

**Combining proton and silaborane-based superhalogen anions - an
effective route to new superacid as verified by systematic DFT
calculations**

Lan Luo,^a Fu-Qiang Zhou,^a Ru-Fang Zhao,^a Jin-Feng Li,^{*ab} Lin-Yu Wu,^{ac}

Jian-Li Li and Bing Yin^{*a}

^a MOE Key Laboratory of Synthetic and Natural Functional Molecule Chemistry,
College of Chemistry and Materials Science, Northwest University, Xi'an 710069,
China.

^b College of Chemistry & Chemical Engineering, Shaanxi Key Laboratory of
Chemical Reaction Engineering, Yan'an University, Yan'an 716000, China.

^c College of Chemistry and Chemical Engineering, Northwest Normal University,
Lanzhou 730070, China.

E-mail: rayinyin@nwu.edu.cn (B. Yin) lijinfengxiaofeng@163.com (J.-F. Li)

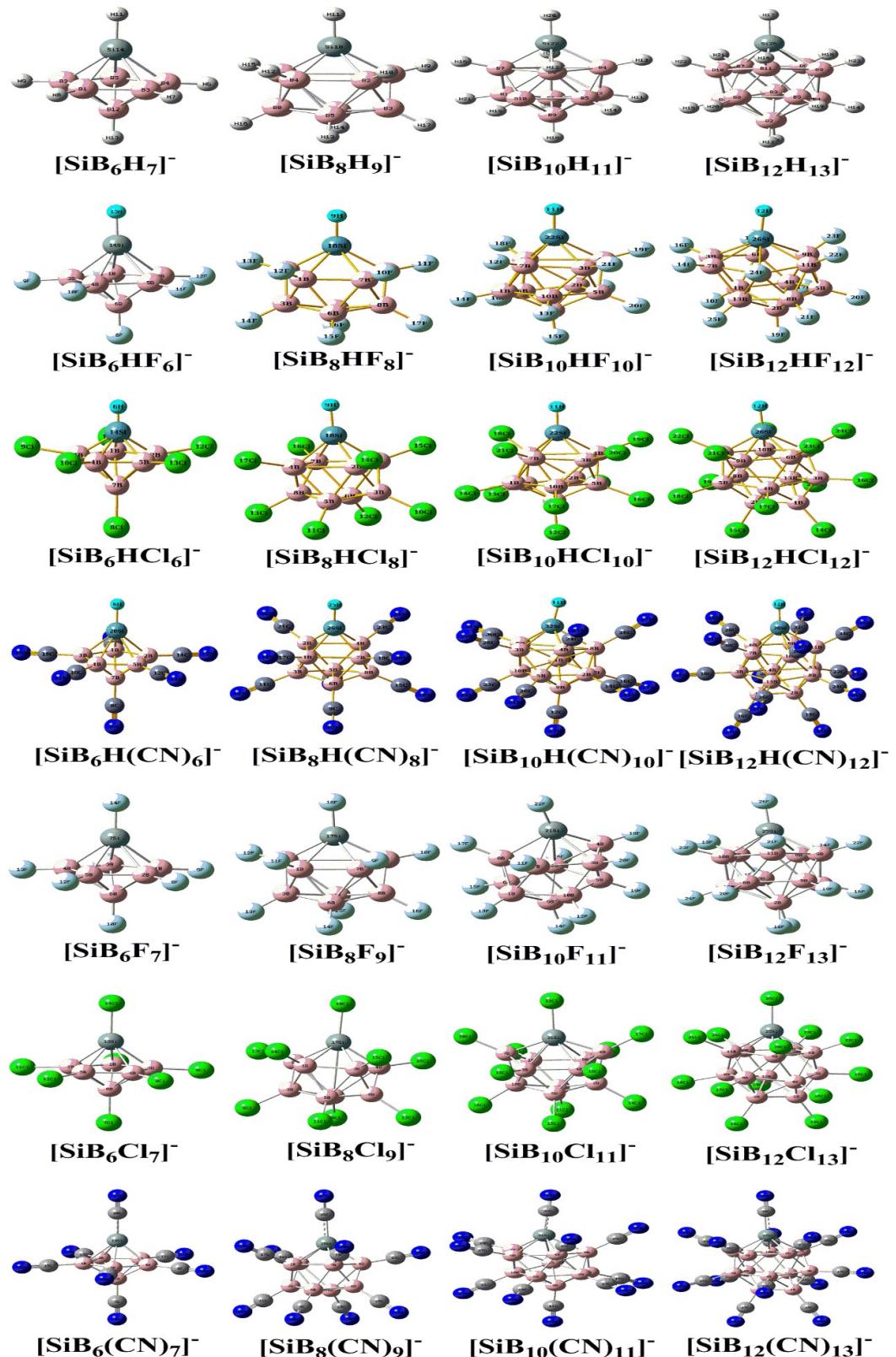


Fig. S1 Equilibrium structures of selected silicon anions and their derivatives $[\text{SiB}_n\text{H}_m\text{X}_{n-m+1}]^-$ ($m=1$ and 0 ; $n=6,8,10,12$; $\text{X}=\text{H}, \text{F}, \text{Cl}, \text{CN}$).

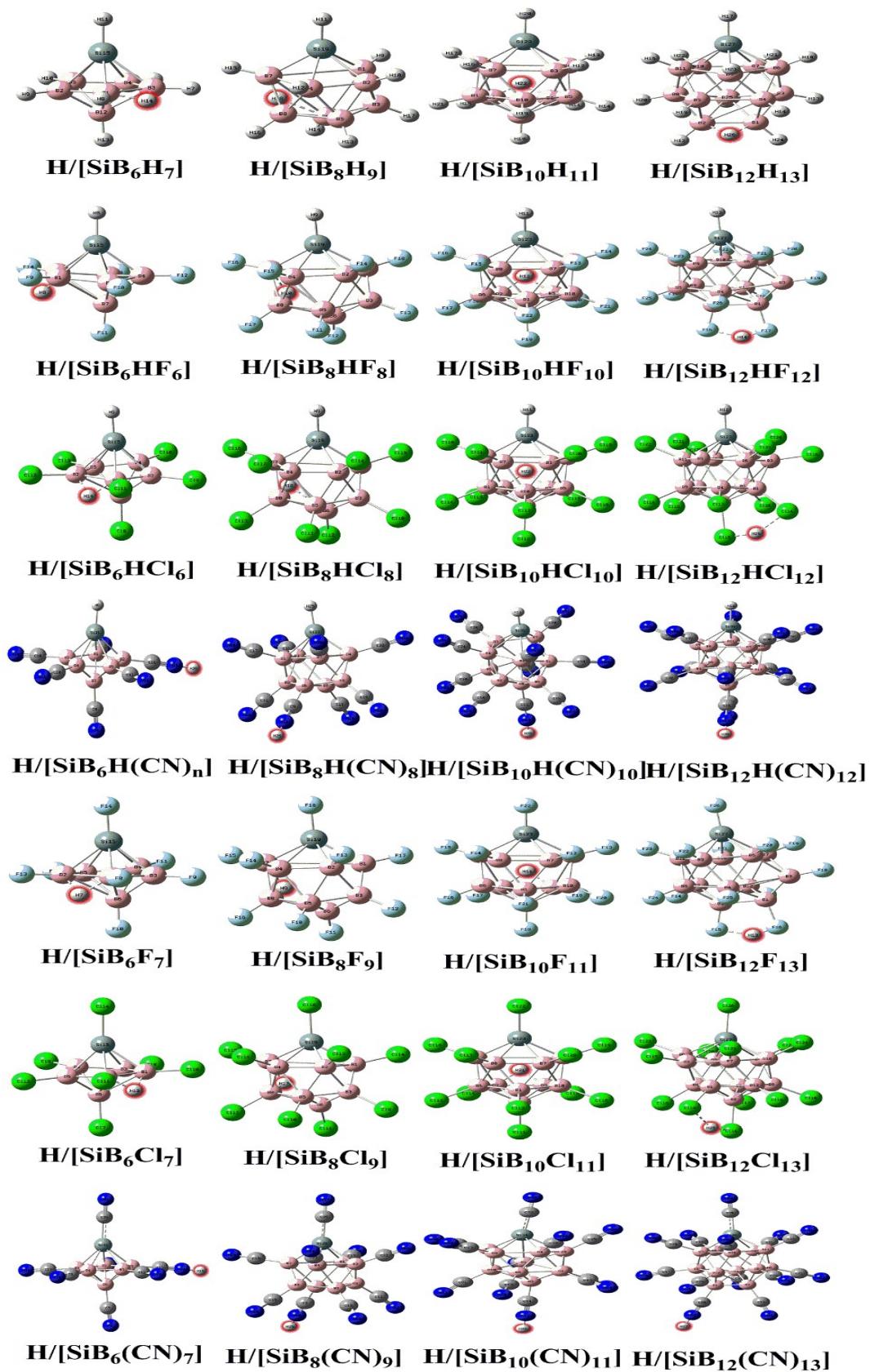


Fig. S2 Equilibrium structures of selected composites of $\text{H}/[\text{SiB}_n\text{H}_m\text{X}_{n-m+1}]$ ($m=1$ and 0 ; $n=6,8,10,12$; $\text{X}=\text{H}, \text{F}, \text{Cl}, \text{CN}$).

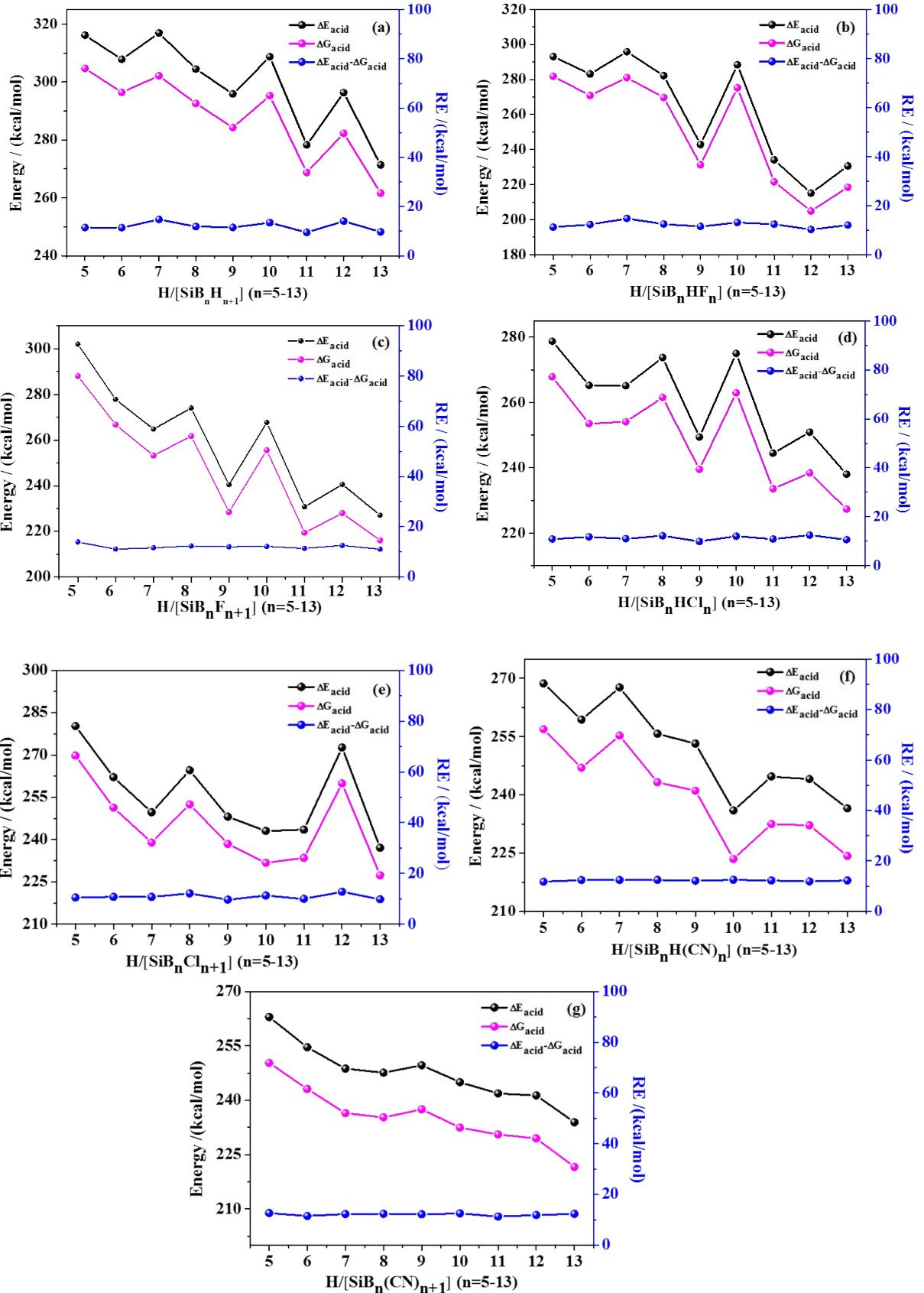


Fig. S3 The comparison between ΔG_{acid} and ΔE_{acid} : (a) H/[SiB_nH_{n+1}] , (b) H/[SiB_nHF_n] , (c) H/[SiB_nHCl_n] , (d) H/[SiB_nH(CN)_n] ,(e) H/[SiB_nF_{n+1}] ,(f) H/[SiB_nCl_{n+1}],(g) H/[SiB_n(CN)_{n+1}] (n = 5 - 13).

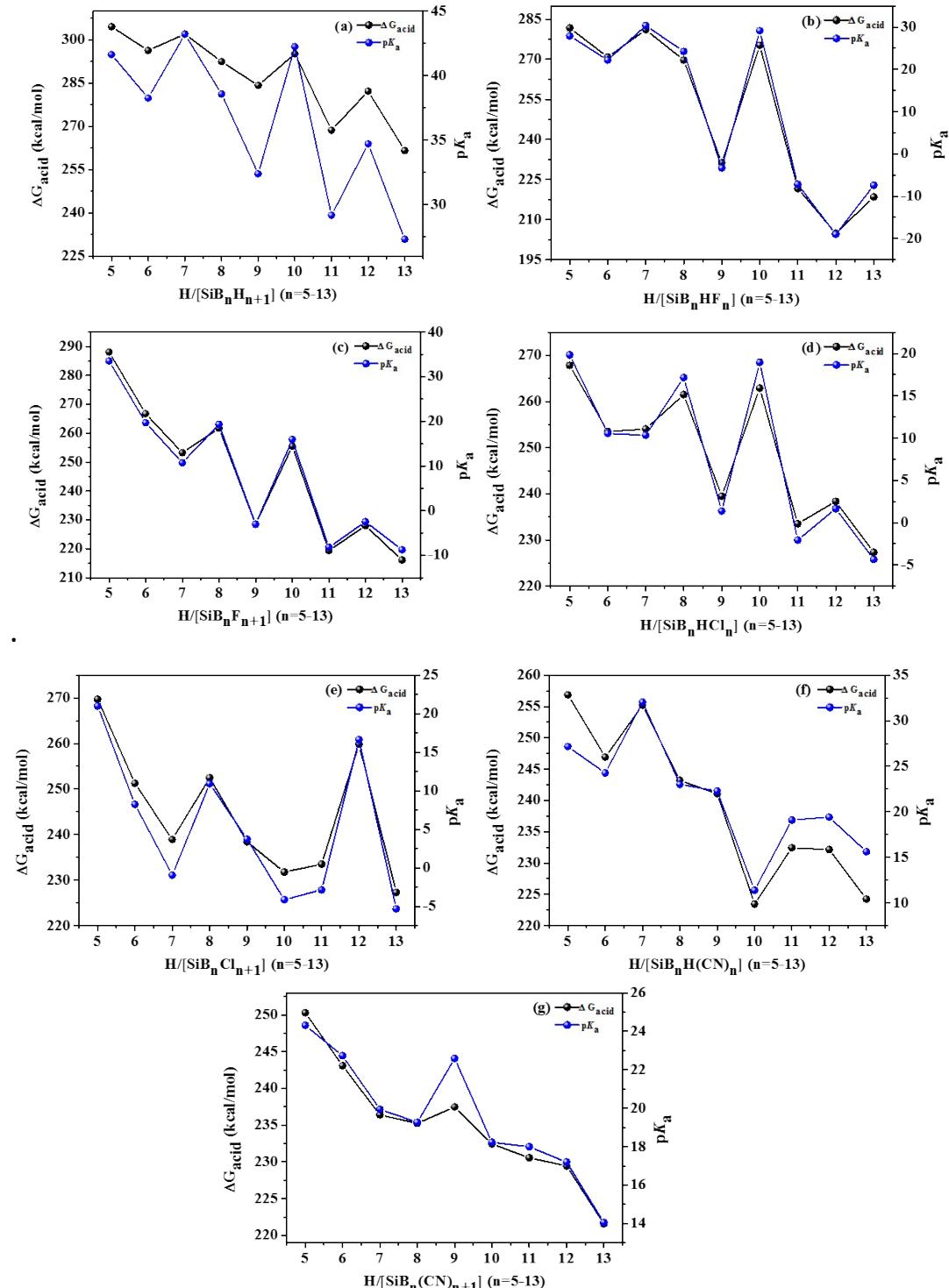


Fig. S4 The comparison between the gas-phase acidity (ΔG_{acid}) and acid dissociation content(pK_a) of the whole composites in DCE (a) H/[SiB_nH_{n+1}] , (b)

H/[SiB_nHF_n],(c)H/[SiB_nF_{n+1}],(d)H/[SiB_nHCl_n],(e)H/[SiB_nCl_{n+1}],(f)H/[SiB_nH(CN)_n],(g) H/[SiB_n(CN)_{n+1}] (n = 5 - 13).

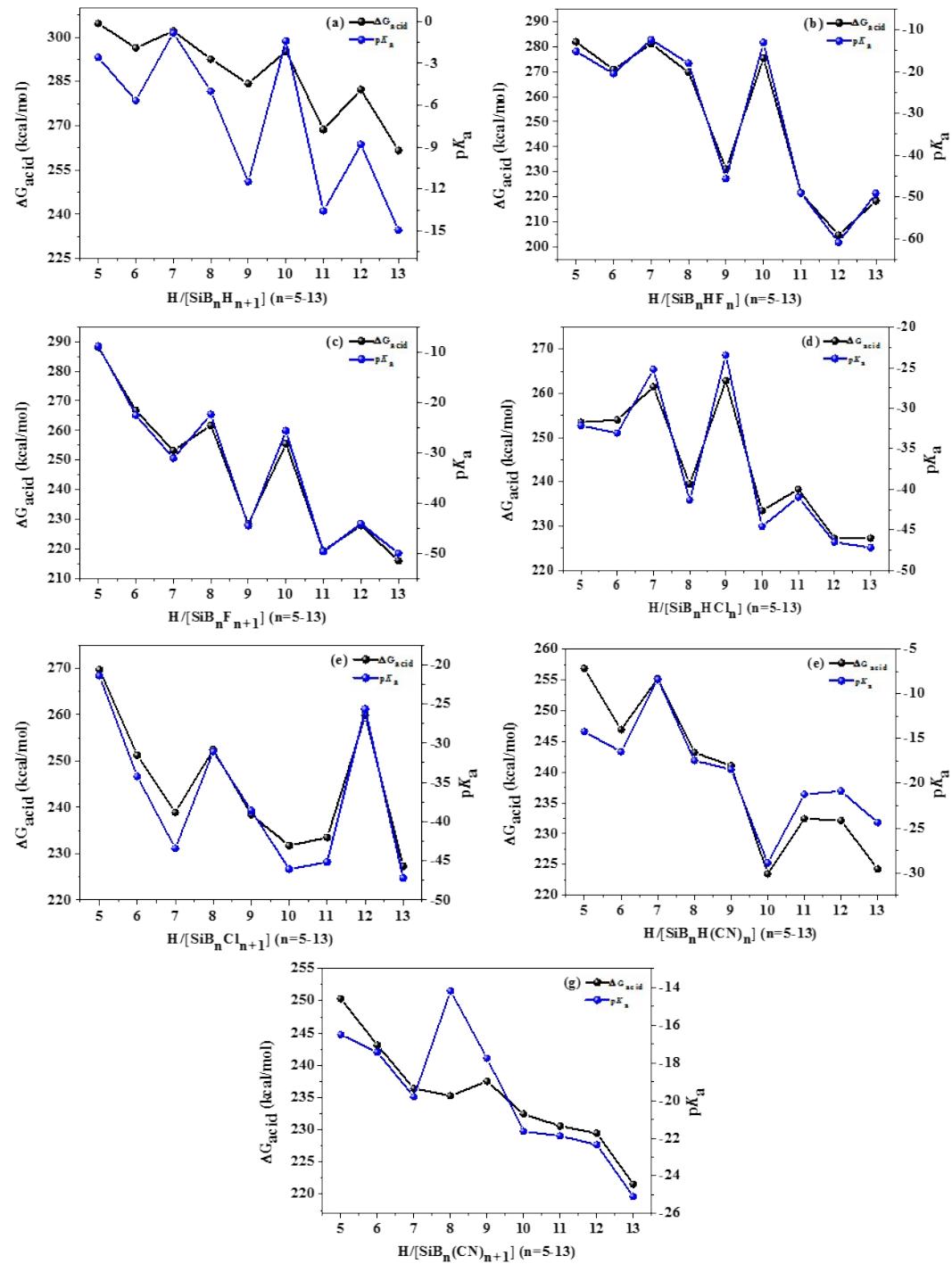


Fig. S5 The comparison between the gas-phase acidity (ΔG_{acid}) and acid dissociation content(pK_a) of the whole composites in H₂O (a) H/[SiB_nH_{n+1}] , (b) H/[SiB_nHF_n],(c)H/[SiB_nF_{n+1}],(d)H/[SiB_nHCl_n],(e)H/[SiB_nCl_{n+1}],(f)H/[SiB_nH(CN)_n],(g) H/[SiB_n(CN)_{n+1}] (n = 5 - 13).

