

**Superhalogen-based composite with strong acidity- a crossing point
between two topics**

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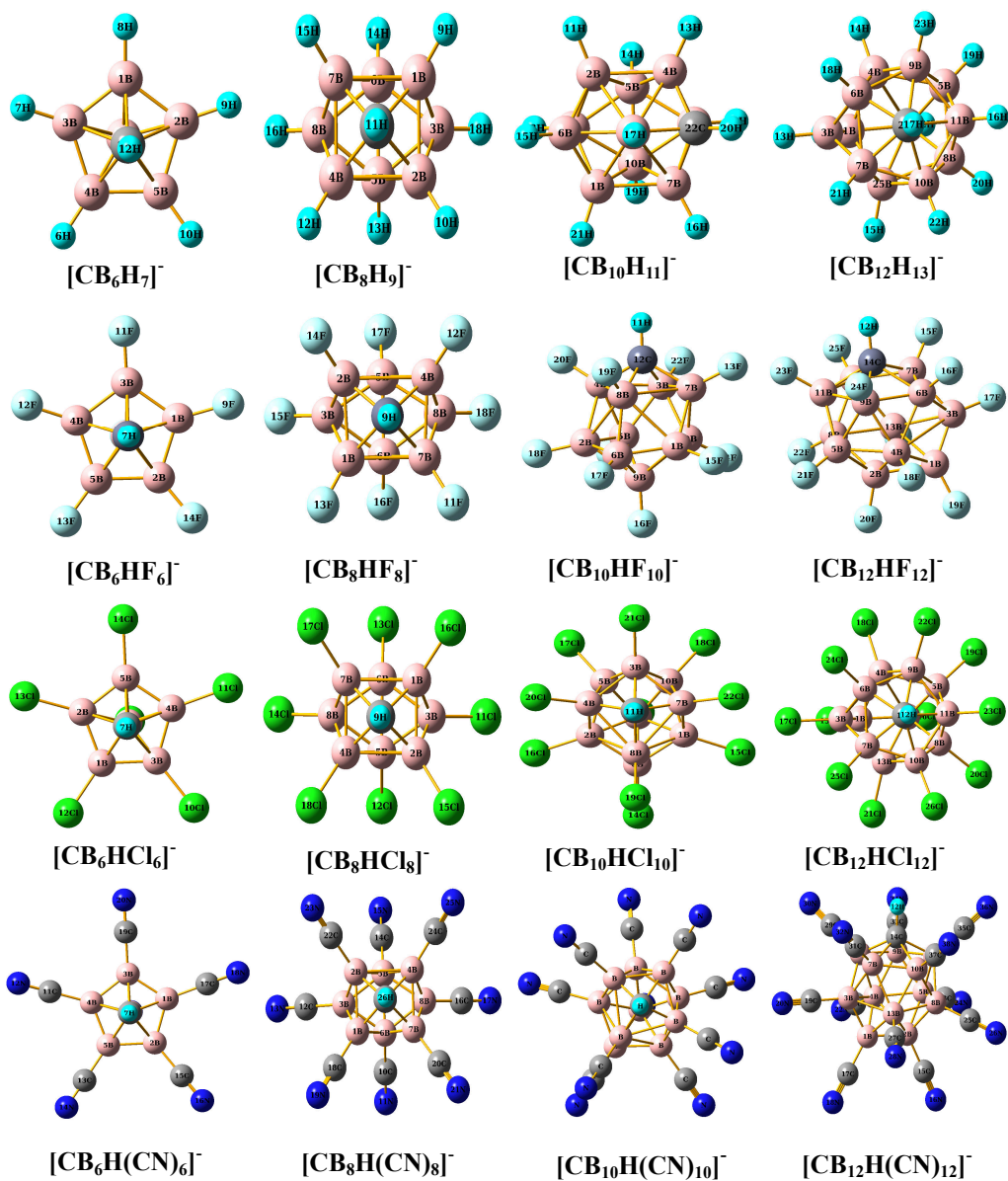


Fig .S1 Equilibrium structures of the carborane anions and their derivatives

$[\text{CB}_n\text{HX}_n]^-$ ($n = 6, 8, 10, 12$; $X = \text{H}, \text{F}, \text{Cl}, \text{CN}$).

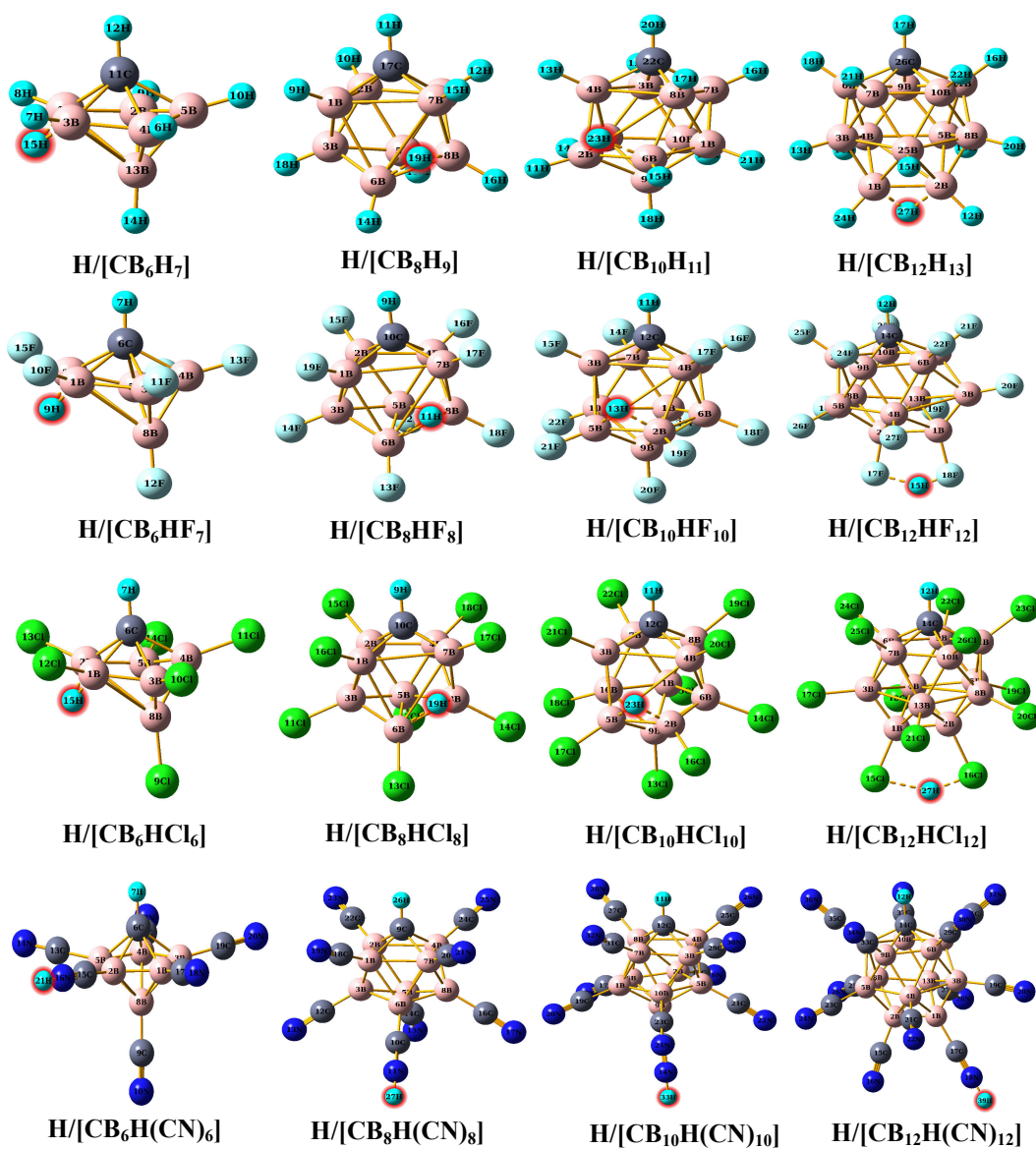


Fig. S2 Equilibrium structures of the composites of H/[CB_nHX_n] (n = 6, 8, 10, 12 ; X= H, F, Cl, CN).

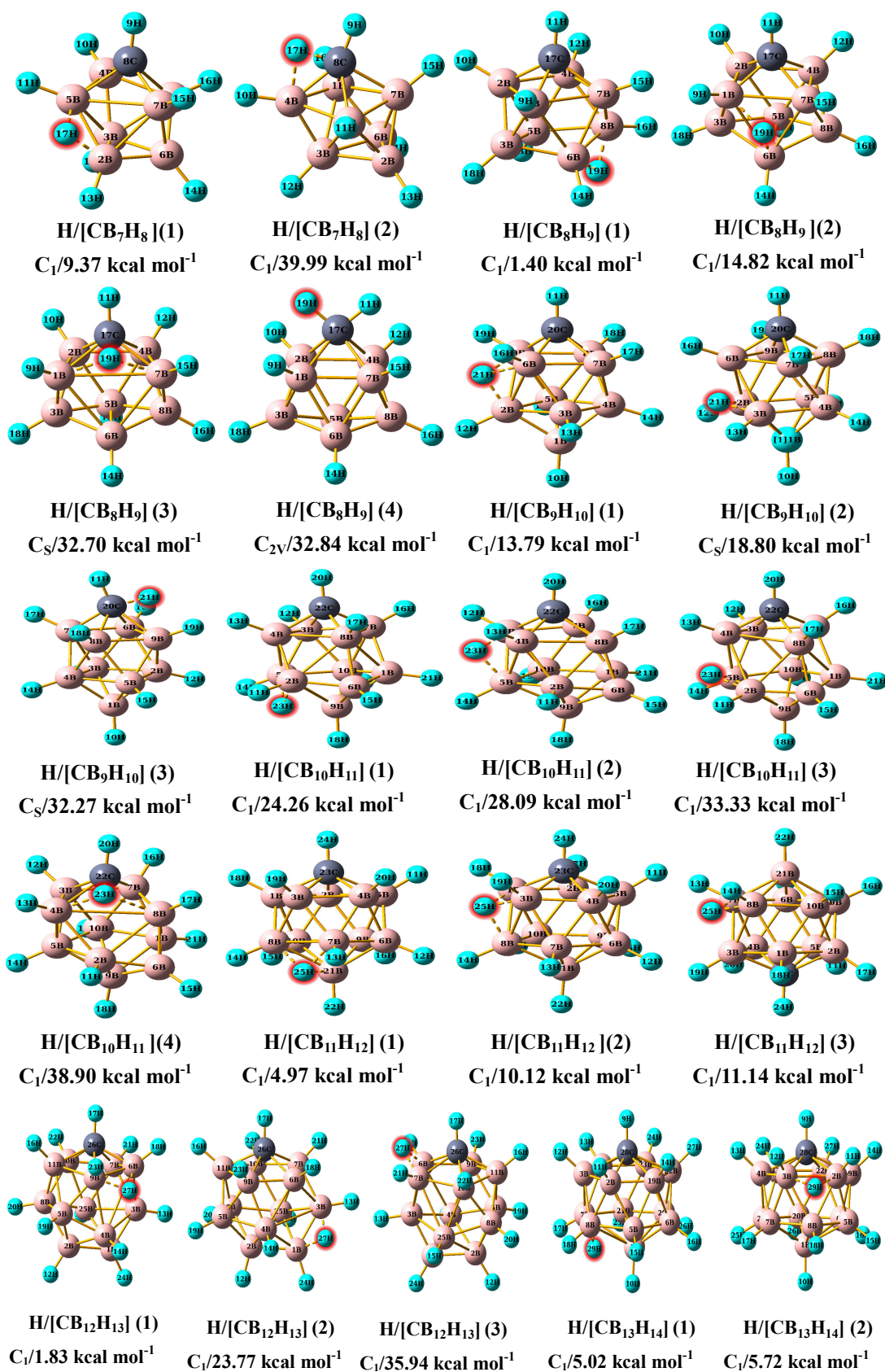


Fig. S3 Equilibrium structures of proration isomer of the composites of

H/[CB_nH_{n+1}] (n = 5-13 ;), point group and relative energy (kcal/mol).

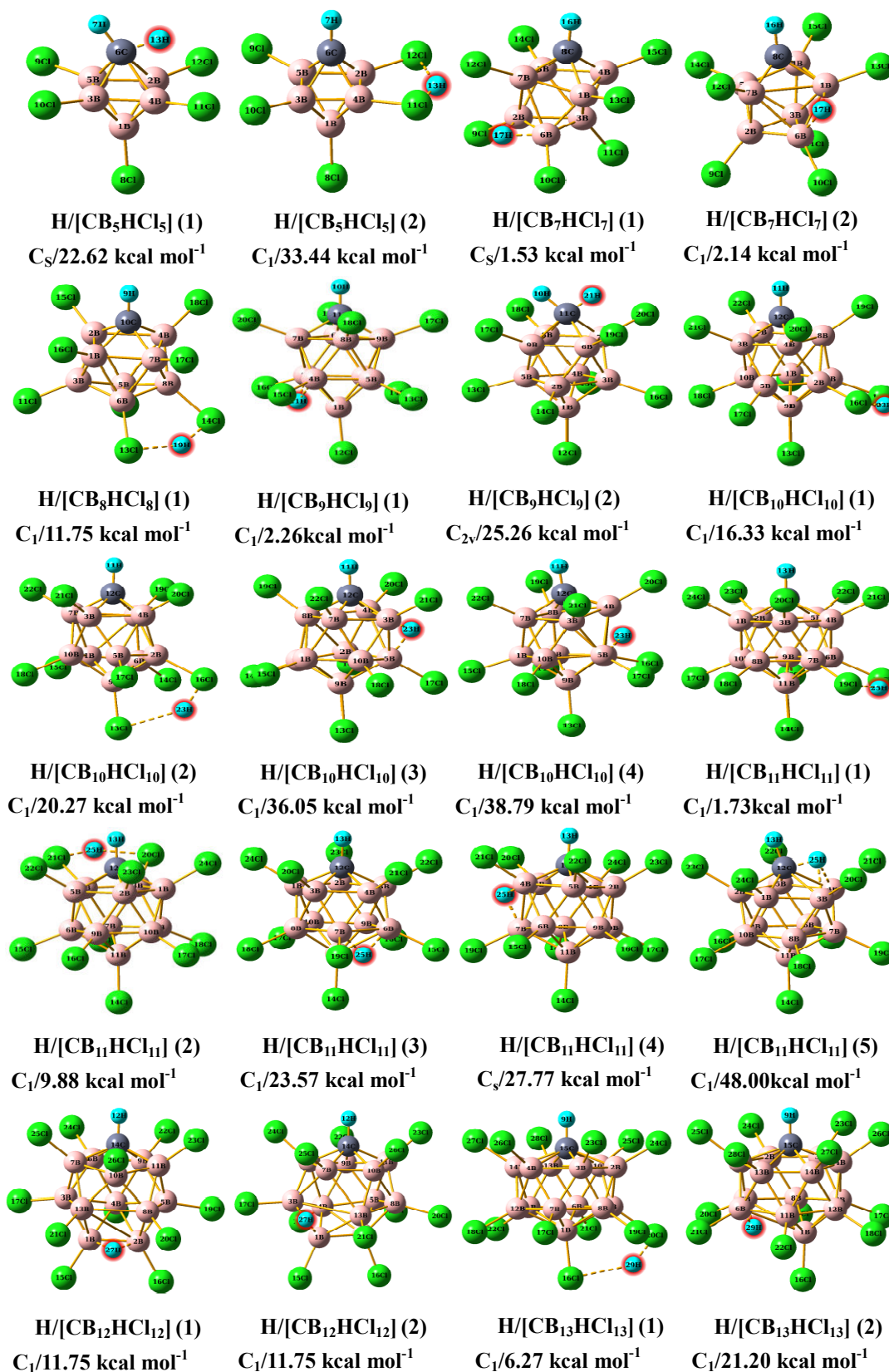


Fig. S4 Equilibrium structures of proration isomer of the composites of
H/[CB_nHCl_n] (n = 5-13), point group and relative energy (kcal/mol).

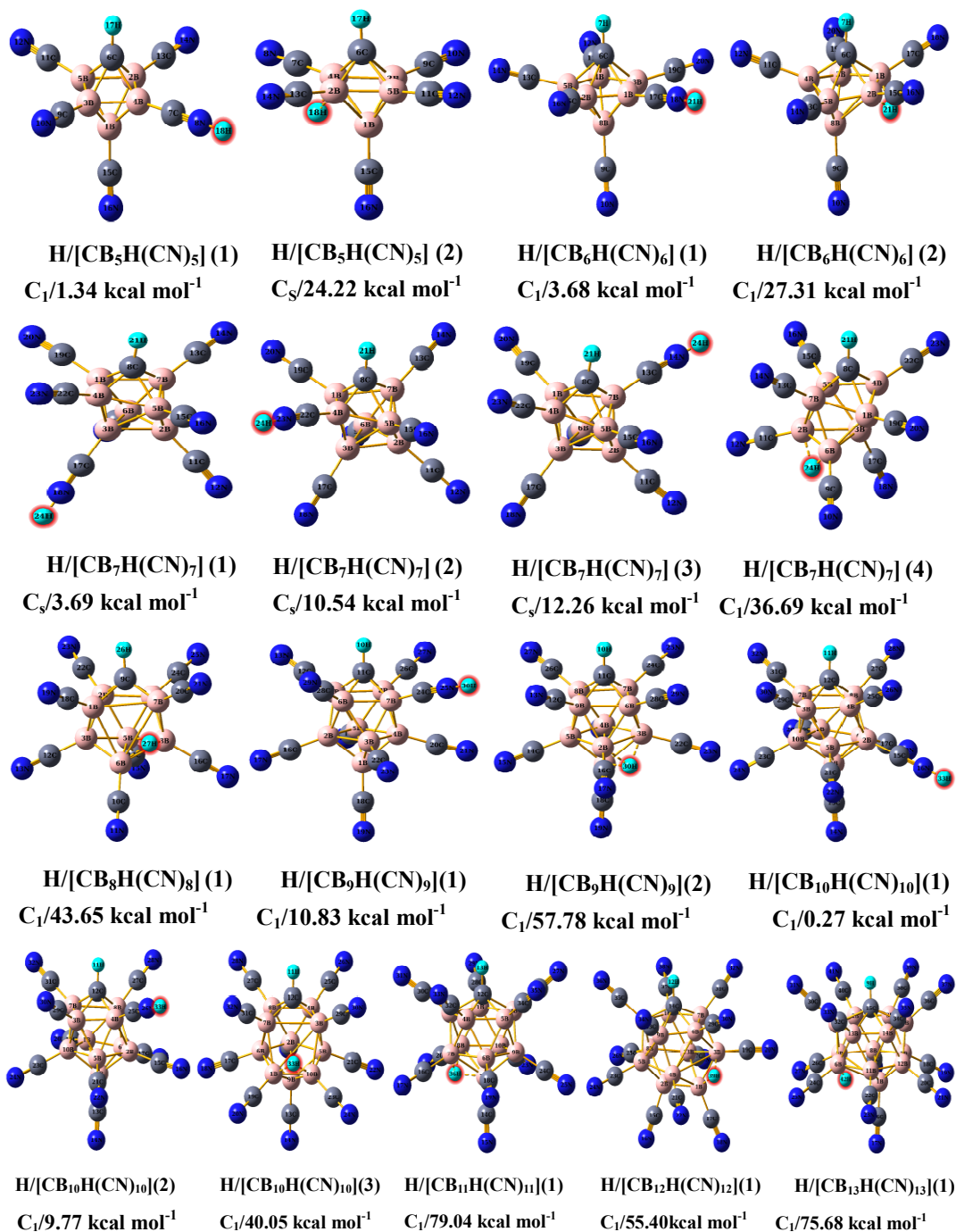


Fig. S5 Equilibrium structures of proration isomer of the composites of H/[CB_nH(CN)_n] (n = 5-13), point group and relative energy (kcal/mol).

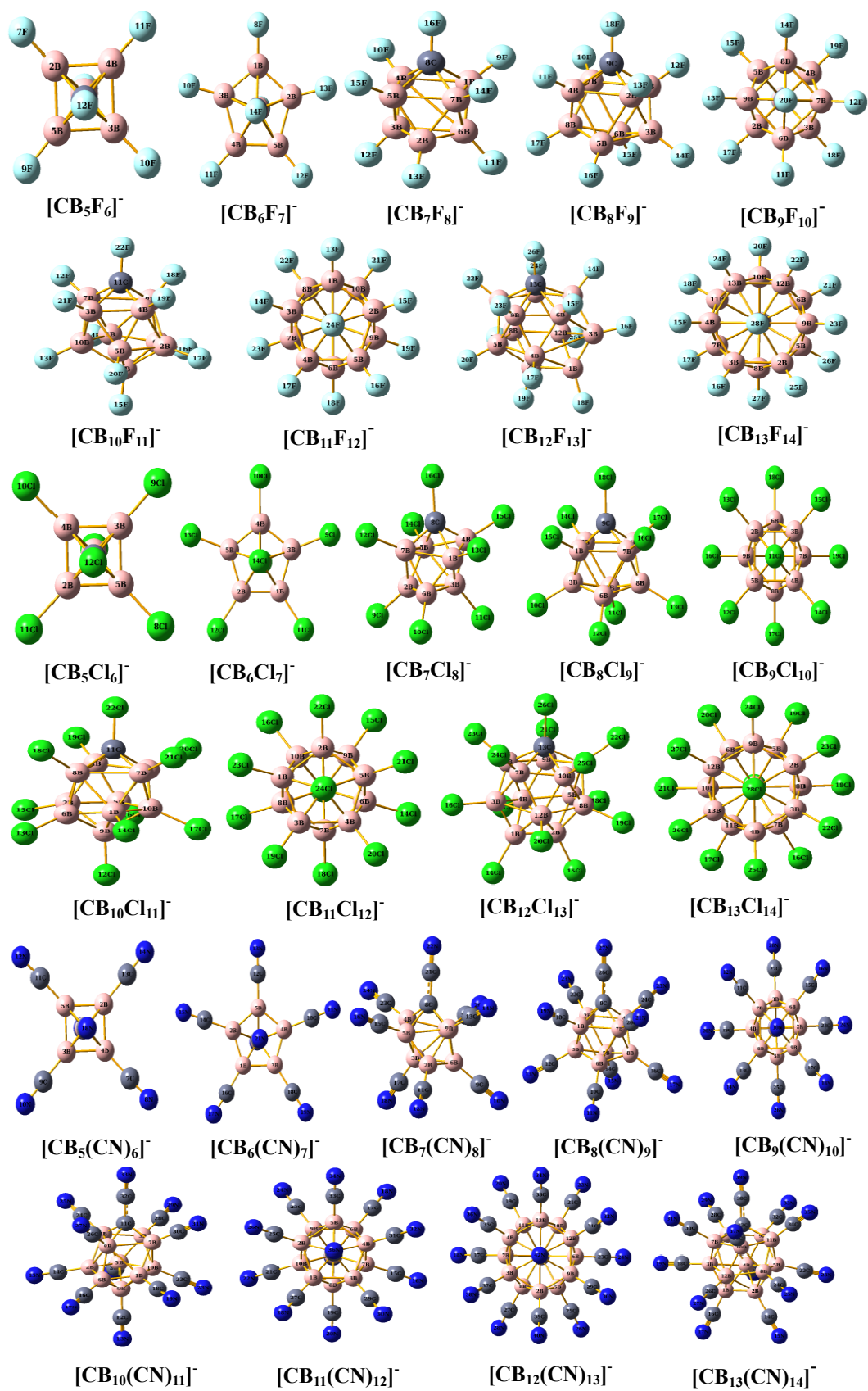


Fig .S6 Equilibrium structures of the carborane anions and their derivatives

$[\text{CB}_n\text{X}_{n+1}]^-$ ($n = 5 - 13$; $\text{X} = \text{F}, \text{Cl}, \text{CN}$).

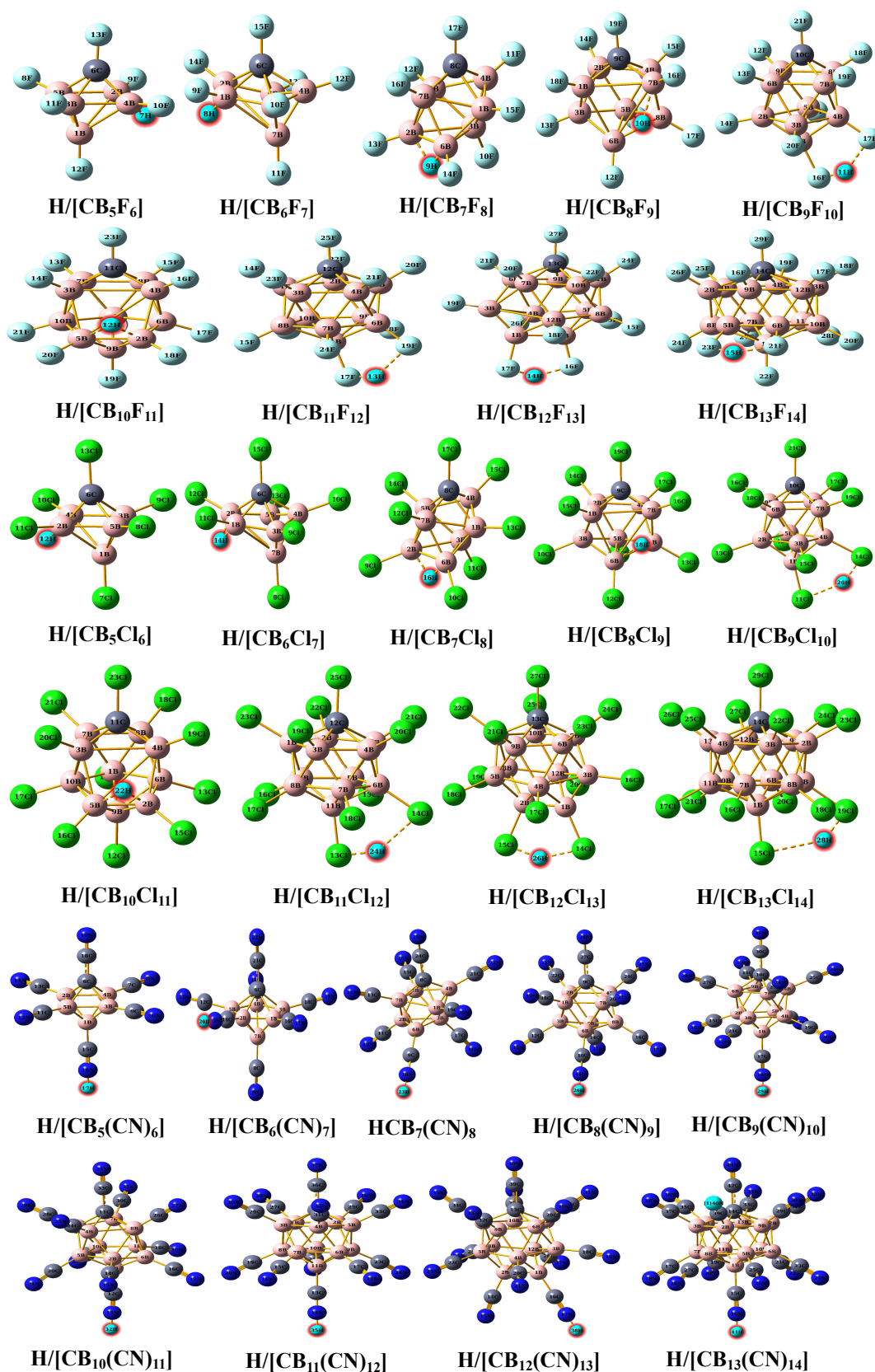


Fig. S7 Equilibrium structures of the composites of $\text{H}/[\text{CB}_n\text{HX}_n]$ ($n = 5 - 13$; $\text{X} = \text{F, Cl, CN}$).

