts of 20–110 cm<sup>−1</sup> have also been observed experimentally. In the

study by McDowell [28] on the HF···HKrCl, a blue-shift of 262 cm<sup>−1</sup> was predicted. This is compared to our predicted blue-shifts of 261 and 364 cm<sup>−1</sup> for the HF···HKrF and HKrF···HF, respectively.

### 3.9. Dissociation barriers

In the gas phase, the thermal stability of HNgF molecules depends on their dissociation rates. The two main dissociation pathways are (1) to the constituent atoms, H + Ng + F, and (2) to the global minimum, HF + Ng. The energy barriers for these two pathways have been estimated to be approximately 24 and 13 kcal/mol for HArF and 32 and 26 kcal/mol for HKrF [33]. Due to the strong interaction between HF and HNgF in the complexes, the first pathway will be inhibited by large endoergicities. For example, the calculated energy of reactions for HNgF···HF → H + Ng + F + HF are 25, 44, and 67 kcal/mol for Ng = Ar, Kr, and Xe, respectively. The dissociation through second pathway, however, is expected to be enhanced due to the stabilization of the transition state by the HF molecule. The calculated dissociation transition states (TS) geometry and the barrier heights through the second (or ‘bending’) pathway for the HNgF monomers and the complexes are shown in Table 6, and a general structure of the TS is depicted in Fig. 2. (All the TS calculation on the hydrogen-side complexes converged to the TS of the corresponding fluorine-side complexes.) The calculated barriers for the HArF and HKrF monomers are almost

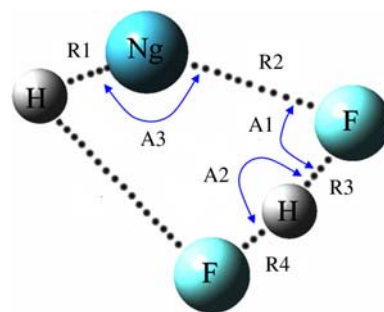


Fig. 2. The general structure of the dissociation transition state through the bending coordinate.

Table 6  
Calculated transition state geometry and barrier heights<sup>a</sup> (in kcal/mol) at MP2/aug-cc-pVTZ level

	HNgF				HNgF···HF							
	R1	R2	A3	$\Delta V^\ddagger$	R1	R2	R3	R4	A1	A2	A3	$\Delta V^\ddagger$
Ar	1.257	2.263	106.7	23.0 (24.0)	1.264	2.374	1.192	1.103	73.5	165.3	138.5	4.4 (5.2)
Kr	1.401	2.329	102.1	31.4 (32.4)	1.398	2.521	1.160	1.129	73.0	166.0	128.4	11.4 (12.3)
Xe	1.579	2.399	100.3	37.6 (38.5)	1.583	2.725	1.121	1.167	71.9	166.4	121.6	18.9 (19.7)

Bond lengths (Å) and the bond angles (°).

Numbers in parentheses are QCISD(T)/aug-cc-pVTZ values.

<sup>a</sup> Born–Oppenheimer energies.

identical to those obtained by Chaban et al. [33]. In the TS structures of the complexes, the Ng–F bonds (R2) are significantly longer (by 0.1–0.3 Å) and the H–Ng–F angles (A3) are significantly larger (by 20°–30°) than those in the TS of the monomers. The F···H distances (R3) in the TS are significantly shorter (by 0.2–0.4 Å) than those in the complexes, indicating the formation of HF dimers in the products. Compared to the monomers, the barriers of the complexes are ~20 kcal/mol lower. Similar lowering of the barrier heights (by 13–39 kcal/mol) has also been predicted in a recent study of the HXeOH–(H<sub>2</sub>O)<sub>1–3</sub> complexes [11]. The small barrier of 5.2 kcal/mol for HArF···HF (or 3.4 kcal/mol including ZPE) indicates that this complex might not be thermally stable. However, the dissociation barriers for HKrF···HF and HXeF···HF (12.3 and 19.7 kcal/mol) are still quite high, and thus these two complexes might be stable enough to be observed in the future experiments. It is noted that in the matrix environment, secondary reactions with reactive radicals [9] can also affect the stability of the monomers and complexes.

#### 4. Summary

We have studied the hydrogen-bond complexes of HNgF (Ng = Ar, Kr, and Xe) with hydrogen fluoride by correlating electronic structure methods with extended basis sets. The fluorine-side complexes (HNgF···HF) show very strong hydrogen bonding strengths for neutral molecules, while the bonding strengths for the hydrogen-side complexes (HF···HNgF) are normal. The H–Ng bonds in both HNgF···HF and HF···HNgF complexes are significantly stronger, and this in turn causes significant increases in the H–Ng stretching frequencies. The dissociation barriers of the complexes through the bending coordinates are predicted to be significantly lower than those of the monomers. The results also indicated that HKrF···HF and HXeF···HF might still be thermally stable. It would be interesting to see if these hydrogen-bond complexes with large blue-shifts can be experimentally identified.