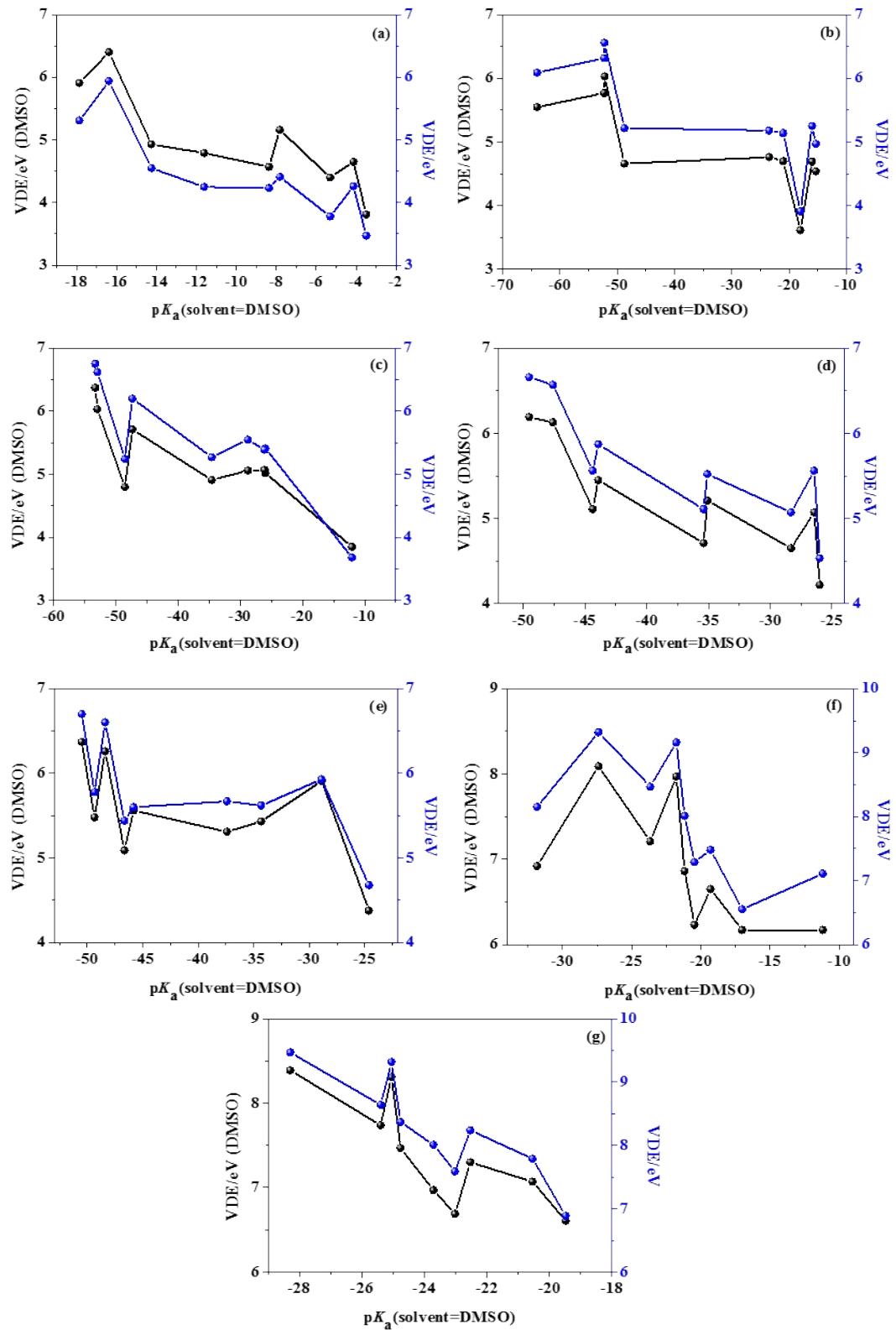


Fig. S6 The relationship between the acidity of the whole composite and the VDE of the superhalogen component: (a) $\text{H}/[\text{SiB}_n\text{H}_{n+1}]$, (b) $\text{H}/[\text{SiB}_n\text{HF}_n]$, (c) $\text{H}/[\text{SiB}_n\text{HCl}_n]$, (d) $\text{H}/[\text{SiB}_n\text{H}(\text{CN})_n]$,(e) $\text{H}/[\text{SiB}_n\text{F}_{n+1}]$,(f) $\text{H}/[\text{SiB}_n\text{Cl}_{n+1}]$,(g) $\text{H}/[\text{SiB}_n(\text{CN})_{n+1}]$ ($n = 5 - 13$).

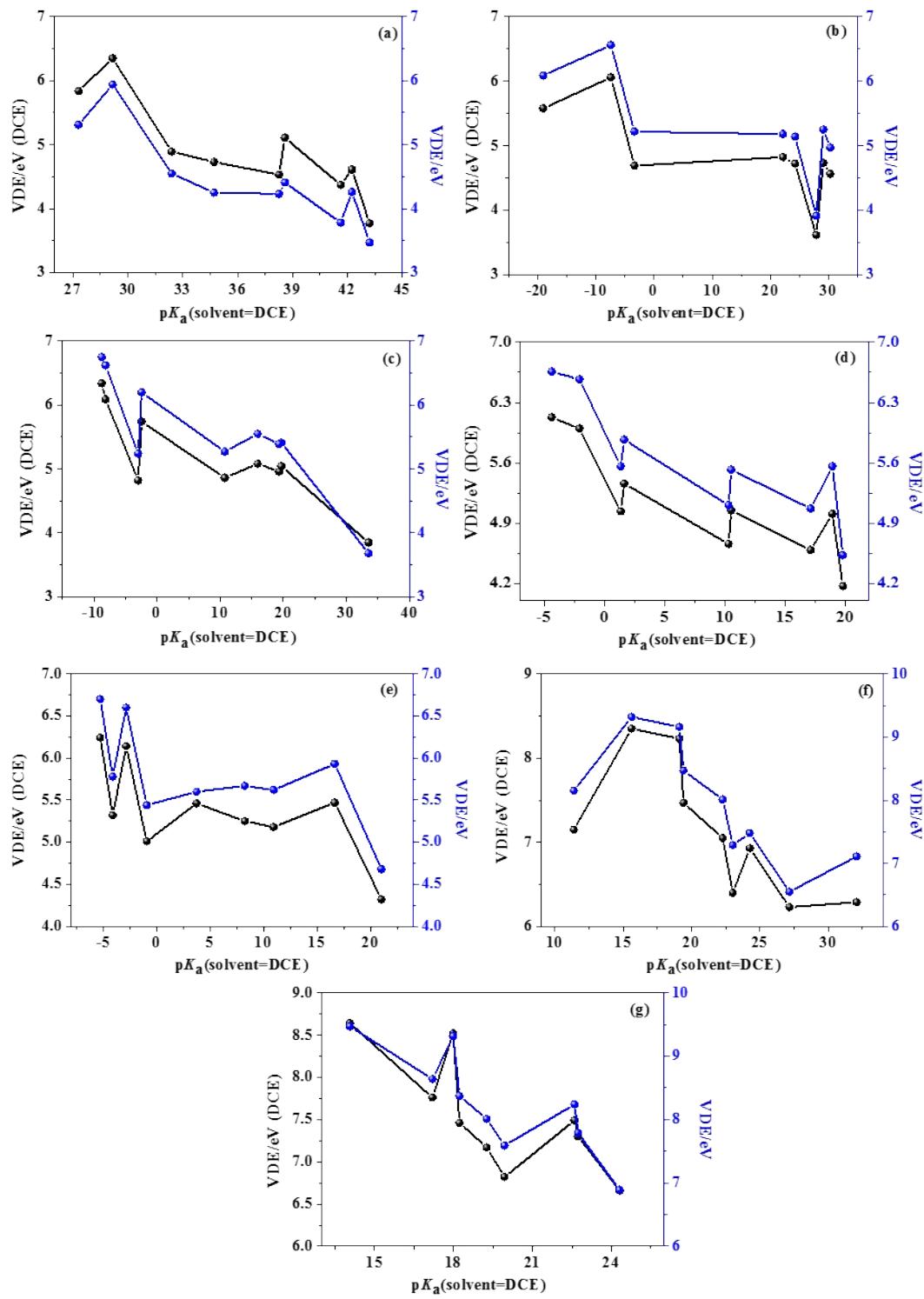


Fig. S7 The relationship between the acidity of the whole composite and the VDE of the superhalogen component: (a) H/[SiB_nH_{n+1}] , (b) H/[SiB_nHF_n] , (c) H/[SiB_nHCl_n] , (d) H/[SiB_nH(CN)_n] ,(e) H/[SiB_nF_{n+1}] ,(f) H/[SiB_nCl_{n+1}],(g) H/[SiB_n(CN)_{n+1}] (n = 5 - 13).

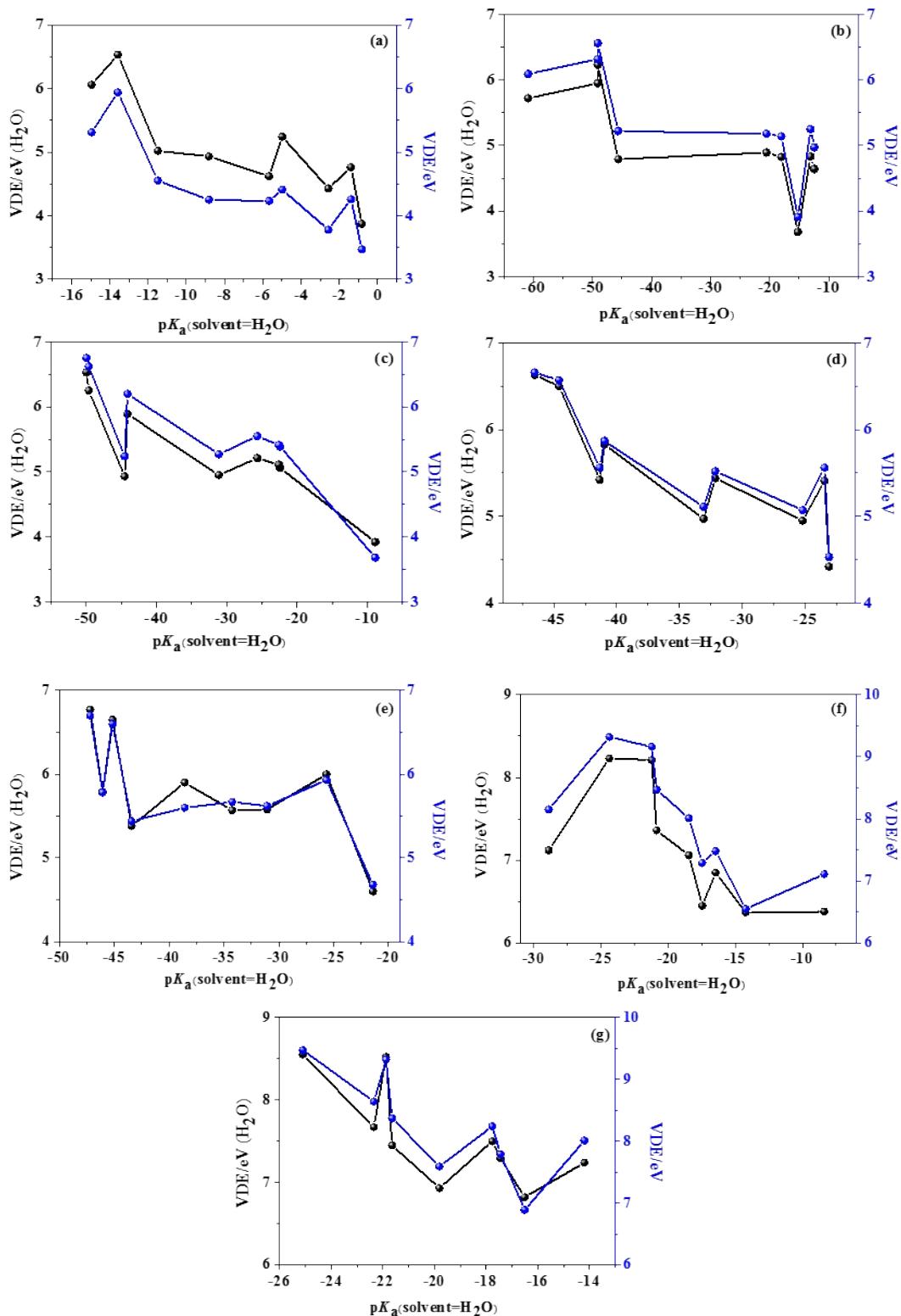


Fig. S8 The relationship between the acidity of the whole composite and the VDE of the superhalogen component: (a) $H/[SiB_nH_{n+1}]$, (b) $H/[SiB_nHF_n]$, (c) $H/[SiB_nHCl_n]$, (d) $H/[SiB_nH(CN)_n]$, (e) $H/[SiB_nF_{n+1}]$, (f) $H/[SiB_nCl_{n+1}]$, (g) $H/[SiB_n(CN)_{n+1}]$ ($n = 5 - 13$).

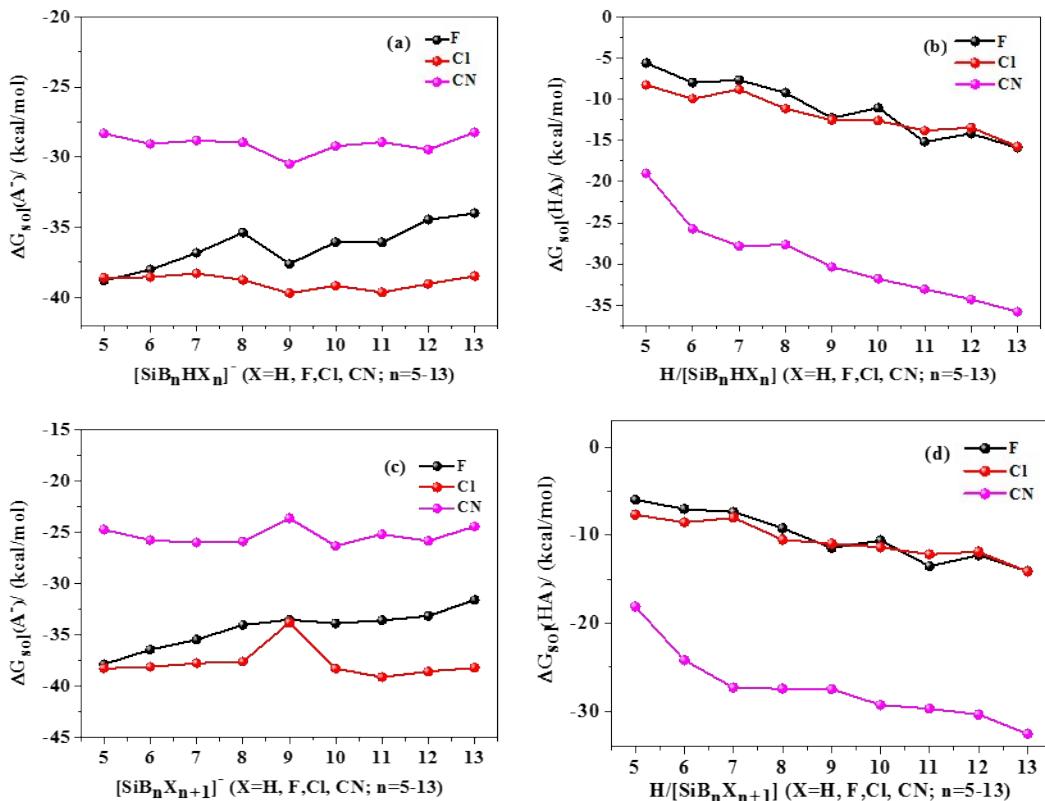


Fig.S9 The solvation free energies of both the conjugate acid (HA) and conjugate base (A^-) in DCE solvent.

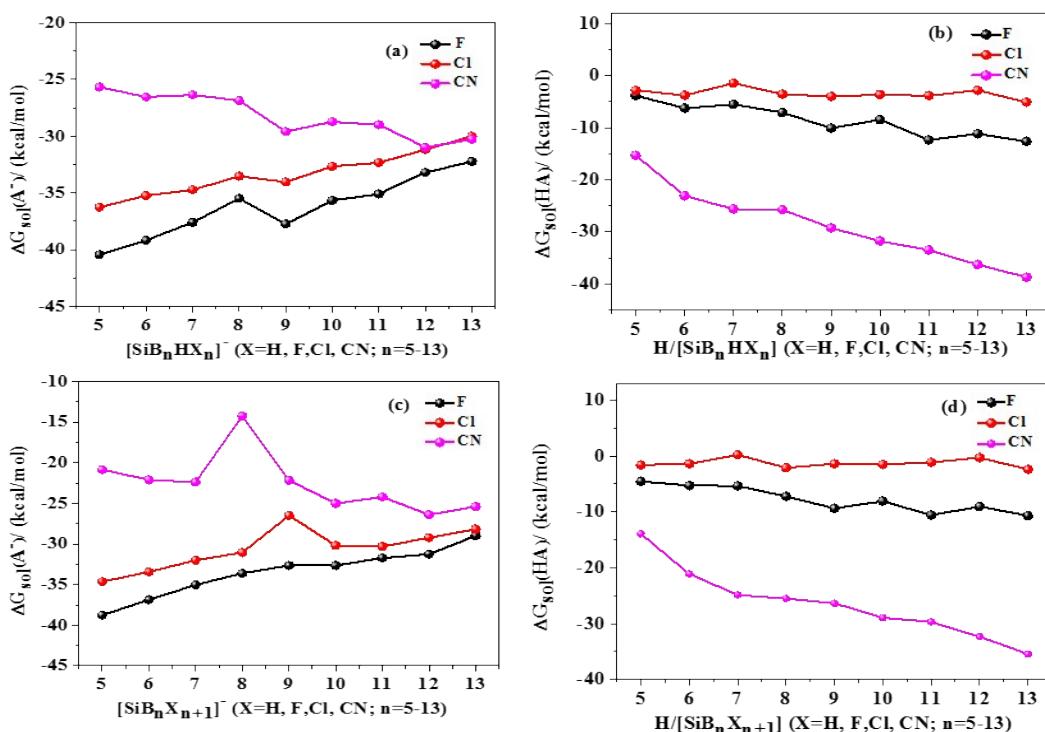


Fig.S10 The solvation free energies of both the conjugate acid (HA) and conjugate base (A^-) in H_2O solvent.