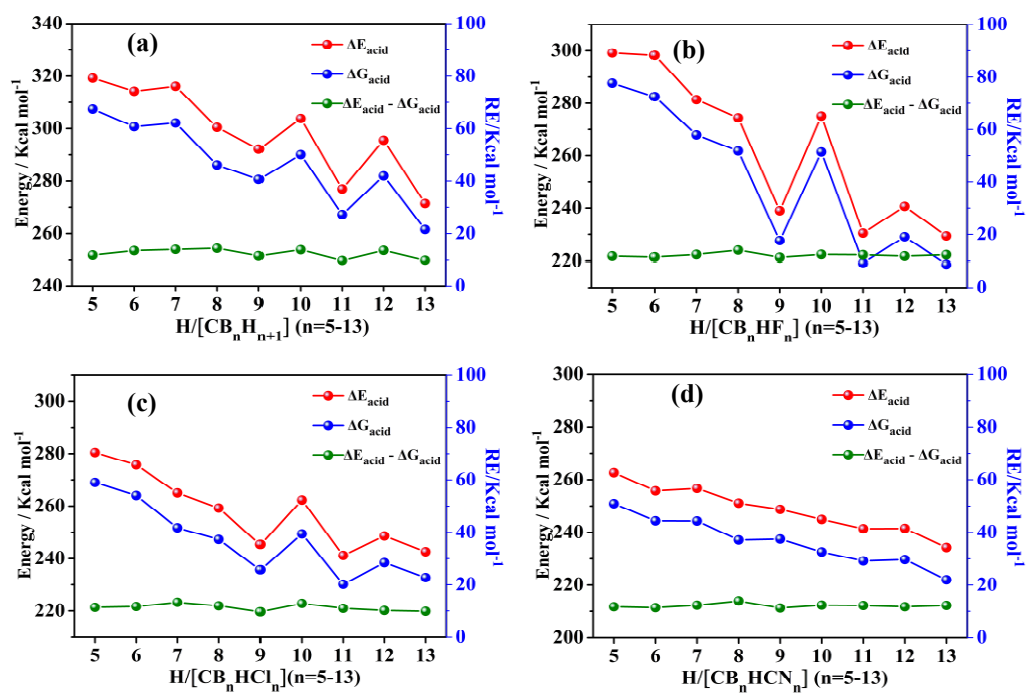


Fig. S8 The comparison between ΔG_{acid} and ΔE_{acid} (a) $\text{H}/[\text{CB}_n\text{H}_{n+1}]$, (b) $\text{H}/[\text{CB}_n\text{HF}_n]$, (c) $\text{H}/[\text{CB}_n\text{HCl}_n]$, (d) $\text{H}/[\text{CB}_n\text{H(CN)}_n]$ ($n = 5 - 13$)

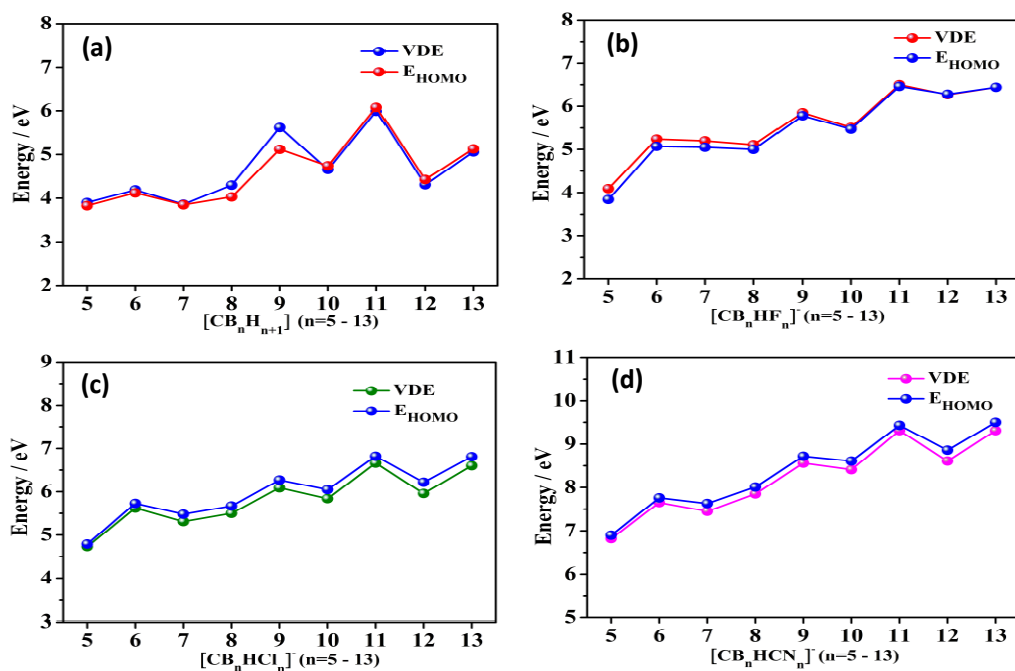


Fig. S9 The comparison between VDE and absolute value of HOMO energy (E_{HOMO}) for the selected Wade-Mingos superhalogens (a) $[\text{CB}_n\text{H}_{n+1}]^-$, (b) $[\text{CB}_n\text{HF}_n]^-$, (c) $[\text{CB}_n\text{HCl}_n]^-$, (d) $[\text{CB}_n\text{H(CN)}_n]^-$ ($n = 5 - 13$)

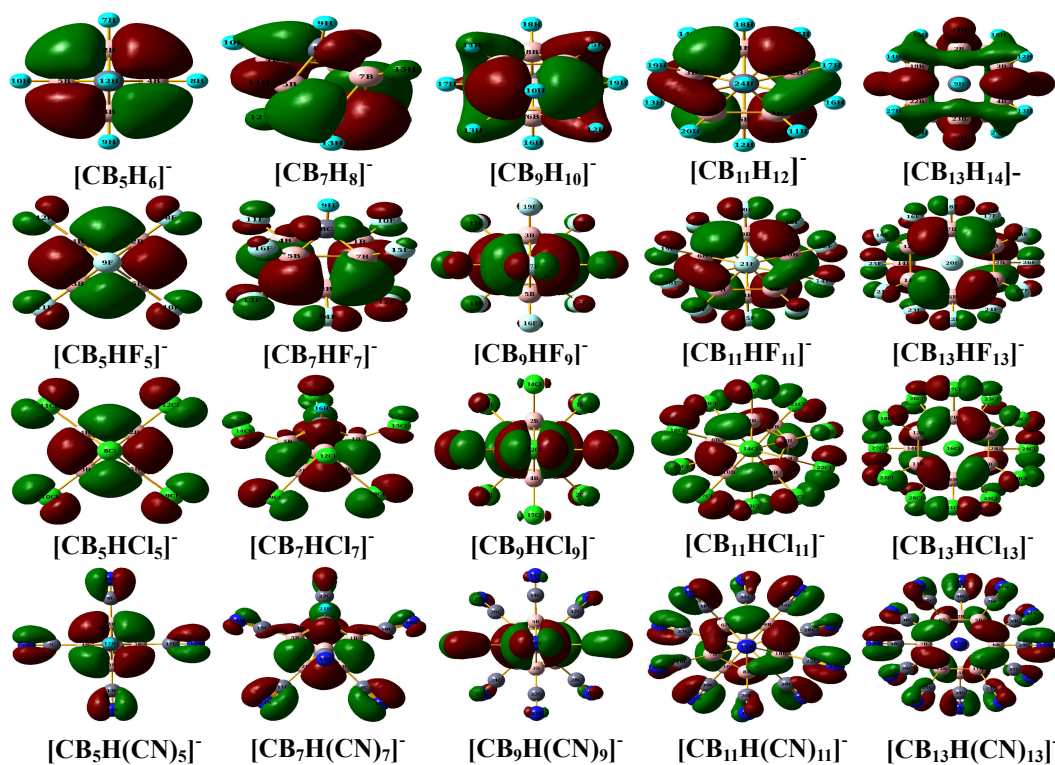


Fig. S10 The distribution HOMO orbital of carborane anions and their derivatives of

[CB_nHX_n]⁻ (n = 5, 7, 9, 11, 13; X = H, F, Cl, CN)

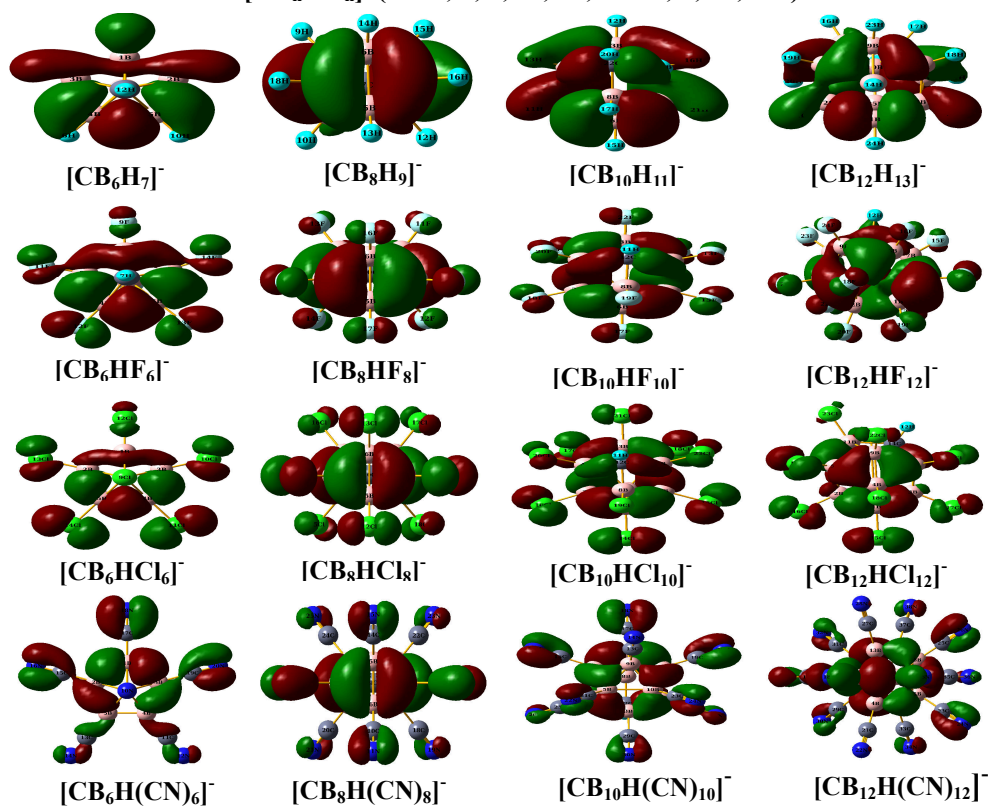


Fig. S11 The distribution HOMO orbital of carborane anions and their derivatives of

[CB_nHX_n]⁻ (n = 6, 8, 10, 12 ; X = H, F, Cl, CN)

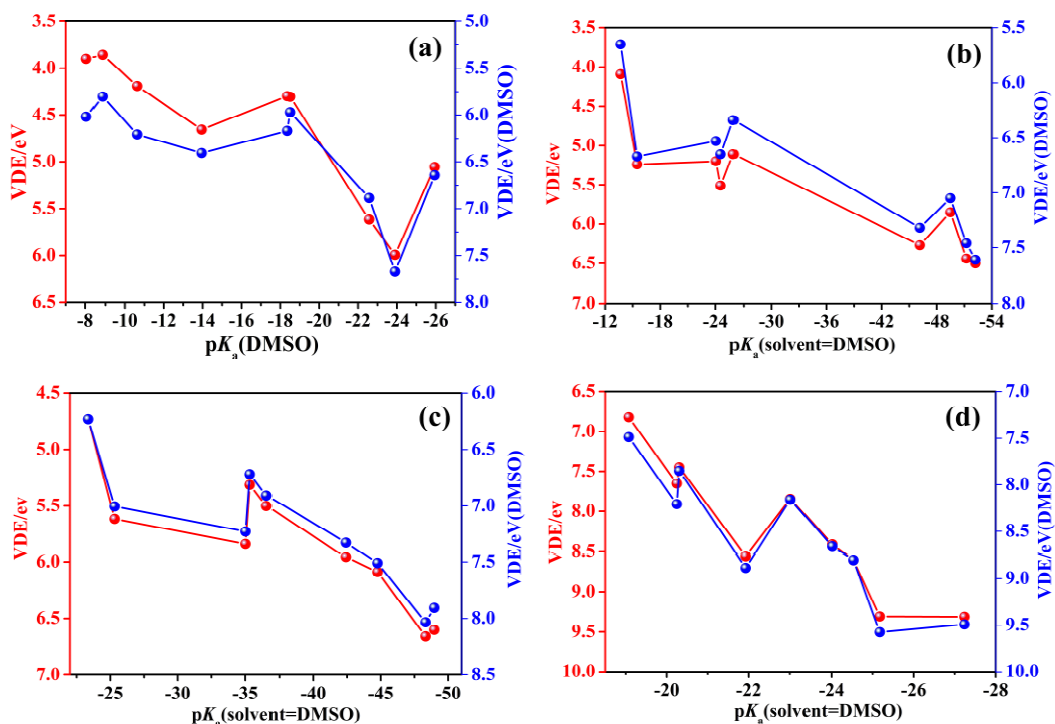


Fig. S12 The relationship between the acidity of the whole composite and the VDE of the superhalogen component (a) $H/[CB_nH_{n+1}]$, (b) $H/[CB_nHF_n]$, (c) $H/[CB_nHCl_n]$, (d) $H/[CB_nH(CN)_n]$ (n = 5 - 13)

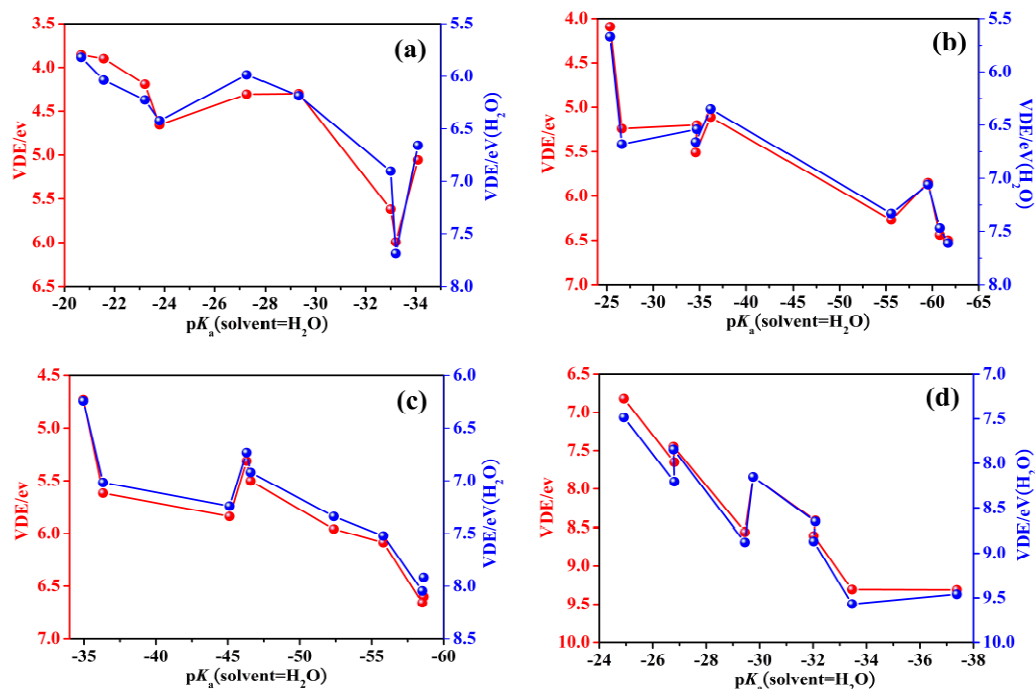


Fig. S13 The relationship between the acidity of the whole composite and the VDE of the superhalogen component (a) $H/[CB_nH_{n+1}]$, (b) $H/[CB_nHF_n]$, (c) $H/[CB_nHCl_n]$, (d) $H/[CB_nH(CN)_n]$ (n = 5 - 13)

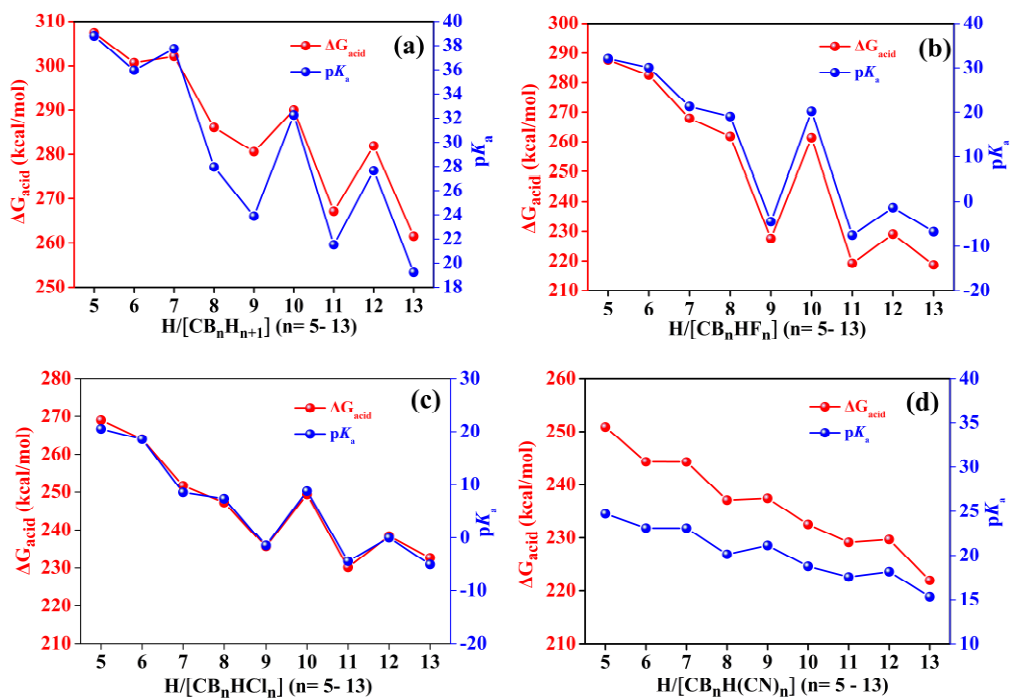


Fig. S14 The comparison between the gas-phase acidity (ΔG_{acid}) and acid dissociation content(pK_a) of the whole composites in DCE solvent (a) $H/[CB_nH_{n+1}]$, (b) $H/[CB_nHF_n]$, (c) $H/[CB_nHCl_n]$, (d) $H/[CB_nH(CN)_n]$ ($n = 5 - 13$)

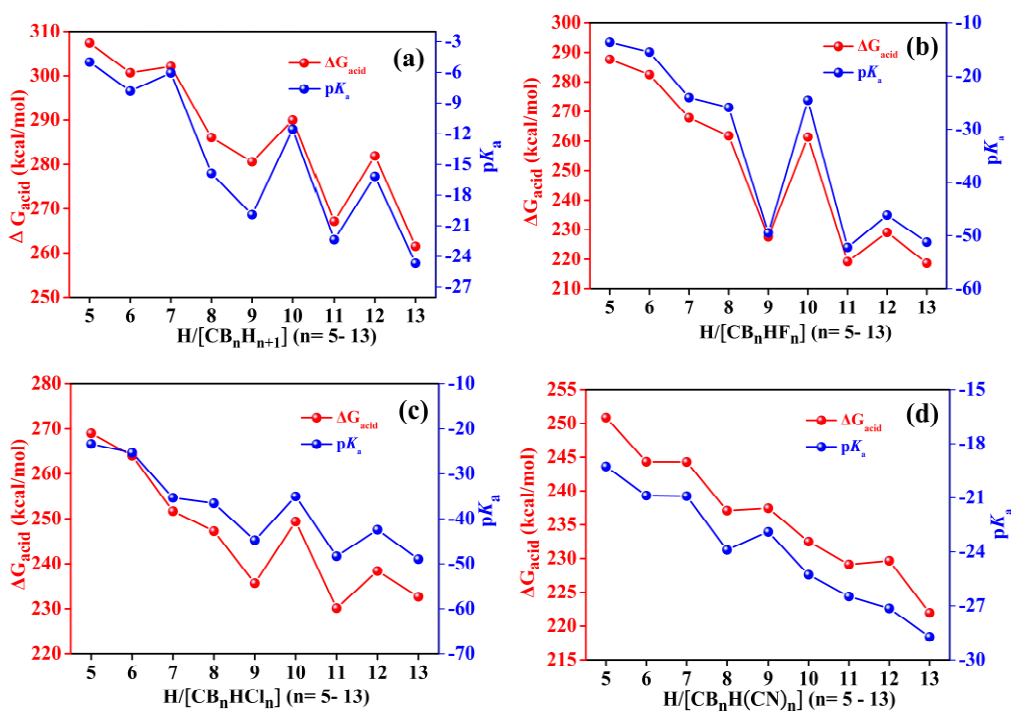


Fig. S15 The comparison between the gas-phase acidity (ΔG_{acid}) and acid dissociation content(pK_a) of the whole composites in DMSO solvent (a) $H/[CB_nH_{n+1}]$, (b) $H/[CB_nHF_n]$, (c) $H/[CB_nHCl_n]$, (d) $H/[CB_nH(CN)_n]$ ($n = 5 - 13$)

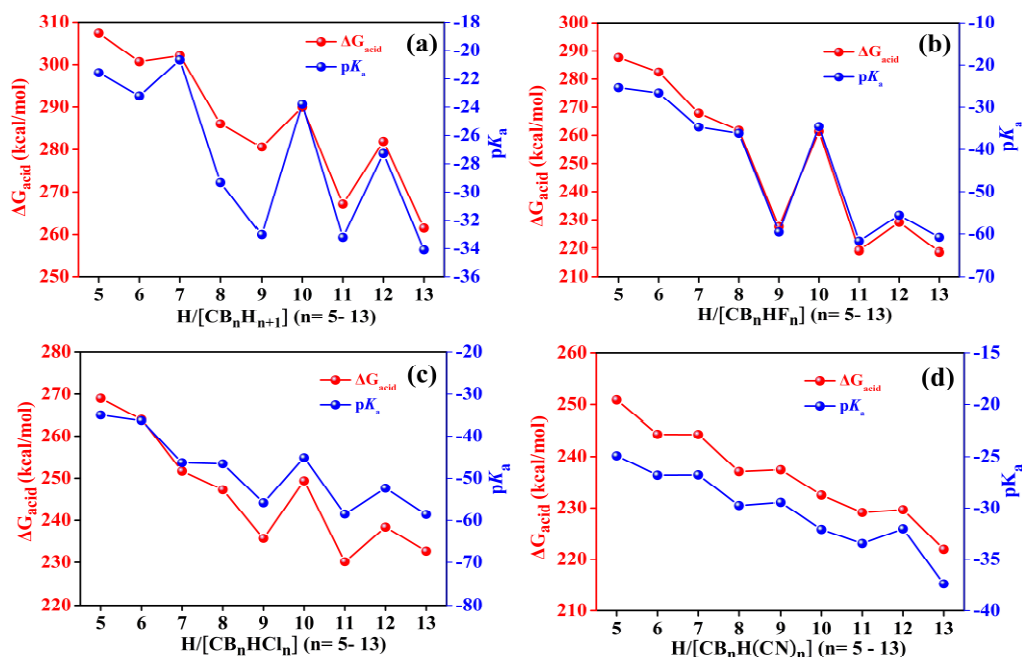


Fig. S16 The comparison between the gas-phase acidity (ΔG_{acid}) and acid dissociation content (pK_a) of the whole composites in H_2O (a) $\text{H}/[\text{CB}_n\text{H}_{n+1}]$, (b) $\text{H}/[\text{CB}_n\text{HF}_n]$, (c) $\text{H}/[\text{CB}_n\text{HCl}_n]$, (d) $\text{H}/[\text{CB}_n\text{H}(\text{CN})_n]$ ($n = 5 - 13$)

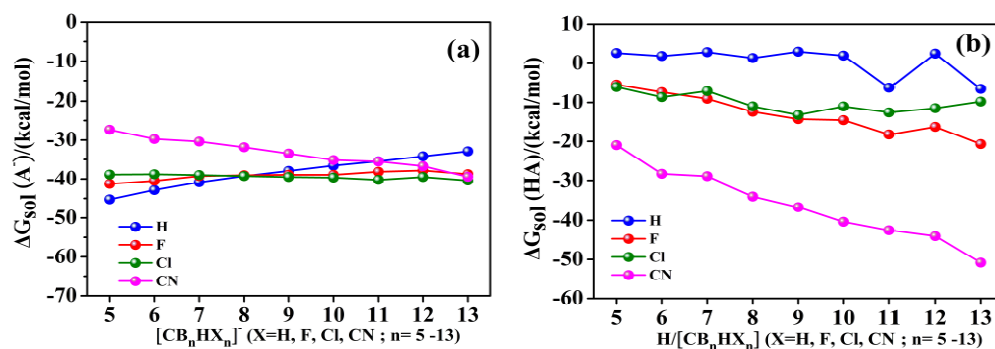


Fig. S17 The solvation free energies of both the conjugate acid (HA) and conjugate base (A^-) in DMSO solvent