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#### References

- [1] N. Bartlett, Proc. Chem. Soc. (1962) 218.
- [2] R.N. Perutz, J.J. Turner, J. Am. Chem. Soc. 97 (1975) 4791.
- [3] J.H. Holloway, G.J. Schrobilgen, Inorg. Chem. 20 (1981) 3363.
- [4] P. Laszlo, G.J. Schrobilgen, Angew. Chem. Int. Ed. Engl. 27 (1988) 479.
- [5] M. Pettersson, J. Lundell, M. Räsänen, J. Chem. Phys. 102 (1995) 6423.
- [6] M. Pettersson, J. Lundell, M. Räsänen, J. Chem. Phys. 103 (1995) 205.
- [7] M. Pettersson, J. Lundell, L. Khriachtchev, M. Räsänen, J. Chem. Phys. 103 (1995) 205.
- [8] L. Khriachtchev, M. Pettersson, N. Runeberg, J. Lundell, M. Räsänen, Nature 406 (2000) 874.
- [9] L. Khriachtchev, M. Pettersson, A. Lignell, M. Räsänen, J. Am. Chem. Soc. 123 (2001) 8610.
- [10] M. Pettersson, L. Khriachtchev, A. Lignell, M. Räsänen, J. Chem. Phys. 116 (2002) 2508.
- [11] A.V. Nemukhin, B.L. Grigorenko, L. Khriachtchev, H. Tanskanen, M. Pettersson, M. Räsänen, J. Am. Chem. Soc. 124 (2002) 10706.
- [12] L. Khriachtchev, H. Tanskanen, J. Lundell, M. Pettersson, H. Kiljunen, M. Räsänen, J. Am. Chem. Soc. 125 (2003) 4696.
- [13] V.I. Feldman, F.F. Sukhov, A.Y. Orlov, I.V. Tyulpina, J. Am. Chem. Soc. 125 (2003) 4698.
- [14] L. Khriachtchev, H. Tanskanen, A. Cohen, R.B. Gerber, J. Lundell, M. Pettersson, H. Kiljunen, M. Räsänen, J. Am. Chem. Soc. 125 (2003) 6876.
- [15] S. Seidel, K. Seppelt, Science 290 (2000) 117.
- [16] T. Drews, S. Seidel, K. Seppelt, Angew. Chem. Int. Ed. Engl. 41 (2002) 454.
- [17] J. Li, B.E. Bursten, B. Liang, L. Andrews, Science 295 (2002) 2242.
- [18] L. Andrews, B. Liang, J. Li, B.E. Bursten, J. Am. Chem. Soc. 125 (2003) 3126.
- [19] K.O. Christe, Angew. Chem. Int. Ed. 40 (2001) 1419.
- [20] N. Runeberg, M. Pettersson, L. Khriachtchev, J. Lundell, M. Räsänen, J. Chem. Phys. 114 (2001) 836.
- [21] J. Lundell, G.M. Chaban, R.B. Gerber, Chem. Phys. Lett. 331 (2000) 308.
- [22] A. Lignell, L. Khriachtchev, M. Pettersson, M. Räsänen, J. Chem. Phys. 117 (2002) 961.
- [23] A. Lignell, L. Khriachtchev, M. Pettersson, M. Räsänen, J. Chem. Phys. 118 (2003) 11120.
- [24] S.A.C. McDowell, J. Chem. Phys. 118 (2003) 7283.
- [25] S.A.C. McDowell, Phys. Chem. Chem. Phys. 5 (2003) 808.
- [26] S.A.C. McDowell, Chem. Phys. Lett. 368 (2003) 649.
- [27] S.A.C. McDowell, Chem. Phys. Lett. 377 (2003) 143.
- [28] S.A.C. McDowell, J. Chem. Phys. 119 (2003) 3711.
- [29] D. Schröder, H. Schwarz, J. Hrušák, P. Pyykkö, Inorg. Chem. 37 (1998) 624.
- [30] W.-P. Hu, C.H. Huang, J. Am. Chem. Soc. 123 (2001) 2340.
- [31] A. Nicklass, M. Dolg, H. Stoll, H. Preuss, J. Chem. Phys. 102 (1995) 8942.
- [32] M.J. Frisch et al., GAUSSIAN 98, Rev. A.11.3, Gaussian Inc., Pittsburgh, PA, 2002.
- [33] G.M. Chaban, J. Lundell, R.B. Gerber, Chem. Phys. Lett. 364 (2002) 628.