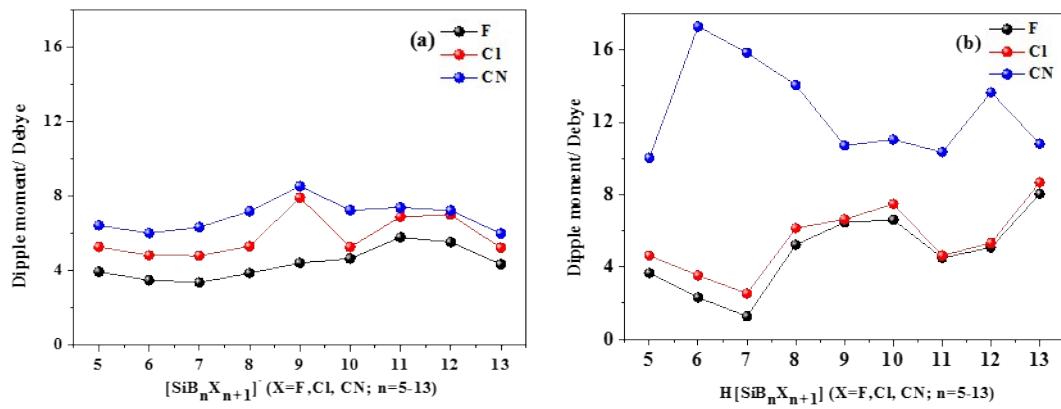


Fig.S11 The dipole moment of both the conjugate acid (HA) and conjugate base (A^-) in DMSO solvent.

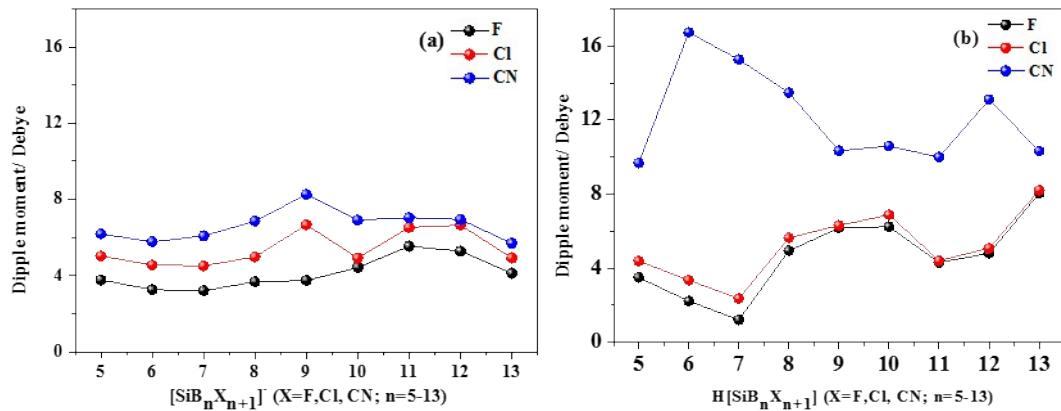


Fig.S12 The dipole moment of both the conjugate acid (HA) and conjugate base (A^-) in DCE solvent.

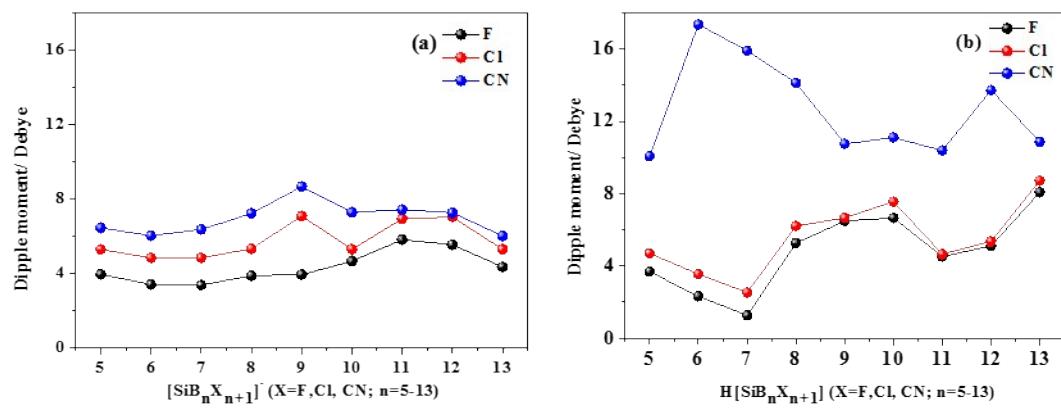


Fig.S13 The dipole moment of both the conjugate acid (HA) and conjugate base (A^-) in H_2O solvent.

Table S1 The calculated VDE values of the superhalogen of $[SiB_nH_mX_{n-m+1}]^-$ (m= 1and 0; n=5-13; X=H, F, Cl, CN)(eV)

n	H/[SiB _n H _{n+1}]	H/[SiB _n HF _n]	H/[SiB _n HCl _n]	H/[SiB _n H(CN) _n]	H/[SiB _n F _{n+1}]	H/[SiB _n Cl _{n+1}]	H/[SiB _n (CN) _{n+1}]
n=5	3.8	3.9	4.5	6.6	3.7	4.7	6.9
n=6	4.2	5.2	5.5	7.5	5.4	5.7	7.8
n=7	3.5	5.0	5.1	7.1	5.3	5.4	7.6
n=8	4.4	5.1	5.1	7.3	5.4	5.6	8.0
n=9	4.6	5.2	5.6	8.0	5.2	5.6	8.2
n=10	4.3	5.3	5.6	8.2	5.6	5.8	8.4
n=11	5.9	6.3	6.6	9.2	6.6	6.6	9.3
n=12	4.3	6.1	5.9	8.5	6.2	5.9	8.6
n=13	5.3	6.6	6.7	9.3	6.8	6.7	9.5

Table S2 The calculated ΔE_{acid} values of the composites of H/[SiB_nH_mX_{n-m+1}](m= 1and 0; n=5-13; X=H, F, Cl, CN).

n	H/[SiB _n H _{n+1}]	H/[SiB _n HF _n]	H/[SiB _n HCl _n]	H/[SiB _n H(CN) _n]	H/[SiB _n F _{n+1}]	H/[SiB _n Cl _{n+1}]	H/[SiB _n (CN) _{n+1}]
n=5	316.1	293.0	278.8	268.7	302.0	280.2	263.0
n=6	307.8	283.1	265.3	259.4	277.9	262.1	254.6
n=7	316.9	295.8	265.1	267.7	264.9	249.6	248.7
n=8	304.5	282.2	273.8	255.7	274.0	264.6	247.6
n=9	295.8	242.8	249.4	253.2	240.5	248.1	249.6
n=10	308.7	288.4	275.0	236.0	267.7	243.0	245.0
n=11	278.2	234.1	244.4	244.7	230.8	243.5	241.9
n=12	296.3	215.1	250.9	244.1	240.5	272.6	241.3
n=13	271.4	230.6	238.0	236.5	227.1	237.1	233.9

Table S3 The calculated bond dissociation energy of the composites of H/[SiB_nH_mX_{n-m+1}](m= 1and 0; n=5-13; X=H, F, Cl, CN).

n	H/[SiB _n H _{n+1}]	H/[SiB _n HF _n]	H/[SiB _n HCl _n]	H/[SiB _n H(CN) _n]	H/[SiB _n F _{n+1}]	H/[SiB _n Cl _{n+1}]	H/[SiB _n (CN) _{n+1}]
n=5	91.4	72.5	72.5	113.3	85.0	83.3	115.6
n=6	92.3	87.1	81.7	124.4	86.5	80.9	126.1
n=7	84.5	78.9	73.9	108.4	78.7	73.1	112.0
n=8	94.7	89.7	85.6	118.2	88.8	85.2	116.7
n=9	84.1	79.0	73.0	125.5	81.8	72.7	127.0
n=10	93.3	84.3	81.8	123.5	83.5	81.2	126.4

n=11	102.8	90.2	89.3	144.4	94.6	89.4	145.1
n=12	87.5	93.0	77.9	127.7	94.4	77.3	128.9
n=13	103.8	89.4	83.8	140.4	89.9	84.0	141.2

Table S4 The calculated deformation energy of the composites of H/[SiB_nH_mX_{n-m+1}](m= 1and 0; n=5-13; X=H, F, Cl, CN) (kcal/mol)

n	H/[SiB _n H _{n+1}]	H/[SiB _n HF _n]	H/[SiB _n HCl _n]	H/[SiB _n H(CN) _n]	H/[SiB _n F _{n+1}]	H/[SiB _n Cl _{n+1}]	H/[SiB _n (CN) _{n+1}]
n=5	-1.7	-2.9	-2.8	-7.2	-11.7	-8.9	-7.3
n=6	-0.6	2.0	-2.8	-6.1	2.5	-1.6	-5.4
n=7	-1.2	17.9	-4.5	9.7	-5.9	-11.7	-1.9
n=8	-2.2	-2.6	-8.6	-8.1	-4.0	-4.8	2.1
n=9	3.2	-29.4	-8.9	-1.0	-34.1	-9.0	-1.0
n=10	-0.1	11.7	7.8	-13.2	-1.4	-18.5	-2.2
n=11	-1.2	-24.0	-7.0	-2.0	-24.8	-7.3	-1.9
n=12	-6.6	-51.1	-5.3	-1.9	-24.5	18.4	-1.9
n=13	-23.6	-21.2	-5.9	-2.5	-20.7	-5.9	-2.5

Table S5 The calculated acid dissociation constants(pK_a) of the composites of H/[SiB_nH_mX_{n-m+1}](m= 1and 0; n=5-13; X=H, F, Cl, CN) in DMSO solvent

n	H/[SiB _n H _{n+1}]	H/[SiB _n HF _n]	H/[SiB _n HCl _n]	H/[SiB _n H(CN) _n]	H/[SiB _n F _{n+1}]	H/[SiB _n Cl _{n+1}]	H/[SiB _n (CN) _{n+1}]
n=5	-5.3	-18.0	-26.0	-17.0	-12.1	-24.6	-19.5
n=6	-8.4	-23.5	-35.1	-19.3	-26.0	-37.4	-20.5
n=7	-3.5	-15.3	-35.4	-11.2	-34.6	-46.7	-23.0
n=8	-7.8	-21.0	-28.3	-20.5	-26.1	-34.3	-23.7
n=9	-14.3	-48.7	-44.4	-21.2	-48.6	-45.8	-22.5
n=10	-4.1	-16.0	-26.4	-31.8	-28.8	-49.4	-24.8
n=11	-16.4	-52.2	-47.6	-21.8	-53.0	-48.4	-25.1
n=12	-11.6	-64.0	-43.9	-23.7	-47.3	-28.9	-25.4
n=13	-17.9	-52.2	-49.5	-27.4	-53.3	-50.5	-28.3

Table S6 The calculated acid dissociation constants(pK_a) of the composites of H/[SiB_nH_mX_{n-m+1}](m= 1and 0; n=5-13; X=H, F, Cl, CN) in DCE solvent

n	H/[SiB _n H _{n+1}]	H/[SiB _n HF _n]	H/[SiB _n HCl _n]	H/[SiB _n H(CN) _n]	H/[SiB _n F _{n+1}]	H/[SiB _n Cl _{n+1}]	H/[SiB _n (CN) _{n+1}]
n=5	41.6	27.9	19.8	27.2	41.6	27.9	19.8

n=6	38.3	22.2	10.6	24.3	38.3	22.2	10.6
n=7	43.2	30.3	10.3	32.1	43.2	30.3	10.3
n=8	38.6	24.2	17.2	23.0	38.6	24.2	17.2
n=9	32.4	-3.4	1.4	22.3	32.4	-3.4	1.4
n=10	42.3	29.1	18.9	11.4	42.3	29.1	18.9
n=11	29.2	-7.2	-2.1	19.1	29.2	-7.2	-2.1
n=12	34.7	-19.0	1.7	19.4	34.7	-19.0	1.7
n=13	27.3	-7.4	-4.4	15.6	27.3	-7.4	-4.4

Table S7 The calculated acid dissociation constants(pK_a) of the composites of H/[SiB_nH_mX_{n-m+1}](m= 1and 0; n=5-13; X=H, F, Cl, CN) in H₂O solvent

n	H/[SiB _n H _{n+1}]	H/[SiB _n HF _n]	H/[SiB _n HCl _n]	H/[SiB _n H(CN) _n]	H/[SiB _n F _{n+1}]	H/[SiB _n Cl _{n+1}]	H/[SiB _n (CN) _{n+1}]
n=5	-2.6	-15.2	-23.1	-14.2	-8.9	-21.4	-16.5
n=6	-5.7	-20.5	-32.1	-16.5	-22.6	-34.2	-17.4
n=7	-0.8	-12.4	-33.1	-8.4	-31.1	-43.4	-19.8
n=8	-5.0	-18.0	-25.2	-17.5	-22.4	-31.1	-14.2
n=9	-11.5	-45.7	-41.4	-18.5	-44.5	-38.6	-17.8
n=10	-1.4	-13.1	-23.5	-28.9	-25.6	-46.1	-21.6
n=11	-13.6	-49.1	-44.6	-21.2	-49.6	-45.2	-21.9
n=12	-8.8	-60.9	-41.0	-20.9	-44.1	-25.7	-22.4
n=13	-15.0	-49.1	-46.5	-24.4	-50.0	-47.2	-25.1

Table S8 The calculated VDE values of the superhalogen of [SiB_nH_mX_{n-m+1}]⁻ (m= 1and 0; n=5-13; X=H, F, Cl, CN)(eV)

in DCE solvent

n	[SiB _n H _{n+1}] ⁻	[SiB _n HF _n] ⁻	[SiB _n HCl _n] ⁻	[SiB _n H(CN) _n] ⁻	[SiB _n F _{n+1}] ⁻	[SiB _n Cl _{n+1}] ⁻	[SiB _n (CN) _{n+1}] ⁻
n=5	4.4	3.6	4.2	6.2	3.9	4.3	6.7
n=6	4.5	4.8	5.1	6.9	5.0	5.3	7.3
n=7	3.8	4.6	4.7	6.3	4.9	5.0	6.8
n=8	5.1	4.7	4.6	6.4	5.0	5.2	7.2

n=9	4.9	4.7	5.0	7.1	4.8	5.5	7.5
n=10	4.6	4.7	5.0	7.2	5.1	5.3	7.5
n=11	6.4	4.7	6.0	8.2	6.1	6.1	8.5
n=12	4.7	5.6	5.4	7.5	5.7	5.5	7.8
n=13	5.8	6.1	6.1	8.4	6.3	6.2	8.6

Table S9 The calculated VDE values of the superhalogen of $[\text{SiB}_n\text{H}_m\text{X}_{n-m+1}]^-$ ($m=1$ and 0 ;

$n=5-13$; X=H, F, Cl, CN)(eV)

in DMSO solvent

n	$[\text{SiB}_n\text{H}_{n+1}]^-$	$[\text{SiB}_n\text{HF}_n]^-$	$[\text{SiB}_n\text{HCl}_n]^-$	$[\text{SiB}_n\text{H}(\text{CN})_n]^-$	$[\text{SiB}_n\text{F}_{n+1}]^-$	$[\text{SiB}_n\text{Cl}_{n+1}]^-$	$[\text{SiB}_n(\text{CN})_{n+1}]^-$
n=5	4.4	3.6	4.2	6.2	3.9	4.4	6.6
n=6	4.6	4.8	5.2	6.7	5.0	5.3	7.1
n=7	3.8	4.5	4.7	6.2	4.9	5.1	6.7
n=8	5.2	4.7	4.7	6.2	5.1	5.4	7.0
n=9	4.9	4.7	5.1	6.9	4.8	5.6	7.3
n=10	4.7	4.7	5.1	6.9	5.1	5.5	7.5
n=11	6.4	5.8	6.1	8.0	6.0	6.3	8.3
n=12	4.8	5.6	5.5	7.2	5.7	5.9	7.7
n=13	5.9	6.0	6.2	8.1	6.4	6.4	8.4

Table S10 The calculated VDE values of the superhalogen of $[\text{SiB}_n\text{H}_m\text{X}_{n-m+1}]^-$ ($m=1$ and 0 ;

$n=5-13$; X=H, F, Cl, CN)(eV)

in H_2O solvent.

n	$[\text{SiB}_n\text{H}_{n+1}]^-$	$[\text{SiB}_n\text{HF}_n]^-$	$[\text{SiB}_n\text{HCl}_n]^-$	$[\text{SiB}_n\text{H}(\text{CN})_n]^-$	$[\text{SiB}_n\text{F}_{n+1}]^-$	$[\text{SiB}_n\text{Cl}_{n+1}]^-$	$[\text{SiB}_n(\text{CN})_{n+1}]^-$
n=5	4.4	3.7	4.4	6.4	3.9	4.6	6.8
n=6	4.6	4.9	5.4	6.9	5.1	5.6	7.3
n=7	3.9	4.6	5.0	6.4	5.0	5.4	6.9
n=8	5.2	4.8	5.0	6.5	5.1	5.6	7.2
n=9	5.0	4.8	5.4	7.1	4.9	5.9	7.5
n=10	4.8	4.8	5.4	7.1	5.2	5.8	7.5
n=11	6.5	6.0	6.5	8.2	6.3	6.7	8.5
n=12	4.9	5.7	5.8	7.4	5.9	6.0	7.7

n=13	6.1	6.2	6.6	8.2	6.5	6.8	8.6
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Table S11 The calculated solvation free energies(ΔG_{sol}) of the conjugate acid H/[SiB_nH_mX_{n-m+1}](m= 1and 0; n=5-13; X=H, F, Cl, CN) (kcal/mol) in DCE solvent.

n	H/[SiB _n H _{n+1}]	H/[SiB _n HF _n]	H/[SiB _n HCl _n]	H/[SiB _n H(CN) _n]	H/[SiB _n F _{n+1}]	H/[SiB _n Cl _{n+1}]	H/[SiB _n (CN) _{n+1}]
n=5	1.0	-5.6	-8.3	-19.0	-6.0	-7.7	-18.1
n=6	0.5	-8.0	-9.9	-25.7	-7.1	-8.6	-24.2
n=7	1.1	-7.7	-8.8	-27.8	-7.4	-8.0	-27.3
n=8	1.1	-9.2	-11.1	-27.7	-9.2	-10.5	-27.4
n=9	0.9	-12.3	-12.5	-30.4	-11.4	-11.0	-27.5
n=10	0.8	-11.0	-12.6	-31.8	-10.6	-11.4	-29.2
n=11	-6.1	-15.2	-13.8	-33.0	-13.5	-12.2	-29.7
n=12	1.5	-14.2	-13.4	-34.3	-12.3	-11.9	-30.3
n=13	-5.9	-15.9	-15.7	-35.8	-14.1	-14.1	-32.5

Table S12 The calculated solvation free energies(ΔG_{sol}) of the conjugate acid H/[SiB_nH_mX_{n-m+1}](m= 1and 0; n=5-13; X=H, F, Cl, CN) (kcal/mol) in DMSO solvent.

n	H/[SiB _n H _{n+1}]	H/[SiB _n HF _n]	H/[SiB _n HCl _n]	H/[SiB _n H(CN) _n]	H/[SiB _n F _{n+1}]	H/[SiB _n Cl _{n+1}]	H/[SiB _n (CN) _{n+1}]
n=5	1.7	-5.6	-7.4	-20.3	-6.2	-6.6	-19.4
n=6	1.2	-8.3	-9.1	-28.3	-7.3	-7.2	-26.8
n=7	2.0	-7.9	-7.5	-31.1	-7.7	-6.3	-30.8
n=8	2.0	-9.8	-10.1	-31.2	-10.0	-9.2	-31.4
n=9	1.9	-13.1	-11.2	-34.6	-12.3	-9.0	-31.9
n=10	1.7	-12.0	-11.4	-36.7	-11.6	-9.8	-34.3
n=11	-6.1	-16.3	-12.2	-38.3	-14.5	-10.0	-34.9
n=12	2.7	-15.2	-11.6	-40.4	-13.1	-9.5	-36.8
n=13	-5.9	-17.2	-14.2	-42.2	-15.2	-12.0	-39.5