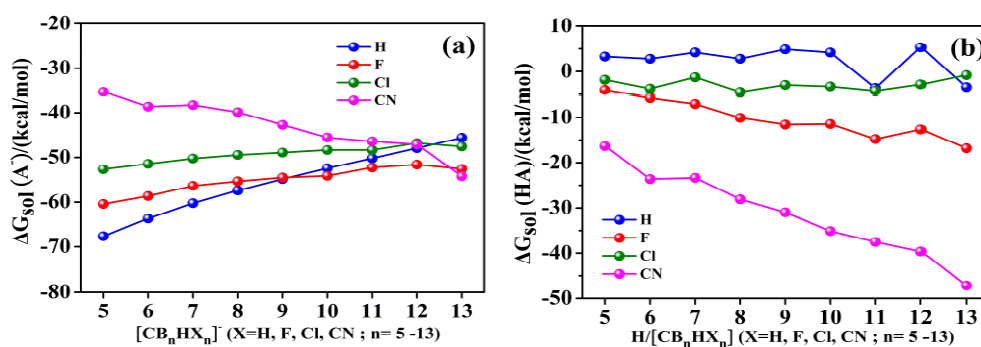


Fig. S18 The solvation free energies of both the conjugate acid (HA) and conjugate base (A^-) in H_2O

Table S1 The calculated VDE values of the superhalogen of $[\text{CB}_n\text{HX}_n]^-$ ($n = 5 - 13$; $\text{X}=\text{H}, \text{F}, \text{Cl}, \text{CN}$) (eV)

$[\text{CB}_n\text{H}_{n+1}]^-$	$[\text{CB}_n\text{H}_{n+1}]^-$	$[\text{CB}_n\text{HF}_n]^-$	$[\text{CB}_n\text{HCl}_n]^-$	$[\text{CB}_n\text{H}(\text{CN})_n]^-$
n = 5	3.90	4.09	4.73	6.82
n = 6	4.19	5.24	5.62	7.65
n = 7	3.86	5.20	5.31	7.45
n = 8	4.30	5.11	5.50	7.85
n = 9	5.62	5.85	5.41	8.56
n = 10	4.66	5.51	5.84	8.41
n = 11	5.99	6.50	6.66	9.31
n = 12	4.31	6.27	5.96	8.61
n = 13	5.06	6.44	6.60	9.31

Table S2 The calculated ΔE_{acid} values of the composites of $\text{H}/[\text{CB}_n\text{HX}_n]$ ($n = 5 - 13$; $\text{X}=\text{H}, \text{F}, \text{Cl}, \text{CN}$) (kcal/mol)

	$\text{H}/[\text{CB}_n\text{H}_{n+1}]$	$\text{H}/[\text{CB}_n\text{HF}_n]$	$\text{H}/[\text{CB}_n\text{HCl}_n]$	$\text{HCB}_n\text{H}(\text{CN})_n$
n = 5	319.23	299.14	280.44	262.68
n = 6	314.23	298.23	275.74	255.77
n = 7	316.12	281.36	265.04	256.69
n = 8	300.48	274.42	259.28	251.11
n = 9	292.16	238.96	245.39	248.74
n = 10	303.85	275.11	262.30	244.92
n = 11	276.96	230.48	241.19	241.38
n = 12	295.53	240.62	248.61	241.48
n = 13	271.41	229.39	242.59	234.26

Table S3 The calculated bond dissociation energy of the composites of $\text{H}/[\text{CB}_n\text{HX}_n]$ ($n = 5 - 13$; $\text{X}=\text{H}, \text{F}, \text{Cl}, \text{CN}$) (kcal/mol)

	$\text{HCB}_n\text{H}_{n+1}$	HCB_nHF_n	HCB_nHCl_n	$\text{H}/[\text{CB}_n\text{H}(\text{CN})_n]$
n = 5	93.44	72.49	70.95	104.34
n = 6	88.41	47.90	83.79	112.71
n = 7	84.53	72.33	65.93	109.31
n = 8	74.73	62.85	61.67	110.45
n = 9	83.78	46.00	63.28	126.16
n = 10	88.33	77.36	75.87	120.05
n = 11	91.46	58.44	76.69	139.93
n = 12	70.63	55.61	66.55	121.34
n = 13	68.64	51.80	73.12	130.15

Table S4 The calculated deformation energy of the composites of H/[CB_nHX_n] (n = 5 - 13;

X=H, F, Cl, CN) (kcal/mol)

	[CB _n H _{n+1}] ⁻	[CB _n HF _n] ⁻	[CB _n HCl _n] ⁻	[CB _n H(CN) _n] ⁻
n = 5	2.13	7.28	4.98	2.02
n = 6	8.87	57.50	7.86	5.91
n = 7	6.93	15.28	8.04	5.54
n = 8	11.30	15.85	10.87	8.00
n = 9	24.30	14.28	8.91	6.33
n = 10	9.27	11.18	7.43	5.27
n = 11	10.10	8.44	4.42	2.51
n = 12	10.58	15.99	5.82	5.00
n = 13	5.75	12.57	8.07	5.25

Table S5 The absolute value of HOMO energy of superhalogen [CB_nHX_n]⁻ (n = 5 - 13; X=H,

F, Cl, CN) (eV)

	[CB _n H _{n+1}] ⁻	[CB _n HF _n] ⁻	[CB _n HCl _n] ⁻	[CB _n H(CN) _n] ⁻
n = 5	3.83	4.79	3.84	6.90
n = 6	4.12	5.73	5.07	7.76
n = 7	3.85	5.48	5.05	7.63
n = 8	4.03	5.67	5.00	8.01
n = 9	5.12	6.27	5.78	8.72
n = 10	4.74	6.05	5.47	8.61
n = 11	6.08	6.82	6.46	9.43
n = 12	4.43	6.22	6.28	8.86
n = 13	5.13	6.81	6.44	9.50

Table S6 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 _n H _{n+1}]	H/[CB _n HF _n]	H/[CB _n HCl _n]	H/[CB _n H(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 S7 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

	$H/[CB_nH_{n+1}]$	$H/[CB_nHF_n]$	$H/[CB_nHCl_n]$	$H/[CB_nH(CN)_n]$
$n = 5$	-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 S8 The calculated acid dissociation constants(pK_a) of the composites of $H/[CB_nHX_n]$
($n = 5 - 13$; $X=H, F, Cl, CN$) in H_2O

	$H/[CB_nH_{n+1}]$	$H/[CB_nHF_n]$	$H/[CB_nHCl_n]$	$H/[CB_nH(CN)_n]$
$n = 5$	-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 S9 The calculated VDE values of the superhalogen of $[CB_nHX_n]^-$ ($n = 5 - 13$; $X=H, F, Cl, CN$) (eV) in DCE solvent

	$[CB_nH_{n+1}]^-$	$[CB_nHF_n]^-$	$[CB_nHCl_n]^-$	$[CB_nH(CN)_n]^-$
$n = 5$	5.84	5.55	6.12	7.50
$n = 6$	6.04	6.58	6.91	8.23
$n = 7$	5.64	6.45	6.61	7.90
$n = 8$	6.01	6.27	6.80	8.23
$n = 9$	6.73	6.98	7.39	8.94
$n = 10$	6.26	6.59	7.12	8.73
$n = 11$	7.53	7.55	7.93	9.62
$n = 12$	5.83	7.27	7.22	8.87
$n = 13$	6.51	7.41	7.80	9.56

Table S10 The calculated VDE values of the superhalogen of $[\text{CB}_n\text{HX}_n]^-$ ($n = 5 - 13$; $\text{X}=\text{H}, \text{F}$, Cl, CN) (eV) in DMSO solvent

	$[\text{CB}_n\text{H}_{n+1}]^-$	$[\text{CB}_n\text{HF}_n]^-$	$[\text{CB}_n\text{HCl}_n]^-$	$[\text{CB}_n\text{H}(\text{CN})_n]^-$
$n = 5$	6.02	5.65	6.23	7.49
$n = 6$	6.21	6.67	7.01	8.21
$n = 7$	5.80	6.53	6.72	7.85
$n = 8$	6.17	6.34	6.91	8.16
$n = 9$	6.89	7.05	7.51	8.89
$n = 10$	6.41	6.65	7.23	8.66
$n = 11$	7.67	7.61	8.03	9.58
$n = 12$	5.97	7.32	7.33	8.81
$n = 13$	6.64	7.46	7.91	9.49

Table S11 The calculated VDE values of the superhalogen of $[\text{CB}_n\text{HX}_n]^-$ ($n = 5 - 13$; $\text{X}=\text{H}, \text{F}$, Cl, CN) (eV) in H_2O

	$[\text{CB}_n\text{H}_{n+1}]^-$	$[\text{CB}_n\text{HF}_n]^-$	$[\text{CB}_n\text{HCl}_n]^-$	$[\text{CB}_n\text{H}(\text{CN})_n]^-$
$n = 5$	6.04	5.67	6.24	7.49
$n = 6$	6.23	6.68	7.02	8.21
$n = 7$	5.82	6.54	6.73	7.84
$n = 8$	6.19	6.35	6.92	8.15
$n = 9$	6.90	7.06	7.52	8.88
$n = 10$	6.42	6.66	7.24	8.65
$n = 11$	7.69	7.61	8.04	9.57
$n = 12$	5.99	7.33	7.34	8.87
$n = 13$	6.66	7.47	7.92	9.46

Table S12 The calculated solvation free energies(ΔG_{sol}) of the conjugate acid $\text{H}/[\text{CB}_n\text{HX}_n]$ $(n = 5 - 13; \text{X}=\text{H}, \text{F}, \text{Cl}, \text{CN})$ (kcal/mol) in DCE solvent

	$\text{H}/[\text{CB}_n\text{H}_{n+1}]$	$\text{H}/[\text{CB}_n\text{HF}_n]$	$\text{H}/[\text{CB}_n\text{HCl}_n]$	$\text{H}/[\text{CB}_n\text{H}(\text{CN})_n]$
$n = 5$	1.82	-5.36	-7.01	-19.50
$n = 6$	1.10	-7.06	-9.46	-25.55
$n = 7$	1.89	-8.55	-8.46	-25.84
$n = 8$	0.63	-11.33	-11.75	-29.79
$n = 9$	1.92	-13.28	-11.71	-31.73
$n = 10$	1.08	-13.09	-12.21	-34.34
$n = 11$	-6.14	-16.70	-14.07	-36.03
$n = 12$	1.37	-14.96	-11.35	-36.85
$n = 13$	-6.42	-18.64	-10.93	-42.24

Table S13 The calculated solvation free energies(ΔG_{sol}) of the conjugate acid $\text{H}/[\text{CB}_n\text{HX}_n]$

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

	$\text{H}/[\text{CB}_n\text{H}_{n+1}]$	$\text{H}/[\text{CB}_n\text{HF}_n]$	$\text{H}/[\text{CB}_n\text{HCl}_n]$	$\text{H}/[\text{CB}_n\text{H}(\text{CN})_n]$
n = 5	2.63	-5.44	-6.06	-20.97
n = 6	1.86	-7.36	-8.63	-28.29
n = 7	2.86	-9.06	-7.09	-28.91
n = 8	1.36	-12.41	-11.01	-33.89
n = 9	2.98	-14.29	-13.23	-36.62
n = 10	1.97	-14.56	-11.04	-40.37
n = 11	-6.21	-18.22	-12.57	-42.54
n = 12	2.48	-16.28	-11.49	-44.05
n = 13	-6.52	-20.67	-9.79	-50.82

Table S14 The calculated solvation free energies(ΔG_{sol}) of the conjugate acid $\text{H}/[\text{CB}_n\text{HX}_n]$ (n = 5 - 13; X=H, F, Cl, CN) (kcal/mol) in H_2O

	$\text{H}/[\text{CB}_n\text{H}_{n+1}]$	$\text{H}/[\text{CB}_n\text{HF}_n]$	$\text{H}/[\text{CB}_n\text{HCl}_n]$	$\text{H}/[\text{CB}_n\text{H}(\text{CN})_n]$
n = 5	3.27	-4.06	-1.83	-16.31
n = 6	2.79	-5.72	-3.77	-23.62
n = 7	4.19	-7.02	-1.28	-23.34
n = 8	2.79	-10.06	-4.51	-28.07
n = 9	4.88	-11.56	-2.98	-30.97
n = 10	4.17	-11.44	-3.30	-35.13
n = 11	-3.64	-14.75	-4.25	-37.52
n = 12	5.32	-12.63	-2.84	-39.62
n = 13	-3.46	-16.78	-0.81	-47.16

Table S15 The calculated solvation free energies(ΔG_{sol}) of the conjugate base $[\text{CB}_n\text{HX}_n]^-$ (n

= 5 - 13; X=H, F, Cl, CN) (kcal/mol) in DCE solvent

	$\text{H}/[\text{CB}_n\text{H}_{n+1}]$	$\text{H}/[\text{CB}_n\text{HF}_n]$	$\text{H}/[\text{CB}_n\text{HCl}_n]$	$\text{H}/[\text{CB}_n\text{H}(\text{CN})_n]$
n = 5	-42.15	-38.78	-37.55	-26.16
n = 6	-40.03	-38.06	-37.66	-27.86
n = 7	-38.23	-36.91	-38.02	-28.13
n = 8	-36.80	-36.66	-38.51	-28.92
n = 9	-35.60	-36.48	-38.89	-29.85
n = 10	-34.43	-36.40	-39.14	-30.74
n = 11	-33.45	-35.66	-39.78	-30.70
n = 12	-32.31	-35.36	-39.30	-31.24
n = 13	-31.21	-36.00	-40.02	-32.78

Table S16 The calculated solvation free energies(ΔG_{sol}) of the conjugate base $[\text{CB}_n\text{HX}_n]^-$ ($n = 5 - 13$; $\text{X}=\text{H}, \text{F}, \text{Cl}, \text{CN}$) (kcal/mol) in DMSO solvent

	$[\text{CB}_n\text{H}_{n+1}]^-$	$[\text{CB}_n\text{HF}_n]^-$	$[\text{CB}_n\text{HCl}_n]^-$	$[\text{CB}_n\text{H}(\text{CN})_n]^-$
n = 5	-45.23	-41.24	-38.88	-27.36
n = 6	-42.84	-40.47	-38.78	-29.73
n = 7	-40.84	-39.25	-38.99	-30.40
n = 8	-39.25	-39.04	-39.26	-31.87
n = 9	-37.92	-38.91	-39.50	-33.48
n = 10	-36.57	-38.94	-39.65	-35.14
n = 11	-35.47	-38.16	-40.23	-35.52
n = 12	-34.18	-37.82	-39.51	-36.69
n = 13	-32.92	-38.76	-40.39	-39.45

Table S17 The calculated solvation free energies(ΔG_{sol}) of the conjugate base $[\text{CB}_n\text{HX}_n]^-$ ($n = 5 - 13$; $\text{X}=\text{H}, \text{F}, \text{Cl}, \text{CN}$) (kcal/mol) in H_2O

	$[\text{CB}_n\text{H}_{n+1}]^-$	$[\text{CB}_n\text{HF}_n]^-$	$[\text{CB}_n\text{HCl}_n]^-$	$[\text{CB}_n\text{H}(\text{CN})_n]^-$
n = 5	-67.64	-60.41	-52.63	-35.28
n = 6	-63.68	-58.63	-51.44	-38.62
n = 7	-60.23	-56.36	-50.24	-38.27
n = 8	-57.39	-55.33	-49.43	-39.86
n = 9	-54.85	-54.49	-48.91	-42.69
n = 10	-52.42	-54.10	-48.33	-45.52
n = 11	-50.20	-52.25	-48.34	-46.39
n = 12	-47.91	-51.60	-46.78	-47.08
n = 13	-45.58	-52.57	-47.54	-54.22

Table S18 The comparison between ΔG_{acid} values at DFT level and those at MP2 level for selected systems (kcal/mol)

	$\text{H}/[\text{CB}_{11}\text{H}_{12}]$	$\text{H}/[\text{CB}_{11}\text{HF}_{11}]$	$\text{H}/[\text{CB}_{11}\text{F}_{12}]$	$\text{H}/[\text{CB}_{11}\text{HCl}_{11}]$	$\text{H}/[\text{CB}_{11}\text{Cl}_{12}]$	$\text{H}/[\text{CB}_{11}\text{H}(\text{CN})_{11}]$	$\text{H}/[\text{CB}_{11}(\text{CN})_{12}]$
$\omega\text{B97XD}/6\text{-}311+\text{G}^{**}$	267.20	219.21	214.78	230.19	229.15	229.17	225.66
$\text{MP2}/6\text{-}311+\text{G}^{**}$	262.94	218.20	213.94	230.22	229.90	225.52	216.32
Relative error (%)	-1.59	-0.46	-0.39	0.01	0.33	-1.59	-4.14

Table S19 The comparison between VDE values at DFT and OVGF level (eV)

	$[\text{CB}_{11}\text{H}_{12}]^-$	$[\text{CB}_{11}\text{HF}_{11}]^-$	$[\text{CB}_{11}\text{HCl}_{11}]^-$	$[\text{CB}_{11}\text{H}(\text{CN})_{11}]^-$
ωB97XD	5.99	6.50	6.66	9.31
OVGF	5.814(-2.94%) ^a	6.100(-6.15%)	6.122(-8.08%)	8.932(-4.06%)

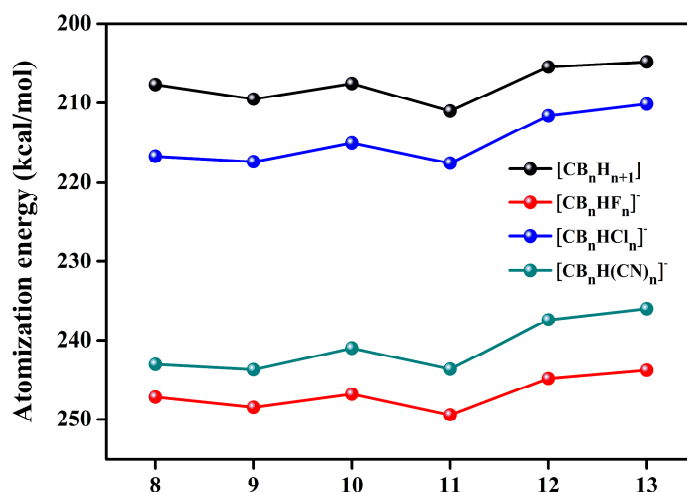
^a relative error in percentage

$$\Delta E_{\text{at}} = \{[E(\text{C}) + E(\text{H}) + n \times E(\text{B}) + n \times E(\text{X})] - E([\text{CB}_n\text{HX}_n]^-)\} / (n+1) \quad (\text{S-1})$$

Table S20 The calculated averaged atomization energy (ΔE_{at}) of $[\text{CB}_n\text{HX}_n]^-$ ($n = 8 - 13$;

X=H, F, Cl, CN) (kcal/mol).

	$[\text{CB}_n\text{H}_{n+1}]^-$	$[\text{CB}_n\text{HF}_n]^-$	$[\text{CB}_n\text{HCl}_n]^-$	$[\text{CB}_n\text{H}(\text{CN})_n]^-$
n = 8	207.67	247.15	216.70	242.97
n = 9	209.51	248.43	217.38	243.62
n = 10	207.55	246.77	215.06	240.94
n = 11	211.03	249.40	217.56	243.56
n = 12	205.43	244.76	211.62	237.42
n = 13	204.78	243.71	210.13	236.02

**Fig.S19** The variation of the averaged atomization energy of $[\text{CB}_{11}\text{HX}_{11}]^-$ (X= F, Cl, CN, $n = 8 \sim 13$) at $\omega\text{B97XD}/6\text{-}311+\text{G}(\text{d}, \text{p})$ level

$$\Delta E_{\text{bind}} = E(X^-) + E([\text{HCB}_n\text{HX}_{n-1}]^+) - E(\text{H}/[\text{CB}_n\text{HX}_n]) \quad (\text{S-2})$$

Table S21 The calculated ΔE_{bind} of the electron withdrawing groups X of $\text{H}/[\text{CB}_n\text{HX}_n]^-$ (n = 8 - 13; X= F, Cl, CN) (kcal/mol).

	X = F	X = Cl	X = CN
n = 8	271.82	194.50	258.43
n = 9	257.38	214.04	258.52
n = 10	270.11	227.67	257.64
n = 11	251.42	220.75	273.14
n = 12	189.38	140.02	265.95
n = 13	255.37	201.54	264.33

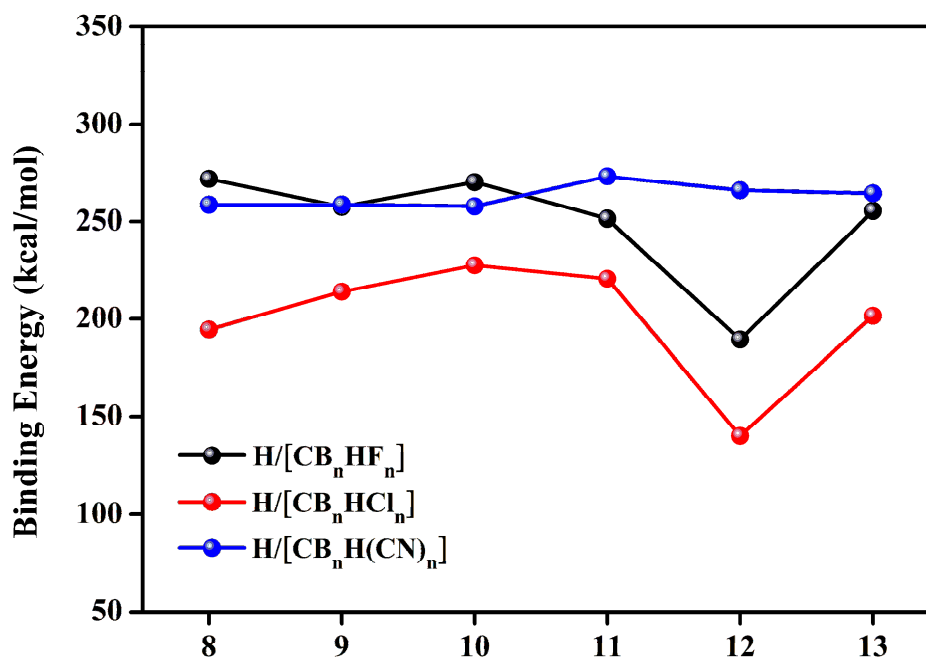


Fig.S20 The variation of the binding energy of various X ligands of $[\text{CB}_{11}\text{HX}_{11}]^-$ (X= F, Cl, CN, n = 8 ~ 13) at $\omega\text{B97XD}/6\text{-}311\text{+G(d, p)}$ level

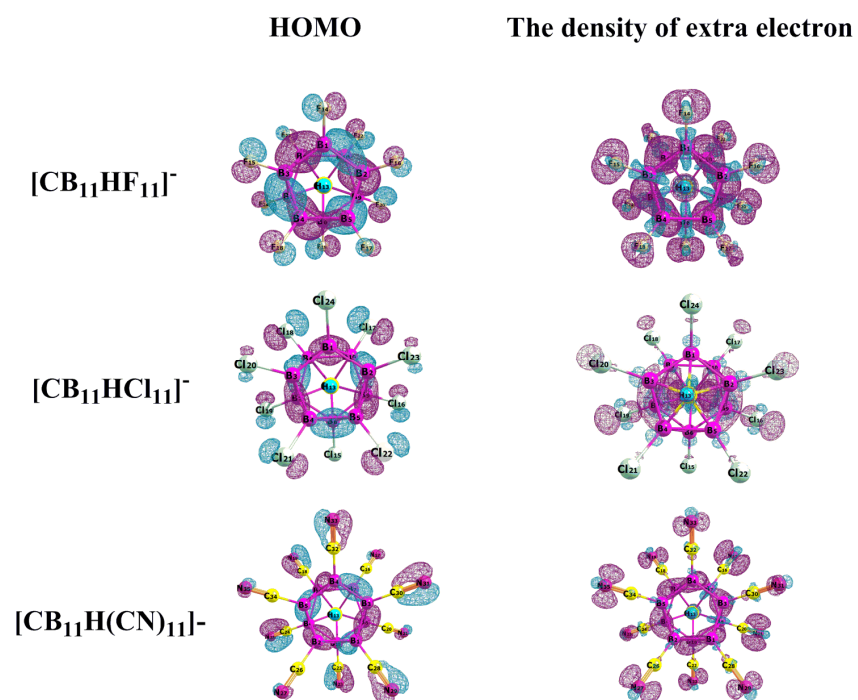


Fig.S21 The comparison of HOMO and the density of extra electron of carborane anions and their derivatives of $[\text{CB}_{11}\text{HX}_{11}]^-$ (X= F, Cl, CN)

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

H/[CB₅H₆]

Lowest normal mode frequency: 354.61 cm⁻¹

B	0.00494400	0.66505800	1.08931900
B	0.85904400	0.79141300	-0.38079200
B	-0.95168300	-0.75369800	0.30646000
B	-0.85238000	0.79992100	-0.37814100
B	0.94440500	-0.76262400	0.30554000
H	0.00802900	1.14400000	2.16983800
H	1.71049200	1.45299700	-0.86170200
H	-1.69801000	1.47006800	-0.85750700
H	-1.76852400	-1.56555100	0.56190200
H	1.75478900	-1.58205700	0.55736100
C	-0.00335200	-0.47632400	-0.95269200
H	-0.00636100	-0.96917400	-1.91265100
H	-0.00195300	-0.79268900	1.34698300

H/[CB₆H₇]

Lowest normal mode frequency: 281.2 cm⁻¹

B	1.13999000	0.88281000	0.06782900
B	-0.46297000	1.30405000	0.05317700
B	1.14472900	-0.87771300	0.06795700
B	-0.45607200	-1.30618500	0.05432400
B	-1.41345900	-0.00368000	-0.24217300
H	-0.68274900	-2.43795400	-0.20009800
H	2.00599700	-1.66755000	-0.13227400
H	1.99690000	1.67737900	-0.13237800
H	-0.69386400	2.43489600	-0.20149000
H	-2.51534700	-0.00723700	-0.66748500
C	0.12297000	0.00008300	-0.98376200
H	0.25062100	0.00000500	-2.05995500
B	-0.43149300	-0.00015300	1.22224800
H	-0.48528200	-0.00003200	2.40495700
H	1.78228200	0.00435200	0.77447700

H/[CB₇H₈]