Table S13 The calculated solvation free energies(ΔG_{sol}) of the conjugate acid H/[SiB_nH_mX_{n-m+1}](m= 1and 0; n=5-13; X=H, F, Cl, CN) (kcal/mol) in H₂O solvent.

n	H/[SiB _n H _{n+1}]	H/[SiB _n HF _n]	H/[SiB _n HCl _n]	H/[SiB _n H(CN) _n]	H/[SiB _n F _{n+1}]	H/[SiB _n Cl _{n+1}]	H/[SiB _n (CN) _{n+1}]
n=5	2.7	-3.9	-2.8	-15.3	-4.5	-1.6	-13.9
n=6	2.4	-6.3	-3.8	-23.1	-5.3	-1.4	-21.1
n=7	3.7	-5.5	-1.5	-25.6	-5.3	0.3	-24.9

n=8	3.7	-7.1	-3.6	-25.8	-7.2	-2.1	-25.5
n=9	4.2	-10.1	-4.0	-29.3	-9.4	-1.4	-26.4
n=10	4.2	-8.5	-3.7	-31.8	-8.0	-1.5	-29.0
n=11	-3.2	-12.4	-3.9	-33.5	-10.6	-1.1	-29.7
n=12	5.9	-11.2	-2.8	-36.3	-9.0	-0.3	-32.4
n=13	-2.4	-12.7	-5.1	-38.7	-10.7	-2.4	-35.5

Table S14 The calculated solvation free energies(ΔG_{sol}) of the conjugate base $[\text{SiB}_n\text{H}_m\text{X}_{n-m+1}]^-$

(m= 1and 0; n=5-13; X=H, F, Cl, CN) (kcal/mol) in DCE solvent

n	$[\text{SiB}_n\text{H}_{n+1}]^-$	$[\text{SiB}_n\text{HF}_n]^-$	$[\text{SiB}_n\text{HCl}_n]^-$	$[\text{SiB}_n\text{H}(\text{CN})_n]^-$	$[\text{SiB}_n\text{F}_{n+1}]^-$	$[\text{SiB}_n\text{Cl}_{n+1}]^-$	$[\text{SiB}_n(\text{CN})_{n+1}]^-$
n=5	-36.4	-38.8	-38.6	-28.3	-37.8	-38.3	-24.7
n=6	-33.2	-38.0	-38.5	-29.1	-36.4	-38.1	-25.8
n=7	-31.5	-36.8	-38.3	-28.8	-35.4	-37.7	-26.0
n=8	-28.3	-35.4	-38.8	-29.0	-34.0	-37.6	-25.9
n=9	-28.7	-37.6	-39.7	-30.5	-33.5	-33.8	-23.6
n=10	-26.3	-36.1	-39.2	-29.2	-33.9	-38.3	-26.3
n=11	-24.5	-36.1	-39.6	-28.9	-33.6	-39.1	-25.2
n=12	-22.9	-34.5	-39.0	-29.5	-33.1	-38.5	-25.8
n=13	-19.7	-34.0	-38.5	-28.2	-31.6	-38.2	-24.4

Table S15 The calculated solvation free energies(ΔG_{sol}) of the conjugate base $[\text{SiB}_n\text{H}_m\text{X}_{n-m+1}]^-$

(m= 1and 0; n=5-13; X=H, F, Cl, CN) (kcal/mol) in DMSO solvent

n	$[\text{SiB}_n\text{H}_{n+1}]^-$	$[\text{SiB}_n\text{HF}_n]^-$	$[\text{SiB}_n\text{HCl}_n]^-$	$[\text{SiB}_n\text{H}(\text{CN})_n]^-$	$[\text{SiB}_n\text{F}_{n+1}]^-$	$[\text{SiB}_n\text{Cl}_{n+1}]^-$	$[\text{SiB}_n(\text{CN})_{n+1}]^-$
n=5	-39.6	-41.5	-40.2	-29.9	-40.2	-39.4	-25.8
n=6	-36.1	-40.6	-39.9	-31.1	-39.0	-39.0	-27.4
n=7	-34.3	-39.3	-39.3	-31.1	-37.6	-38.3	-28.1
n=8	-30.7	-37.7	-39.8	-31.8	-36.8	-38.0	-28.5
n=9	-31.3	-40.3	-40.7	-34.0	-36.5	-39.5	-29.6
n=10	-28.7	-38.6	-39.9	-33.1	-35.9	-38.4	-30.0
n=11	-26.7	-38.7	-40.2	-30.0	-35.7	-39.1	-29.1
n=12	-24.9	-36.8	-39.4	-34.4	-35.2	-38.3	-30.4

n=13	-21.3	-36.4	-38.6	-33.3	-33.5	-37.7	-29.2
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Table S16 The calculated solvation free energies(ΔG_{sol}) of the conjugate base $[SiB_nH_mX_{n-m+1}]^-$ ($m=1$ and 0 ; $n=5-13$; $X=H, F, Cl, CN$) (kcal/mol) in H_2O solvent

n	$[SiB_nH_{n+1}]^-$	$[SiB_nHF_n]^-$	$[SiB_nHCl_n]^-$	$[SiB_nH(CN)_n]^-$	$[SiB_nF_{n+1}]^-$	$[SiB_nCl_{n+1}]^-$	$[SiB_n(CN)_{n+1}]^-$
n=5	-39.5	-40.4	-36.3	-25.7	-38.8	-34.6	-20.9
n=6	-35.8	-39.2	-35.2	-26.6	-36.9	-33.5	-22.1
n=7	-33.6	-37.6	-34.7	-26.4	-35.1	-32.0	-22.4
n=8	-29.7	-35.5	-33.5	-26.9	-33.6	-31.1	-14.2
n=9	-29.9	-37.7	-34.1	-29.6	-32.7	-26.5	-22.2
n=10	-27.0	-35.7	-32.7	-28.7	-32.7	-30.2	-25.0
n=11	-24.5	-35.1	-32.3	-29.0	-31.7	-30.3	-24.2
n=12	-22.4	-33.2	-31.2	-31.0	-31.3	-29.2	-26.4
n=13	-18.5	-32.2	-30.0	-30.3	-29.0	-28.2	-25.4

Table S17 The calculated acid dissociation constants(pK_a) of the composites of $H/[CB_nHX_n]$ ($n = 5 - 13$; $X=H, F, Cl, CN$) in DCE solvent.

	$H/[CB_nH_{n+1}]$	$H/[CB_nHF_n]$	$H/[CB_nHCl_n]$	$H/[CB_nH(CN)_n]$
n = 5	38.82	32.06	20.53	24.74
n = 6	35.99	30.04	18.58	23.12
n = 7	37.77	21.28	8.55	23.12
n = 8	27.98	19.03	7.36	20.16
n = 9	23.91	-4.47	-1.42	21.16
n = 10	32.29	20.20	8.79	18.80
n = 11	21.54	-7.51	-4.41	17.59
n = 12	27.68	-1.33	0.00	18.19
n = 13	19.25	-6.72	-5.04	15.37

Table S18 The calculated acid dissociation constants(pK_a) of the composites of $H/[CB_nHX_n]$ ($n = 5 - 13$; $X=H, F, Cl, CN$) in DMSO solvent.

	H/[CB _n H _{n+1}]	H/[CB _n HF _n]	H/[CB _n HCl _n]	H/[CB _n H(CN) _n]
n = 5	-8.02	-13.67	-25.12	-19.05
n = 6	-10.60	-15.48	-26.83	-20.22
n = 7	-8.83	-24.05	-37.14	-20.28
n = 8	-18.33	-25.90	-37.71	-22.98
n = 9	-22.54	-49.48	-44.73	-21.90
n = 10	-13.92	-24.55	-36.41	-23.99
n = 11	-23.87	-52.21	-49.82	-25.14
n = 12	-18.48	-46.16	-44.04	-24.50
n = 13	-25.91	-51.23	-50.12	-27.21

Table S19 The calculated acid dissociation constants(pK_a) of the composites of H/[CB_nHX_n]

(n = 5 - 13; X=H, F, Cl, CN) in H₂O

	H/[CB _n H _{n+1}]	H/[CB _n HF _n]	H/[CB _n HCl _n]	H/[CB _n H(CN) _n]
n = 5	-21.54	-25.34	-34.92	-24.89
n = 6	-23.18	-26.61	-36.30	-26.78
n = 7	-20.64	-34.70	-46.27	-26.75
n = 8	-29.30	-36.19	-46.55	-29.73
n = 9	-32.97	-59.53	-55.77	-29.42
n = 10	-23.77	-34.58	-45.08	-32.06
n = 11	-33.17	-61.68	-58.48	-33.43
n = 12	-27.25	-55.56	-52.33	-31.99
n = 13	-34.06	-60.80	-58.58	-37.35

Table S20 The calculated ΔG_{acid} values of the composites of H/[CB_nHX_n] (n = 5 - 13; X= H, F, Cl, CN) (kcal/mol).

HCB _n H _{n+1}	ΔG_{acid}	HCB _n HF _n	ΔG_{acid}	HCB _n HCl _n	ΔG_{acid}	HCB _n HCN _n	ΔG_{acid}
HCB ₅ H ₆	307.4	HCB ₅ HF ₅	287.7	HCB ₅ HCl ₅	269.1	HCB ₅ HCN ₅	250.9
HCB ₆ H ₇	300.7	HCB ₆ HF ₆	282.5	HCB ₆ HCl ₆	264.1	HCB ₆ HCN ₆	244.4
HCB ₇ H ₈	302.2	HCB ₇ HF ₇	267.9	HCB ₇ HCl ₇	251.7	HCB ₇ HCN ₇	244.3
HCB ₈ H ₉	286.1	HCB ₈ HF ₈	261.8	HCB ₈ HCl ₈	247.3	HCB ₈ HCN ₈	237.1

HCB₉H₁₀	280.6	HCB₉HF₉	227.6	HCB₉HCl₉	235.7	HCB₉HCN₉	237.5
HCB₁₀H₁₁	290.1	HCB₁₀HF₁₀	261.4	HCB₁₀HCl₁₀	249.4	HCB₁₀HCN₁₀	232.6
HCB₁₁H₁₂	267.2	HCB₁₁HF₁₁	219.2	HCB₁₁HCl₁₁	230.2	HCB₁₁HCN₁₁	229.2
HCB₁₂H₁₃	282.0	HCB₁₂HF₁₂	229.1	HCB₁₂HCl₁₂	238.4	HCB₁₂HCN₁₂	229.7
HCB₁₃H₁₄	261.6	HCB₁₃HF₁₃	218.7	HCB₁₃HCl₁₃	232.7	HCB₁₃HCN₁₃	222.0

Table S21 The difference between the ΔG_{sol} , ΔG_{acid} and $\Delta \Delta G_{\text{sol}}$ in DCE solvent

(kcal/mol).

	ΔG_{sol}	ΔG_{acid}	$\Delta \Delta G_{\text{sol}}$
strongest carbo	-13.3	214.8	-228.1
strongest sila	-26.0	204.9	-230.8
difference	-12.7	-9.9	-2.8

Table S22 The difference between the ΔG_{sol} , ΔG_{acid} and $\Delta \Delta G_{\text{sol}}$ in DMSO solvent

(kcal/mol).

	ΔG_{sol}	ΔG_{acid}	$\Delta \Delta G_{\text{sol}}$
strongest carbo	-74.0	214.8	-288.8
strongest sila	-87.3	204.9	-292.1
difference	-13.3	-9.9	-3.4

Table S23 The difference between the ΔG_{sol} , ΔG_{acid} and $\Delta \Delta G_{\text{sol}}$ in H₂O solvent

(kcal/mol).

	ΔG_{sol}	ΔG_{acid}	$\Delta \Delta G_{\text{sol}}$
strongest carbo	-69.4	214.8	-284.1
strongest sila	-83.1	204.9	-287.9
difference	-13.7	-9.9	-3.8

Table S24 The difference of single point energy between the basis 6-311+G**and 6-

311++G*(kcal/mol).

	SiB5F6	HSiB5F6	Error
6-311+G**	-635782.1	-636084.2	-302.0
6-311++G**	-635782.1	-636084.2	-302.0
Different	0.0	0.0	0.0

Table S25 The difference of single point energy between the basis 6-311+G**and 6-

311++G*(kcal/mol).

	SiB5HF5	HSiB5HF5	Error
6-311+G**	-573475.3	-573768.4	-293.0
6-311++G**	-573475.4	-573768.4	-293.0
Different	0.0	0.0	0.0

Table S26 The difference of key position bond length between the basis 6-311+Gand 6-311++G*(kcal/mol).**

HSiB5F6	6-311+G**	6-311++G**	Error
B2-H6	1.328	1.328	0
B1-H6	1.348	1.348	0
Si13-F12	1.607	1.607	0
Frequency	58.79	58.74	-0.05

Table S27The difference of key position bond length between the basis 6-311+Gand 6-311++G*(kcal/mol).**

HSiB5HF5	6-311+G**	6-311++G**	Error
B2-H7	1.368	1.368	0
B4-H7	1.368	1.368	0
Si13-H6	1.463	1.463	0
Frequency	80.95	81.48	0.53

Lowest normal mode frequencies and optimized coordinates at ω B97XD/6-311+G(d, p) level of the composites of H/[SiB_nH_mX_{n-m+1}] (m= 1and 0; n=5 - 13; X=H, F, Cl, CN) .

H/[SiB₅H₆]

Lowest normal mode frequency: 233.910 cm⁻¹

B	1.50694900	-0.00001300	0.01114100
B	0.36258500	0.87816600	0.92059400
B	0.27564200	-1.06062600	-0.81639600
B	0.36257100	-0.87816000	0.92060100
B	0.27561400	1.06064700	-0.81638700
H	2.68916300	0.00000400	-0.00515900

H	0.47925800	1.72423400	1.73989900
H	0.47919000	-1.72421200	1.73993100
H	0.34605500	-1.87561000	-1.67112300
H	0.34609200	1.87557400	-1.67116100
H	-2.66150800	-0.00001300	0.03698500
H	1.12245300	-0.00005500	-1.33100500
Si	-1.19410800	0.00000100	0.00456200

H/[SiB₆H₇]

Lowest normal mode frequency: 221.610 cm⁻¹

B	1.20834300	-0.01780500	0.90155000
B	-0.40559700	-0.42645200	1.34683300
B	1.20826600	-0.01796400	-0.90162300
B	-0.40571600	-0.42668800	-1.34673600
B	-1.40970400	-0.57848300	0.00009700
H	-0.59185900	-0.50898800	-2.51170800
H	2.00712800	0.11991100	-1.77082000
H	2.00730100	0.12022400	1.77063400
H	-0.59171300	-0.50856800	2.51182200
H	-2.56830700	-0.81728300	0.00021800
H	-0.56885900	2.58519300	-0.00019000
B	0.15861600	-1.38634500	0.00011200
H	0.48231600	-2.52676300	0.00019600
H	2.12704000	-0.15998500	-0.00007100
Si	-0.29100600	1.14035300	-0.00008900

H/[SiB₇H₈]

Lowest normal mode frequency: 235.380 cm⁻¹

B	0.01970700	0.25874200	-1.27215300
B	-1.55860600	-0.35671800	0.83991900
B	-0.88166400	1.19222600	-0.00000100
B	0.81229700	1.35131300	-0.00000200
B	0.01970800	0.25874600	1.27215200
B	-1.55860600	-0.35672000	-0.83991800
B	-0.24680500	-1.26353700	0.00000100
H	2.77507400	-1.15505700	0.00000200
H	1.29197700	2.43260100	-0.00000300
H	0.14477300	0.30590100	2.45114900
H	-1.50723700	2.19977400	-0.00000200
H	-2.24876900	-0.60828800	1.77271200
H	-2.24877000	-0.60829200	-1.77271000
H	-0.15816000	-2.45244400	0.00000200
H	0.14477300	0.30589500	-2.45115000
H	-2.54360300	-0.40749800	0.00000100
Si	1.52284200	-0.38806100	0.00000000

H/[SiB₈H₉]

Lowest normal mode frequency: 148.75 cm⁻¹

B	0.19171200	-1.48876000	-0.77461800
B	0.01716300	-0.94610000	1.02863200
B	-1.28799700	-1.34415500	-0.04599000
B	0.27304700	0.86791600	1.01866700
B	-1.38023200	0.17178500	0.82464500
B	-1.59591400	0.04525700	-0.92113100
B	0.77398900	1.48972100	-0.59558900
B	-0.88825400	1.57187400	-0.11812900
H	0.43660700	-2.40824500	-1.48274500
H	0.32317600	-1.60753600	1.96805200
H	2.98872500	-0.45165300	0.28304200
H	0.64757800	1.47160000	1.97053100
H	-2.24548600	0.40798800	1.60267300
H	-2.30057500	0.23416600	-1.85298000
H	1.31634200	2.38038600	-1.15708700
H	-1.45860500	2.60874800	-0.13750800
H	-2.07815300	-2.23022900	-0.03701100
H	-0.47629500	1.22312700	-1.31605800
Si	1.59493700	-0.24757400	-0.13738200

H/[SiB₉H₁₀]**Lowest normal mode frequency: 309.88 cm⁻¹**

B	2.15973300	-0.00011600	0.07351900
B	1.01946900	1.03490600	-0.87613400
B	1.01971800	-1.03235900	-0.87886800
B	1.00962200	-0.93742000	0.92164900
B	1.00957200	0.93504100	0.92392100
B	-0.42087100	0.00193100	-1.34643000
B	-0.47801400	-1.35701100	0.04469900
B	-0.46323000	-0.00179600	1.36239600
B	-0.47818700	1.35690700	0.04807800
H	3.33319600	0.00000200	0.20884900
H	-3.34427400	-0.00008700	-0.08821500
H	1.39389300	1.81384500	-1.68886000
H	1.39322700	-1.80969400	-1.69358700
H	1.45688400	-1.69050000	1.72114700
H	1.45705200	1.68599700	1.72529200
H	-0.76624100	0.00335200	-2.48459500
H	-0.83567800	-2.48994600	0.00316400
H	-0.80251800	-0.00324100	2.50041600
H	-0.83599100	2.48990900	0.00962900
H	2.02483600	0.00057700	-1.22191300
Si	-1.88310300	-0.00004400	-0.02539100

H/[SiB₁₀H₁₁]

Lowest normal mode frequency: 154.11 cm⁻¹

B	-0.78794600	1.39713100	0.47923000
B	-1.48340900	-0.87645900	-1.04851500
B	0.85451700	-0.92248300	1.02798800
B	0.43021100	-1.32858300	-0.75976800
B	-0.78810400	-1.39707700	0.47926400
B	-1.48326100	0.87651400	-1.04855700
B	0.85460600	0.92241200	1.02802200
B	0.43041000	1.32860100	-0.75975400
B	-1.89917800	0.00008900	0.42683000
B	-0.55787700	0.00002400	1.57343500
H	-2.11662700	-1.63185500	-1.70543100
H	1.45242100	-1.63907400	1.76186500
H	0.71483000	-2.12844100	-1.59336000
H	-1.17351300	-2.48608500	0.76109900
H	-2.11633200	1.63195300	-1.70556600
H	1.45255400	1.63890700	1.76195500
H	0.71505500	2.12857900	-1.59322000
H	-3.00220800	0.00017100	0.85978800
H	-0.83957600	0.00003900	2.72452900
H	3.28917300	-0.00023000	-0.76542600
H	-1.17329400	2.48617200	0.76102600
H	-1.04514100	-0.00005200	-1.92813700
Si	1.85663000	-0.00006600	-0.45214200