Lowest normal mode frequency: 281.2 cm⁻¹

B	0.36005600	1.23128200	-0.01147800
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B	-1.33254100	-0.83495200	0.02282700
B	-0.28741600	0.00054200	1.27806100
B	1.34388200	0.00039300	0.82540900
B	0.36007500	-1.23126900	-0.01030000
B	-1.33253400	0.83501700	0.02213100
B	-0.23780200	-0.00064200	-1.26866200
C	1.24055300	-0.00034100	-0.70541300
H	2.06429300	-0.00062200	-1.40289400
H	2.31195200	0.00076300	1.50034800
H	0.61580700	-2.38492100	-0.06120800
H	-0.55587600	0.00111600	2.43441000
H	-2.05173600	-1.77839700	0.06547300
H	-2.05160500	1.77859400	0.06391100
H	-0.46041600	-0.00119600	-2.43115400
H	0.61587800	2.38486600	-0.06344300
H	-2.30021900	-0.00001300	-0.16289200

H/[CB₇H₈](1)

Lowest normal mode frequency: 217.68 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 292.98 kcal/mol

B	-0.32287800	-1.16420200	0.57499100
B	1.33413500	0.81077600	-0.26707300
B	0.22519600	0.48717900	1.20504000
B	-1.36904600	0.24543600	0.65274200
B	-0.41660200	1.22629000	-0.46543400
B	1.29711400	-0.69626800	0.39924100
B	0.42463100	-0.77830600	-1.06693100
C	-1.06695800	-0.33432200	-0.75650900
H	-1.85631300	-0.62391600	-1.43720400
H	-2.42634500	0.52097700	1.09902000
H	-0.98521600	2.20815500	-0.82912900
H	0.43295700	0.96828700	2.26847900
H	2.37820000	1.36162900	-0.38460800
H	2.31409800	-1.17854000	0.75956000
H	0.71117800	-1.32944700	-2.07653200
H	-0.73149200	-2.18127400	1.02239600
H	0.70193300	1.60554300	-1.04580700

H/[CB₇H₈](2)

Lowest normal mode frequency: 296.65 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 263.42 kcal/mol

B	0.26808300	-0.05064600	-1.25879100
B	-1.38787700	0.04585100	0.81684200
B	-0.38165100	1.25398300	-0.01094300

B	1.27604400	0.87489400	-0.00773800
B	0.26880700	-0.02904400	1.25943100
B	-1.38857400	0.03197800	-0.81660100
B	-0.49791800	-1.20896400	0.01008700
C	1.20321600	-0.73505200	0.00624000
H	1.71824200	-1.69431500	0.01384500
H	2.21063800	1.60416000	-0.01361000
H	0.66232400	-0.06755500	2.37726200
H	-0.50002300	2.43550200	-0.02094900
H	-2.22389700	0.11777300	1.65162600
H	-2.22497600	0.08961900	-1.65212200
H	-0.53398100	-2.39318100	0.02141500
H	0.65988100	-0.10944700	-2.37629900
H	2.22792500	-0.16250300	-0.00004600

H/[CB₈H₉]

Lowest normal mode frequency: 291.36 cm⁻¹

B	-0.37764800	-1.19369900	-0.91228300
B	-0.32017600	-1.05371700	0.89802800
B	-1.61644700	-0.43753400	-0.06941200
B	0.97929000	0.21051100	0.95973800
B	-0.76277700	0.71999800	0.94140400
B	-1.08323700	0.97529000	-0.76634500
B	1.45661900	0.28399000	-0.72842100
B	0.44968300	1.57087700	-0.01846200
H	-0.49269700	-1.99196200	-1.77908900
H	-0.41144000	-1.90019100	1.72115600
H	1.70927100	-1.88594000	-0.08838400
H	1.76909800	0.32091400	1.83371900
H	-1.24725200	1.32326200	1.84011700
H	-1.66682800	1.62981000	-1.56208800
H	2.35710200	0.43385500	-1.47806400
H	0.78849600	2.70274500	0.02203200
C	1.00029400	-1.07055400	-0.11338300
H	-2.75852400	-0.75171200	-0.08315000
H	0.32447700	1.16396500	-1.26718300

H/[CB₈H₉](1)

Lowest normal mode frequency: 244.0cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 284.97 kcal/mol

B	-1.19712200	0.18514100	-0.90718200
B	-1.17367400	0.15541300	0.87856400
B	-0.57510700	1.51775900	-0.03553200
B	0.32386600	-0.95589400	0.96171200
B	0.54225100	0.84473700	1.03812800

B	0.78540200	0.85575200	-0.91037000
B	0.39750600	-1.02190200	-0.92119200
B	1.66592000	-0.31554200	0.03086800
H	-1.98391500	0.20627100	-1.79012600
H	-2.05051600	0.17633500	1.67258700
H	-1.54076100	-2.01991200	-0.08620600
H	0.56406700	-1.79074600	1.76460100
H	1.10987000	1.48651100	1.85588000
H	1.18064200	1.60928300	-1.74129600
H	0.65633400	-1.86914000	-1.70708400
H	2.72515100	-0.83449100	0.13980700
C	-0.93332400	-1.12948500	-0.06460200
H	-0.94087600	2.64021500	-0.11053500
H	2.03473600	0.84526100	-0.28498900

H/[CB₈H₉](2)

Lowest normal mode frequency: 107.68 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 273.33 kcal/mol

B	0.81681800	0.96575800	0.84977500
B	0.66213600	0.88965100	-0.91119500
B	-0.62709100	1.55170100	-0.01227900
B	0.38009500	-1.04382400	-0.91107900
B	-1.09196900	0.15889000	-0.90378100
B	-1.34140200	0.18861900	0.82020900
B	0.49658200	-1.15270000	0.85565800
B	-1.04263600	-1.30970700	-0.00751300
H	1.41562500	1.53040900	1.69792000
H	1.26421300	1.51042000	-1.71967600
H	2.52925800	-0.37322300	-0.10523900
H	0.78050900	-1.80767100	-1.72214600
H	-1.96310200	0.28786700	-1.69806200
H	-2.10430100	0.30822800	1.71664000
H	0.90667900	-1.85387400	1.71403100
H	-1.74340700	-2.25904500	-0.07259500
C	1.46531800	-0.21565500	-0.03124200
H	-1.02837200	2.66178000	-0.06625100
H	-0.11168500	0.04710300	1.54385300

H/[CB₈H₉](3)

Lowest normal mode frequency: 259.75 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 253.68 kcal/mol

B	1.34645400	0.60146400	-0.74992800
B	0.93004700	0.44147100	0.94660800
B	1.43183800	-0.87838400	-0.07059900

B	-0.93100100	0.43932900	0.94666100
B	0.00118100	-1.13504000	0.87318600
B	0.00148700	-1.19023300	-0.94627600
B	-1.34811000	0.59913100	-0.74966700
B	-1.42987000	-0.88125200	-0.07101500
H	2.03082700	1.21966900	-1.49161000
H	1.48391700	1.00400200	1.82965300
H	-0.00233300	2.51740800	0.14598200
H	-1.48580500	1.00016700	1.83019800
H	0.00210900	-1.97124200	1.71480900
H	0.00210200	-1.96840700	-1.84036000
H	-2.03388200	1.21626700	-1.49092100
H	-2.42796000	-1.51757900	-0.09274600
C	-0.00152900	1.45059600	-0.03511800
H	2.43129000	-1.51254500	-0.09269300
H	-0.00122400	1.32625500	-1.19645200

H/[CB₈H₉](4)

Lowest normal mode frequency: 209.34 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 253.58 kcal/mol

B	-0.97066500	0.92725900	0.46232900
B	0.97066500	0.92725900	0.46232900
B	0.00000000	1.42219200	-0.84862500
B	0.97066500	-0.92725900	0.46232900
B	0.89930700	0.00000000	-1.17686500
B	-0.89930700	0.00000000	-1.17686500
B	-0.97066500	-0.92725900	0.46232900
B	0.00000000	-1.42219200	-0.84862500
H	-1.77321400	1.62304700	0.98785500
H	1.77321400	1.62304700	0.98785500
H	0.00000000	-0.82326000	2.26550700
H	1.77321400	-1.62304700	0.98785500
H	1.75040800	0.00000000	-2.00291900
H	-1.75040800	0.00000000	-2.00291900
H	-1.77321400	-1.62304700	0.98785500
H	0.00000000	-2.49718000	-1.33999400
C	0.00000000	0.00000000	1.53528500
H	0.00000000	2.49718000	-1.33999400
H	0.00000000	0.82326000	2.26550700

H/[CB₉H₁₀]

Lowest normal mode frequency: 384.22 cm⁻¹

B	-1.88633200	-0.00067800	-0.12132800
B	-0.75289700	1.02594300	0.86194100
B	-0.75594500	-1.01732000	0.87071000

B	-0.70880600	-0.93324200	-0.92938200
B	-0.70860900	0.92546000	-0.93786300
B	0.71535900	0.00732200	1.31859300
B	0.79246900	-1.30232300	-0.01413900
B	0.79542900	-0.00580800	-1.29483900
B	0.79358100	1.30127200	-0.02594900
H	-3.06233900	0.00162100	-0.22905600
H	2.76798300	-0.00158600	0.10631400
H	-1.14349700	1.80940400	1.66247200
H	-1.14159500	-1.79507100	1.67926600
H	-1.12719500	-1.69901100	-1.73228200
H	-1.12742900	1.68432000	-1.74694400
H	1.16319500	0.01146200	2.41382100
H	1.26610400	-2.38450300	0.04331600
H	1.29663000	-0.01133100	-2.36557000
H	1.26818300	2.38353700	0.02208300
C	1.69200700	-0.00082200	0.05146600
H	-1.73332600	0.00296000	1.19906900

H/[CB₉H₁₀](1)

Lowest normal mode frequency: 263.04 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 268.15 kcal/mol

B	-1.88033500	-0.05447800	0.00017200
B	-0.83832900	1.29730000	0.04159800
B	-0.76638100	-0.05927100	1.30664800
B	-0.75893300	-1.32068200	-0.04142300
B	-0.77035800	0.02378400	-1.30652700
B	0.78250500	0.82263700	1.04883600
B	0.72522200	-0.99465300	0.87522100
B	0.72312600	-0.93524800	-0.93895400
B	0.77894400	0.88972400	-0.99343000
H	-3.05789300	0.01679200	0.00423000
H	2.74433800	-0.01179000	-0.00370300
H	-1.40476100	2.34327400	0.07672400
H	-1.17552700	-0.07948700	2.42030700
H	-1.20154000	-2.42120900	-0.07591100
H	-1.18150200	0.07475000	-2.41842400
H	1.28628400	1.56872300	1.81626700
H	1.21976900	-1.75270500	1.63665600
H	1.21655100	-1.64198600	-1.74889800
H	1.28289400	1.68067100	-1.71459500
C	1.66654300	-0.00581400	-0.00140500
H	0.29482100	1.91228600	0.05507600

H/[CB₉H₁₀](2)

Lowest normal mode frequency: 232.97 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 263.38 kcal/mol

B	-0.05288700	-1.89062498	0.00000000
B	0.85457145	-0.80410484	1.03973664
B	0.85457145	-0.80410484	-1.03973664
B	-0.93701723	-0.76172511	-0.90648271
B	-0.93701723	-0.76172511	0.90648271
B	1.30728906	0.84345699	0.00000000
B	-0.02312762	0.75627181	-1.31386417
B	-1.31542493	0.75101805	0.00000000
B	-0.02312762	0.75627181	1.31386417
H	-0.03883502	-3.07117898	0.00000000
H	-0.02456589	2.75904802	0.00000000
H	1.66386155	-1.19670873	1.81113182
H	1.66386155	-1.19670873	-1.81113182
H	-1.67445592	-1.15914723	-1.74648932
H	-1.67445592	-1.15914723	1.74648932
H	2.38287307	1.33228496	0.00000000
H	-0.03808978	1.24257063	-2.39133434
H	-2.39674792	1.22943407	0.00000000
H	-0.03808978	1.24257063	2.39133434
C	-0.03072991	1.68126902	0.00000000
H	1.72677203	-0.53579402	0.00000000

H/[CB₉H₁₀](3)

Lowest normal mode frequency: 368.96 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 249.22 kcal/mol

B	-0.01534088	-1.90329997	0.00000000
B	-1.30110404	-0.75134415	0.00000000
B	0.02476617	-0.82119509	1.30393687
B	1.29747197	-0.79483279	0.00000000
B	0.02476617	-0.82119509	-1.30393687
B	-0.89166891	0.66262981	1.03280897
B	0.90646282	0.68944007	0.95027418
B	0.90646282	0.68944007	-0.95027418
B	-0.89166891	0.66262981	-1.03280897
H	-0.06792671	-3.08282898	0.00000000
H	0.42325147	2.73883009	0.00000000
H	-2.42342699	-1.13921331	0.00000000
H	-0.01107019	-1.22516720	2.41952595
H	2.42638802	-1.16003863	0.00000000
H	-0.01107019	-1.22516720	-2.41952595
H	-1.66204863	1.18289063	1.76632449
H	1.68503208	1.20741511	1.67499773

H	1.68503208	1.20741511	-1.67499773
H	-1.66204863	1.18289063	-1.76632449
C	0.05713861	1.71649704	0.00000000
H	-1.06580942	1.95790588	0.00000000

H/[CB₁₀H₁₁]

Lowest normal mode frequency: 246.25 cm⁻¹

B	-0.36835700	1.39268500	0.55730700
B	-1.51392400	-0.87152800	-0.65238200
B	1.35288500	-0.88740200	0.52826300
B	0.40703000	-1.13319300	-1.01621300
B	-0.36657200	-1.39268600	0.55800000
B	-1.51651400	0.86983900	-0.65190900
B	1.35193600	0.88901100	0.52803800
B	0.40569500	1.13331700	-1.01671000
B	-1.45026800	-0.00103600	0.88874500
B	0.18910200	0.00041300	1.53681200
H	-2.27135900	-1.66078700	-1.10666200
H	2.23198400	-1.58351100	0.90356000
H	0.49782600	-1.83548500	-1.96653900
H	-0.61849300	-2.49321500	0.92480600
H	-2.27410800	1.65857600	-1.10682700
H	2.22987100	1.58669800	0.90310800
H	0.49455800	1.83433200	-1.96817000
H	-2.36444700	-0.00123100	1.64332000
H	0.29804600	0.00060400	2.71659100
H	2.37966300	0.00077700	-1.47043700
H	-0.62080800	2.49297000	0.92447400
C	1.50011500	0.00063800	-0.84362100
H	-1.43847800	-0.00066100	-1.63524800

H/[CB₁₀H₁₁](1)

Lowest normal mode frequency: 166.60 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 267.91 kcal/mol

B	0.79658200	-1.42882700	-0.02275400
B	1.05584300	1.23790700	-0.50239600
B	-1.50205300	0.21549600	0.78656700
B	-0.79887800	1.31957700	-0.48754100
B	0.00253400	1.11192400	1.10111400
B	1.66343400	-0.28718400	-0.87638500
B	-1.04250700	-1.30574400	0.02481700
B	-0.02629900	-0.31155700	-1.41231200

B	1.50906200	-0.05400600	0.86511200
B	-0.09100900	-0.68714700	1.37593500
H	1.55661000	2.26439000	-0.82365200
H	-2.48957900	0.44552400	1.39297900
H	-1.22824000	2.33215000	-0.92487900
H	-0.03269700	1.96653900	1.92548900
H	2.57394100	-0.49047400	-1.60174700
H	-1.62266000	-2.33525600	-0.01409100
H	0.00529100	-0.43603900	-2.59209000
H	2.43963500	-0.01448200	1.59900400
H	-0.12541600	-1.22748700	2.43072300
H	-2.37536800	-0.06012000	-1.47024100
H	1.12760000	-2.56760300	0.00240000
C	-1.49868000	-0.05104400	-0.84171600
H	1.32942200	1.37691800	0.86562100

H/[CB₁₀H₁₁](2)

Lowest normal mode frequency: 238.83 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 264.19 kcal/mol

B	1.08564200	-1.29113900	-0.10458800
B	0.81247600	1.37903700	-0.26509500
B	-1.53332300	-0.18513400	0.77429800
B	-0.99109100	1.28642700	-0.39921300
B	-0.07556000	0.94717100	1.23381300
B	1.74200000	0.09085500	-0.81921500
B	-0.72002800	-1.41164800	-0.27829600
B	0.13431600	-0.07435300	-1.43558600
B	1.46584100	0.10616900	0.89610500
B	0.03144300	-0.88365200	1.27165200
H	1.15545500	2.49600700	-0.47925200
H	-2.57757800	-0.31130000	1.31676600
H	-1.60625900	2.26150200	-0.66643600
H	-0.08323000	1.69674500	2.15626500
H	2.70439700	0.19180500	-1.49686700
H	-1.14823900	-2.48668600	-0.52339800
H	0.16426400	-0.09515100	-2.62178700
H	2.32814700	0.26262200	1.69443800
H	0.00493100	-1.55739200	2.24719300
H	-2.27003800	-0.25066300	-1.55951100
H	1.57232600	-2.37037500	-0.18319200
C	-1.43296400	-0.14169300	-0.88715300
H	-1.40497400	1.19439000	1.06932300

H/[CB₁₀H₁₁](3)

Lowest normal mode frequency: 166.80 cm⁻¹

The value of ΔG_{acid} at $\omega B97XD/6-311+G(d, p)$ level: 258.92 kcal/mol

B	0.98984800	-1.36019000	0.03065900
B	1.03857000	1.31116400	-0.41576700
B	-1.50888500	0.03316500	0.79730100
B	-1.12984200	1.24722900	-0.42474000
B	-0.06716000	1.06288400	1.14535500
B	1.69835700	-0.14134800	-0.85665800
B	-0.86011200	-1.40133400	-0.03956600
B	0.07943400	-0.25909900	-1.43751800
B	1.48505000	0.13563600	0.86490700
B	0.00644300	-0.74161500	1.34793700
H	1.45600500	2.36111500	-0.78632700
H	-2.52959100	0.07333600	1.39242800
H	-1.64807300	2.23641600	-0.81247500
H	-0.13895000	1.88079600	2.00126800
H	2.64378700	-0.15828500	-1.56593100
H	-1.34663300	-2.47418800	-0.14337200
H	0.08634000	-0.41476200	-2.61417700
H	2.37447600	0.28759800	1.63460500
H	-0.02107300	-1.23706100	2.42447400
H	-2.29887600	-0.34656400	-1.52288900
H	1.44946500	-2.45317600	0.04829600
C	-1.44991200	-0.19645200	-0.87285100
H	0.01408200	1.99102300	0.12166100

H/[CB₁₀H₁₁](4)

Lowest normal mode frequency: 295.54 cm⁻¹

The value of ΔG_{acid} at $\omega B97XD/6-311+G(d, p)$ level: 252.17 kcal/mol

B	-1.29824500	0.97587600	0.51554100
B	-0.53448800	-1.15409000	-0.95215600
B	1.47434800	-0.02841600	0.81660400
B	1.38504100	-1.00673700	-0.63054700
B	0.30720700	-1.37929700	0.61908200
B	-1.73823500	-0.00722200	-0.84868500
B	0.43346500	1.40007100	0.47133300
B	-0.39962600	1.01414600	-1.09601500
B	-1.38756200	-0.80242700	0.65136200
B	-0.14397500	0.09588900	1.53938500
H	-0.62440300	-1.91743400	-1.86078700
H	2.49936400	0.03272700	1.40347000
H	2.18356700	-1.64441000	-1.22159300
H	0.50830000	-2.48709500	1.00046000
H	-2.69493100	0.05807900	-1.54128500
H	0.78842400	2.49987200	0.72659500

H	-0.43545000	1.72162500	-2.04832000
H	-2.18616900	-1.46695500	1.22315100
H	-0.15786300	0.17091100	2.72197500
H	2.18099400	1.35897900	-1.03535100
H	-2.00239700	1.81227600	0.97485700
C	1.38816500	0.70617600	-0.68948100
H	1.12191500	0.08540100	-1.63580400

H/[CB₁₁H₁₂]

Lowest normal mode frequency: 49.95 cm⁻¹

B	-0.77178600	-1.41535200	-0.55055900
B	-0.76578300	0.09026500	-1.51246500
B	-0.76040500	-0.96730800	1.17349000
B	-0.76075200	0.81852900	1.28058600
B	-0.77553500	1.46952200	-0.37807100
B	0.72601000	1.44009800	0.55552500
B	0.73933100	-0.09229700	1.53340700
B	0.72832200	-1.49469000	0.38135100
B	0.72490000	0.98700500	-1.18718900
B	0.72767200	-0.83574200	-1.29634800
H	-1.42400200	2.42620800	-0.62872300
H	1.28803800	2.41052800	0.94071500
H	1.29845800	-0.15348400	2.57716000
H	1.29253600	-2.50340300	0.64627000
H	1.28306200	-1.39181500	-2.18409100
H	1.28001100	1.64540300	-2.00213700
H	-1.40679900	0.14820700	-2.50462700
H	-1.41781200	-2.33638400	-0.91516600
H	-1.39817300	-1.59334400	1.94803900
H	-1.39846900	1.34711100	2.12469000
B	1.54280300	0.00183100	-0.00544900
H	2.83440600	0.00407200	-0.42049700
H	-2.61789200	-0.00308600	0.00894500
H	2.83509800	0.00152700	0.40660100
C	-1.53705700	-0.00180800	0.00523800

H/[CB₁₁H₁₂](1)

Lowest normal mode frequency: 468.88 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 261.13 kcal/mol

B	0.27757800	-1.41424800	-0.87569900
B	1.39205400	-0.90419900	0.39131900
B	-0.44834400	0.04022900	-1.62586000
B	0.28314800	1.45405900	-0.80640100
B	1.39544600	0.87888900	0.43438500

B	-0.22355900	1.43438200	0.90046500
B	-1.36664800	0.98521200	-0.41315300
B	-1.37061800	-0.95859600	-0.45942500
B	0.49442700	-0.04042800	1.63284800
B	-0.22892800	-1.47539400	0.83026500
H	2.40690600	1.46570600	0.60780800
H	-0.38512800	2.43598600	1.51172100
H	-2.31197600	1.63541700	-0.71065500
H	-2.31747000	-1.59099100	-0.78865700
H	-0.39451900	-2.50499400	1.39192300
H	0.77937600	-0.06823000	2.78176500
H	2.40133700	-1.50247800	0.53591800
H	0.49417900	-2.34646300	-1.56877900
H	-0.64177100	0.06836600	-2.79130900
H	0.50378800	2.41798500	-1.45327000
B	-1.22278600	-0.02791300	1.22799400
H	-2.08772800	-0.04558200	2.03952500
C	1.14320900	0.02265900	-1.02763400
H	1.93464900	0.03889900	-1.76369100
H	-2.14973200	0.00046000	0.18980700

H/[CB₁₁H₁₂](2)

Lowest normal mode frequency: 444.34 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 256.16 kcal/mol

B	1.30214400	0.97850400	-0.53492400
B	-0.37739000	1.44320900	-0.80814700
B	1.30342400	-0.97883700	-0.53188500
B	-0.37554700	-1.44631900	-0.80340100
B	-1.36210300	-0.00255700	-1.01586200
B	-1.37799800	-0.89573200	0.52804100
B	0.28794500	-1.45735800	0.84861300
B	1.31693400	0.00282400	1.12125400
B	-1.37924200	0.89564100	0.52507300
B	0.28590500	1.46057600	0.84390100
H	-2.18445000	-0.00458200	-1.86596800
H	-2.31498900	-1.53497500	0.87035800
H	0.53363000	-2.46744700	1.41698900
H	2.25632700	0.00442800	1.84554000
H	0.53037000	2.47293600	1.40874500
H	-2.31713400	1.53471700	0.86521800
H	-0.50162200	2.37855100	-1.52078300
H	2.20126300	1.56368200	-1.03555700
H	2.20386400	-1.56385900	-1.03028400
H	-0.49870100	-2.38424400	-1.51282800
B	-0.36850200	0.00253200	1.66367000

H	-0.52180900	0.00421600	2.83867100
C	0.28275300	-0.00232200	-1.48951100
H	0.48241400	-0.00382000	-2.55187500
H	2.15646800	0.00191200	0.02717800

HCB₁₁H₁₂(3)

Lowest normal mode frequency: 453.79 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 255.41 kcal/mol

B	0.22769200	-0.78661400	-1.47369100
B	-1.39882200	-0.34768000	-0.90885800
B	1.21801300	-1.19191900	-0.04868100
B	0.22683300	-0.90584600	1.40381200
B	-1.39920100	-0.42132100	0.87638900
B	-0.29040600	0.81480000	1.47000600
B	1.36376400	0.41109200	0.97831900
B	1.36430800	0.49127400	-0.94061600
B	-1.28378500	1.15356700	0.04739900
B	-0.28973400	0.93363200	-1.39788500
H	-2.32960800	-0.86074300	1.45887800
H	-0.40626800	1.33879600	2.52578100
H	2.30346700	0.63779500	1.66715600
H	2.30512600	0.77338500	-1.60713700
H	-0.40537300	1.54274200	-2.40698800
H	-2.17252500	1.93627100	0.07972700
H	-2.32891700	-0.73737700	-1.52616700
H	0.36015900	-1.44515700	-2.44636500
H	2.01434100	-2.06408000	-0.08474900
H	0.35921100	-1.64262500	2.31866800
B	0.42084500	1.65979100	0.06884500
H	0.75902000	2.79461000	0.11608300
C	-0.45280200	-1.45985900	-0.06057000
H	-0.72437100	-2.50574300	-0.10398900
H	2.18501400	-0.06260400	-0.00267700

H/[CB₁₂H₁₃]

Lowest normal mode frequency: 93.09 cm⁻¹

B	1.89198400	0.86438600	0.03096700
B	1.89657100	-0.85865600	0.02829100
B	0.45273500	1.65341400	-0.40235700
B	0.43316200	1.00504700	1.26139000
B	0.43843400	-0.99335600	1.26691400

B	-1.06724900	1.44657500	0.39402800
B	-0.82302000	0.86826700	-1.27027800
B	0.45890100	-1.65503900	-0.39172000
B	-0.98864000	0.00299600	1.43414200
B	-0.82077300	-0.88000400	-1.26419300
B	-1.06148900	-1.44732700	0.40376100
H	2.80061400	-1.62952200	-0.03393300
H	0.78657100	2.73608400	-0.74576500
H	0.81829700	1.57609300	2.22930800
H	1.31677400	-0.00396200	-2.44265600
H	-1.77814100	-2.35635000	0.64410800
H	-2.80012400	-0.00590000	-0.24201700
H	-1.78838800	2.35369600	0.62803100
H	0.82761100	-1.55483700	2.23873300
H	0.79398300	-2.73926100	-0.72891700
H	-1.34409700	1.38824300	-2.19499600
H	-1.34004900	-1.40873400	-2.18495100
H	-1.64117700	0.00463600	2.42084300
H	2.79351700	1.63859600	-0.03049300
B	0.84014800	-0.00238800	-1.35525600
C	-1.72450600	-0.00357200	-0.13518500
H	2.64782200	0.00308200	0.57536700