H/[SiB₁₁H₁₂]**Lowest normal mode frequency: 25.78 cm⁻¹**

B	-0.53124400	-1.48905300	-0.58115700
B	-0.52116900	0.09614600	-1.59300900
B	-0.52412800	-1.01800900	1.23140400
B	-0.52262300	0.86322300	1.34411300
B	-0.53197700	1.54786100	-0.39981000
B	0.94921300	1.44293600	0.55849000
B	0.95705100	-0.09339100	1.53903900
B	0.94865600	-1.49926800	0.38390100
B	0.95175700	0.98868800	-1.18811200
B	0.95257900	-0.83883300	-1.29758000
H	-1.03835000	2.58679000	-0.67276500
H	1.54120000	2.39835700	0.93925100
H	1.54033500	-0.15441400	2.57061200
H	1.54114500	-2.49343900	0.64634600
H	1.53816700	-1.38811000	-2.17134600
H	1.53859800	1.63758500	-1.98976900
H	-1.01856100	0.16005400	-2.66946600
H	-1.03674800	-2.48778100	-0.97773300

H	-1.02333400	-1.69700100	2.06805200
H	-1.02089600	1.43787200	2.25611000
B	1.75639500	0.00002500	-0.00141800
H	3.04120800	0.00109800	-0.41400200
H	-3.23777600	-0.00025400	-0.00112400
H	3.03911900	-0.00144700	0.41713600
Si	-1.77333300	-0.00006700	0.00138600

H/[SiB₁₂H₁₃]

Lowest normal mode frequency: 206.36 cm⁻¹

B	-2.12976600	-0.85392700	-0.05441200
B	-2.12878300	0.85413500	-0.05350700
B	-0.67607900	-1.68175900	-0.37979700
B	-0.67969200	-1.04178800	1.26634500
B	-0.67885000	1.04479400	1.26476000
B	0.82022000	-1.53445400	0.46627300
B	0.59956900	-0.91259800	-1.28506900
B	-0.67509000	1.68128800	-0.38255300
B	0.70637100	0.00115900	1.54253500
B	0.59981500	0.91005800	-1.28674100
B	0.82111500	1.53504200	0.46374100
H	-3.07026700	1.56785400	-0.16220000
H	-1.03380500	-2.75219600	-0.74069000
H	-1.14204600	-1.57257300	2.22290700
H	-1.49441000	-0.00119500	-2.45089500
H	1.42275300	2.51718200	0.75418000
H	3.42273400	-0.00112400	-0.22003100
H	1.42112000	-2.51654700	0.75840700
H	-1.14014500	1.57802800	2.22048500
H	-1.03344200	2.75102800	-0.74486100
H	1.00078200	-1.48577900	-2.24405700
H	1.00117200	1.48125300	-2.24685000
H	1.17894800	0.00189900	2.63208700
H	-3.07165600	-1.56699100	-0.16348600
B	-1.04701700	-0.00054400	-1.35054400
H	-2.61240500	0.00001900	0.77970100
Si	1.96368600	-0.00056300	-0.10356100

H/[SiB₁₃H₁₄]

Lowest normal mode frequency: 54.83 cm⁻¹

B	-0.00165400	0.00021300	1.56583600
B	0.80573800	1.63859200	-0.57280800
B	-1.01927500	1.51436300	-0.57497400
B	-1.82244700	-0.12372400	-0.58265500
B	1.46761600	0.97928400	0.91075700
B	1.58673700	-0.77215600	0.91031700

B	-1.58778700	0.77242500	0.90826600
B	-0.12057700	1.75705200	0.91436100
H	0.00150500	-0.00087600	-3.12183500
H	0.00673200	-0.40852900	2.89035000
H	1.26489000	2.58568300	-1.11921000
H	-1.60127800	2.39025600	-1.12310900
H	-2.86693100	-0.19521700	-1.13982600
H	2.86902200	0.19480500	-1.13553500
H	2.28472800	1.53413200	1.56738600
H	2.47172400	-1.21112300	1.56670600
H	-2.47403200	1.21186800	1.56261100
H	-0.18822200	2.74294600	1.57020200
B	1.82356700	0.12349600	-0.58018700
B	0.11933500	-1.75671200	0.91521800
B	-1.46876900	-0.97880400	0.90950400
B	1.02010300	-1.51474900	-0.57300900
B	-0.80490800	-1.63860400	-0.57323800
H	-1.26370000	-2.58566200	-1.12000600
H	-2.28721700	-1.53369700	1.56442900
H	0.18578500	-2.74241500	1.57147100
H	1.60248400	-2.39114500	-1.11992100
H	-0.01041300	0.41025400	2.88986000
Si	0.00118100	-0.00033300	-1.65646600

H/[SiB₅HF₅]

Lowest normal mode frequency: 80.95 cm⁻¹

B	-1.14096000	-0.19546200	0.00000000
B	0.08592300	0.91599700	0.99660100
B	0.08592300	-0.90360900	-0.88209900
B	0.08592300	0.91599700	-0.99660100
B	0.08592300	-0.90360900	0.88209900
H	3.09670100	0.02869200	0.00000000
H	-0.57089000	1.58491600	0.00000000
F	0.08882700	-1.72980700	1.94415700
F	-0.04363500	1.67213400	2.09803100
F	-0.04363500	1.67213400	-2.09803100
F	0.08882700	-1.72980700	-1.94415700
F	-2.47256000	-0.12132300	0.00000000
Si	1.63572200	0.09784500	0.00000000

H/[SiB₆HF₆]

Lowest normal mode frequency: 48.41 cm⁻¹

B	-0.92946400	-1.27235800	0.06120400
B	0.93091800	-1.27070300	0.06114600
B	-1.34424000	0.43026800	-0.00503000
B	-0.00113500	1.47501400	-0.31011500

B	1.34369100	0.43274100	-0.00561700
H	0.00011300	-0.43072200	-2.93482400
B	0.00014000	0.47811100	1.12103900
H	0.00121000	-1.64581600	0.92076200
F	-1.87155500	-2.22626500	0.07398900
F	-2.66430700	0.73370500	-0.00817200
F	0.00018200	0.59472600	2.44094800
F	-0.00280800	2.79802000	-0.54844300
F	2.66352100	0.73700500	-0.00916600
F	1.87500000	-2.22266200	0.07389900
Si	-0.00008400	-0.21568500	-1.48618400

H/[SiB₇HF₇]

Lowest normal mode frequency: 31.45 cm⁻¹

B	0.57618200	1.31471300	-0.00783200
B	-1.07091700	-0.88119200	0.60070000
B	0.76115400	0.00000600	1.15479300
B	1.69361800	0.00003600	-0.25410500
B	0.57624900	-1.31469700	-0.00784700
B	-1.07095600	0.88112600	0.60072900
B	-1.36399800	-0.00000700	-1.00597900
H	1.08886300	0.00003600	-3.08699200
H	-1.18923600	-0.00004800	1.59195000
F	1.02867000	0.00000100	2.46196300
F	3.02545500	0.00007200	-0.47306700
F	0.81936200	-2.63849400	-0.02672400
F	-1.87368200	-1.89269300	0.96788200
F	-1.87376200	1.89258500	0.96793800
F	0.81923400	2.63852200	-0.02669600
F	-2.59529600	-0.00000300	-1.52001100
Si	0.38884900	0.00001300	-1.79063000

H/[SiB₈HF₈]

Lowest normal mode frequency: 85.22 cm⁻¹

B	-1.46640000	-0.89141800	-0.87021300
B	-0.80736200	-0.68514500	0.93347500
B	-1.63990200	0.56405300	-0.01662300
B	0.97733800	-0.48710100	0.83631200
B	-0.10824600	1.01517700	0.79129800
B	-0.45645400	1.37002100	-0.88026200
B	1.73677500	-0.72833200	-0.83180300
B	1.33479800	0.89635200	-0.28597300
H	0.33793800	-3.36087800	-0.17719400
H	1.14394600	0.39925000	-1.48877800
F	0.02723100	1.90440000	1.79424800
F	-0.48634800	2.34625100	-1.75563500

F	-2.87134600	1.08343900	0.23182600
F	-1.34349500	-1.25445100	2.02627400
F	1.73878200	-0.78438400	1.90954900
F	2.97522900	-0.99187500	-1.24164400
F	2.29051900	1.84093000	-0.19994200
F	-2.56314400	-1.35750200	-1.47285400
Si	0.19703800	-1.95626500	-0.59581900

H/[SiB₉HF₉]

Lowest normal mode frequency: 71.3 cm⁻¹

B	-1.36131600	-0.00001400	0.98391600
B	0.14671600	0.00001200	1.62563100
B	-0.52248900	-1.33973200	0.42303700
B	-1.14164100	-0.00001700	-0.68224300
B	-0.52251400	1.33971700	0.42302400
B	1.23269500	-0.96318200	0.40145400
B	0.21067000	-1.05287500	-1.28229100
B	0.21065500	1.05287100	-1.28229400
B	1.23267700	0.96321400	0.40144200
H	3.26718100	0.00002500	-1.79247400
H	-3.10985600	-0.00005300	0.14600400
F	2.10513100	1.84229100	0.96180900
F	2.10516500	-1.84223600	0.96183400
F	0.59284100	0.00002300	2.89257900
F	-0.97944700	2.60655800	0.60929300
F	-2.89512800	-0.00001400	1.12648900
F	-2.48246700	-0.00002200	-1.20481700
F	-0.07659500	2.02315000	-2.17857200
F	-0.07655600	-2.02317200	-2.17855700
F	-0.97937700	-2.60658600	0.60931500
Si	1.89952200	0.00001000	-1.27187600

H/[SiB₁₀HF₁₀]

Lowest normal mode frequency: 100.94 cm⁻¹

B	0.00000000	-0.32455300	1.39716700
B	0.87774600	1.55734900	-0.67525900
B	-1.56097500	-0.43743100	-1.10063700
B	1.56097400	-0.43743100	-1.10063700
B	-0.87774600	1.55734900	-0.67525900
B	1.45882900	0.30324800	0.48058300
B	-0.89029200	-1.47527700	0.31544600
B	0.89029200	-1.47527700	0.31544600
B	0.00000000	1.35571900	0.85612300
B	-1.45882900	0.30324800	0.48058300
H	0.00000000	-2.97480100	-2.17979200
H	0.00000000	1.27578900	-1.63941000

F	-1.64887100	-2.46642300	0.82507400
F	-2.70893400	-0.42998700	-1.76861600
F	1.64887100	-2.46642300	0.82507400
F	2.70893400	-0.42998700	-1.76861600
F	2.62438300	0.59328900	1.10732500
F	1.70196800	2.52970100	-1.06107300
F	0.00000000	2.30834800	1.81339900
F	-1.70196800	2.52970100	-1.06107300
F	-2.62438300	0.59328900	1.10732500
F	0.00000000	-0.55449100	2.71881900
Si	0.00000000	-1.62849000	-1.59195100

H/[SiB₁₁HF₁₁]

Lowest normal mode frequency: 144.36 cm⁻¹

B	1.82657300	-0.00002600	-0.12425400
B	0.80778900	1.54429600	-0.56758100
B	0.80774400	-1.54431700	-0.56758900
B	-0.87541400	-0.96146700	-1.28598000
B	-0.87538600	0.96150000	-1.28597500
B	-1.60455700	0.00002400	0.01122700
B	-0.65802300	-1.46988400	0.42607200
B	0.91762900	-0.91840700	1.13139200
B	-0.65798100	1.46990200	0.42607900
B	0.91765600	0.91837500	1.13139600
B	-0.54502400	0.00000400	1.38578800
H	1.41060000	-0.00001200	-3.28490700
H	-2.40926300	-0.00002000	2.10366000
F	3.18277500	-0.00004600	-0.13903300
F	1.56899200	-1.62939600	2.08162500
F	1.56903900	1.62934100	2.08163300
F	-1.55570400	0.00001600	2.57605800
F	-1.31656400	2.55592300	0.91774400
F	-2.92860200	0.00004300	0.49657700
F	-1.59297400	1.70552100	-2.16313700
F	-1.59302400	-1.70546300	-2.16314500
F	1.38065000	2.72288600	-0.91756900
F	1.38057000	-2.72292100	-0.91758200
F	-1.31663900	-2.55588800	0.91773100
Si	0.83478300	-0.00000700	-1.93998200

H/[SiB₁₂HF₁₂]

Lowest normal mode frequency: 20.41 cm⁻¹

B	1.49062300	1.25556400	-0.01109100
B	-0.16766600	1.61919200	-0.03181000
B	2.25211100	-0.10297200	0.00583900
B	0.41325200	0.60142000	-1.43534600

B	-1.37756900	0.71963400	-0.92672500
B	1.02385600	-1.19804600	-0.91110500
B	1.01351700	-1.15609000	0.96973800
B	-1.39050200	0.75656400	0.88159500
B	-0.71818100	-0.83156400	-1.48286700
B	-0.73599000	-0.77095000	1.50783600
B	-1.88568700	-0.70964800	0.00336300
H	-0.80577600	-3.64297900	0.06742600
B	0.39132400	0.66007700	1.41764200
H	1.17275300	3.23578100	-0.05028500
F	-2.29519200	1.47755600	1.58932200
F	-0.21310100	3.05061200	-0.06116200
F	2.03848000	2.71945500	-0.03214300
F	0.74093200	1.18507000	2.61719100
F	3.48393700	-0.57455800	0.01265600
F	1.79079600	-1.80088400	1.88121500
F	1.80505500	-1.88768800	-1.78635200
F	-1.08995300	-1.20369500	2.74295700
F	-1.05855400	-1.31403300	-2.70322800
F	-3.17758500	-1.12109100	0.00352000
F	-2.27066600	1.41262600	-1.67591400
F	0.77594000	1.08040800	-2.64988500
Si	-0.47737700	-2.21590800	0.04313800

H/[SiB₁₃HF₁₃]

Lowest normal mode frequency: 136.03 cm⁻¹

B	-0.03751500	0.00829200	1.51829700
B	-0.91072100	-1.57565400	-0.91183200
B	0.91770100	-1.66223800	-0.75947700
B	1.90968400	-0.09513200	-0.68493600
B	-1.46250400	-0.76546100	0.53034500
B	-1.43828700	0.94798300	0.56569000
B	1.45300500	-0.96714600	0.80140500
B	-0.10735200	-1.80336100	0.69176500
H	0.24857200	-0.00133100	-3.39145100
B	-1.72346500	0.10226700	-0.97560400
B	0.06537100	1.79602700	0.70953900
B	1.53857200	0.80665500	0.80869700
B	-0.76015100	1.67267200	-0.88594400
B	1.07462700	1.56404800	-0.74192100
H	-3.02880700	-0.10463600	1.53969700
F	-2.93084400	0.13599100	-1.59454500
F	-1.28071600	2.72602700	-1.55174100
F	1.77531600	2.55706100	-1.33453900
F	3.13760000	-0.15243500	-1.24809200

F	0.05991100	2.94273900	1.42614500
F	-2.60064200	1.30219600	1.30529300
F	-0.23368600	-0.00596800	2.85866700
F	-2.75321900	-1.04348100	1.33074200
F	-0.26055300	-2.94168500	1.40598400
F	1.51461500	-2.71754600	-1.35735100
F	-1.56232500	-2.55371800	-1.57581100
F	2.36973300	-1.58554200	1.57958500
F	2.51222200	1.32172200	1.59245700
Si	0.17562200	0.00664000	-1.92925000

H/[SiB₅HCl₅]

Lowest normal mode frequency: 55.17 cm⁻¹

B	-1.45844800	0.58385800	0.48555200
B	0.11912000	-1.33578600	-0.71546800
B	1.44595200	1.10286400	-0.16686200
B	1.73127400	-0.49805000	-1.05849700
B	1.27408300	-0.50113900	0.58125200
B	-1.53661900	-1.03490600	-0.20200500
B	-0.32054300	1.59633100	-0.46816000
B	-1.27388200	0.22222300	-1.26571400
B	-0.46206100	-0.76734300	1.05006600
B	0.21463700	0.86275500	1.09230300
H	0.67950700	1.39909800	-3.34837300
C	-0.65457800	-1.52048500	2.38556700
N	-0.81639300	-2.07666200	3.36798000
C	0.21852100	-2.76909200	-1.24395700
N	0.29425800	-3.85147600	-1.62990000
C	-2.68337400	-2.03703300	-0.18383500
N	-3.53840300	-2.80379200	-0.10340300
C	-2.66167100	1.17821000	1.22344600
N	-3.56712000	1.58053400	1.80866600
C	2.19758300	-1.22768200	1.57190000
N	2.79282000	-1.80888400	2.36781000
C	0.38820200	1.55677200	2.44943500
N	0.49862300	2.00358000	3.50428100
C	3.02464400	-1.16916900	-1.50139600
N	4.00203400	-1.65830000	-1.86346600
C	-2.17945300	0.39046400	-2.48933700
N	-2.80010200	0.51593600	-3.45226300
C	2.56991900	2.12212800	0.03068000
N	3.42135700	2.88830000	0.14380100
C	-0.68503800	3.06227600	-0.73179800
N	-0.94390800	4.15859100	-0.96907600
H	-0.93584500	-2.55844200	4.24293500

Si 0.64129100 0.70372800 -2.06015200

H/[SiB₆HCl₆]

Lowest normal mode frequency: 70.79 cm⁻¹

B	0.92404600	1.28123600	-0.13752400
B	-0.92429300	1.28103200	-0.13747700
B	1.34666000	-0.40157300	-0.16513900
B	0.00012800	-1.43264800	-0.42661900
B	-1.34660000	-0.40186800	-0.16512000
H	-0.00020000	0.40359200	-3.10392400
B	0.00002000	-0.37373200	0.95506400
Cl	0.00009300	-0.51821600	2.69397200
Cl	3.05542400	-0.87013100	-0.13508600
Cl	0.00036000	-3.18140100	-0.64909700
Cl	2.11992400	2.58446600	-0.12415100
Cl	-2.12045700	2.58400300	-0.12408300
Cl	-3.05529000	-0.87069200	-0.13509800
H	-0.00016100	1.69935600	0.69225000
Si	-0.00002600	0.19702300	-1.65385800

H/[SiB₇HCl₇]

Lowest normal mode frequency: 14.64 cm⁻¹

B	0.59097200	1.32303200	-0.20212000
B	-0.99441600	-0.88016000	0.49776300
B	0.81026700	-0.00008800	0.93677900
B	1.66585000	-0.00027100	-0.52018700
B	0.59042400	-1.32315700	-0.20210100
B	-0.99410400	0.88062000	0.49761200
B	-1.37156900	0.00009900	-1.08051700
Cl	-2.05488300	-2.15341900	1.13002200
Cl	-2.05418700	2.15431900	1.12962800
Cl	1.36975300	-0.00016200	2.60546500
Cl	-3.00681300	0.00013900	-1.73035100
Cl	0.99652400	3.03945500	-0.27571400
Cl	0.99537100	-3.03972700	-0.27565600
Cl	3.41223000	-0.00063400	-0.82912100
H	0.87787300	-0.00011200	-3.33414300
H	-1.09667300	0.00032000	1.46721600
Si	0.32469800	-0.00000400	-1.97084700

H/[SiB₈HCl₈]

Lowest normal mode frequency: 58.82 cm⁻¹

B	-1.50052000	-0.68870200	-1.17736600
B	-0.81755300	-1.02536400	0.59584400
B	-1.59290900	0.45986700	0.04159600
B	0.98212700	-0.86028600	0.52373200

B	-0.05824400	0.59262600	0.92188500
B	-0.39100800	1.44921600	-0.57072200
B	1.67291000	-0.63335400	-1.15608300
B	1.36669500	0.77264700	-0.15680700
H	0.21203000	-3.30861100	-1.21985000
Cl	-3.13847400	1.14734200	0.60817900
Cl	0.06478200	1.37800500	2.50841500
Cl	-0.45901300	2.99425700	-1.32614300
Cl	2.69788800	1.87618200	0.22746300
Cl	-1.58997700	-2.12516100	1.75061800
Cl	-2.91052600	-1.03943600	-2.15924000
Cl	3.23304500	-0.90411900	-1.90147700
Cl	2.02828900	-1.67228500	1.70929100
H	1.12435300	0.64264700	-1.44134700
Si	0.11527700	-1.84276000	-1.18142800

H/[SiB₉HCl₉]

Lowest normal mode frequency: 74.96 cm⁻¹

B	-0.55886300	-0.00001800	1.46452800
B	1.05786600	0.00002900	1.04718800
B	-0.14156100	-1.32756000	0.50285100
B	-1.27618000	-0.00003500	-0.04510500
B	-0.14163400	1.32755000	0.50285500
B	1.31808900	-0.97119300	-0.51243900
B	-0.47177100	-0.99628600	-1.29528500
B	-0.47182800	0.99626000	-1.29528600
B	1.31803300	0.97127000	-0.51243300
H	1.58740300	0.00004800	-3.53925800
Cl	-1.61335300	-0.00004800	2.92567700
Cl	-0.46264000	2.98024800	1.09295400
Cl	2.35180900	0.00006300	2.26927700
Cl	-3.14244000	-0.00008400	0.18527800
Cl	-0.46246600	-2.98027900	1.09294600
Cl	2.64925400	2.16607700	-0.57531300
Cl	-1.43707200	2.19383500	-2.21539300
Cl	2.64937400	-2.16592800	-0.57531500
Cl	-1.43694900	-2.19391000	-2.21539800
H	-2.90869800	-0.00009100	1.56571600
Si	0.96691000	0.00002900	-2.21792600

H/[SiB₁₀HCl₁₀]

Lowest normal mode frequency: 60.25 cm⁻¹

B	1.45920600	0.10730600	0.40917900
B	-0.87901200	1.58811000	-0.42757900
B	-0.89165500	-1.55232100	-0.19821200
B	-1.56060100	-0.21165300	-1.31156400

B	-1.45920800	0.10732400	0.40918200
B	0.87903400	1.58810400	-0.42757300
B	0.89162900	-1.55233500	-0.19821000
B	1.56060500	-0.21168100	-1.31156400
B	0.00000600	1.03581200	1.00998400
B	-0.00000600	-0.72769300	1.13453900
H	-0.00002800	-2.36661000	-2.98864200
Cl	0.00001600	2.01491100	2.48890200
Cl	1.88132400	3.01025400	-0.64451900
Cl	2.98582100	0.25348200	1.31457100
Cl	-1.88128500	3.01027400	-0.64453100
Cl	-2.98581700	0.25352400	1.31457400
Cl	-0.00001100	-1.45817900	2.74258500
Cl	3.02966700	-0.03492800	-2.24002700
Cl	-3.02966700	-0.03489900	-2.24002300
Cl	-1.89116200	-2.99794800	0.06220900
Cl	1.89112200	-2.99797200	0.06220600
H	0.00001400	1.53142700	-1.41728300
Si	-0.00000900	-1.23817800	-2.05043600

H/[SiB₁₁HCl₁₁]

Lowest normal mode frequency: 103.56 cm⁻¹

B	-0.00013600	1.73445600	-0.71270200
B	-1.52706400	0.63922100	-0.86976800
B	1.52696000	0.63944700	-0.86979200
B	0.94771600	-1.14460900	-1.11276000
B	-0.94756900	-1.14474900	-1.11274400
B	0.00012000	-1.55140100	0.33242900
B	1.46834700	-0.51781900	0.47966900
B	0.90897300	1.18152400	0.72785800
B	-1.46826500	-0.51803700	0.47969700
B	-0.90914300	1.18138900	0.72787100
B	0.00001800	-0.16182200	1.39693500
H	-0.00009900	0.50949400	-3.63680300
Cl	0.00006800	-0.66268200	3.20699800
Cl	0.00024600	-3.16558400	1.15341000
Cl	-2.94270000	-1.13478800	1.27409600
Cl	-1.82940900	2.31220400	1.75177000
Cl	1.82908800	2.31247300	1.75175000
Cl	2.94289200	-1.13434700	1.27405100
Cl	3.06139400	1.23554100	-1.55514800
Cl	1.89567000	-2.35239100	-2.02041600
Cl	-1.89534600	-2.35269400	-2.02039100
Cl	-3.06160300	1.23507000	-1.55510800
Cl	-0.00027500	3.43402500	-1.25148600

H	0.00046500	-1.96270000	2.80102700
Si	-0.00004000	0.31493900	-2.18997600

H/[SiB₁₂HCl₁₂]

Lowest normal mode frequency: 50.51 cm⁻¹

B	0.18809100	-1.51380900	0.59172000
B	0.51592700	0.00790200	1.36367800
B	-1.13749800	-1.57052300	-0.60635300
B	1.68035600	-0.66162500	0.18344400
B	1.42528300	1.11887400	0.32012000
B	0.71045900	-1.40049500	-1.09072700
B	-2.16175200	-0.25649000	-0.70224100
B	-0.24099100	1.47653300	0.83195100
B	1.38721400	0.30914500	-1.28664800
B	-1.54403400	1.27615200	-0.43274200
B	0.25629700	1.70816900	-0.86196400
H	-0.77238300	0.13129200	-3.43213600
B	-1.23487500	-0.21576200	0.90380400
Cl	0.34203100	-2.93714800	1.72708400
Cl	0.94233200	-0.24556500	3.16610900
Cl	-1.83024500	-3.19170700	-0.85728600
Cl	3.26672200	-1.33732200	0.63565200
Cl	2.78364900	2.12509000	0.87394600
Cl	-0.53475900	2.76183500	2.03218800
Cl	-2.34903200	-0.49296600	2.27285800
Cl	2.61437400	0.57180500	-2.54910500
Cl	0.48164900	3.27755800	-1.67140100
Cl	1.35124800	-2.73157900	-2.08398200
Cl	-3.86668500	-0.48275900	-1.10353300
Cl	-2.68852100	2.63127000	-0.54653000
H	0.77667000	-1.62550000	2.91950800
Si	-0.56740300	0.06994000	-1.98497100

H/[SiB₁₃HCl₁₃]

Lowest normal mode frequency: 70.89 cm⁻¹

B	0.05588400	-0.00006900	1.41246900
B	1.50658200	0.92622500	-1.02568400
B	-0.08015000	1.84256200	-0.92630400
B	-1.66351100	0.92130700	-0.81149300
B	1.67055100	-0.00134900	0.45019400
B	0.88289700	-1.55034600	0.52793800
B	-0.86842800	1.54410700	0.65495300
B	0.88533400	1.54885900	0.52796000
H	-0.21777600	0.00014000	-3.48256800
B	1.50518500	-0.92863000	-1.02566300
B	-0.87084100	-1.54273500	0.65492200

B	-1.74200300	0.00137000	0.72063100
B	-0.08302200	-1.84243600	-0.92633500
B	-1.66494600	-0.91867200	-0.81150400
Cl	0.35242300	-0.00025100	3.19633900
Cl	-1.56891300	2.88839800	1.58422800
Cl	-3.22019200	0.00243500	1.70819900
Cl	1.75627200	2.85804800	1.37687500
Cl	3.28265500	-0.00257300	1.47323400
Cl	1.75183800	-2.86074900	1.37697400
Cl	-1.57348500	-2.88593400	1.58418500
Cl	-0.11561900	3.40965700	-1.76546100
Cl	2.86774700	1.69533200	-1.87888400
Cl	2.86514100	-1.69977200	-1.87887400
Cl	-3.07194000	1.70462700	-1.56161500
Cl	-3.07459200	-1.69978100	-1.56171300
Cl	-0.12093600	-3.40945000	-1.76552600
H	2.54838700	-0.00246700	2.58665200
Si	-0.15821800	0.00011000	-2.02213000

H/[SiB₅H(CN)₅]

Lowest normal mode frequency: 53.91 cm⁻¹

B	-0.00005800	-0.00006500	0.74054100
B	0.89784100	0.89948800	-0.37154100
B	-0.89779800	-0.89933000	-0.37191400
B	-0.89931200	0.89794500	-0.37170100
B	0.89942100	-0.89778200	-0.37174800
C	-1.97309600	1.96935500	-0.21886700
N	-2.78375800	2.77815700	-0.08885500
C	-1.96960200	-1.97273700	-0.21918900
N	-2.77873900	-2.78307200	-0.08922100
C	1.97311400	-1.96928700	-0.21894500
N	2.78369500	-2.77817400	-0.08895700
C	1.96968700	1.97282400	-0.21862200
N	2.77887100	2.78309900	-0.08858100
C	-0.00036500	-0.00043600	2.24632600
N	-0.00029900	-0.00041600	3.39352100
H	0.00033700	0.00054100	-3.37619600
H	0.00011300	-0.00002600	4.39537900
Si	0.00016200	0.00019500	-1.91263900

H/[SiB₆H(CN)₆]

Lowest normal mode frequency: 52.77 cm⁻¹

B	0.34716300	-1.38299600	-0.30010700
B	1.29865800	-0.00172700	-0.37865000
B	-1.25498000	-0.85468000	-0.20205000
B	-1.25283100	0.85775800	-0.20206200

B	0.35063800	1.38198500	-0.30017200
H	-0.22502900	0.00021200	-3.23735400
B	-0.03973300	0.00001500	0.80487700
C	0.13296700	-0.00014500	2.32748100
N	0.31167900	-0.00033800	3.46494200
C	-2.47221800	1.75888200	-0.04058100
N	-3.39171500	2.44563000	0.05675400
C	0.92529900	2.79459200	-0.22948900
N	1.41989900	3.83486400	-0.19925200
C	2.80654900	-0.00306200	-0.23725000
N	3.94396600	-0.00457100	-0.09661300
C	0.91802100	-2.79713800	-0.22940000
N	1.40965500	-3.83881500	-0.19918500
C	-2.47666100	-1.75269700	-0.04056900
N	-3.39788900	-2.43712300	0.05676000
H	4.93584700	-0.00487100	0.05255200
Si	-0.21630700	0.00019700	-1.77209900

H/[SiB₇H(CN)₇]

Lowest normal mode frequency: 53.3 cm⁻¹

B	-1.23755800	-0.89934300	-0.56338400
B	1.16110300	0.13377800	0.61635600
B	-0.53763400	-0.11386600	0.91040300
B	-1.51809500	0.73684500	-0.28193800
B	0.06668800	1.41028200	0.11943400
B	0.41865400	-1.13024600	-0.25403800
B	1.37107500	0.41002200	-1.01465800
C	0.97182300	-2.55256800	-0.11201800
N	1.36347000	-3.62127500	0.00654200
C	2.30567000	0.03048500	1.62146600
N	3.17251500	-0.11817000	2.36498100
C	2.76866500	0.56751400	-1.59941300
N	3.81616900	0.64256000	-2.07472600
C	0.25671100	2.87797900	0.49899500
N	0.41077600	3.98977100	0.75670600
C	-1.05137800	-0.47065400	2.31143300
N	-1.42830500	-0.78023500	3.35423600
C	-2.21984800	-2.03744300	-0.81661000
N	-2.90355800	-2.94018200	-1.03155400
H	-0.77108800	0.92396100	-3.24457200
C	-2.85563400	1.46393100	-0.23366900
N	-3.86762300	2.01419300	-0.23119100
H	1.70725900	-4.55566200	0.13564900
Si	-0.32553500	0.52230300	-1.89914300

H/[SiB₈H(CN)₈]

Lowest normal mode frequency: 46.1 cm⁻¹

B	0.95084600	-0.75652600	-0.88814400
B	1.36856000	1.05418100	-0.73908600
B	1.44959900	0.06345700	0.56977600
B	-1.36875400	1.05400300	-0.73895800
B	-0.00004400	0.93417000	0.94795700
B	0.00003700	-0.84880900	0.65311100
B	-0.95085800	-0.75662200	-0.88808500
B	-1.44962800	0.06327000	0.56989800
C	0.00019600	-2.06139800	1.60855500
N	0.00041700	-2.94469700	2.33199900
C	2.63465700	-0.18950900	1.49997400
N	3.48503200	-0.45813700	2.22866700
C	-0.00006500	1.86514700	2.15624200
N	-0.00006000	2.57216900	3.06592200
C	-2.63458800	-0.18981400	1.50018500
N	-3.48489100	-0.45850000	2.22894000
C	1.73138600	-1.90315700	-1.54212100
N	2.30474600	-2.78005600	-2.02024400
C	-1.73128200	-1.90331400	-1.54209400
N	-2.30454300	-2.78025100	-2.02026500
C	2.48137300	2.05056600	-1.03014500
N	3.30441100	2.81807000	-1.27898400
C	-2.48165500	2.05029400	-1.03000600
N	-3.30475600	2.81773000	-1.27884900
H	-0.00030100	0.61492700	-3.56148200
H	0.00054600	-3.71517200	2.97741200
Si	-0.00011700	0.66053000	-2.09800800

H/[SiB₉H(CN)₉]

Lowest normal mode frequency: 56.09 cm⁻¹

B	-0.00058600	-0.00031400	1.56874500
B	-1.17272100	-0.60516200	0.52592400
B	-0.60525400	1.17243400	0.52652200
B	1.17235000	0.60496200	0.52709800
B	0.60487000	-1.17263700	0.52650000
B	-1.29853400	0.41486700	-0.96940100
B	0.41504600	1.29912300	-0.96854600
B	1.29929900	-0.41445900	-0.96856200
B	-0.41427800	-1.29871000	-0.96941700
H	0.00154300	0.00083700	-3.87425200
C	-0.85587900	-2.68253500	-1.45981400
N	-1.18339200	-3.70898900	-1.86602100
C	1.25237800	-2.42802700	1.12239800
N	1.72592100	-3.34625500	1.63006400

C	-2.42820000	-1.25303000	1.12124600
N	-3.34651000	-1.72686400	1.62849100
C	-0.00126700	-0.00069200	3.08544400
N	-0.00181400	-0.00097700	4.22789400
C	2.42739600	1.25259600	1.12358200
N	3.34534400	1.72624300	1.63165500
C	-1.25325100	2.42756700	1.12243100
N	-1.72720500	3.34558000	1.63010000
C	0.85701800	2.68314500	-1.45805200
N	1.18486900	3.70974400	-1.86361900
C	2.68341100	-0.85613500	-1.45808200
N	3.71008300	-1.18374200	-1.86366000
C	-2.68226900	0.85676000	-1.45978600
N	-3.70865000	1.18451200	-1.86598400
H	-0.00228100	-0.00117900	5.23258600
Si	0.00094500	0.00051200	-2.41509200

H/[SiB₁₀H(CN)₁₀]

Lowest normal mode frequency: 55.20 cm⁻¹

B	-0.11843100	-1.33714300	-0.71376100
B	1.45799800	0.58536600	0.48443100
B	-1.44681000	1.10135900	-0.16835700
B	0.31952200	1.59580200	-0.47074100
B	-0.21510300	0.86400200	1.09102100
B	1.53715000	-1.03426700	-0.20063400
B	-1.73105100	-0.50109600	-1.05755300
B	1.27352200	0.22107800	-1.26627200
B	0.46270700	-0.76569800	1.05127300
B	-1.27357100	-0.50138100	0.58216000
H	-0.68131500	1.39440500	-3.34994200
C	0.65620100	-1.51567200	2.38839600
N	0.81882400	-2.06910700	3.37222400
C	2.66079600	1.18153700	1.22160000
N	3.56577500	1.58538700	1.80649800
C	2.68483500	-2.03533000	-0.18124500
N	3.54058900	-2.80119300	-0.09999400
C	-0.21621600	-2.77119500	-1.24048500
N	-0.29070100	-3.85398700	-1.62552900
C	-0.38908700	1.55967000	2.44726300
N	-0.49967200	2.00763400	3.50160300
C	-2.19687300	-1.22654200	1.57399500
N	-2.79207600	-1.80636400	2.37093700
C	0.68279200	3.06163700	-0.73645400
N	0.94069000	4.15785300	-0.97525400
C	2.17887000	0.38798600	-2.49022900

N	2.79928300	0.51245400	-3.45344000
C	-2.57152700	2.12001500	0.02797200
N	-3.42343600	2.88579000	0.14024700
C	-3.02400100	-1.17358700	-1.49957000
N	-4.00085900	-1.66406300	-1.86125900
H	0.93908800	-2.54832400	4.24847600
Si	-0.64222200	0.70013400	-2.06114700

H/[SiB₁₁H(CN)₁₁]

Lowest normal mode frequency: 61.71 cm⁻¹

B	-1.58999500	0.13501300	-0.94840500
B	-0.61976300	-1.47028700	-0.94852600
B	-0.36293500	1.55389900	-0.94844600
B	1.36556100	0.82531900	-0.94859200
B	1.20680500	-1.04369800	-0.94866600
B	1.52920300	-0.12991200	0.54638700
B	0.59607900	1.41414800	0.54657400
B	-1.16076900	1.00387000	0.54663300
B	0.34904300	-1.49445400	0.54643600
B	-1.31340900	-0.79376800	0.54660100
B	0.00009100	-0.00007700	1.42504600
H	-0.00028900	0.00016400	-3.70135600
C	0.00019700	-0.00015100	2.97269200
N	0.00042300	-0.00024900	4.11172300
C	1.10937900	2.63182100	1.32394400
N	1.47786200	3.50566700	1.97548000
C	2.84600000	-0.24179200	1.32363200
N	3.79111700	-0.32208000	1.97490300
C	-2.16026600	1.86829700	1.32404500
N	-2.87751800	2.48876900	1.97552900
C	-2.44434300	-1.47728800	1.32407500
N	-3.25581700	-1.96792400	1.97573000
C	0.64958800	-2.78137500	1.32372400
N	0.86543900	-3.70482200	1.97526600
C	-1.15795400	-2.74705100	-1.60129200
N	-1.55508800	-3.68893700	-2.13001600
C	-2.97060500	0.25223100	-1.60107700
N	-3.98926700	0.33864500	-2.12957100
C	-0.67807600	2.90313700	-1.60113700
N	-0.91079400	3.89867900	-2.12948800
C	2.55131700	1.54194600	-1.60143100
N	3.42614600	2.07086500	-2.12996200
C	2.25471900	-1.95003100	-1.60157000
N	3.02797700	-2.61866900	-2.13021100
H	0.00036900	-0.00010100	5.11860100

Si -0.00019500 0.00011500 -2.24155500

H/[SiB₁₂H(CN)₁₂]

Lowest normal mode frequency: 25.77 cm⁻¹

B	1.31259600	-0.08055100	1.34541600
B	-0.25259300	-0.10373000	1.72708000
B	1.86699700	0.01037100	-0.16475500
B	0.49429200	1.36344000	0.54104900
B	-1.37882200	0.85080400	0.71621800
B	0.92420300	1.01057700	-1.30404100
B	0.92466000	-0.84694300	-1.41555900
B	-1.37867800	-0.93079700	0.60942000
B	-0.75118600	1.53660400	-0.78331500
B	-0.75062100	-1.43213700	-0.96142100
B	-1.90249000	0.04467000	-0.75022000
H	-0.93039700	0.22381200	-3.72830900
B	0.49468700	-1.41815600	0.37410800
C	-0.54589000	-0.19420700	3.23100500
N	-0.63159000	-0.26324200	4.37733200
C	2.33113700	-0.14968400	2.49263200
N	3.08513900	-0.20128500	3.34637000
C	3.39410200	0.01987900	-0.31713800
N	4.54573300	0.01977700	-0.31189500
C	0.99645200	2.67398700	1.16407900
N	1.43272600	3.60124700	1.68839300
C	-2.36929900	1.67734100	1.54076300
N	-3.09916000	2.31104600	2.16518900
C	-2.36897900	-1.85029800	1.32906000
N	-3.09869300	-2.55434200	1.87315500
C	0.99739900	-2.79360100	0.83603100
N	1.43419900	-3.77661900	1.24582900
C	1.78652500	1.95038500	-2.15439700
N	2.41282000	2.65199300	-2.81831400
C	1.78740700	-1.67816200	-2.37191000
N	2.41412700	-2.29519400	-3.11472100
C	-1.22746200	2.92643200	-1.21910400
N	-1.58681500	3.95164100	-1.59925500
C	-3.35492800	0.07379800	-1.23699200
N	-4.42340200	0.09949600	-1.66405100
C	-1.22666300	-2.75991400	-1.56040300
N	-1.58613300	-3.73216400	-2.06059500
H	3.74506700	-0.24717600	4.10481400
Si	-0.59438300	0.13859900	-2.31001600