H/[CB₁₂H₁₃](1)

Lowest normal mode frequency: 189.04 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 279.64 kcal/mol

B	-1.92531500	0.83346400	0.01741600
B	-0.49395200	1.65717000	-0.37194000
B	-1.86552400	-0.88148000	0.05201100
B	-0.43181800	0.99503100	1.27063300
B	1.05443600	1.48641300	0.38814500
B	-0.38261800	-0.99208400	1.26652800
B	-0.41424600	-1.64985500	-0.38559600
B	0.79425200	0.91225200	-1.28146100
B	1.03295800	0.03972200	1.40791500
B	0.82583800	-0.82755800	-1.29648100
B	1.88404500	0.05517900	-0.18970300
H	-0.88102700	2.72386000	-0.71149200
H	-2.74276000	-1.67965000	-0.02998300
H	-0.84366500	1.50522600	2.26165400
H	-1.36533100	-0.06196200	-2.41137700
H	3.05768800	-0.04832900	-0.28828700
H	1.61548000	-2.16162300	0.57508800
H	-0.63233600	-1.65874600	2.21429600
H	1.66869900	2.46503400	0.64990200

H	1.15903900	1.47559900	-2.25786100
H	-0.65622000	-2.77041900	-0.67067400
H	1.26421500	-1.48405200	-2.17632800
H	1.61884500	-0.07019400	2.42973800
H	-2.87117100	1.54705600	-0.06098900
B	-0.87170900	-0.02553600	-1.33235000
C	1.01917200	-1.29207500	0.33652100
H	-2.53822500	-0.04293600	0.73160000

H/[CB₁₂H₁₃](2)

Lowest normal mode frequency: 115.26 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 259.66 kcal/mol

B	1.96035600	0.82487900	-0.07794100
B	1.75577100	-0.82902700	-0.05309100
B	0.60920800	1.76431500	-0.04495900
B	1.14804800	0.21353400	1.30666300
B	0.38764600	-1.37789100	0.98084600
B	-1.06038800	1.46582100	0.68650700
B	-0.76032900	1.17704700	-0.99409700
B	0.34313900	-1.57161000	-0.78551400
B	-0.90315900	-0.23771100	1.45958500
B	-0.90342500	-0.51312600	-1.39400300
B	-1.14078200	-1.43990100	0.09621700
H	2.71727200	-1.52131300	-0.11687300
H	0.84430200	2.92622500	-0.13404200
H	1.50288500	0.52511400	2.39666000
H	1.21571800	0.32849200	-2.48429700
H	-1.95881200	-2.28305600	0.22619100
H	-2.79922100	0.19876800	-0.09355700
H	-1.76752400	2.33854900	1.05750100
H	0.61590500	-2.23977500	1.76498500
H	0.57919400	-2.57631700	-1.36736600
H	-1.28682100	1.98413600	-1.68185800
H	-1.53907400	-0.73555200	-2.36587100
H	-1.50018900	-0.46025400	2.45789400
H	3.00220400	1.37490700	-0.18432800
B	0.79559400	0.17430200	-1.38414500
C	-1.72114900	0.13999300	-0.03544000
H	-0.45733600	1.04696000	1.75726100

H/[CB₁₂H₁₃](3)

Lowest normal mode frequency: 159.57 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 248.03 kcal/mol

B	-1.90230500	1.01098600	0.00028400
B	-1.88139700	-0.63661200	0.00007500

B	-0.42614000	1.70739900	0.00032800
B	-0.89249300	0.36488800	-1.31253400
B	-0.56717400	-1.40421600	-0.89379200
B	1.07998500	1.26528700	-0.83770600
B	1.08056100	1.26509000	0.83738200
B	-0.56688100	-1.40439400	0.89362500
B	0.83988400	-0.50621800	-1.38220900
B	0.84045900	-0.50693400	1.38213400
B	0.92587300	-1.63273000	-0.00044500
H	-2.91680800	-1.21719500	-0.00012700
H	-0.54802100	2.89286300	0.00021200
H	-1.20612300	0.65140400	-2.42185900
H	-1.20537700	0.65086900	2.42223300
H	1.61167100	-2.59597400	-0.00073100
H	2.78835300	-0.20580800	-0.00049300
H	1.55428400	1.83697200	-1.76368200
H	-0.94658600	-2.24279400	-1.64277900
H	-0.94631300	-2.24303300	1.64254800
H	1.55325600	1.83554800	1.76493600
H	1.39556300	-0.68457900	2.40988700
H	1.39521400	-0.68393100	-2.40985700
H	-2.86712000	1.69282300	0.00018900
B	-0.89272600	0.36449100	1.31258900
C	1.70714500	-0.17150800	-0.00001000
H	1.90691600	1.90669900	0.00092100

H/[CB₁₃H₁₄]

Lowest normal mode frequency: 62.75 cm⁻¹

B	-0.00015400	1.39985000	0.00000000
B	-1.74448400	-0.75119100	0.00000000
B	-0.87042700	-0.76141400	1.50888600
B	0.87029000	-0.76142700	1.50893400
B	-1.52181500	0.73717100	-0.88522800
B	0.00022200	0.73026200	-1.76470100
B	0.00022200	0.73026200	1.76470100
B	-1.52181500	0.73717100	0.88522800
H	-0.00106700	-2.51249000	0.00000000
H	0.40968300	2.72148700	0.00000000
H	-2.70372600	-1.44391900	0.00000000
H	-1.35005400	-1.46458900	2.33082600
H	1.34938300	-1.46454200	2.33125300
H	-1.35005400	-1.46458900	-2.33082600
H	-2.40061300	1.35271700	-1.38913500
H	-0.00022500	1.34287100	-2.77958700
H	-0.00022500	1.34287100	2.77958700

H	-2.40061300	1.35271700	1.38913500
B	-0.87042700	-0.76141400	-1.50888600
B	1.52253100	0.73636800	-0.88532900
B	1.52253100	0.73636800	0.88532900
B	0.87029000	-0.76142700	-1.50893400
B	1.74433900	-0.75131700	0.00000000
H	2.70340700	-1.44432100	0.00000000
H	2.40078000	1.35266600	1.38928200
H	2.40078000	1.35266600	-1.38928200
H	1.34938300	-1.46454200	-2.33125300
C	-0.00049600	-1.42950100	0.00000000
H	-0.41037700	2.72168800	0.00000000

H/[CB₁₃H₁₄](1)

Lowest normal mode frequency: 102.70 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 256.44 kcal/mol

B	-0.26919300	0.00071500	1.64033400
B	0.84550100	-1.50093400	-0.73272100
B	1.73883700	-0.00774000	-0.76422000
B	0.85891100	1.49375900	-0.73226300
B	-0.03659200	-1.73993800	0.76484200
B	-1.56650500	-0.88099600	0.71672900
B	1.60071600	0.92718900	0.72723600
B	1.59178000	-0.94128000	0.72751900
H	0.04405700	0.00000400	-2.50617600
H	-0.19511100	0.00016400	2.82342500
H	1.36034600	-2.34410500	-1.38396300
H	2.67053200	-0.01177000	-1.49103100
H	1.38152000	2.33242600	-1.38313600
H	-1.33056000	-2.33181600	-1.48131700
H	-0.03867700	-2.78494300	1.32339800
H	-2.47429000	-1.41696200	1.25743600
H	2.50027200	1.49718700	1.24577200
H	2.48625600	-1.51915400	1.24613800
B	-0.88374600	-1.51599700	-0.75084000
B	-1.55821900	0.89454400	0.71705500
B	-0.02099000	1.74022400	0.76512000
B	-1.72078300	0.00776300	-0.79506900
B	-0.87003200	1.52364400	-0.75072600
H	-1.30953400	2.34345300	-1.48117900
H	-0.01376400	2.78483700	1.32433900
H	-2.46110400	1.43844100	1.25806500
H	-2.63545500	0.01197100	-1.54540100
C	0.02420700	0.00016300	-1.42310400
H	1.32185100	-0.00548900	1.66727300

H/[CB₁₃H₁₄](2)**Lowest normal mode frequency: 57.65 cm⁻¹****The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 251.11 kcal/mol**

B	-0.10022700	0.00353300	1.57297300
B	1.46488300	-1.01380700	-0.71978700
B	1.53470500	0.91780700	-0.71650800
B	0.01888700	1.73417400	-0.73207000
B	0.77938800	-1.54126000	0.79185200
B	-0.96255600	-1.46768000	0.76434000
B	0.88107400	1.48668400	0.79286800
B	1.71996700	-0.05752200	0.86759100
H	0.05984300	-0.00197600	-2.49819200
H	-0.06010200	0.00239000	2.75919400
H	2.27262900	-1.55210500	-1.40229700
H	2.37825300	1.40039600	-1.39727100
H	0.10404500	2.64841100	-1.47850000
H	-0.07349000	-2.65047600	-1.47735300
H	1.26005900	-2.45740000	1.37005300
H	-1.49198500	-2.36965100	1.32160300
H	1.42038300	2.36942200	1.37134100
H	2.75075400	-0.09393100	1.45301900
B	-0.09990900	-1.73241400	-0.73120300
B	-1.80265600	0.06057300	0.72553600
B	-0.86174000	1.52833200	0.76278600
B	-1.56172700	-0.82498200	-0.75442300
B	-1.49821600	0.92296800	-0.75749400
H	-2.26327400	1.41477000	-1.51462800
H	-1.33140400	2.46350200	1.31885600
H	-2.86373500	0.09815400	1.25210100
H	-2.36028200	-1.26439600	-1.50906900
C	0.03880400	-0.00141900	-1.41524600
H	2.40612500	-0.08062800	-0.40968700

H/[CB₅HF₅]**Lowest normal mode frequency: 127.10 cm⁻¹**

B	-0.52806100	1.06474700	0.00000000
B	0.95670400	-0.01835800	0.90253300
B	-0.77989600	-0.33515700	-0.86866300
B	0.95670400	-0.01835800	-0.90253300
B	-0.77989600	-0.33515700	0.86866300
C	0.32083400	-1.18822700	0.00000000
H	0.53453500	-2.24526700	0.00000000
H	1.48833400	0.82441500	0.00000000
F	-1.52470800	-0.75383100	1.89993300

F	1.74011200	-0.05193400	1.98459500
F	1.74011200	-0.05193400	-1.98459500
F	-1.52470800	-0.75383100	-1.89993300
F	-0.77254500	2.36282100	0.00000000

H/[CB₆HF₆]

Lowest normal mode frequency: 90.14 cm⁻¹

B	-1.43486500	-0.15888800	0.14611600
B	-0.36849800	-1.62307800	0.18831400
B	-0.53716500	1.28338800	-0.16456200
B	1.00266100	0.72958900	-0.53792000
B	1.07732800	-0.87104100	0.19942800
C	-0.23337300	-0.24975200	-0.99906000
H	-0.42181100	-0.47063700	-2.04284700
B	0.45822000	0.71147200	1.08153900
H	-1.16159900	-1.00561400	1.08648300
F	-2.75690200	-0.07443400	-0.06051800
F	-1.23958300	2.34253400	-0.59075800
F	0.70839000	1.06144700	2.32155400
F	2.04858800	1.21148200	-1.20555400
F	2.27931700	-1.40283200	-0.10892500
F	-0.81811700	-2.84735800	-0.09067100

H/[CB₇HF₇]

Lowest normal mode frequency: 96.01 cm⁻¹

B	-0.19547300	0.42910500	1.23919500
B	0.50696100	-1.17142500	-0.86731700
B	1.11974800	0.75358800	0.00000000
B	-0.22507100	1.71921000	0.00000000
B	-0.19547300	0.42910500	-1.23919500
B	0.50696100	-1.17142500	0.86731700
B	-1.05897100	-0.88863400	0.00000000
C	-1.34745300	0.65487400	0.00000000
H	-2.38282500	0.96928700	0.00000000
H	1.47798000	-1.34126700	0.00000000
F	2.43816000	0.93836400	0.00000000
F	-0.38073500	3.04831100	0.00000000
F	-0.43891000	0.63772400	-2.54512600
F	0.81376600	-1.96597900	-1.89524700
F	0.81376600	-1.96597900	1.89524700
F	-0.43891000	0.63772400	2.54512600
F	-2.06311800	-1.78070700	0.00000000

H/[CB₈HF₈]

Lowest normal mode frequency: 97.76 cm⁻¹

B	-1.05298900	-0.95533300	-0.95203500
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B	-0.79989900	-0.87424400	0.85519400
B	-1.60616400	0.38222200	-0.06818600
B	0.99372800	-0.55852500	0.83195300
B	-0.16179100	0.85911500	0.90062300
B	-0.42132800	1.33513400	-0.76829700
B	1.43071200	-0.78502700	-0.88132200
B	1.29128400	0.86763800	-0.21042800
H	0.35769000	-2.68176000	-0.24498600
C	0.25361500	-1.60191100	-0.27100700
H	0.88912400	0.52255100	-1.41418100
F	-0.12605500	1.68271700	1.96730600
F	-0.56114500	2.40482400	-1.53456600
F	-2.89828200	0.77769100	0.06860200
F	-1.31789500	-1.61574800	1.84273000
F	1.79481800	-0.96902100	1.82534100
F	2.41136900	-1.24553500	-1.63270300
F	2.30544400	1.74759700	-0.13837200
F	-1.73450600	-1.62521700	-1.87081600

H/[CB₉HF₉]

Lowest normal mode frequency: 116.58 cm⁻¹

B	1.06819800	0.00002900	-1.13359300
B	-0.53893800	-0.00012900	-1.47944300
B	0.37801900	-1.35279700	-0.40847600
B	1.22263200	0.00012000	0.53339800
B	0.37785000	1.35283700	-0.40863300
B	-1.34707900	-0.94454500	-0.04723000
B	-0.09274000	-0.94398100	1.34015400
B	-0.09285800	0.94410800	1.34005100
B	-1.34719300	0.94434900	-0.04733400
H	-2.19319200	-0.00003100	1.96920200
C	-1.38115400	-0.00002700	1.25700200
H	2.99314800	0.00009400	-0.75954200
F	-2.35988400	1.78826200	-0.31525000
F	-2.35966500	-1.78861000	-0.31505700
F	-1.19422300	-0.00024900	-2.65231600
F	0.79441600	2.61536400	-0.68226800
F	2.54138200	0.00004800	-1.63255300
F	2.61709800	0.00019700	0.80077300
F	0.10219600	1.81983900	2.33945700
F	0.10245900	-1.81956700	2.33965800
F	0.79483300	-2.61526900	-0.68201400

H/[CB₁₀HF₁₀]

Lowest normal mode frequency: 119.74 cm⁻¹

B	1.26489100	0.70287500	0.00000000
B	-0.38079600	-1.60088100	0.87199400
B	-1.26078900	0.25085500	-1.23084600
B	-1.26078900	0.25085500	1.23084600
B	-0.38079600	-1.60088100	-0.87199400
B	0.45486800	-0.11406000	1.44227600
B	-0.04520500	1.56163700	-0.88595700
B	-0.04520500	1.56163700	0.88595700
B	1.07626300	-1.06971700	0.00000000
B	0.45486800	-0.11406000	-1.44227600
H	-2.25420600	1.93886600	0.00000000
C	-1.40920300	1.25955900	0.00000000
H	-1.38991200	-1.61504200	0.00000000
F	0.10948600	2.65790300	-1.64084500
F	-2.24347500	0.11149100	-2.11103000
F	0.10948600	2.65790300	1.64084500
F	-2.24347500	0.11149100	2.11103000
F	1.03227900	-0.27626900	2.65388700
F	-0.55872800	-2.57289000	1.76217200
F	2.21288400	-1.79919400	0.00000000
F	-0.55872800	-2.57289000	-1.76217200
F	1.03227900	-0.27626900	-2.65388700
F	2.52052300	1.17844800	0.00000000

H/[CB₁₁HF₁₁]

Lowest normal mode frequency: 130.75 cm⁻¹

B	-0.21430100	1.77797000	0.00000000
B	-0.64140200	0.81148000	1.46474700
B	-0.64140200	0.81148000	-1.46474700
B	-1.32517100	-0.77673300	-0.91188900
B	-1.32517100	-0.77673300	0.91188900
B	-0.06096800	-1.59613000	0.00000000
B	0.35549300	-0.63928000	-1.48440600
B	1.06754600	0.95140800	-0.92601600
B	0.35549300	-0.63928000	1.48440600
B	1.06754600	0.95140800	0.92601600
B	1.30711000	-0.51914900	0.00000000
C	-1.52603500	0.66273300	0.00000000
H	-2.52271000	1.09217100	0.00000000
H	2.09257800	-2.37420700	0.00000000
F	-0.46294800	3.10071500	0.00000000
F	2.02583600	1.58999500	-1.63439500
F	2.02583600	1.58999500	1.63439500
F	2.52189300	-1.50684200	0.00000000
F	0.85022700	-1.29624100	2.56634400

F	0.40245800	-2.91774900	0.00000000
F	-2.36516000	-1.31577700	1.57271700
F	-2.36516000	-1.31577700	-1.57271700
F	-1.19368900	1.43526300	2.52134900
F	-1.19368900	1.43526300	-2.52134900
F	0.85022700	-1.29624100	-2.56634400

H/[CB₁₂HF₁₂]

Lowest normal mode frequency: 5.95 cm⁻¹

B	1.38180800	1.30811700	-0.00917300
B	-0.30517200	1.51603000	-0.02771500
B	2.22466900	-0.00549000	0.00685000
B	0.36971300	0.55141600	-1.45261200
B	-1.45598400	0.53120600	-0.92597500
B	1.04972000	-1.16530700	-0.86595100
B	1.03766800	-1.12737200	0.92337300
B	-1.47092900	0.56446100	0.88601800
B	-0.63817500	-0.94886900	-1.41938900
B	-0.65845700	-0.89635700	1.44478300
B	-1.74942000	-0.93833600	0.00488800
H	-0.36122800	-2.85908100	0.05082400
B	0.34365800	0.60567800	1.44000200
C	-0.24927800	-1.77935100	0.03165200
H	0.87670200	3.23715100	-0.04672100
F	-2.41566500	1.21199200	1.60733000
F	-0.46856000	2.94247900	-0.05548800
F	1.79392600	2.79891100	-0.02998600
F	0.63020900	1.17722000	2.63274400
F	3.48506400	-0.40087100	0.01223900
F	1.74824900	-1.93905900	1.73202500
F	1.76677900	-2.01176600	-1.63245100
F	-0.97484700	-1.55105700	2.57505000
F	-0.93919600	-1.64399200	-2.52945100
F	-2.87437600	-1.67126900	0.01008600
F	-2.38704900	1.15332800	-1.68615400
F	0.67265400	1.08099000	-2.66033500

H/[CB₁₃HF₁₃]

Lowest normal mode frequency: 72.37 cm⁻¹

B	-0.01688000	0.00863400	1.47580400
B	-0.51191600	-1.67870200	-0.92881700
B	1.21779100	-1.41501200	-0.77693300
B	1.75293100	0.27908200	-0.76138300

B	-1.26007800	-1.05858800	0.50018200
B	-1.60466500	0.62928700	0.53028300
B	1.63889400	-0.64258100	0.74617300
B	0.28547300	-1.80653900	0.65673900
H	0.19686300	0.03907700	-2.60671800
B	-1.56276300	-0.23156500	-1.00962400
B	-0.31061800	1.79495800	0.67254600
B	1.34148500	1.11847100	0.74480000
B	-1.07135100	1.46687600	-0.88514500
B	0.67472400	1.69522400	-0.78394200
C	0.11767600	0.02064300	-1.52116300
H	-2.95160700	-0.72496900	1.45718900
F	-2.59694200	-0.43515100	-1.85592500
F	-1.74266700	2.27747700	-1.71156000
F	1.13940100	2.67864800	-1.57174600
F	2.82722400	0.47009700	-1.55191900
F	-0.53935100	2.92598100	1.37726700
F	-2.83993900	0.70624200	1.23990100
F	-0.18991600	-0.04004400	2.81639100
F	-2.48438200	-1.59638900	1.25861400
F	0.37552600	-2.96084000	1.35592600
F	1.97326300	-2.21405600	-1.54442100
F	-0.92466200	-2.63632300	-1.76982200
F	2.69379300	-1.02359700	1.50166600
F	2.21793500	1.82176700	1.49708000

H/[CB₅HCl₅]

Lowest normal mode frequency: 81.46 cm⁻¹

B	-0.39269000	1.00457400	0.00000000
B	0.96630500	-0.17361900	0.91188300
B	-0.76303300	-0.37653500	-0.86804900
B	0.96630500	-0.17361900	-0.91188300
B	-0.76303300	-0.37653500	0.86804900
C	0.26095700	-1.30102300	0.00000000
H	0.41867400	-2.36780300	0.00000000
Cl	-0.63103000	2.72279400	0.00000000
Cl	-1.84750600	-0.80388600	2.18457300
Cl	-1.84750600	-0.80388600	-2.18457300
Cl	2.05903400	-0.26388700	-2.28224900
Cl	2.05903400	-0.26388700	2.28224900
H	1.48186900	0.66937700	0.00000000

H/[CB₅HCl₅](1)

Lowest normal mode frequency: 72.52 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 261.13 kcal/mol

B	0.04843700	-0.00001500	0.92315600
B	0.80546700	-0.95694200	-0.28372500
B	-0.85655800	0.89286400	-0.23974400
B	0.80473900	0.95796500	-0.28308100
B	-0.85590900	-0.89281100	-0.24101400
C	-0.17121000	0.00104000	-1.48787300
H	-0.83083200	0.00334600	-2.35694900
Cl	0.26243900	-0.00209900	2.66002400
Cl	-2.19958700	-2.02530900	-0.35824300
Cl	-2.20090800	2.02449400	-0.35691100
Cl	2.10619500	2.08227700	-0.56375400
Cl	2.10739000	-2.08024100	-0.56583800
H	0.84321900	0.00004200	-1.95351400

H/[CB₅HCl₅](2)

Lowest normal mode frequency: 71.42 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 261.13 kcal/mol

B	0.14672500	0.00838700	0.94412500
B	-0.75137100	0.83122900	-0.27730900
B	0.96949000	-0.88407100	-0.32033700
B	-0.69091300	-0.84641700	-0.27682800
B	0.94207300	0.87884100	-0.31245300
C	0.08728600	0.00575900	-1.39541100
H	0.06347900	0.00556500	-2.47303900
Cl	0.13210600	-0.01052700	2.71405400
Cl	2.24116000	2.05245500	-0.53758400
Cl	2.29581000	-2.02631100	-0.54906200
Cl	-2.36420600	-1.63385000	-0.44859000
Cl	-2.34838500	1.64270900	-0.44233500
H	-2.92746400	-0.39605700	-0.46071400

H/[CB₆HCl₆]

Lowest normal mode frequency: 61.71 cm⁻¹

B	0.88908200	1.27085100	0.07369100
B	-0.88700000	1.27229200	0.07371600
B	1.31941500	-0.33970400	-0.01549900
B	-0.00097200	-1.26089500	-0.49339800
B	-1.31988900	-0.33752500	-0.01552900
C	0.00042600	0.30874000	-1.03553000
H	0.00060800	0.53659600	-2.09477100
B	-0.00048500	-0.65861600	1.12483000
Cl	-0.00104900	-1.07494200	2.79869200
Cl	2.97905000	-0.80126900	-0.41997700
Cl	-0.00231700	-2.82537300	-1.28322600
Cl	1.95523700	2.63811100	-0.23206400

Cl	-1.95108700	2.64115100	-0.23198600
Cl	-2.98014300	-0.79663200	-0.42022400
H	0.00135300	1.60116000	0.97822500

H/[CB₇HCl₇]

Lowest normal mode frequency: 64.97 cm⁻¹

B	0.42607300	1.24700300	-0.31074400
B	-1.07879900	-0.86359600	0.53802300
B	0.81902200	-0.00116500	0.98776300
B	1.68934300	0.00025700	-0.42777300
B	0.42630000	-1.24659800	-0.31179800
B	-1.07955300	0.86458100	0.53768400
B	-0.94833200	0.00027900	-1.04173000
C	0.56628700	0.00066100	-1.47330400
Cl	-2.13810300	-2.15864200	1.08705400
Cl	-2.13969400	2.15893200	1.08636700
Cl	1.33597300	-0.00182600	2.66305200
Cl	-2.24553900	-0.00025900	-2.24359800
Cl	0.75597600	2.94834300	-0.66120100
Cl	0.75477600	-2.94787000	-0.66349900
Cl	3.42595100	0.00077100	-0.67908500
H	0.78431400	0.00105600	-2.53256600
H	-1.19109300	0.00052500	1.50071900

H/[CB₇HCl₇](1)

Lowest normal mode frequency: 60.99 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 250.48 kcal/mol

B	-1.24886600	0.25275100	-0.57195800
B	0.85774100	-0.99668800	0.60853000
B	0.00027100	0.57353200	0.94222900
B	0.00124300	1.56529800	-0.42606700
B	1.24941300	0.25077400	-0.57200500
B	-0.85846900	-0.99575600	0.60829000
B	-0.00104600	-0.92736900	-1.23174600
C	0.00050600	0.58523300	-1.61718700
Cl	2.18701900	-1.75643900	1.48628900
Cl	-2.18897700	-1.75415800	1.48549300
Cl	0.00026400	1.28139500	2.56826100
Cl	-0.00189600	-2.31779300	-2.30226900
Cl	-2.94320900	0.58757900	-0.93017800
Cl	2.94412300	0.58342800	-0.93068600
Cl	0.00242700	3.31465900	-0.49457400
H	0.00081100	0.89080600	-2.65426000
H	-0.00103700	-1.97230500	0.57130000

H/[CB₇HCl₇](2)

Lowest normal mode frequency: 64.06 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 249.62 kcal/mol

B	0.93429500	-0.96870800	0.81513400
B	-1.26205800	0.21074500	-0.39326100
B	0.41511100	-0.23974700	-0.93921100
B	1.51173600	0.56150800	0.08500100
B	-0.04292100	1.35921700	-0.07841700
B	-0.74120600	-1.30589200	0.10102500
B	-0.94061600	0.43919700	1.25807500
C	0.63836000	0.63350300	1.38698000
Cl	-2.70495800	0.40727400	-1.38536300
Cl	-1.57117500	-2.79413100	-0.32372200
Cl	0.79010000	-0.70384100	-2.60588500
Cl	-2.06858300	0.78292500	2.54938300
Cl	2.20974200	-2.04151300	1.41537800
Cl	-0.06515800	3.08145500	-0.45149700
Cl	3.16803000	1.05923400	-0.14114400
H	1.03344400	1.10419500	2.28011500
H	-0.12128300	-1.64065700	1.18474000

H/[CB₈HCl₈]

Lowest normal mode frequency: 66.78 cm⁻¹

B	-1.08457700	-0.86808900	-1.08809000
B	-0.81824600	-1.01750400	0.71790700
B	-1.55576400	0.36955700	-0.03864700
B	0.98349700	-0.77315600	0.70646600
B	-0.11099200	0.65772700	0.96039200
B	-0.34329900	1.34860600	-0.64503900
B	1.36542700	-0.80351600	-1.02816500
B	1.31660600	0.75645300	-0.14783800
H	0.24924100	-2.73274600	-0.58430500
C	0.17970100	-1.65556100	-0.48835400
Cl	-3.21469400	0.94930300	0.22056400
Cl	-0.07750000	1.58193700	2.47340100
Cl	-0.53545900	2.86303200	-1.47754800
Cl	2.72745200	1.80512700	0.02096400
Cl	-1.59905000	-2.08488500	1.88728000
Cl	-2.02423900	-1.52103900	-2.40309800
Cl	2.58596700	-1.29615800	-2.15514800
Cl	2.08196700	-1.49092700	1.88623300
H	0.85375500	0.60708100	-1.36549400

H/[CB₈HCl₈](1)

Lowest normal mode frequency: 60.13 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 242.83 kcal/mol

B	0.83760900	-0.95021900	-0.90768900
B	1.38326400	0.74024700	-0.62257500
B	1.37351600	-0.38664800	0.64261800
B	-0.71227100	1.33797200	-0.84848800
B	0.18849800	0.72264000	1.11595200
B	-0.26682200	-0.92067000	0.60894500
B	-0.99626600	-0.45780400	-1.05454200
B	-1.30246800	0.42579200	0.38800700
H	0.39437900	0.53248300	-2.75702000
C	0.24577000	0.38272200	-1.69599100
Cl	2.74876700	-0.96737500	1.59809600
Cl	0.30166400	1.67785800	2.60543800
Cl	-1.04244000	-2.22668400	1.62669700
Cl	-2.90292100	0.26627300	1.32840900
Cl	2.73311800	1.79267800	-1.03257100
Cl	1.50585400	-2.32211100	-1.80765100
Cl	-2.18482300	-1.36801100	-2.00489500
Cl	-1.27635500	2.88950200	-1.45474600
H	-2.40300000	-1.00153700	1.72260900

H/[CB₉HCl₉]

Lowest normal mode frequency: 91.14cm⁻¹

B	-0.60162400	-0.00169400	1.41012000
B	1.03326000	0.00240100	1.05225800
B	-0.15071400	-1.33180400	0.45621900
B	-1.26941500	-0.00298800	-0.12200400
B	-0.15702500	1.33086100	0.45661500
B	1.32693100	-0.93107100	-0.52536800
B	-0.34971600	-0.94461300	-1.33766000
B	-0.35427300	0.94311100	-1.33754100
B	1.32242200	0.93757800	-0.52513200
H	1.34172300	0.00350000	-2.72065700
C	0.86542300	0.00221000	-1.75248400
Cl	-1.71639400	-0.00441600	2.82675700
Cl	-0.50842800	2.98748100	1.01234200
Cl	2.28773100	0.00515200	2.31259500
Cl	-3.13678800	-0.00703300	0.02659800
Cl	-0.49379100	-2.99025900	1.01164700
Cl	2.66617600	2.07180700	-0.70639100
Cl	-1.11507600	2.07107200	-2.47123100
Cl	2.67597900	-2.05903500	-0.70662300
Cl	-1.10528800	-2.07589000	-2.47159200
H	-2.95352900	-0.00662300	1.41828700

H/[CB₉HCl₉](1)

Lowest normal mode frequency: 87.02 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 233.08kcal/mol

B	-0.00122000	-0.43108300	1.59579900
B	-0.94963000	-0.97882900	0.24709600
B	-1.10529000	0.75966600	0.73354600
B	1.10855000	0.75109500	0.73876500
B	0.94255500	-0.98713800	0.24733200
B	-1.32237300	0.27858800	-1.01316700
B	0.00332200	1.56752200	-0.58133800
B	1.32444500	0.26853200	-1.01026000
B	-0.00229200	-0.96659300	-1.32145600
H	0.00570200	0.87591700	-2.86769200
C	0.00306500	0.56724000	-1.83340400
Cl	-0.00745900	-1.08724100	3.22805300
Cl	2.04940800	-2.33485000	0.57257500
Cl	-2.06622200	-2.31827400	0.57312500
Cl	2.33887500	1.69101200	1.57417000
Cl	-2.32452700	1.70591000	1.57670100
Cl	-0.00707400	-2.32200700	-2.44463000
Cl	2.92323600	0.47442700	-1.72257600
Cl	-2.91867100	0.49344900	-1.72850700
Cl	0.01100100	3.31858000	-0.80808800
H	0.00992500	0.85475700	1.73254100

H/[CB₉HCl₉](2)

Lowest normal mode frequency: 75.34 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 210.39 kcal/mol

B	0.00000000	0.00000000	1.59781895
B	-1.33743738	0.00000000	0.55092688
B	0.00000000	1.32000227	0.47674696
B	1.33743738	0.00000000	0.55092688
B	0.00000000	-1.32000227	0.47674696
B	-1.02491483	0.89006886	-0.97127754
B	1.02491483	0.89006886	-0.97127754
B	1.02491483	-0.89006886	-0.97127754
B	-1.02491483	-0.89006886	-0.97127754
H	0.00000000	-0.81920316	-2.76414943
C	0.00000000	0.00000000	-2.02851305
Cl	0.00000000	0.00000000	3.34313895
Cl	0.00000000	-2.99229630	1.06657820
Cl	-2.98580091	0.00000000	1.21365456
Cl	2.98580091	0.00000000	1.21365456
Cl	-0.00000000	2.99229630	1.06657820
Cl	-2.13458991	-2.04376379	-1.69912323
Cl	2.13458991	-2.04376379	-1.69912323

Cl	-2.13458991	2.04376379	-1.69912323
Cl	2.13458991	2.04376379	-1.69912323
H	-0.00000000	0.81920316	-2.76414943

H/[CB₁₀HCl₁₀]

Lowest normal mode frequency: 76.69 cm⁻¹

B	-0.00334900	0.88450800	1.08675700
B	-0.86870200	-1.58511500	-0.26219300
B	1.24904100	0.11793000	-1.36249000
B	-1.24922700	0.10888900	-1.36286500
B	0.88046900	-1.57984300	-0.26082000
B	-1.44170400	-0.02768000	0.39834600
B	0.87708500	1.56224400	-0.32178700
B	-0.88836100	1.55607300	-0.32208900
B	0.00293300	-0.89399700	1.12131500
B	1.44202600	-0.01747700	0.39908200
H	-0.00558400	1.66272000	-2.54624200
C	-0.00366600	1.07258300	-1.63818800
Cl	0.00553000	-1.73011200	2.68585700
Cl	-3.03284500	-0.08573500	1.18831800
Cl	-0.00756800	1.75689400	2.62281700
Cl	-1.91989700	-2.98431400	-0.36434000
Cl	1.94224600	-2.97061400	-0.36371000
Cl	3.03312600	-0.06413700	1.18961200
Cl	-1.88785200	3.00871000	-0.33266000
Cl	-2.42429100	-0.19193200	-2.61571000
Cl	2.42588200	-0.17495000	-2.61551200
Cl	1.86683100	3.02162700	-0.33221200
H	0.00676800	-1.67830000	-1.25272500

H/[CB₁₀HCl₁₀](1)

Lowest normal mode frequency: 42.37 cm⁻¹

The value of ΔG_{acid} at ωB97XD/6-311+G(d, p) level: 235.47 kcal/mol

B	0.02614200	-1.69138400	-0.00867000
B	1.25507700	0.75930600	0.24308100
B	-1.58910100	0.86760100	-0.32075700
B	-0.03122900	1.64986400	-0.70934900
B	-0.34996800	1.05731500	0.95103700
B	1.42152400	-0.85820200	-0.15455900
B	-1.29123800	-0.74389200	-1.09027000

B	0.73541400	-0.05946900	-1.53061600
B	0.49710500	-0.49145100	1.26592200
B	-1.21120500	-0.60272200	0.68393200
H	-1.04254800	0.92072300	-2.68661900
C	-0.71792800	0.59563800	-1.70788100
Cl	1.04784800	-0.95274100	2.89798400
Cl	3.18984100	-1.42076000	-0.09852200
Cl	-0.10594400	-3.45355800	0.04386300
Cl	2.82366300	1.59414100	0.63351600
Cl	-0.63105600	2.17676700	2.30022100
Cl	-2.48323000	-1.25521400	1.74183400
Cl	1.71677200	-0.17262500	-3.00753900
Cl	0.23982900	3.33152000	-1.18578300
Cl	-3.15348000	1.69313000	-0.36332300
Cl	-2.37863200	-1.76465800	-2.02112400
H	3.52212700	-0.12142300	0.28598200

H/[CB₁₀HCl₁₀](2)

Lowest normal mode frequency: 47.96 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 231.12 kcal/mol

B	-0.17516400	-1.61456900	-0.31150700
B	-1.19034300	0.80852700	0.16421100
B	1.67994300	0.68842500	0.31708600
B	0.22601200	1.38954800	1.11372200
B	0.31286700	1.22571400	-0.66988700
B	-1.56123100	-0.81847100	0.16039400
B	1.38125800	-1.04240700	0.69285200
B	-0.53175900	-0.50171300	1.55615800
B	-0.69798400	-0.15808300	-1.20880800
B	1.06000200	-0.46556900	-0.94855400
H	1.42537800	0.15735800	2.68142600
C	0.96231200	0.10276100	1.70598100
Cl	-1.57682400	0.00022800	-2.77338300
Cl	-3.20911000	-1.47834100	0.22676900
Cl	-0.19071600	-3.32918600	-0.74039900
Cl	-2.64200900	1.99888100	-0.19010700
Cl	0.46705300	2.64711700	-1.73309400
Cl	2.09823100	-0.88602800	-2.33027400
Cl	-1.26698500	-0.99742900	3.08862400
Cl	0.09326300	2.90813800	2.02048000
Cl	3.28503700	1.43327900	0.34350300
Cl	2.53158100	-2.28656200	1.15694800
H	-2.73910800	1.49742300	-1.41978500

H/[CB₁₀HCl₁₀](3)

Lowest normal mode frequency: 44.78 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 215.97 kcal/mol

B	-0.23621100	-1.55339600	0.22087000
B	1.50618000	0.59404500	0.02081800
B	-1.49669800	1.14407500	-0.35419300
B	0.47442100	1.43020300	-1.17284200
B	0.03090300	1.31927800	0.86340500
B	1.37348000	-1.10625100	-0.03380700
B	-1.43113000	-0.59829900	-0.82737600
B	0.48863600	-0.61382600	-1.46685500
B	0.54431100	-0.38274000	1.30096400
B	-1.19229300	-0.18267100	0.88997700
H	-1.07279100	0.71485500	-2.69953300
C	-0.70179000	0.54072800	-1.69770600
Cl	1.08299900	-0.64475700	2.96444600
Cl	2.74820100	-2.19843700	-0.03647100
Cl	-0.68520600	-3.24028900	0.51908900
Cl	3.11181500	1.32314200	0.25383200
Cl	0.24155200	2.56839500	2.10021000
Cl	-2.43781100	-0.39118700	2.13299500
Cl	1.07211900	-1.30302400	-2.98196500
Cl	1.01615900	2.85380600	-2.01504200
Cl	-2.98960800	2.08062500	-0.51698800
Cl	-2.82606400	-1.42029000	-1.50226900
H	-0.70513600	2.11295700	0.07774600

H/[CB₁₀HCl₁₀](4)

Lowest normal mode frequency: 52.67 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 213.51 kcal/mol

B	1.09614200	-1.14154700	0.24448900
B	0.80095100	1.63450200	0.01317400
B	-1.75279000	-0.41745000	-0.24359900
B	-1.34783000	1.03047300	-1.15388400
B	-0.95630400	0.91708500	0.74789000
B	1.78653500	0.33403400	-0.23139000
B	-0.46160200	-1.55705500	-0.69485500
B	0.77192900	-0.12206200	-1.55743400
B	0.77242500	0.32367700	1.22517100
B	-0.50913300	-0.92564400	0.95648900
H	-1.25976600	-0.63758000	-2.64376100
C	-0.85153200	-0.33596900	-1.68626800
Cl	1.36616500	0.63769000	2.87019700
Cl	3.53560600	0.61387800	-0.33482400
Cl	2.13440800	-2.51171200	0.66675200
Cl	1.16316400	3.33942800	0.02280100

Cl	-1.89221800	1.88803000	1.87474100
Cl	-1.09990100	-1.84774600	2.34437900
Cl	1.59533700	-0.27790800	-3.10624100
Cl	-2.26401100	2.26409500	-1.96312200
Cl	-3.46385800	-0.86189300	-0.18659700
Cl	-0.72569500	-3.21499900	-1.21503800
H	-0.56561600	1.78265400	-0.31069000

H/[CB₁₁HCl₁₁]

Lowest normal mode frequency: 106.74 cm⁻¹

B	-0.22115200	1.67591600	-0.68747600
B	-1.52858800	0.45445200	-0.87508800
B	1.35803400	0.83476700	-0.87589000
B	1.03142300	-0.91312600	-1.16552500
B	-0.76059000	-1.14924100	-1.16506100
B	0.20404700	-1.54884700	0.26532000
B	1.52772700	-0.33640400	0.44499400
B	0.75151900	1.26877300	0.75190600
B	-1.38837100	-0.72067600	0.44587500
B	-1.05423700	1.03079900	0.75242800
B	0.02752000	-0.20597200	1.37657500
C	-0.04102600	0.30658900	-1.71689700
H	-0.06567400	0.49067900	-2.78447900
Cl	0.10211400	-0.76611000	3.17160900
Cl	0.42012600	-3.18402800	1.00071500
Cl	-2.77802000	-1.55203400	1.18803700
Cl	-2.11890800	2.00961700	1.78758500
Cl	1.52686200	2.49046300	1.78667100
Cl	3.08612400	-0.77934000	1.18633300
Cl	2.69913900	1.63278000	-1.70789800
Cl	2.04742300	-1.84921100	-2.27049600
Cl	-1.49995400	-2.31651300	-2.26959000
Cl	-3.03101300	0.87794900	-1.70627000
Cl	-0.43590300	3.30438100	-1.34228000
H	0.26934600	-2.03765300	2.73050100

H/[CB₁₁HCl₁₁](1)

Lowest normal mode frequency: 106.10 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 228.78 kcal/mol

B	1.38495500	-0.86679600	-0.81151100
B	1.33226000	0.93393400	-0.82831500
B	-0.29094400	-1.48523100	-0.98036800
B	-1.36738900	-0.06097800	-1.11333000
B	-0.37529000	1.44007600	-1.01098800

B	-1.20664900	0.82753600	0.40371100
B	-1.19028700	-0.92788600	0.43575100
B	0.50294100	-1.45109300	0.63079400
B	0.41831600	1.48360400	0.60498900
B	1.51603900	0.04990300	0.71885000
B	-0.08370700	0.00275500	1.50216600
C	0.20824000	-0.01073500	-1.72706700
H	0.32163900	-0.01757500	-2.80456000
Cl	-0.33500400	0.03054000	3.26649000
Cl	-2.78824700	1.50074000	1.13987000
Cl	0.72738700	3.03327600	1.42255100
Cl	3.02859600	0.10913200	1.64623900
Cl	0.93703700	-2.95492700	1.47161900
Cl	-2.67993900	-1.67663200	1.15219400
Cl	-0.64427900	-2.93711700	-1.92774100
Cl	-2.82153400	-0.09473700	-2.12992500
Cl	-0.83659000	2.86005900	-1.96326200
Cl	2.60333600	1.85654400	-1.64127500
Cl	2.71418000	-1.71662500	-1.61050600
H	-3.15631800	0.17854700	1.36190000

H/[CB₁₁HCl₁₁](2)

Lowest normal mode frequency: 108.30 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 220.86 kcal/mol

B	0.50625600	-1.43752800	-0.95085000
B	1.47561600	0.08193100	-1.04710200
B	-1.19147200	-0.95937300	-0.76792000
B	-1.25208000	0.79132500	-0.74880500
B	0.35108800	1.48400300	-0.94415500
B	-0.45410700	1.43950400	0.66759100
B	-1.41613100	-0.08724800	0.77133200
B	-0.29600900	-1.49074600	0.65732500
B	1.27939800	0.97714300	0.49247900
B	1.37744300	-0.83278100	0.48757400
B	0.18937000	0.00393500	1.54929100
C	-0.10319600	-0.00843500	-1.68577700
H	-0.20957600	-0.01084000	-2.76401700
Cl	0.34684500	0.01358800	3.31744400
Cl	-1.00987000	2.94076600	1.44290300
Cl	2.58322700	1.99643700	1.13495700
Cl	2.78899600	-1.69862500	1.12733500
Cl	-0.65955900	-3.03938900	1.44906200
Cl	-2.98376800	-0.15622300	1.61664800
Cl	-2.58856700	-1.71847100	-1.63993300
Cl	-2.77680200	1.41335500	-1.62027000

Cl	0.57133900	2.93452300	-1.94079100
Cl	2.87355300	0.16575200	-2.12766800
Cl	0.91975700	-2.84304500	-1.94565900
H	-3.12566400	0.06328300	-1.79359300

H/[CB₁₁HCl₁₁](3)

Lowest normal mode frequency: 104.10 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 207.56 kcal/mol

B	-0.88947500	-1.16322500	-1.03371500
B	0.90895000	-1.14765000	-1.03376100
B	-1.44940800	0.51991800	-0.90583800
B	-0.01370600	1.61755000	-0.79034700
B	1.44020900	0.54482700	-0.90632900
B	1.01013900	1.24576600	0.66634400
B	-1.03072800	1.22857200	0.66637500
B	-1.46886700	-0.54220700	0.54672900
B	1.47774200	-0.51672500	0.54658000
B	0.01345000	-1.59349400	0.42541900
B	0.00261000	-0.24402700	1.59227400
C	-0.00146500	0.15939900	-1.70053900
H	-0.00248000	0.26145700	-2.77948200
Cl	0.00435400	-0.44981700	3.34218200
Cl	1.97526300	2.46410100	1.49612400
Cl	3.00221300	-1.06775900	1.26603800
Cl	0.02794800	-3.23250900	1.08863500
Cl	-2.98338800	-1.11823300	1.26729500
Cl	-2.01777200	2.43031000	1.49483400
Cl	-2.88793100	1.08198800	-1.75510100
Cl	-0.02755000	3.19500500	-1.58399500
Cl	2.86911600	1.13093800	-1.75551100
Cl	1.80737600	-2.26420400	-2.06221200
Cl	-1.76859200	-2.29475800	-2.06247400
H	-0.01094500	1.15957100	1.60518600

H/[CB₁₁HCl₁₁](4)

Lowest normal mode frequency: 101.96 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 203.39 kcal/mol

B	1.46095200	0.56343600	-0.87912200
B	-0.00018800	1.57532500	-0.84126300
B	1.01168500	-1.15883000	-1.05165800
B	-1.01130100	-1.15908200	-1.05156300

B	-1.46112000	0.56310200	-0.87907400
B	-1.47868600	-0.50694900	0.56127200
B	0.00013400	-1.59837300	0.60956900
B	1.47879100	-0.50667400	0.56119600
B	-0.90619900	1.21203000	0.66552500
B	0.90596900	1.21221500	0.66551000
B	0.00001500	-0.05396900	1.52419900
C	-0.00000100	0.07236400	-1.70586600
H	-0.00005600	0.15116800	-2.78713500
Cl	0.00008700	-0.21389500	3.28416200
Cl	-2.99111300	-1.05123100	1.31131500
Cl	-1.84847200	2.44947200	1.51233900
Cl	1.84799700	2.44984200	1.51231100
Cl	2.99134800	-1.05061200	1.31123900
Cl	0.00035900	-3.19759900	1.35508800
Cl	1.90733000	-2.27960100	-2.07058400
Cl	-1.90696300	-2.27984400	-2.07054300
Cl	-2.88123900	1.05283500	-1.79832600
Cl	-0.00034100	3.11285900	-1.70838600
Cl	2.88098800	1.05345200	-1.79838500
H	0.00012700	-2.07303100	-0.68452300

H/[CB₁₁HCl₁₁](5)

Lowest normal mode frequency: 82.00 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 185.29 kcal/mol

B	-0.57170900	1.41744600	-0.94702400
B	-1.61511800	-0.09203000	-0.85566800
B	1.24561700	1.08634700	-0.87183100
B	1.36422600	-0.93896400	-0.86913300
B	-0.40571800	-1.47193600	-0.94897300
B	0.52868300	-1.43695500	0.59078500
B	1.54724600	0.08834700	0.55516600
B	0.36180800	1.48689000	0.59145100
B	-1.19345300	-0.98095000	0.60246100
B	-1.29719800	0.83790000	0.60330300
B	0.00628300	-0.00005000	1.52157300
C	-0.13805700	-0.00604700	-1.81839200
H	-0.48086500	-0.02330600	-2.85915500
Cl	0.05850900	0.00251200	3.28887900
Cl	1.12826000	-2.92841200	1.33373600
Cl	-2.40514600	-2.00802400	1.38803200
Cl	-2.61810700	1.71979700	1.38948900
Cl	0.78932000	3.03656700	1.33384700
Cl	3.15015800	0.18159000	1.31628000
Cl	2.37928400	2.02219800	-1.81519500

Cl	2.59636000	-1.73889300	-1.81252300
Cl	-0.80216100	-2.93977700	-1.86063700
Cl	-3.11563900	-0.17770700	-1.76008300
Cl	-1.13243000	2.83150700	-1.85681400
H	0.97294000	0.05627900	-2.15620900

H/[CB₁₂HCl₁₂]

Lowest normal mode frequency: 5.24 cm⁻¹

B	1.19215100	1.49805700	-0.03870400
B	-0.42053800	1.53961100	-0.04661400
B	1.95325000	0.09271700	0.00238900
B	0.45483700	0.44980700	-1.43993500
B	-1.43292700	0.38866400	-0.91800500
B	1.11067000	-1.25780500	-0.85443800
B	1.10004400	-1.19871600	0.94326800
B	-1.44529000	0.44363500	0.87650500
B	-0.56528400	-1.06123900	-1.41257600
B	-0.58179700	-0.97268800	1.46897400
B	-1.67002400	-1.07294000	0.02346800
H	-0.24885800	-2.95624100	0.09035900
B	0.43385400	0.53965400	1.41556400
C	-0.16358900	-1.87626700	0.05733500
Cl	2.03090600	3.09612800	-0.08223900
Cl	-1.00849500	3.33332600	-0.10137200
Cl	3.72915000	0.06935900	0.00778600
Cl	0.87133700	1.10488000	-3.04028800
Cl	-2.71587000	1.07285000	-1.94801600
Cl	-2.74305200	1.18605800	1.84610300
Cl	0.83451400	1.29178000	2.97676100
Cl	-1.04123300	-1.94865500	-2.86867500
Cl	-3.15411900	-2.03235700	0.04431500
Cl	2.15077400	-2.36462600	-1.76761400
Cl	2.13320600	-2.24021800	1.93707300
Cl	-1.07385100	-1.77017700	2.97108300
H	0.36012900	3.69814700	-0.10746000

H/[CB₁₂HCl₁₂](1)

Lowest normal mode frequency: 5.24 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 233.77 kcal/mol

B	1.19215100	1.49805700	-0.03870400
B	-0.42053800	1.53961100	-0.04661400
B	1.95325000	0.09271700	0.00238900

B	0.45483700	0.44980700	-1.43993500
B	-1.43292700	0.38866400	-0.91800500
B	1.11067000	-1.25780500	-0.85443800
B	1.10004400	-1.19871600	0.94326800
B	-1.44529000	0.44363500	0.87650500
B	-0.56528400	-1.06123900	-1.41257600
B	-0.58179700	-0.97268800	1.46897400
B	-1.67002400	-1.07294000	0.02346800
H	-0.24885800	-2.95624100	0.09035900
B	0.43385400	0.53965400	1.41556400
C	-0.16358900	-1.87626700	0.05733500
Cl	2.03090600	3.09612800	-0.08223900
Cl	-1.00849500	3.33332600	-0.10137200
Cl	3.72915000	0.06935900	0.00778600
Cl	0.87133700	1.10488000	-3.04028800
Cl	-2.71587000	1.07285000	-1.94801600
Cl	-2.74305200	1.18605800	1.84610300
Cl	0.83451400	1.29178000	2.97676100
Cl	-1.04123300	-1.94865500	-2.86867500
Cl	-3.15411900	-2.03235700	0.04431500
Cl	2.15077400	-2.36462600	-1.76761400
Cl	2.13320600	-2.24021800	1.93707300
Cl	-1.07385100	-1.77017700	2.97108300
H	0.36012900	3.69814700	-0.10746000

H/[CB₁₂HCl₁₂](2)

Lowest normal mode frequency: 68.98 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 231.32 kcal/mol

B	0.85733300	-1.38457000	-1.10087100
B	-0.85988900	-1.38253400	-1.10236800
B	1.76708600	-0.45356700	0.06306600
B	-0.00378300	-1.43655300	0.59248900
B	-1.76586700	-0.45103100	0.06381800
B	0.88461300	-0.07193400	1.56994200
B	1.47397400	1.22832700	0.46508900
B	-1.16324200	0.66001700	-1.17946300
B	-0.88385000	-0.06979800	1.57042400
B	0.00183000	1.79451100	-0.44579100
B	-1.47091500	1.23144200	0.46512700
H	0.00237000	2.12370000	2.02294900
B	1.16470200	0.65774200	-1.17966200
C	0.00167900	1.35566100	1.25745100
Cl	1.72529800	-2.60979500	-2.01250600
Cl	-1.73077200	-2.60467800	-2.01529800
Cl	3.41976500	-1.07203600	0.25807900

Cl	-0.00604100	-3.03343200	1.36354200
Cl	-3.42016000	-1.06616000	0.25903700
Cl	-1.95846100	1.10259800	-2.67658500
Cl	1.95998900	1.09775200	-2.67754100
Cl	-1.68550500	-0.31870700	3.12549100
Cl	-2.77245700	2.34250700	0.90581100
Cl	1.68584500	-0.32365200	3.12474500
Cl	2.77732200	2.33737900	0.90585300
Cl	0.00388800	3.49837500	-0.94585900
H	-0.00052100	-0.82050200	-1.92773200