H/[SiB₁₃H(CN)₁₃]

Lowest normal mode frequency: 62.42 cm⁻¹

B	0.00000000	-0.00001300	1.32078000
B	-1.33758800	1.24963100	-0.93877800
B	-1.75103300	-0.53361700	-0.93877100
B	-0.41346400	-1.78326000	-0.93878600
B	-0.51415600	1.68713100	0.56463800
B	1.20395300	1.28876800	0.56472800
B	-1.20395200	-1.28877900	0.56470100
B	-1.71808900	0.39830100	0.56466400
H	-0.00000500	0.00003400	-3.53317900
B	0.41345800	1.78328300	-0.93874300
B	1.71808900	-0.39831200	0.56464400
B	0.51415600	-1.68714300	0.56459100
B	1.75102700	0.53364100	-0.93876600
B	1.33758100	-1.24960700	-0.93881600
C	0.00001900	-0.00007900	2.88259300
N	0.00001400	-0.00009400	4.02095900
C	-2.07495800	-2.22114700	1.41289200
N	-2.69956700	-2.88972000	2.11084900
C	0.88613400	-2.90765700	1.41274800
N	1.15280300	-3.78291200	2.11068600
C	2.96106200	-0.68647700	1.41280200
N	3.85228700	-0.89315700	2.11083900
C	2.07496600	2.22111600	1.41293300
N	2.69957900	2.88968000	2.11089400
C	-0.88613400	2.90763600	1.41280700
N	-1.15280800	3.78289800	2.11073400
C	-2.96106400	0.68644300	1.41282600
N	-3.85229400	0.89311700	2.11085700
C	0.71872500	3.10005700	-1.65377300
N	0.94490600	4.07534900	-2.22140400
C	3.04400200	0.92762000	-1.65378400
N	4.00186900	1.21953800	-2.22104900
C	2.32531900	-2.17232000	-1.65384600
N	3.05713600	-2.85571500	-2.22124800
C	-0.71873200	-3.10001700	-1.65384500
N	-0.94489200	-4.07530300	-2.22149600
C	-3.04401200	-0.92757900	-1.65379300
N	-4.00187900	-1.21948500	-2.22106300
C	-2.32532700	2.17236300	-1.65378200
N	-3.05714100	2.85578100	-2.22115900
H	0.00009800	-0.00012200	5.02932500
Si	-0.00000700	0.00002700	-2.07186100

H/[SiB₅F₆]

Lowest normal mode frequency: 58.79 cm⁻¹

B	0.15187600	-1.40334700	-0.53374800
B	-1.22533600	-0.46246600	-0.87275700
B	1.08463100	-0.23274100	0.60486400
B	1.46769600	0.93675800	-0.54373600
B	-0.63521600	-0.59495200	0.73517000
H	-0.24001400	-0.82446900	-1.68671400
F	-1.30160100	-1.01736500	1.82796900
F	-2.38626500	-0.47526700	-1.52577300
F	2.47399500	1.38410900	-1.25080000
F	1.91553600	-0.71403500	1.56407400
F	0.66654900	-2.59633800	-0.80862600
F	-1.29622500	2.43705700	0.66491300
Si	-0.33043800	1.31748300	0.03513800

H/[SiB₆F₇]

Lowest normal mode frequency: 36.89 cm⁻¹

B	0.93478700	-1.16034800	-0.53114000
B	-0.93185400	-1.16351200	-0.53226900
B	1.34883700	0.50800700	-0.11359700
B	-0.00221300	1.46723000	0.40109900
B	-1.34978800	0.50331500	-0.11615400
B	0.00046900	0.76707900	-1.19380000
H	0.00262100	-1.35700700	-1.44991500
F	1.88654900	-2.07612900	-0.73873000
F	2.66735400	0.79682400	-0.06047400
F	0.00088500	1.12600000	-2.47265800
F	-0.00586600	2.70587100	0.91479000
F	-2.66870400	0.79105000	-0.06431800
F	-1.87951300	-2.08322500	-0.74096500
F	-0.00062700	-0.95736100	2.66606300
Si	-0.00032200	-0.42707900	1.16756000

H/[SiB₇F₈]

Lowest normal mode frequency: 16.45 cm⁻¹

B	-0.43665200	-0.40652300	-1.32360100
B	1.30654200	-0.33843300	0.89036200
B	-0.18227200	-1.53506600	0.00721800
B	-1.54732000	-0.51852500	0.00469800
B	-0.43280700	-0.39577900	1.32793800
B	1.30339400	-0.34258800	-0.89587500
B	1.12609400	1.30037000	-0.00509500
H	1.75191100	-1.22623900	-0.00062400
F	0.02281100	-2.84980700	0.01150800
F	-2.87745600	-0.71778900	0.00619300
F	-0.67667100	-0.46792700	2.64789700
F	2.20515400	-0.39191800	1.88657400

F	2.19978500	-0.40178600	-1.89358400
F	-0.68986300	-0.49028400	-2.64136700
F	2.14095100	2.14866400	-0.00719100
F	-1.94638100	2.44045900	-0.00546600
Si	-0.77441300	1.35589000	-0.00490600

H/[SiB₈F₉]

Lowest normal mode frequency: 79.54 cm⁻¹

B	1.13183800	1.27635100	-0.78408600
B	0.60905200	0.67824300	1.00391500
B	1.81953600	-0.08684700	-0.03756800
B	-0.96309100	-0.14917100	0.88767300
B	0.59548500	-1.14624300	0.72719200
B	0.99534300	-1.21453700	-0.97112500
B	-1.83058600	-0.11274200	-0.76903300
B	-0.83404200	-1.49226600	-0.32036800
H	-0.88734000	-0.88997600	-1.49700800
F	0.84057300	-2.09678500	1.64714200
F	1.35507800	-2.03306900	-1.92581700
F	3.16242000	-0.14076100	0.15895800
F	0.90391500	1.34652700	2.12796600
F	-1.75702400	-0.20087400	1.97420800
F	-3.09876200	-0.30666000	-1.11685500
F	-1.36253200	-2.72893600	-0.29497100
F	1.99560200	2.15417300	-1.29280500
F	-1.53106000	2.92859400	-0.12441400
Si	-0.80744400	1.55901200	-0.54047800

H/[SiB₉F₁₀]

Lowest normal mode frequency: 87.49 cm⁻¹

B	-1.83954500	0.00000000	0.51575900
B	-0.62267900	0.00000100	1.62613200
B	-0.81614600	-1.35578900	0.34350400
B	-0.92369200	0.00000000	-0.91912400
B	-0.81614500	1.35579000	0.34350300
B	0.84431200	-0.90928400	0.79349200
B	0.43056000	-1.24144600	-1.08006900
B	0.43056100	1.24144600	-1.08006900
B	0.84431300	0.90928400	0.79349200
H	-2.90681700	0.00000000	-1.35792100
F	1.64664800	1.68837400	1.55734100
F	1.64664700	-1.68837400	1.55734200
F	-0.59761300	0.00000100	2.96636200
F	-1.35336700	2.59860600	0.36565700
F	-3.21606500	0.00000100	0.22124300
F	-2.14421100	0.00000000	-1.96887000

F	0.27766100	2.29348800	-1.89422600
F	0.27766000	-2.29348900	-1.89422500
F	-1.35336800	-2.59860500	0.36565800
F	3.51106300	0.00000000	-0.60627100
Si	1.92811600	-0.00000100	-0.81109000

H/[SiB₁₀F₁₁]

Lowest normal mode frequency: 86.93 cm⁻¹

B	1.49449900	-0.34343100	0.00000000
B	-1.10257500	-1.41505500	0.87740100
B	-0.83153400	0.61404500	-1.59003300
B	-0.83153400	0.61404500	1.59003300
B	-1.10257500	-1.41505500	-0.87740100
B	0.41055900	-0.61219400	1.45836800
B	0.86725900	1.11058400	-0.88039100
B	0.86725900	1.11058400	0.88039100
B	0.40774100	-1.73422700	0.00000000
B	0.41055900	-0.61219400	-1.45836800
H	-1.92185600	-0.83308200	0.00000000
F	1.64896400	1.89777300	-1.64055000
F	-1.41565800	0.82770500	-2.75975400
F	1.64896400	1.89777300	1.64055000
F	-1.41565800	0.82770500	2.75975400
F	0.90562600	-1.09895200	2.62151500
F	-1.78645900	-2.20066700	1.70481300
F	0.99022800	-2.95203600	0.00000000
F	-1.78645900	-2.20066700	-1.70481300
F	0.90562600	-1.09895200	-2.62151500
F	2.81124600	-0.59178500	0.00000000
F	-1.16648600	3.41845400	0.00000000
Si	-0.93470200	1.83645800	0.00000000

H/[SiB₁₁F₁₂]

Lowest normal mode frequency: 125.43 cm⁻¹

B	-1.38813100	-1.09881900	0.00000000
B	-0.31398500	-0.79399700	1.55387100
B	-0.31398500	-0.79399700	-1.55387100
B	1.45497100	-0.28110500	-0.96769900
B	1.45497100	-0.28110500	0.96769900
B	1.19047400	1.18073200	0.00000000
B	0.19401800	0.90316300	-1.47026500
B	-1.47110300	0.45191700	-0.91904600
B	0.19401800	0.90316300	1.47026500
B	-1.47110300	0.45191700	0.91904600
B	-0.50083800	1.57424000	0.00000000
H	0.48061700	3.31695000	0.00000000

F	-2.42680200	-1.96572100	0.00000000
F	-2.57826200	0.77192700	-1.62752800
F	-2.57826200	0.77192700	1.62752800
F	-0.47649300	3.13289600	0.00000000
F	0.39424400	1.70110900	2.55471900
F	1.90842700	2.39206700	0.00000000
F	2.56186500	-0.50758100	1.71079300
F	2.56186500	-0.50758100	-1.71079300
F	-0.53330000	-1.42980300	2.72797300
F	-0.53330000	-1.42980300	-2.72797300
F	0.39424400	1.70110900	-2.55471900
F	0.96807200	-3.36336500	0.00000000
Si	0.52944300	-1.84301000	0.00000000

H/[SiB₁₂F₁₃]

Lowest normal mode frequency: 25.89 cm⁻¹

B	-1.90010300	0.81359400	0.00273900
B	-1.56618800	-0.85033400	-0.00436500
B	-0.97599600	2.07035300	0.00239300
B	-0.89714000	0.07418700	-1.42716800
B	-0.26279100	-1.59265100	-0.91480900
B	0.50968900	1.39312000	-0.93807400
B	0.50565500	1.38586600	0.94924900
B	-0.26483700	-1.60024900	0.90285700
B	0.87209100	-0.36758200	-1.50365900
B	0.86827200	-0.37878800	1.50377000
B	1.26827200	-1.46466500	-0.00368300
B	-0.90030200	0.06173200	1.42661700
H	-3.59341300	-0.26959200	-0.00202000
F	-0.54006400	-2.72275500	1.60973700
F	-2.85265300	-1.47295500	-0.00830700
F	-3.46355400	0.72623400	0.00259600
F	-1.50312500	0.19261900	2.63199400
F	-1.05945700	3.38523400	0.00298800
F	0.78090600	2.35678900	1.85617100
F	0.79199200	2.36960300	-1.83712300
F	1.43403200	-0.50066200	2.72684400
F	1.44158800	-0.48073100	-2.72583600
F	2.16741500	-2.47544000	-0.00651100
F	-0.53714200	-2.70915800	-1.63149500
F	-1.49781500	0.21285600	-2.63264300
F	3.59260500	0.72651300	0.00661500
Si	2.03698200	0.43381100	0.00481700

H/[SiB₁₃F₁₄]

Lowest normal mode frequency: 135.67 cm⁻¹

B	-0.17459200	-0.00683100	-1.64243500
B	-0.86434300	1.57957600	0.84721500
B	0.95313100	1.66845200	0.55609600
B	1.94343900	0.09717900	0.40712200
B	-1.52102600	0.76674300	-0.54914300
B	-1.49497000	-0.94904900	-0.58744100
B	1.36568400	0.96840100	-1.04072900
B	-0.18181500	1.80427900	-0.81349100
B	-1.66991300	-0.10382900	0.97383700
B	-0.00676600	-1.79667400	-0.84662400
B	1.45347600	-0.80582200	-1.05513900
B	-0.71217500	-1.67921600	0.80754300
B	1.11209900	-1.57029000	0.52532200
H	-3.15472100	0.10034700	-1.44087600
F	-2.82350100	-0.14041300	1.68175700
F	-1.17840900	-2.72845000	1.51310000
F	1.85415300	-2.55997300	1.06350900
F	3.20750800	0.15567800	0.87335000
F	-0.06754600	-2.94055500	-1.56332600
F	-2.70856700	-1.30143900	-1.23922400
F	-0.47198600	0.00768700	-2.96353300
F	-2.86467800	1.04036100	-1.25054600
F	-0.38784800	2.94147200	-1.51420200
F	1.58977800	2.72159500	1.10810600
F	-1.45941800	2.55312200	1.56281200
F	2.21932900	1.58516900	-1.88752300
F	2.36528800	-1.31559700	-1.91146900
F	0.50035700	-0.00307100	3.31549200
Si	0.29810300	-0.00751600	1.74539100

H/[SiB₅Cl₆]

Lowest normal mode frequency: 44.84 cm⁻¹

B	0.63405500	-1.13987600	-0.40933500
B	-0.92592600	-0.72582500	-0.98753900
B	0.91696300	0.22381700	0.73093800
B	1.13153900	1.17891200	-0.64418800
B	-0.57075700	-0.63240100	0.69032200
Cl	1.74761800	-2.48833100	-0.56297500
Cl	-1.48683600	-1.40296900	1.99231300
Cl	2.02875300	0.27209400	2.11892000
Cl	2.37889700	1.83759800	-1.62754500
Cl	-2.22994800	-1.34647500	-1.98390700
H	0.21577800	-0.81068700	-1.64430900
Cl	-2.19551300	2.48344200	0.47369200
Si	-0.73397600	1.23188900	-0.15965400

H/[SiB₆Cl₇]**Lowest normal mode frequency: 65.73 cm⁻¹**

B	0.92425600	-1.14330100	-0.53166200
B	-0.92424300	-1.14331600	-0.53165700
B	1.35156200	0.48629300	-0.07340400
B	-0.00001000	1.41856200	0.44737800
B	-1.35157000	0.48627200	-0.07339900
B	-0.00000700	0.73250800	-1.15118100
Cl	-0.00001700	1.31512900	-2.79984900
Cl	3.05788200	0.94669400	0.00799700
Cl	-0.00002200	3.04736600	1.11459900
Cl	2.12298200	-2.39964000	-0.85705600
Cl	-2.12295100	-2.39967500	-0.85704500
Cl	-3.05789600	0.94665000	0.00800800
H	0.00000600	-1.33618100	-1.44128300
Cl	0.00002000	-1.23644700	3.04784400
Si	0.00000600	-0.47073000	1.19389000

H/[SiB₇Cl₈]**Lowest normal mode frequency: 4.64 cm⁻¹**

B	0.43933600	1.35349400	-0.24960300
B	-1.29881900	-0.66092800	0.66606800
B	0.16741100	0.61809200	1.31947800
B	1.52954800	0.18315600	0.40681100
B	0.42458000	-1.06062300	0.87959900
B	-1.28868800	0.94621300	-0.09108700
B	-1.08674700	-0.55003200	-1.17583000
Cl	-2.53877000	-1.72870600	1.35246600
Cl	-2.51576100	2.16603500	-0.48420500
Cl	0.01448400	1.36232100	2.90559600
Cl	-2.35766800	-1.06127500	-2.26340200
Cl	0.86010500	2.94358400	-0.87848300
Cl	0.82875600	-2.56585000	1.69947300
Cl	3.26408900	0.32202600	0.72770400
H	-1.76754500	0.50613300	1.05400600
Cl	2.20515400	-1.21936400	-2.58867800
Si	0.81484400	-0.59800700	-1.27351300

H/[SiB₈Cl₉]**Lowest normal mode frequency: 54.39 cm⁻¹**

B	1.30278000	1.06812800	-0.92741900
B	0.65795800	0.71816800	0.87367000
B	1.76128500	-0.29236400	-0.05924800
B	-1.02395500	0.09481200	0.76179500
B	0.38771800	-1.07215000	0.75275900
B	0.82464000	-1.38807200	-0.91529000

B	-1.77860000	0.11128100	-0.91685700
B	-1.02510500	-1.35244200	-0.32275800
Cl	3.46879000	-0.65908800	0.30560000
Cl	0.60350500	-2.24500400	2.06584800
Cl	1.23043800	-2.59950300	-2.06452500
Cl	-1.97658500	-2.84305700	-0.23268500
Cl	1.17612600	1.67841400	2.26358200
Cl	2.50961600	2.04973600	-1.72825500
Cl	-3.41838400	0.13136000	-1.51972100
Cl	-2.15275000	0.28778000	2.11660000
H	-0.94403600	-0.84194700	-1.53506000
Cl	-1.24076500	3.51553300	-0.32820600
Si	-0.57067300	1.64501800	-0.68773100

H/[SiB₉Cl₁₀]

Lowest normal mode frequency: 56.32 cm⁻¹

B	-0.42919300	-1.82159000	0.00000000
B	-1.52535800	-0.56376100	0.00000000
B	-0.22953500	-0.79744300	1.32931600
B	1.02213400	-0.99009000	0.00000000
B	-0.22953500	-0.79744300	-1.32931600
B	-0.85243500	0.86534500	0.97268200
B	1.07706900	0.48821100	1.01057100
B	1.07706900	0.48821100	-1.01057100
B	-0.85243500	0.86534500	-0.97268200
Cl	-0.38294400	-3.62471800	0.00000000
Cl	-0.30535700	-1.46568300	-2.98115500
Cl	-3.28461300	-0.82834600	0.00000000
Cl	2.41808300	-2.24631000	0.00000000
Cl	-0.30535700	-1.46568300	2.98115500
Cl	-1.90021900	1.69901200	-2.15534600
Cl	2.38552100	0.69617800	-2.21050000
Cl	-1.90021900	1.69901200	2.15534600
Cl	2.38552100	0.69617800	2.21050000
H	1.42368100	-3.24702900	0.00000000
Cl	0.73805400	4.01242700	0.00000000
Si	0.41881700	2.04556500	0.00000000

H/[SiB₁₀Cl₁₁]

Lowest normal mode frequency: 56.43 cm⁻¹

B	-0.20156800	0.00000000	1.45278000
B	-1.41592500	0.87970300	-1.06581300
B	0.58306600	-1.58138400	-0.92346000
B	0.58306600	1.58138400	-0.92346000
B	-1.41592500	-0.87970300	-1.06581300
B	-0.55484400	1.46050400	0.40394800

B	1.18252400	-0.88721500	0.71495600
B	1.18252400	0.88721500	0.71495600
B	-1.66010000	0.00000000	0.45476900
B	-0.55484400	-1.46050400	0.40394800
Cl	-3.25044700	0.00000000	1.23919500
Cl	-1.13707200	2.98401400	1.11880000
Cl	-0.38099000	0.00000000	3.20904100
Cl	-2.53710700	1.88157900	-1.96619000
Cl	-2.53710700	-1.88157900	-1.96619100
Cl	-1.13707100	-2.98401400	1.11880000
Cl	2.32181900	1.87694900	1.64478100
Cl	0.90428100	3.05874900	-1.78973800
Cl	0.90428100	-3.05874800	-1.78973800
Cl	2.32181900	-1.87694900	1.64478100
H	-0.87392200	0.00000000	-1.89508500
Cl	3.76355300	0.00000000	-1.52029600
Si	1.80162500	0.00000000	-1.06958000

H/[SiB₁₁Cl₁₂]