H/[CB₁₃HCl₁₃]

Lowest normal mode frequency: 56.87 cm⁻¹

B	0.00677700	-0.00030700	1.44797200
B	-1.65162400	-0.00649400	-1.01754400
B	-0.80001500	-1.55189500	-0.95603500
B	0.95657600	-1.54741100	-0.86827200
B	-1.46111900	0.85589600	0.51389500
B	0.00267200	1.77674600	0.60910500
B	0.01649200	-1.77661200	0.60910600
B	-1.45477100	-0.86760100	0.51391700
H	0.13631100	0.00011600	-2.69804900
B	-0.81252000	1.54591700	-0.95573400
B	1.53361300	0.89235300	0.66431200
B	1.54043300	-0.88019200	0.66433100
B	0.94415900	1.55478000	-0.86828900
B	1.80602200	0.00701500	-0.85022800
C	0.08308500	-0.00023300	-1.61284400
Cl	-0.12938700	-0.00062400	3.22622400
Cl	-0.08510200	-3.33409600	1.46716800
Cl	2.86319900	-1.66380800	1.55513500
Cl	-2.95731400	-1.52085000	1.36208800
Cl	-2.96898400	1.49789300	1.36175100
Cl	-0.11108600	3.33325200	1.46732000
Cl	2.85030100	1.68605300	1.55508400
Cl	-1.54172500	-2.84320800	-1.91585800
Cl	-3.14017800	-0.01196500	-1.99312900
Cl	-1.56429600	2.83158900	-1.91512400
Cl	1.73479500	-2.83330500	-1.80063100
Cl	3.31094400	0.01284500	-1.78663500
Cl	1.71240400	2.84632900	-1.80114000
H	-3.31902100	-0.01148800	1.54412000

H/[CB₁₃HCl₁₃](1)

Lowest normal mode frequency: 55.13 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 225.53 kcal/mol

B	-0.05669500	-0.00198400	1.41331400
B	-1.41951900	-0.91613500	-1.03303200
B	0.12146700	-1.76576200	-0.93245800
B	1.62936400	-0.85567800	-0.81015000
B	-1.66715100	-0.02954600	0.44647300
B	-0.91030400	1.53124100	0.51752700
B	0.89529500	-1.52623300	0.65055500
B	-0.85554500	-1.56277700	0.51815300
H	0.18223100	0.00212900	-2.70018800
B	-1.45173000	0.86521300	-1.03320900
B	0.84046400	1.55741900	0.64967800
B	1.73994800	0.03121700	0.72111300
B	0.05821000	1.76864200	-0.93311400
B	1.59737400	0.91240400	-0.81102700
C	0.10643600	0.00083200	-1.61626400
Cl	-0.35841500	-0.00569100	3.19371800
Cl	1.62872500	-2.87822400	1.54203400
Cl	3.23653900	0.05838000	1.67950000
Cl	-1.71751200	-2.90547700	1.32060000
Cl	-3.30335900	-0.05753500	1.42242700
Cl	-1.81865000	2.84275000	1.32050800
Cl	1.52576000	2.93465700	1.54043200
Cl	0.19274300	-3.24107600	-1.90938600
Cl	-2.68270500	-1.67206500	-2.02368300
Cl	-2.74117800	1.57461300	-2.02408800
Cl	2.98557800	-1.57290900	-1.69198000
Cl	2.92722500	1.67689600	-1.69343300
Cl	0.07701300	3.24520500	-1.91055900
H	-2.60673100	-0.03917200	2.55513200

H/[CB₁₃HCl₁₃](2)

Lowest normal mode frequency: 25.68 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 211.44 kcal/mol

B	-0.53386700	-0.02232700	1.59368500
B	0.82962300	1.58183800	-0.79747200
B	-0.91954800	1.49459500	-0.90891000
B	-1.65907700	-0.10765100	-1.03130500
B	1.59347500	1.04516200	0.68568200
B	1.72226000	-0.83948100	0.68190300
B	-1.68731200	0.80209900	0.51625400
B	-0.14963400	1.72551900	0.69043000
H	0.16578300	0.00967200	-2.64588300
B	1.81398800	0.11388600	-0.85082600
B	0.07707500	-1.73172200	0.69225700
B	-1.56453000	-1.00476200	0.52367500

B	1.02828400	-1.47197700	-0.79292800
B	-0.71861200	-1.59860800	-0.90587900
C	0.09764800	0.00697000	-1.56116800
Cl	-0.53427600	-0.02424500	3.33117300
Cl	-3.16625000	1.52839600	1.16785500
Cl	-2.93689400	-1.91498600	1.17953500
Cl	-0.28511700	3.27407900	1.55038900
Cl	2.87343400	1.96228400	1.47129500
Cl	3.11433700	-1.58219400	1.46175300
Cl	0.13553100	-3.27935100	1.56048300
Cl	-1.66576200	2.73835000	-1.91478600
Cl	1.54653000	2.95138200	-1.65489200
Cl	3.26557200	0.20784600	-1.85472900
Cl	-3.02366100	-0.19688500	-2.14959400
Cl	-1.30370600	-2.92906200	-1.90820000
Cl	1.91210000	-2.73883200	-1.65095100
H	1.24642800	0.07038200	1.51147100

H/[CB₅H(CN)₅]

Lowest normal mode frequency: 56.66 cm⁻¹

B	-0.00037800	-0.00029500	0.80268800
B	0.85310100	0.86970100	-0.38953000
B	-0.85237400	-0.86807500	-0.39223100
B	-0.86837400	0.85367500	-0.39067800
B	0.86932200	-0.85209600	-0.39086700
C	0.00119900	0.00152900	-1.47003100
C	-1.95318900	1.91586700	-0.50007600
N	-2.77556600	2.72046300	-0.55146000
C	-1.91647800	-1.95089200	-0.50305900
N	-2.72266600	-2.77165600	-0.55536400
C	1.95387600	-1.91451700	-0.50062500
N	2.77557800	-2.71978700	-0.55231200
C	1.91772900	1.95223600	-0.49811000
N	2.72455700	2.77244600	-0.54916000
C	-0.00226100	-0.00244400	2.31931800
N	-0.00329400	-0.00455400	3.46538600
H	0.00199800	0.00258500	-2.54915900
H	-0.00401000	-0.00618600	4.46812100

H/[CB₅H(CN)₅](1)

Lowest normal mode frequency: 53.28 cm⁻¹

The value of ΔG_{acid} at ωB97XD/6-311+G(d, p) level: 248.73 kcal/mol

B	-0.06875800	-0.00138600	0.94143200
B	-0.05749400	-1.21998800	-0.29760000
B	-0.13754300	1.21507400	-0.29790300

B	1.07356900	0.03628000	-0.33500700
B	-1.30993300	-0.04240000	-0.23803800
C	-0.14823600	-0.00439600	-1.38634800
C	2.57139800	0.08189000	-0.50420400
N	3.71433500	0.11550900	-0.59531200
C	-0.12393800	2.72722100	-0.48486800
N	-0.07380900	3.86780400	-0.63614400
C	-2.82693000	-0.09151400	-0.36681100
N	-3.97297600	-0.12866300	-0.47107100
C	0.05871100	-2.72783000	-0.48387400
N	0.18718400	-3.86235400	-0.63457900
C	0.06445500	0.00311500	2.46188700
N	0.20318600	0.00768500	3.60517900
H	-0.18949100	-0.00573700	-2.46385200
H	4.71207800	0.13705700	-0.69178000

H/[CB₅H(CN)₅](2)

Lowest normal mode frequency: 61.00 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 228.86 kcal/mol

B	0.00006800	-0.19101000	0.98734900
B	0.94254200	0.87369500	-0.28991100
B	-0.85599300	-0.83051100	-0.34020400
B	-0.94208300	0.87412800	-0.28902300
B	0.85567600	-0.83082500	-0.34034600
C	-0.00027100	0.12542400	-1.35172800
C	-2.02793400	1.92717100	-0.39733000
N	-2.85090300	2.72712500	-0.47987900
C	-1.95113900	-1.85432500	-0.58432100
N	-2.78112400	-2.62863100	-0.77320200
C	1.95014400	-1.85522200	-0.58507200
N	2.77963600	-2.62993900	-0.77444100
C	2.02838600	1.92675000	-0.39795800
N	2.85135000	2.72674700	-0.48014200
C	0.00062200	-0.27405700	2.50239600
N	0.00109800	-0.33375800	3.65175000
H	-0.00065200	0.21816500	-2.42688500
H	0.00035400	1.29919500	0.66303300

H/[CB₆H(CN)₆]

Lowest normal mode frequency: 51.78 cm⁻¹

B	0.35003600	-1.33624600	-0.16870200
B	1.25849200	0.00630100	-0.18071500
B	-1.20048300	-0.82817300	-0.15972800
B	-1.20828200	0.81689600	-0.15951700
B	0.33722400	1.34000500	-0.16794600

C	-0.10155600	-0.00014400	-1.22262600
H	-0.10292400	0.00028500	-2.30510000
B	-0.10868700	-0.00055200	1.03309300
C	-0.02932100	-0.00022800	2.56221900
N	0.06508700	0.00022200	3.70962500
C	-2.43028500	1.69723300	-0.38942000
N	-3.34720700	2.36899200	-0.57263800
C	0.88911900	2.74129500	-0.40979800
N	1.37123400	3.76887600	-0.60589000
C	2.76124200	0.01257600	-0.38621900
N	3.89837400	0.01772300	-0.51874800
C	0.91656900	-2.73177200	-0.41006600
N	1.41024800	-3.75399300	-0.60551600
C	-2.41383300	-1.72038500	-0.38962300
N	-3.32411700	-2.40113000	-0.57278400
H	4.89447700	0.01227000	-0.64246000

H/[CB₆H(CN)₆](1)

Lowest normal mode frequency: 51.76 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 244.37 kcal/mol

B	-1.25840800	0.00484500	-0.18188600
B	-0.34866500	-1.33682000	-0.16895700
B	-0.33899200	1.33978500	-0.16895200
B	1.20715900	0.81832500	-0.15972200
B	1.20120400	-0.82680000	-0.15967500
C	0.10194800	-0.00024600	-1.22324600
H	0.10366900	-0.00020600	-2.30571700
B	0.10830000	-0.00014400	1.03244300
C	0.02839900	-0.00041900	2.56156600
N	-0.06647800	-0.00081400	3.70893000
C	2.42817300	1.70029100	-0.38871800
N	3.34434500	2.37338600	-0.57078200
C	2.41603300	-1.71723100	-0.38882400
N	3.32755700	-2.39659200	-0.57095400
C	-0.91274400	-2.73326300	-0.41074500
N	-1.40407800	-3.75645800	-0.60689400
C	-2.76120200	0.00923800	-0.38745800
N	-3.89855800	0.01278300	-0.51806300
C	-0.89238300	2.74053500	-0.41037500
N	-1.37560000	3.76769500	-0.60597100
H	-4.89632700	0.01083000	-0.62759900

H/[CB₆H(CN)₆](2)

Lowest normal mode frequency: 57.45 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 218.06 kcal/mol

B	-0.87598500	-1.22660500	-0.01032600
B	0.88008100	-1.22309800	-0.01007600
B	-1.31092600	0.38507100	-0.01405000
B	-0.00269800	1.34136900	-0.36975400
B	1.30938000	0.39017000	-0.01495000
C	0.00018800	-0.19416100	-1.06021600
H	0.00036900	-0.34420400	-2.13375600
B	-0.00025500	0.50470800	1.16204600
C	-0.00039300	0.63659300	2.66752800
N	-0.00056400	0.71959800	3.81659100
C	-0.00593900	2.75209400	-0.92787700
N	-0.00839700	3.82206800	-1.35194800
C	2.74501300	0.76545400	-0.34902500
N	3.83181200	1.05020900	-0.59927300
C	1.84964700	-2.35977300	-0.30966200
N	2.57909100	-3.22121100	-0.53418000
C	-1.84069900	-2.36729700	-0.31023400
N	-2.56645200	-3.23177400	-0.53504800
C	-2.74784700	0.75582300	-0.34765100
N	-3.83564200	1.03711700	-0.59749900
H	0.00289500	-1.67832200	0.85163600

H/[CB₇H(CN)₇]

Lowest normal mode frequency: 53.06 cm⁻¹

B	-0.23706800	-1.24716700	-0.57564300
B	0.83818700	0.98276400	0.44592800
B	-0.48524000	-0.19610200	1.01641900
B	-1.68920100	-0.23756100	-0.16663200
B	-0.65025200	1.28267100	-0.28572000
B	1.07963300	-0.60057800	0.24035600
B	0.66289000	0.30921800	-1.24183900
C	-0.89887100	0.05669500	-1.44393300
C	2.28553100	-1.36809800	0.74235400
N	3.20215900	-1.92511200	1.14274100
C	1.75651600	1.97259900	1.14886000
N	2.48684900	2.68274300	1.68677200
C	1.60989500	0.57965300	-2.41484000
N	2.35269100	0.75483700	-3.27659800
C	-1.32323200	2.64842300	-0.42271000
N	-1.82901200	3.67666300	-0.53216300
C	-0.72394700	-0.47982600	2.50223100
N	-0.85214000	-0.72176900	3.62089400
C	-0.34709100	-2.71002100	-1.01182600
N	-0.37833600	-3.81926800	-1.31878700
H	-1.33436400	0.11145800	-2.43164300

C	-3.18387700	-0.49743300	-0.05404000
N	-4.31320800	-0.70327700	0.03232300
H	4.00705100	-2.40336400	1.50445600

H/[CB₇H(CN)₇](1)

Lowest normal mode frequency: 48.01 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 240.77 kcal/mol

B	-0.26200200	-1.29261000	-0.54406500
B	1.05476500	0.81423100	0.41181700
B	-0.49530400	0.00021000	0.86112000
B	-1.59132200	0.00176100	-0.40307800
B	-0.25957900	1.29375400	-0.54277100
B	1.05320400	-0.81653800	0.41097400
B	0.94343400	-0.00015900	-1.19502400
C	-0.62760700	0.00144100	-1.58247700
C	1.92987200	-1.78553800	1.19432500
N	2.55058200	-2.51349000	1.83615500
C	1.93348900	1.78079300	1.19587400
N	2.55576700	2.50706500	1.83808800
C	2.00282300	-0.00062300	-2.30028500
N	2.79813800	-0.00098600	-3.13205500
C	-0.68671100	2.73060100	-0.84166200
N	-1.02544100	3.81091100	-1.05024300
C	-0.98340300	-0.00051000	2.31870400
N	-1.33352600	-0.00115800	3.40739500
C	-0.69187200	-2.72833700	-0.84440400
N	-1.03266600	-3.80779100	-1.05405100
H	-0.92910000	0.00224900	-2.62025100
C	-3.11266100	0.00312400	-0.38721900
N	-4.26167200	0.00410800	-0.31091600
H	-1.62874500	-0.00180500	4.36763700

H/[CB₇H(CN)₇](2)

Lowest normal mode frequency: 53.13 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 233.90 kcal/mol

B	0.22756200	1.29720700	-0.44301300
B	-1.07511000	-0.81397800	0.53112600
B	0.49008800	0.00001800	0.97862200
B	1.46374800	0.00010200	-0.38705500
B	0.22771700	-1.29714700	-0.44303400
B	-1.07520100	0.81386800	0.53114100
B	-1.02412700	-0.00004200	-1.09469000
C	0.50008000	0.00005400	-1.55298000
C	-2.00587600	1.79165100	1.23509900
N	-2.69809800	2.54432400	1.76518400

C	-2.00567200	-1.79188500	1.23506000
N	-2.69782600	-2.54462400	1.76514000
C	-2.12624500	-0.00010300	-2.15689100
N	-2.94467100	-0.00014200	-2.96616500
C	0.69668400	-2.70952600	-0.80519100
N	1.11683100	-3.74391000	-1.08721200
C	1.16775800	0.00003200	2.35322100
N	1.75304700	0.00003500	3.34526100
C	0.69635000	2.70965100	-0.80514900
N	1.11639000	3.74408200	-1.08715500
H	0.76589000	0.00007700	-2.60056900
C	2.99121000	0.00013800	-0.39962500
N	4.13173100	0.00017100	-0.32757000
H	5.13316700	0.00016500	-0.23856400

H/[CB₇H(CN)₇](3)

Lowest normal mode frequency: 50.08 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 232.21 kcal/mol

B	0.38610700	1.29406300	-0.38364000
B	-0.90821800	-0.81309900	0.60714600
B	0.67325500	-0.00001800	1.03112900
B	1.67873800	-0.00008700	-0.34371100
B	0.38597900	-1.29410400	-0.38359200
B	-0.90813300	0.81322700	0.60711500
B	-0.82249800	0.00001900	-0.97728500
C	0.67349700	-0.00005300	-1.48939100
C	-1.91151900	1.78461400	1.21534600
N	-2.70970600	2.51424700	1.61254700
C	-1.91169700	-1.78436600	1.21541400
N	-2.71001800	-2.51380200	1.61270700
C	-2.02797600	0.00004800	-1.94743800
N	-2.97638400	-0.00001200	-2.58439300
C	0.70859400	-2.72949900	-0.80080800
N	0.92728300	-3.80386900	-1.15204900
C	1.25064200	-0.00002600	2.44786500
N	1.68216500	-0.00003100	3.51531400
C	0.70888600	2.72940600	-0.80091200
N	0.92770800	3.80373600	-1.15219500
H	0.94439300	-0.00008200	-2.53592900
C	3.19312100	-0.00016100	-0.48576500
N	4.33835700	-0.00021700	-0.60274200
H	-3.82766900	-0.00006500	-3.12005700

H/[CB₇H(CN)₇](4)

Lowest normal mode frequency: 60.60 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 208.52 kcal/mol

B	-0.41057900	-1.23395700	-0.36306000
B	1.04919100	0.84461700	0.57860600
B	-0.76695800	0.00551300	0.95923200
B	-1.67373500	0.01435700	-0.44722700
B	-0.38942700	1.24101400	-0.36194400
B	1.03443800	-0.86222500	0.57820900
B	0.95412000	-0.00749100	-1.01910000
C	-0.56259100	0.00545500	-1.50206300
C	1.85972900	-2.04194300	1.08049300
N	2.48700500	-2.92971100	1.45886400
C	1.89469700	2.00966800	1.08148900
N	2.53722300	2.88628900	1.46027700
C	2.08536100	-0.01653900	-2.04684500
N	2.94513900	-0.02339900	-2.81201400
C	-0.61931500	2.71907800	-0.65947200
N	-0.80656800	3.82958700	-0.89534900
C	-1.23235600	0.00860500	2.40644300
N	-1.55706500	0.01066400	3.51090400
C	-0.66488900	-2.70774900	-0.66178400
N	-0.87059800	-3.81479200	-0.89858600
H	-0.73933100	0.00744300	-2.56877100
C	-3.17724700	0.02735800	-0.65062000
N	-4.31774900	0.03725200	-0.80307300
H	1.33202200	-0.01141300	1.51217600

H/[CB₈H(CN)₈]

Lowest normal mode frequency: 53.84 cm⁻¹

B	0.98080100	-0.60852100	-1.04893500
B	1.04535500	1.13484100	-0.63898600
B	1.43191000	-0.03927100	0.51389700
B	-1.02491400	1.15095500	-0.64226000
B	0.00486500	0.72206700	1.07408300
B	-0.00746100	-0.96931300	0.53655800
B	-0.98593600	-0.59331700	-1.05151400
B	-1.43235000	-0.01682100	0.50987100
C	0.00687500	0.51179200	-1.69770200
C	-0.02198500	-2.27844300	1.33543900
N	-0.03509400	-3.24258700	1.94873400
C	2.71316300	-0.33341400	1.28400300
N	3.65226000	-0.62366100	1.88389900
C	0.00861800	1.44701500	2.41694800
N	0.01126000	1.98012900	3.43760400
C	-2.71971100	-0.29238400	1.27672100
N	-3.66406400	-0.57019400	1.87426200

C	1.79386200	-1.58578700	-1.89745600
N	2.39182000	-2.35752300	-2.50700300
C	-1.81204300	-1.55823700	-1.90157900
N	-2.42061900	-2.32114500	-2.51172800
C	1.91489400	2.33509700	-0.99707200
N	2.56693100	3.24454700	-1.26649400
C	-1.87487200	2.36437000	-1.00289700
N	-2.51218800	3.28363100	-1.27423500
H	0.01046300	0.77452400	-2.74572600
H	-0.05675900	-4.09004100	2.48845300

H/[CB₈H(CN)₈](1)

Lowest normal mode frequency: 57.62 cm⁻¹

The value of ΔG_{acid} at ωB97XD/6-311+G(d, p) level: 195.51 kcal/mol

B	1.11136000	-0.68659300	-1.13891600
B	0.82671300	1.05869900	-0.67728700
B	1.54753100	-0.10958800	0.39171500
B	-0.97581500	0.93717000	-0.49984800
B	0.08175200	0.69895600	0.96042800
B	0.32360000	-1.04704900	1.04160300
B	-1.28821000	-0.69117400	-1.12240000
B	-1.31861100	-0.37502300	0.64609500
C	-0.12382800	0.15430200	-1.71890700
C	0.48856400	-2.22711300	1.97136400
N	0.60633100	-3.14678200	2.65531300
C	2.95599200	-0.08443500	0.97333200
N	4.02139400	-0.06842900	1.40829100
C	0.00152200	1.64051100	2.16189700
N	-0.05649200	2.34948800	3.06608900
C	-2.56347600	-0.56992100	1.50286400
N	-3.50752100	-0.72290600	2.14198600
C	1.94558500	-1.58076900	-2.03182000
N	2.55369400	-2.28737000	-2.70856700
C	-2.27803300	-1.53807400	-1.88614000
N	-3.02036100	-2.19984800	-2.46711300
C	1.50789100	2.32397500	-1.19335700
N	2.02188300	3.26993100	-1.59893000
C	-1.94551700	2.08397300	-0.76695300
N	-2.68324100	2.93841500	-0.98847700
H	-0.17685900	0.41923800	-2.76845900
H	-0.84676400	-1.48842300	0.12767000

H/[CB₉H(CN)₉]

Lowest normal mode frequency: 56.73 cm⁻¹

B	0.00350300	-0.00169200	1.49900700
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B	1.05832600	-0.78799000	0.44888300
B	-0.78650700	-1.05790300	0.45315500
B	-1.05645400	0.78701700	0.45603700
B	0.78848900	1.05690000	0.45176000
B	0.18743100	-1.29836400	-1.06938900
B	-1.30238900	-0.18890700	-1.06438100
B	-0.19290700	1.30093400	-1.06536200
B	1.29689700	0.19144800	-1.07037700
H	-0.00773300	0.00365800	-3.06396700
C	-0.00502000	0.00237100	-1.98453200
C	2.67593500	0.39407400	-1.69609200
N	3.71535300	0.54668300	-2.16507300
C	1.63542400	2.19081300	1.03949100
N	2.25497600	3.01957100	1.54377100
C	2.19453600	-1.63377800	1.03384700
N	3.02524900	-2.25225300	1.53623100
C	0.00809100	-0.00386800	3.02243600
N	0.01179300	-0.00558200	4.16398000
C	-2.18981800	1.63175000	1.04796300
N	-3.01816500	2.24949500	1.55512400
C	-1.63027500	-2.19341300	1.04236300
N	-2.24703600	-3.02360200	1.54771000
C	-2.68451100	-0.39005300	-1.68374400
N	-3.72625200	-0.54160400	-2.14788800
C	-0.39634600	2.68224100	-1.68579200
N	-0.54955700	3.72337500	-2.15075300
C	0.38778700	-2.67821800	-1.69403900
N	0.53876600	-3.71825500	-2.16217400
H	0.01506800	-0.00717900	5.16940000

H/[CB₉H(CN)₉](1)

Lowest normal mode frequency: 58.47 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 226.39 kcal/mol

B	0.14488300	-0.00043500	1.64896800
B	1.02540500	-0.92715600	0.51532700
B	-0.81817700	-0.92573700	0.59568700
B	-0.82037500	0.92334500	0.59645600
B	1.02320800	0.92926800	0.51602500
B	0.05602600	-1.31333000	-0.97628400
B	-1.21174100	-0.00117500	-0.89527200
B	0.05283200	1.31412600	-0.97527500
B	1.35110100	0.00200300	-1.02519900
H	-0.03195500	0.00111400	-2.98730100
C	0.00591400	0.00068000	-1.90896700
C	2.70669800	0.00384400	-1.72820900

N	3.71691500	0.00524400	-2.27858600
C	2.05346500	1.96076200	0.98266000
N	2.82295900	2.74582800	1.32299200
C	2.05818500	-1.95645300	0.98124800
N	2.82963900	-2.73981500	1.32106300
C	0.18021700	-0.00109800	3.16740500
N	0.18957900	-0.00151700	4.31834700
C	-1.91379300	1.88918600	1.07201500
N	-2.80820000	2.55961600	1.34823200
C	-1.90899000	-1.89471600	1.07082800
N	-2.80156000	-2.56762100	1.34690600
C	-2.68955800	-0.00244000	-1.35596800
N	-3.80207800	-0.00338100	-1.60373600
C	-0.05490800	2.69535000	-1.62060900
N	-0.18776700	3.71672200	-2.13349900
C	-0.04785000	-2.69442200	-1.62251300
N	-0.17757400	-3.71586800	-2.13606500
H	-4.79352800	-0.00428100	-1.78178900

H/[CB₉H(CN)₉](2)

Lowest normal mode frequency: 65.67 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 182.25 kcal/mol

B	-0.00399500	-0.37024200	1.61920800
B	-1.06490700	0.79286000	0.68522400
B	1.07317600	0.77847200	0.68892400
B	0.92860400	-0.98586900	0.30247100
B	-0.94227800	-0.97292600	0.30053600
B	0.00990900	1.51002600	-0.68881700
B	1.31392000	0.19194200	-1.02440500
B	-0.00554700	-1.05292400	-1.26403800
B	-1.30926000	0.20961700	-1.02779600
H	0.00826100	0.69312700	-2.93521300
C	0.00511000	0.44327200	-1.88432400
C	-2.70298400	0.38156100	-1.61863900
N	-3.75445900	0.51488700	-2.06602300
C	-1.92509800	-2.09422700	0.63490400
N	-2.67171100	-2.93492700	0.87869400
C	-2.09991200	1.69370500	1.34568300
N	-2.87468100	2.38082900	1.84814200
C	-0.01000200	-0.84527900	3.06179600
N	-0.01438800	-1.18956900	4.15935100
C	1.89571400	-2.12031200	0.63827900
N	2.63038600	-2.97109900	0.88336500
C	2.12043200	1.66618100	1.34816600
N	2.90436400	2.34353700	1.84965700