Lowest normal mode frequency: 88.12 cm⁻¹

B	1.42266800	1.05129900	0.00000000
B	0.34061000	0.80114500	1.53243200
B	0.34061000	0.80114500	-1.53243200
B	-1.41678000	0.38249600	-0.95079700
B	-1.41678000	0.38249600	0.95079700
B	-1.27114700	-1.10945500	0.00000000
B	-0.25373000	-0.87386400	-1.46869500
B	1.42100900	-0.49192400	-0.90950500
B	-0.25373000	-0.87386400	1.46869500
B	1.42100900	-0.49192400	0.90950500
B	0.40949400	-1.60032100	0.00000000
Cl	0.59614900	-3.46803300	0.00000000
Cl	-2.47944900	-2.45814300	0.00000000
Cl	-0.54184100	-1.83677600	2.94336200
Cl	2.84579400	-1.03738200	1.82911900
Cl	2.84579400	-1.03738200	-1.82911900
Cl	-0.54184100	-1.83677600	-2.94336200
Cl	0.64557000	1.65892900	-3.06203800
Cl	-2.86762900	0.79851800	-1.89536100
Cl	-2.86762900	0.79851800	1.89536100
Cl	0.64557000	1.65892900	3.06203800
Cl	2.80868300	2.16738200	0.00000000
H	-0.76284500	-3.56041100	0.00000000
Cl	-0.90394200	3.83204200	0.00000000
Si	-0.43587300	1.89980000	0.00000000

H/[SiB₁₂Cl₁₃]**Lowest normal mode frequency: 47.42 cm⁻¹**

B	0.66324700	-1.52609900	-0.50108400
B	1.15822700	-0.01904400	-1.21140200
B	-1.02834000	-1.66691400	0.06344300
B	-0.60436700	-0.40549500	-1.47152800
B	0.13789400	1.38432200	-1.16198900
B	-2.10431400	-0.46617200	-0.38038100
B	0.44684800	-1.27460400	1.23295900
B	1.47346000	1.23528400	0.00387800
B	-1.55094000	1.11172300	-0.51497900
B	0.85055800	0.50978900	1.52848900
B	-0.11628500	1.75834200	0.56051700
B	1.78825200	-0.49848000	0.39167600
Cl	1.37505300	-2.98053900	-1.34713200
Cl	2.29791600	-0.31818000	-2.66128100
Cl	-1.63533600	-3.33539800	0.16203600
Cl	-1.04236900	-0.87074600	-3.14044100
Cl	0.25704000	2.56811900	-2.48949700
Cl	2.85746600	2.35126300	-0.04863300
Cl	3.46849100	-1.02162700	0.67507600
Cl	-2.74298300	2.33745400	-0.98963100
Cl	-0.36717100	3.37730700	1.24881800
Cl	-3.79810500	-0.85411600	-0.67835000
Cl	0.72157100	-2.47341600	2.51604200
Cl	1.43425500	0.96659000	3.14302300
H	2.15250700	-1.69425100	-2.37836300
Cl	-2.29919900	0.23418300	3.03945300
Si	-1.19117100	0.09327000	1.38422400

H/[SiB₁₃Cl₁₄]**Lowest normal mode frequency: 67.09 cm⁻¹**

B	-1.60116700	-0.21240300	0.00000000
B	0.95582500	-1.44305300	0.92946100
B	0.71486400	0.13301500	1.84711600
B	0.45961200	1.70291000	0.92227000
B	-0.49953900	-1.73567300	0.00000000
B	-0.64635700	-0.95846600	-1.54932300
B	-0.92932700	0.77726600	1.54347400
B	-0.64635700	-0.95846600	1.54932300
B	0.95582500	-1.44305300	-0.92946100
B	-0.92932700	0.77726600	-1.54347400
B	-1.07264300	1.63977200	0.00000000
B	0.71486400	0.13301500	-1.84711600
B	0.45961200	1.70291000	-0.92227000

Cl	-3.35132500	-0.66864000	0.00000000
Cl	-1.91785600	1.39265500	2.88676700
Cl	-2.18724000	3.02451200	0.00000000
Cl	-1.41479100	-1.89853000	2.86030100
Cl	-1.38381000	-3.42637000	0.00000000
Cl	-1.41479100	-1.89853000	-2.86030100
Cl	-1.91785600	1.39265500	-2.88676700
Cl	1.54777400	0.24376400	3.41051900
Cl	1.93003700	-2.71748200	1.69662800
Cl	1.93003700	-2.71748200	-1.69662800
Cl	1.08093300	3.17032000	1.70367900
Cl	1.08093300	3.17032000	-1.70367900
Cl	1.54777400	0.24376400	-3.41051900
H	-2.55435700	-2.78314800	0.00000000
Cl	3.75919700	0.56857300	0.00000000
Si	1.78297600	0.30399300	0.00000000

H/[SiB₅(CN)₆]

Lowest normal mode frequency: 52.91 cm⁻¹

B	0.00000000	0.00000000	-1.17312000
B	0.00000000	1.27810000	-0.07026100
B	0.00000000	-1.27810000	-0.07026100
B	1.27810000	0.00000000	-0.07026100
B	-1.27810000	0.00000000	-0.07026100
C	2.79223100	0.00000000	-0.22793300
N	3.93582200	0.00000000	-0.36888100
C	0.00000000	-2.79223100	-0.22793300
N	0.00000000	-3.93582200	-0.36888100
C	-2.79223100	0.00000000	-0.22793300
N	-3.93582200	0.00000000	-0.36888100
C	0.00000000	2.79223100	-0.22793300
N	0.00000000	3.93582200	-0.36888100
C	0.00000000	0.00000000	-2.67950700
N	0.00000000	0.00000000	-3.82593000
H	0.00000000	0.00000000	-4.82842700
C	0.00000000	0.00000000	3.25657900
N	0.00000000	0.00000000	4.40875800
Si	0.00000000	0.00000000	1.45400500

H/[SiB₆(CN)₇]

Lowest normal mode frequency: 52.94 cm⁻¹

B	-0.06425700	0.36873700	1.38673700
B	0.04455400	1.31781600	0.00000000
B	-0.21167900	-1.23744500	0.86029500
B	-0.21167900	-1.23744500	-0.86029500
B	-0.06425700	0.36873700	-1.38673700

B	-1.17328200	0.01141500	0.00000000
C	-2.68919600	0.22133600	0.00000000
N	-3.82200800	0.42662100	0.00000000
C	-0.41707300	-2.45057300	-1.75748000
N	-0.55408200	-3.36679800	-2.44152200
C	-0.12009800	0.94029200	-2.79928700
N	-0.14381800	1.43107400	-3.84130100
C	-0.02245700	2.83254700	0.00000000
N	-0.09895200	3.97517900	0.00000000
C	-0.12009800	0.94029200	2.79928700
N	-0.14381800	1.43107400	3.84130100
C	-0.41707300	-2.45057300	1.75748000
N	-0.55408200	-3.36679800	2.44152200
H	-0.18476700	4.97522200	0.00000000
C	3.17549000	-0.26899700	0.00000000
N	4.32776300	-0.26188200	0.00000000
Si	1.36955600	-0.24282400	0.00000000

H/[SiB₇(CN)₈]

Lowest normal mode frequency: 36.49 cm⁻¹

B	0.99804100	0.98764000	-0.59507800
B	-1.49161800	-0.01433100	0.45504700
B	-0.17500900	1.08347300	0.75885800
B	1.35960400	0.19086900	0.83871000
B	-0.11108800	-0.65809300	1.30405600
B	-0.63302800	0.58242800	-0.91738500
B	-0.94056400	-1.29661500	-0.44639500
C	-1.38606700	1.33897200	-2.01871900
N	-1.94192600	1.92387000	-2.82934000
C	-2.96109600	0.21489400	0.80081500
N	-4.07532600	0.42614900	1.00051200
C	-1.88822100	-2.35740100	-0.98466700
N	-2.59491300	-3.14388700	-1.44333900
C	-0.21153500	-1.45535800	2.59967400
N	-0.28447700	-2.07981600	3.56460000
C	-0.41456400	2.41290300	1.48517500
N	-0.60799400	3.42889900	1.99047100
C	1.77768600	2.00193100	-1.42402900
N	2.31129700	2.75921500	-2.10940500
C	2.62237900	0.28399800	1.68451100
N	3.58899300	0.33315900	2.30887400
H	-2.43852500	2.45178700	-3.52533300
C	2.20324200	-2.08528100	-1.55094400
N	2.98225400	-2.70364700	-2.13346900
Si	0.95075300	-1.11172700	-0.67549700

H/[SiB₈(CN)₉]**Lowest normal mode frequency: 48.2 cm⁻¹**

B	0.94845900	0.37036400	1.33780700
B	-0.88030300	0.64593900	0.96070100
B	-0.17573600	-0.84968400	1.45071600
B	-0.88030300	0.64593900	-0.96070100
B	-1.12545400	-0.91930400	0.00000000
B	0.65470300	-1.21559700	0.00000000
B	0.94845900	0.37036400	-1.33780700
B	-0.17573600	-0.84968400	-1.45071600
C	1.45925800	-2.52767000	0.00000000
N	2.04273900	-3.51054300	0.00000000
C	-0.30613400	-1.79364000	2.64190100
N	-0.34928400	-2.55520200	3.50454100
C	-2.36975000	-1.81374000	0.00000000
N	-3.29117600	-2.50339600	0.00000000
C	-0.30613400	-1.79364000	-2.64190100
N	-0.34928400	-2.55520200	-3.50454100
C	2.04665200	0.48609300	2.38437600
N	2.91625700	0.55622600	3.13748500
C	2.04665200	0.48609300	-2.38437600
N	2.91625700	0.55622600	-3.13748500
C	-1.90139700	1.44649600	1.77092700
N	-2.65001500	2.07257000	2.38194100
C	-1.90139700	1.44649600	-1.77092700
N	-2.65001500	2.07257000	-2.38194100
H	2.53641300	-4.38621000	0.00000000
C	0.69645200	3.55459700	0.00000000
N	0.78445200	4.70323800	0.00000000
Si	0.60845900	1.75661500	0.00000000

H/[SiB₉(CN)₁₀]**Lowest normal mode frequency: 53.18 cm⁻¹**

B	0.00000000	0.00000000	-1.87015200
B	0.93392600	0.93392600	-0.82952900
B	-0.93392600	0.93392600	-0.82952900
B	-0.93392600	-0.93392600	-0.82952900
B	0.93392600	-0.93392600	-0.82952900
B	0.00000000	1.37411900	0.66322000
B	-1.37411900	0.00000000	0.66322000
B	0.00000000	-1.37411900	0.66322000
B	1.37411900	0.00000000	0.66322000
C	2.82548900	0.00000000	1.15045700
N	3.90586200	0.00000000	1.54847400
C	1.93175900	-1.93175900	-1.42706100

N	2.66169500	-2.66169500	-1.93639700
C	1.93175900	1.93175900	-1.42706100
N	2.66169500	2.66169500	-1.93639700
C	0.00000000	0.00000000	-3.38762700
N	0.00000000	0.00000000	-4.52975800
C	-1.93175900	-1.93175900	-1.42706100
N	-2.66169500	-2.66169500	-1.93639700
C	-1.93175900	1.93175900	-1.42706100
N	-2.66169500	2.66169500	-1.93639700
C	-2.82548900	0.00000000	1.15045700
N	-3.90586200	0.00000000	1.54847400
C	0.00000000	-2.82548900	1.15045700
N	0.00000000	-3.90586200	1.54847400
C	0.00000000	2.82548900	1.15045700
N	0.00000000	3.90586200	1.54847400
H	0.00000000	0.00000000	-5.53481500
C	0.00000000	0.00000000	3.87808000
N	0.00000000	0.00000000	5.02993900
Si	0.00000000	0.00000000	2.09057800

H/[SiB₁₀(CN)₁₁]

Lowest normal mode frequency: 44.8 cm⁻¹

B	-0.37073700	0.35045500	-1.44281100
B	-0.89198500	-1.31705300	0.69091400
B	0.99686300	1.02808000	0.96214000
B	0.79873000	-0.82184100	1.05493300
B	-0.56699800	0.30910700	1.39736500
B	-1.22624800	-1.12170300	-1.02548300
B	0.98340000	1.49683200	-0.84703200
B	0.34007600	-1.52962100	-0.60727100
B	-1.63254400	0.13673900	0.00016500
B	-0.45915500	1.52095400	0.06835900
C	-3.11682700	0.54045200	0.15522800
N	-4.21661600	0.81943100	0.26792700
C	-1.61919800	-2.38593100	1.51094500
N	-2.21460000	-3.16748200	2.10996500
C	-2.19592300	-1.89323800	-1.90977300
N	-2.98170100	-2.44320200	-2.54655900
C	-0.65545300	0.71053100	-2.90122800
N	-0.88360700	0.98737200	-3.99560600
C	-1.18713600	0.64625100	2.75873900
N	-1.72816700	0.91295400	3.73888600
C	-1.22540800	2.85210700	0.11355700
N	-1.89938700	3.78495700	0.14445800
C	1.60328800	-1.64254500	2.06680100

N	2.23221500	-2.25711400	2.80960600
C	0.98880300	-2.75407000	-1.25560800
N	1.51802200	-3.64222900	-1.76452700
C	1.79821900	1.83312100	1.98442100
N	2.42445400	2.43877900	2.73650300
C	1.46556400	2.75760500	-1.54748900
N	1.85445200	3.70116700	-2.08036200
H	-5.18064900	1.08524100	0.38052600
C	3.61104600	-0.70476000	-0.70126100
N	4.70159200	-1.04754300	-0.84448800
Si	1.91965700	-0.12226900	-0.52239500

H/[SiB₁₁(CN)₁₂]

Lowest normal mode frequency: 59.02 cm⁻¹

B	0.70048400	0.00013500	-1.60388600
B	0.70055900	-1.52531900	-0.49573500
B	0.70053000	1.52547700	-0.49561000
B	0.70054200	0.94283800	1.29768900
B	0.70065500	-0.94291300	1.29750600
B	-0.79289900	-0.00011900	1.53527600
B	-0.79302500	1.46006400	0.47449900
B	-0.79301500	0.90245600	-1.24196100
B	-0.79290600	-1.46013800	0.47436800
B	-0.79294700	-0.90232200	-1.24203600
B	-1.67083400	0.00000000	0.00000000
C	-3.21873500	0.00000000	0.00013100
N	-4.35759000	0.00000000	0.00017500
C	-1.57059900	2.71614700	0.88264900
N	-2.22312300	3.61737300	1.17556900
C	-1.57043900	-0.00028200	2.85603400
N	-2.22298700	-0.00050500	3.80365100
C	-1.57080600	1.67872700	-2.31030800
N	-2.22371100	2.23577600	-3.07661700
C	-1.57064800	-1.67850900	-2.31051000
N	-2.22336800	-2.23544100	-3.07706800
C	-1.57060200	-2.71618500	0.88237200
N	-2.22341200	-3.61723900	1.17522600
C	1.35344700	-2.84093300	-0.92342100
N	1.87583300	-3.81605100	-1.24043800
C	1.35334400	0.00015800	-2.98728200
N	1.87574200	0.00016900	-4.01263400
C	1.35341000	2.84117600	-0.92309800
N	1.87596200	3.81628100	-1.23990900
C	1.35349100	1.75590700	2.41689600
N	1.87612900	2.35847200	3.24637800

C	1.35364200	-1.75616400	2.41656500
N	1.87630800	-2.35895100	3.24586100
H	-5.36476200	0.00000000	0.00022300
C	3.75927400	0.00000000	-0.00019800
N	4.91093600	-0.00011100	-0.00034500
Si	1.97023800	0.00000000	0.00000000

H/[SiB₁₂(CN)₁₃]

Lowest normal mode frequency: 26.3 cm⁻¹

B	-0.50006400	2.02677800	0.00000000
B	1.06755900	1.65036300	0.00000000
B	-1.68589800	0.93563200	0.00000000
B	-0.17459700	0.86484800	1.39325800
B	1.58589800	0.18886100	0.89315100
B	-1.39482300	-0.55750600	0.93572400
B	-1.39482300	-0.55750600	-0.93572400
B	1.58589800	0.18886100	-0.89315100
B	0.32607100	-0.88935400	1.49529000
B	0.32607100	-0.88935400	-1.49529000
B	1.41214300	-1.31126600	0.00000000
B	-0.17459700	0.86484800	-1.39325800
C	2.01565100	2.85702700	0.00000000
N	2.61546800	3.84003700	0.00000000
C	-0.87906600	3.51571500	0.00000000
N	-1.15793600	4.62109300	0.00000000
C	-3.11385300	1.49617300	0.00000000
N	-4.13583200	2.02703700	0.00000000
C	-0.37276600	1.57711300	2.73844200
N	-0.54691000	2.19299100	3.69520500
C	2.82032100	0.42655000	1.76611600
N	3.73707900	0.61632300	2.43525300
C	2.82032100	0.42655000	-1.76611600
N	3.73707900	0.61632300	-2.43525300
C	-0.37276600	1.57711300	-2.73844200
N	-0.54691000	2.19299100	-3.69520500
C	-2.57212600	-0.97023100	1.82330900
N	-3.45096400	-1.30543100	2.48696800
C	-2.57212600	-0.97023100	-1.82330900
N	-3.45096400	-1.30543100	-2.48696800
C	0.50991300	-1.56818600	2.85473900
N	0.62909400	-2.11899800	3.85823000
C	2.48040200	-2.40691500	0.00000000
N	3.24156600	-3.27013500	0.00000000
C	0.50991300	-1.56818600	-2.85473900
N	0.62909400	-2.11899800	-3.85823000

H	-1.39681500	5.59903000	0.00000000
C	-0.90129900	-3.81133200	0.00000000
N	-1.18546300	-4.92743600	0.00000000
Si	-0.46666400	-2.07747000	0.00000000

H/[SiB₁₃(CN)₁₄]

Lowest normal mode frequency: 60.05 cm⁻¹

B	0.00000000	0.00000000	-1.52558100
B	0.00000000	1.83717300	0.73352400
B	1.59103800	0.91858600	0.73352400
B	1.59103800	-0.91858600	0.73352400
B	-0.88209000	1.52782500	-0.76936000
B	-1.76418000	0.00000000	-0.76936000
B	1.76418000	0.00000000	-0.76936000
B	0.88209000	1.52782500	-0.76936000
B	-1.59103800	0.91858600	0.73352400
B	-0.88209000	-1.52782500	-0.76936000
B	0.88209000	-1.52782500	-0.76936000
B	-1.59103800	-0.91858600	0.73352400
B	0.00000000	-1.83717300	0.73352400
C	0.00000000	0.00000000	-3.08751500
N	0.00000000	0.00000000	-4.22578500
C	3.03964800	0.00000000	-1.61772400
N	3.95383600	0.00000000	-2.31671000
C	1.51982400	-2.63241300	-1.61772400
N	1.97691800	-3.42412300	-2.31671000
C	-1.51982400	-2.63241300	-1.61772400
N	-1.97691800	-3.42412300	-2.31671000
C	-3.03964800	0.00000000	-1.61772400
N	-3.95383600	0.00000000	-2.31671000
C	-1.51982400	2.63241300	-1.61772400
N	-1.97691800	3.42412300	-2.31671000
C	1.51982400	2.63241300	-1.61772400
N	1.97691800	3.42412300	-2.31671000
C	-2.75949600	1.59319600	1.44949200
N	-3.62966400	2.09558700	2.01063900
C	-2.75949600	-1.59319600	1.44949200
N	-3.62966400	-2.09558700	2.01063900
C	0.00000000	-3.18639100	1.44949200
N	0.00000000	-4.19117500	2.01063900
C	2.75949600	-1.59319600	1.44949200
N	3.62966400	-2.09558700	2.01063900
C	2.75949600	1.59319600	1.44949200
N	3.62966400	2.09558700	2.01063900
C	0.00000000	3.18639100	1.44949200

N	0.00000000	4.19117500	2.01063900
H	0.00000000	0.00000000	-5.23442800
C	0.00000000	0.00000000	3.62934900
N	0.00000000	0.00000000	4.78110100
Si	0.00000000	0.00000000	1.83683600