C	2.71125400	0.34597100	-1.61160700
N	3.76549300	0.46564200	-2.05633500
C	-0.01280800	-2.29110900	-2.15160800
N	-0.01825900	-3.21816700	-2.83260000
C	0.02077100	3.00818600	-0.96680900
N	0.02921100	4.14182000	-1.16412200
H	0.00708200	0.94371200	1.70271600

H/[CB₁₀H(CN)₁₀]

Lowest normal mode frequency: 51.63 cm⁻¹

B	0.80568900	-1.36140900	0.05108600
B	0.80340000	1.36280200	0.05117600
B	-1.80764900	-0.00150000	-0.39021600
B	-0.77612000	1.34991700	-0.97473900
B	-0.79522100	0.92914100	0.74835200
B	1.77562200	0.00152000	-0.13998200
B	-0.77386100	-1.35115900	-0.97479500
B	0.72164600	0.00064800	-1.52829700
B	0.65502500	0.00053900	1.17391500
B	-0.79366100	-0.93048100	0.74831100
H	-1.29375600	-0.00101100	-2.79167500
C	-0.89435800	-0.00070200	-1.78667500
C	1.12598500	0.00083100	2.64756800
N	1.45995800	0.00099900	3.73752300
C	1.41536700	2.74361500	0.28585700
N	1.89347500	3.76800500	0.50365500
C	3.29794100	0.00278900	-0.11377500
N	4.44534800	0.00373800	-0.01978500
C	1.42000700	-2.74118800	0.28571500
N	1.89985000	-3.76477200	0.50348500
C	-1.42363800	1.79268400	1.84925800
N	-1.83641600	2.39783100	2.73699200
C	-1.42059700	-1.79513000	1.84919500
N	-1.83230800	-2.40101900	2.73691900
C	-1.19586400	2.68414600	-1.58232400
N	-1.50869800	3.68618600	-2.05396700
C	1.52322900	0.00129600	-2.83265600
N	2.11400900	0.00177900	-3.82044700
C	-3.33409200	-0.00277900	-0.42539800
N	-4.48395000	-0.00373800	-0.45622100
C	-1.19135800	-2.68606500	-1.58243900
N	-1.50249900	-3.68860200	-2.05414600
H	1.74230200	0.00108200	4.70362400

H/[CB₁₀H(CN)₁₀](1)

Lowest normal mode frequency: 49.49 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 232.28 kcal/mol

B	-0.73485100	-1.43207600	0.29958800
B	1.44744300	0.07431900	0.06195000
B	-1.07192900	1.43595200	-0.47672800
B	0.60214200	1.23483700	-1.08043000
B	0.26466800	1.23080200	0.68200100
B	0.91835200	-1.50926700	0.08635800
B	-1.64101700	-0.22288000	-0.85815600
B	0.30749000	-0.76797400	-1.40121000
B	0.33289500	-0.43668100	1.34828600
B	-1.25874200	0.20708400	0.82394100
H	-0.85268300	0.74082500	-2.82656700
C	-0.61043800	0.51906100	-1.79649600
C	0.73607100	-0.66642300	2.80789000
N	1.10590500	-0.83355400	3.88465700
C	2.95293500	0.34697200	0.24901400
N	4.06917700	0.52410200	0.40578800
C	1.85254600	-2.71052100	0.14143900
N	2.62140500	-3.56583300	0.19512000
C	-1.54868800	-2.69334400	0.57687200
N	-2.14727800	-3.65642500	0.77547100
C	0.74112300	2.39967600	1.55249000
N	1.18059800	3.25878300	2.17968400
C	-2.36493600	0.38743000	1.86733400
N	-3.19112300	0.53426900	2.65448500
C	1.53995800	2.20720700	-1.79851200
N	2.32497200	2.88274600	-2.30112100
C	0.81619400	-1.53521000	-2.62538100
N	1.21607400	-2.08716000	-3.55293100
C	-1.90270300	2.70497300	-0.65101800
N	-2.51775400	3.66527700	-0.80146600
C	-2.99030600	-0.68607000	-1.39442300
N	-3.99926300	-1.02825700	-1.82949900
H	5.05090300	0.68846900	0.55198800

H/[CB₁₀H(CN)₁₀](2)

Lowest normal mode frequency: 52.40 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 222.75 kcal/mol

B	-1.66375200	-0.16976300	0.19079900
B	0.79739900	-1.27881200	0.29493700
B	0.66679400	1.57824800	-0.48443800
B	1.41202500	0.01704500	-0.84458100
B	1.05848200	0.42089700	0.83243200

B	-0.84368400	-1.62676000	0.16893200
B	-0.98104100	1.11453200	-1.03585700
B	-0.35755700	-0.85946400	-1.32551600
B	-0.37335100	-0.47122000	1.40264600
B	-0.61073700	1.17904300	0.71180500
H	0.46436300	0.82620000	-2.82890000
C	0.30211600	0.58667700	-1.78732700
C	-0.55536700	-0.75660700	2.89523200
N	-0.67953400	-0.97994000	4.01704300
C	1.88473200	-2.34368800	0.49426100
N	2.77282700	-3.07558800	0.54187100
C	-1.44222900	-3.02285200	0.24768600
N	-1.88321300	-4.08462100	0.30448000
C	-3.18440900	-0.09536100	0.30251900
N	-4.33266600	-0.04887700	0.37076300
C	2.23512600	0.77608700	1.74993600
N	3.18404000	1.02010900	2.35394900
C	-1.14017900	2.31911500	1.58676900
N	-1.51875100	3.18905700	2.23767500
C	2.88630800	-0.17449300	-1.28747100
N	3.98595400	-0.34015100	-1.53554900
C	-0.57376500	-1.75627800	-2.54914900
N	-0.67924800	-2.43009000	-3.47645500
C	1.37542800	2.91077700	-0.72490700
N	1.96313800	3.87350300	-0.95188700
C	-2.00878900	1.94314800	-1.79703700
N	-2.75894600	2.56929600	-2.40507300
H	4.96369400	-0.51296000	-1.70768300

H/[CB₁₀H(CN)₁₀](3)

Lowest normal mode frequency: 58.22 cm⁻¹

The value of ΔG_{acid} at ωB97XD/6-311+G(d, p) level: 193.67 kcal/mol

B	0.06434016	-1.58065459	0.87218381
B	-0.99464397	1.01645898	0.00000000
B	1.35362364	-0.03291578	-1.19877740
B	0.47225881	1.53271543	-0.88511300
B	-0.41569742	0.04280018	-1.41914994
B	-0.41569742	0.04280018	1.41914994
B	1.35362364	-0.03291578	1.19877740
B	0.47225881	1.53271543	0.88511300
B	-1.23571505	-0.74304500	0.00000000
B	0.06434016	-1.58065459	-0.87218381
H	2.70917805	1.42483881	0.00000000
C	1.73687303	0.94742685	0.00000000
C	-2.65761808	-1.30175394	0.00000000

N	-3.71919510	-1.74524588	0.00000000
C	-2.23672092	1.90378504	0.00000000
N	-3.16415889	2.58478909	0.00000000
C	-1.04959821	0.04773152	2.81190924
N	-1.51765591	0.06527612	3.86274537
C	0.03843838	-2.75281306	1.83870546
N	0.03984654	-3.64921367	2.56085295
C	-1.04959821	0.04773152	-2.81190924
N	-1.51765591	0.06527612	-3.86274537
C	0.03843838	-2.75281306	-1.83870546
N	0.03984654	-3.64921367	-2.56085295
C	0.61239161	2.76629894	-1.76891172
N	0.74425047	3.69175457	-2.43931626
C	0.61239161	2.76629894	1.76891172
N	0.74425047	3.69175457	2.43931626
C	2.43205534	-0.48924836	-2.16007546
N	3.26312912	-0.86324179	-2.86517349
C	2.43205534	-0.48924836	2.16007546
N	3.26312912	-0.86324179	2.86517349
H	1.02032189	-1.87202011	0.00000000

H/[CB₁₁H(CN)₁₁]

Lowest normal mode frequency: 60.99 cm⁻¹

B	-1.38150600	0.64292000	-0.99027300
B	-1.03761500	-1.11534700	-0.99084600
B	0.18448700	1.51336100	-0.98913900
B	1.49624000	0.29295400	-0.98887200
B	0.74090800	-1.33168500	-0.98998900
B	1.39152500	-0.64721100	0.51901900
B	1.04512300	1.12357400	0.51952000
B	-0.74596200	1.34130800	0.51869500
B	-0.18550000	-1.52374200	0.51775100
B	-1.50643500	-0.29482900	0.51762300
B	-0.00068100	-0.00053700	1.40256500
C	0.00094800	0.00077700	-1.77246400
H	0.00151700	0.00123500	-2.85660000
C	-0.00185300	-0.00154100	2.95279100
N	-0.00223600	-0.00205300	4.09164000
C	1.95383000	2.10038400	1.27148400
N	2.60710200	2.80276500	1.90674600
C	2.60134200	-1.21019300	1.27056100
N	3.47127300	-1.61491400	1.90548100
C	-1.39472300	2.50742800	1.27015000
N	-1.86106700	3.34584600	1.90517100
C	-2.81643900	-0.55131800	1.26830200

N	-3.75828900	-0.73547600	1.90290100
C	-0.34700700	-2.84879300	1.26854600
N	-0.46313600	-3.80129700	1.90333400
C	-1.92136200	-2.06524900	-1.79668200
N	-2.58591700	-2.77981800	-2.40529600
C	-2.55803000	1.19038800	-1.79574300
N	-3.44295500	1.60197600	-2.40415700
C	0.34159600	2.80209800	-1.79368600
N	0.45981000	3.77122400	-2.40157300
C	2.77041500	0.54237300	-1.79324500
N	3.72876600	0.72971000	-2.40082400
C	1.37176700	-2.46581500	-1.79525300
N	1.84612600	-3.31878900	-2.40359100
H	-0.00364800	-0.00249400	5.09894100

H/[CB₁₁H(CN)₁₁](1)

Lowest normal mode frequency: 73.96 cm⁻¹

The value of ΔG_{acid} at ω B97XD/6-311+G(d, p) level: 153.65 kcal/mol

B	1.44115900	-0.52894900	-0.89283800
B	0.89124200	1.14895300	-1.04573200
B	0.00562200	-1.60950200	-0.76602900
B	-1.43768100	-0.53961500	-0.89227500
B	-0.90017800	1.14233300	-1.04529600
B	-1.46843300	0.54005800	0.54336900
B	-0.99645600	-1.21141500	0.69218900
B	1.00546000	-1.20414000	0.69169600
B	-0.00574300	1.60104200	0.41124500
B	1.46472800	0.55105300	0.54256200
B	-0.00073700	0.26148200	1.58624700
C	0.00023000	-0.17163700	-1.70284600
H	0.00047500	-0.29218100	-2.78095800
C	-0.00086200	0.47022300	3.09687500
N	-0.00074600	0.60493100	4.23939100
C	-1.84273700	-2.25541300	1.41075100
N	-2.46988700	-3.04744800	1.96104300
C	-2.78018900	1.02226800	1.15818700
N	-3.76970200	1.37645000	1.62557300
C	1.86029900	-2.24174900	1.40948900
N	2.49390200	-3.02896200	1.95930400
C	2.77313000	1.04270000	1.15700300
N	3.76017800	1.40402800	1.62413500
C	-0.01101200	3.01688700	0.97841200
N	-0.01501600	4.08519700	1.40507000
C	1.65622100	2.10200200	-1.95657100
N	2.22901800	2.81127000	-2.65764700

C	2.67881800	-1.04210400	-1.61748600
N	3.60740500	-1.43252300	-2.17267200
C	0.01049900	-2.97677600	-1.43933900
N	0.01411300	-4.00750000	-1.94965100
C	-2.67194600	-1.06150900	-1.61646700
N	-3.59799000	-1.45844900	-2.17127600
C	-1.67274700	2.08980500	-1.95552600
N	-2.25116000	2.79494500	-2.65615500
H	0.00557900	-1.14608500	1.67057500

H/[CB₁₂H(CN)₁₂]

Lowest normal mode frequency: 19.63 cm⁻¹

B	-1.30108500	1.31504200	0.00841500
B	0.26385200	1.70565200	0.01129400
B	-1.83881100	-0.20350800	-0.00156800
B	-0.48678900	0.41076300	1.40014600
B	1.38744200	0.62452700	0.89424800
B	-0.85969100	-1.40689900	0.87898100
B	-0.85834700	-1.39358100	-0.90000300
B	1.38926900	0.63713300	-0.88330300
B	0.74895800	-0.92649800	1.42442700
B	0.75094600	-0.90611600	-1.43630000
B	1.84094400	-0.81171500	-0.00437100
H	0.74074200	-2.90575200	-0.02014700
B	-0.48388600	0.43143200	-1.39487000
C	0.48656600	-1.85165700	-0.01277500
C	0.56227000	3.21039000	0.02146700
N	0.65508600	4.35822400	0.02920700
C	-2.32845000	2.45623500	0.01539200
N	-3.08539200	3.30895800	0.02039900
C	-3.35979700	-0.39490300	-0.00321300
N	-4.51104500	-0.42135600	-0.00379900
C	-0.98428800	0.92553900	2.75710900
N	-1.41639200	1.37198900	3.72602000
C	2.38600000	1.36239200	1.78708700
N	3.12049100	1.92531900	2.47090800
C	2.39007500	1.38691800	-1.76363600
N	3.12633300	1.95884400	-2.43801900
C	-0.97992300	0.96493000	-2.74510900
N	-1.41097300	1.42468300	-3.70825200
C	-1.63339700	-2.44694200	1.68769500
N	-2.22517600	-3.22330800	2.29636100
C	-1.63149600	-2.42111800	-1.72504300
N	-2.22297600	-3.18800000	-2.34589500
C	1.23711400	-1.59212800	2.71004600

N	1.60546200	-2.10133000	3.67334900
C	3.22765900	-1.45137600	-0.00783600
N	4.26292200	-1.95223000	-0.01053000
C	1.24091100	-1.55355200	-2.73050200
N	1.61066500	-2.04910900	-3.70035800
H	-3.74726100	4.06742900	0.02484200

H/[CB₁₂H(CN)₁₂](1)

Lowest normal mode frequency: 52.87 cm⁻¹

The value of ΔG_{acid} at ωB97XD/6-311+G(d, p) level: 174.72 kcal/mol

B	-1.15377900	-1.29096300	1.01387000
B	0.50588000	-0.87251300	1.30750300
B	-2.05508500	-0.34837700	-0.09506500
B	0.39228000	-1.62819900	-0.29517400
B	1.76994800	-0.56752900	0.12921900
B	-0.74478200	-0.42609300	-1.61059300
B	-1.31082500	1.05294200	-0.80351600
B	1.05917000	0.79915800	1.05060400
B	1.02629700	-0.48463100	-1.49968700
B	0.09976200	1.79435000	-0.03383100
B	1.58308700	1.01477600	-0.63151700
H	0.21995700	1.60761400	-2.46754200
B	-0.87716800	0.59573600	1.07043200
C	0.16737500	1.00904700	-1.56361900
C	0.91208900	-1.50449900	2.63996000
N	1.24462800	-1.96744500	3.63964800
C	-1.79828700	-2.24034800	2.01020700
N	-2.33926600	-2.96357100	2.72460200
C	-3.57469400	-0.33739800	-0.18270300
N	-4.72423300	-0.38005800	-0.23021400
C	0.41654000	-3.11371600	-0.62105600
N	0.37554300	-4.23852000	-0.86488300
C	3.17282900	-1.12371100	0.36532100
N	4.22893200	-1.54988300	0.52676000
C	1.75210400	1.50030000	2.21471500
N	2.27149400	2.04036100	3.08790600
C	-1.56992600	1.28413200	2.24898700
N	-2.10757700	1.79001300	3.13151000
C	-1.40062000	-0.99691200	-2.85732400
N	-1.93339000	-1.45127700	-3.77119800
C	-2.35959700	2.01896700	-1.35173200
N	-3.11678800	2.76073400	-1.79885700
C	1.74300100	-0.96967100	-2.75756600

N	2.28318700	-1.31816600	-3.71151000
C	2.75928800	1.85235600	-1.11882900
N	3.63536900	2.48824000	-1.50759300
C	0.02694700	3.31100000	0.09344400
N	-0.02210800	4.45687600	0.18209800
H	-1.74671800	-1.60930500	-0.12038900

H/[CB₁₃H(CN)₁₃]

Lowest normal mode frequency: 54.11 cm⁻¹

B	0.00017700	-0.00015600	1.32474500
B	1.73129800	0.29497900	-0.94370400
B	0.61004900	1.64631400	-0.94365600
B	-1.12095800	1.35163300	-0.94338600
B	1.65310800	-0.61273100	0.56210600
B	0.29601000	-1.73790500	0.56203700
B	-0.29588900	1.73776700	0.56264300
B	1.35716300	1.12519000	0.56239700
H	-0.00036900	0.00039900	-2.71957000
B	1.12064700	-1.35133600	-0.94411500
B	-1.35704000	-1.12532400	0.56245500
B	-1.65298600	0.61259400	0.56276300
B	-0.61036700	-1.64604000	-0.94395400
B	-1.73161800	-0.29468600	-0.94327800
C	-0.00017500	0.00023100	-1.63241900
C	0.00056900	-0.00064300	2.88634200
N	0.00102600	-0.00103600	4.02475900
C	-0.51390100	3.01858400	1.37204400
N	-0.67068900	3.93985500	2.04345500
C	-2.87104500	1.06410400	1.37248000
N	-3.74704900	1.38880600	2.04426500
C	-2.35699400	-1.95480400	1.37191500
N	-3.07603900	-2.55130200	2.04371000
C	0.51424300	-3.01883600	1.37120400
N	0.67123300	-3.94011600	2.04255700
C	2.87129600	-1.06443700	1.37152200
N	3.74734200	-1.38929000	2.04317900
C	2.35735300	1.95442600	1.37181400
N	3.07662400	2.55070100	2.04356500
C	1.92345300	-2.31974700	-1.80882900
N	2.52853200	-3.04948400	-2.46095400
C	-1.04754400	-2.82553800	-1.80862300
N	-1.37702900	-3.71441800	-2.46068600
C	-2.97208600	-0.50582400	-1.80729200

N	-3.90702100	-0.66495400	-2.45878800
C	-1.92398400	2.32027800	-1.80762800
N	-2.52922600	3.05017500	-2.45942200
C	1.04700500	2.82606400	-1.80809700
N	1.37632700	3.71513000	-2.45998800
C	2.97155600	0.50635800	-1.80796700
N	3.90634700	0.66565900	-2.45962600
H	0.00130000	-0.00128800	5.03332900

H/[CB₁₃H(CN)₁₃](1)

Lowest normal mode frequency:30.09 cm⁻¹

The value of ΔG_{acid} at $\omega\text{B97XD/6-311+G(d, p)}$ level: 150.64 kcal/mol

B	-0.47193200	-0.00065200	1.59536800
B	0.89634900	1.51006100	-0.78930200
B	-0.84602500	1.52964400	-0.88432400
B	-1.69392500	-0.00311800	-0.98305800
B	1.63419700	0.94359900	0.69060100
B	1.63788700	-0.93782800	0.69046300
B	-1.62443600	0.89698300	0.55514000
B	-0.05372500	1.73225200	0.69454900
H	0.13561100	0.00017800	-2.62760000
B	1.79423600	0.00324800	-0.82757400
B	-0.04729600	-1.73249500	0.69453000
B	-1.62099000	-0.90276600	0.55526500
B	0.90190700	-1.50692500	-0.78926900
B	-0.84039000	-1.53268000	-0.88427300
C	0.07601200	0.00012100	-1.54141300
C	-0.43494200	-0.00064800	3.10836700
N	-0.38290300	-0.00060700	4.25919400
C	-2.83429900	1.60150500	1.16368600
N	-3.75094600	2.12170400	1.62537700
C	-2.82820800	-1.61177300	1.16388300
N	-3.74290000	-2.13536100	1.62561600
C	-0.06737100	-3.07063800	1.42868800
N	-0.06654600	-4.07168100	1.99640200
C	2.78806400	-1.68540900	1.34825800
N	3.66188000	-2.23525100	1.85698700
C	2.78149100	1.69546300	1.34853700
N	3.65322000	2.24858700	1.85728900
C	-0.07859400	3.07040400	1.42857300
N	-0.08142200	4.07151400	1.99616100
C	3.02697500	0.00556500	-1.72120000
N	3.95463900	0.00730700	-2.40222600
C	1.58435800	-2.62477200	-1.57027000
N	2.10201800	-3.46364300	-2.16429400

C	-1.39055800	-2.61722700	-1.80150500
N	-1.80242200	-3.43264800	-2.50126900
C	-2.85679600	-0.00527100	-1.96730500
N	-3.73041500	-0.00689500	-2.71640400
C	-1.40005300	2.61215200	-1.80163000
N	-1.81482000	3.42603800	-2.50146500
C	1.57473900	2.63042500	-1.57024000
N	2.08937200	3.47121200	-2.16418500
H	1.26891700	0.00187000	1.56815600

H/[CB₅F₆]

Lowest normal mode frequency: 118.55 cm⁻¹

B	1.38841400	-0.28165700	0.00000000
B	-0.35487800	-0.86834700	0.90172100
B	0.42341800	0.73927100	-0.87912700
B	-0.35487800	-0.86834700	-0.90172100
B	0.42341800	0.73927100	0.87912700
C	-0.91064800	0.34830100	0.00000000
H	-0.03636100	-1.81377300	0.00000000
F	0.49066000	1.56696500	1.92260000
F	-0.83114400	-1.44689300	2.00256700
F	-0.83114400	-1.44689300	-2.00256700
F	0.49066000	1.56696500	-1.92260000
F	2.56664700	-0.88510000	0.00000000
F	-2.12203600	0.91418000	0.00000000

H/[CB₆F₇]

Lowest normal mode frequency: 86.85 cm⁻¹

B	-1.42704000	-0.15999300	0.14785500
B	-0.35928800	-1.64165200	0.20791200
B	-0.53302600	1.30874400	-0.16731400
B	1.00897100	0.73643000	-0.54684600
B	1.08147800	-0.87550900	0.19836900
C	-0.23401800	-0.24036500	-1.00295600
B	0.44589500	0.71290700	1.06147600
H	-1.17361000	-1.01794900	1.08571200
F	-2.74285200	-0.04835600	-0.06089600
F	-1.25827300	2.34883400	-0.58229200
F	0.68432100	1.02740600	2.31632600
F	2.05654200	1.18664200	-1.22609500
F	2.29058900	-1.38692900	-0.09669500
F	-0.80845400	-2.85825200	-0.07764700
F	-0.47501000	-0.51003100	-2.29112200

H/[CB₇F₈]

Lowest normal mode frequency: 89.53 cm⁻¹

B	-0.13435754	-0.33858312	1.26315198
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B	-0.25503085	1.39507800	-0.87198108
B	-1.44690199	-0.22134399	0.00000000
B	-0.48230206	-1.56430904	0.00000000
B	-0.13435754	-0.33858312	-1.26315198
B	-0.25503085	1.39507800	0.87198108
B	1.14134205	0.64262688	0.00000000
C	0.92552697	-0.91568311	0.00000000
H	-1.12867889	1.84892199	0.00000000
F	-2.75682298	0.01343108	0.00000000
F	-0.73600112	-2.87437302	0.00000000
F	0.01853311	-0.62661892	-2.56154885
F	-0.27541657	2.26289906	-1.88503505
F	-0.27541657	2.26289906	1.88503505
F	0.01853311	-0.62661892	2.56154885
F	2.37656407	1.15331382	0.00000000
F	2.00896593	-1.69868016	0.00000000

H/[CB₈F₉]

Lowest normal mode frequency: 93.27 cm⁻¹

B	-0.22333600	-1.35933800	-0.88335400
B	-0.15108200	-1.02764900	0.91748200
B	-1.56903600	-0.72835000	-0.06726100
B	0.93171600	0.44634200	0.85952000
B	-0.89452100	0.65935100	0.85364600
B	-1.35894500	0.75040400	-0.83355700
B	1.45532900	0.53521900	-0.84903100
B	0.18372900	1.63168600	-0.26809600
C	1.15639200	-0.86731200	-0.20354500
H	0.18595600	1.05424900	-1.44921100
F	-1.45547800	1.32454700	1.87972400
F	-2.17361300	1.37358600	-1.66418200
F	-2.78044500	-1.33028200	0.04586600
F	-0.01085000	-1.86643100	1.94506400
F	1.74546200	0.75211700	1.87203900
F	2.52240400	0.83624900	-1.55492900
F	0.29411000	2.97077400	-0.23899200
F	-0.21608200	-2.36913600	-1.73533200
F	2.18631600	-1.73461500	-0.10217500

H/[CB₉F₁₀]

Lowest normal mode frequency: 113.07 cm⁻¹

B	-1.64513600	0.00002400	0.57533400
B	-0.37165400	-0.00003500	1.61392100
B	-0.70203400	-1.35293000	0.24144800
B	-1.02492000	0.00004200	-0.98213000
B	-0.70199900	1.35295900	0.24150600

B	0.99640200	-0.95143400	0.70865200
B	0.50537200	-0.95210900	-1.11059700
B	0.50539800	0.95214200	-1.11055700
B	0.99642700	0.95136800	0.70869200
C	1.61787000	-0.00001600	-0.44656600
H	-3.19607700	0.00002200	-0.62843000
F	1.79262600	1.78607300	1.39037500
F	1.79257700	-1.78619000	1.39029900
F	-0.31248200	-0.00007100	2.95458600
F	-1.19390800	2.61569300	0.29466800
F	-3.18094000	0.00002000	0.35351400
F	-2.14367300	0.00006000	-1.85239800
F	0.80211100	1.81962700	-2.08491200
F	0.80204500	-1.81955900	-2.08499600
F	-1.19402400	-2.61563700	0.29455400
F	2.91339900	-0.00002400	-0.78052600

H/[CB₁₀F₁₁]

Lowest normal mode frequency: 114.00 cm⁻¹

B	-0.02420700	-0.00000100	1.50917600
B	1.49515000	-0.87202000	-0.88130500
B	-0.54921600	1.23965600	-0.99550300
B	-0.54921400	-1.23965600	-0.99550400
B	1.49514800	0.87202400	-0.88130400
B	0.42899000	-1.43877600	0.45560100
B	-1.31627600	0.89296400	0.62893600
B	-1.31627500	-0.89296700	0.62893500
B	1.55093400	0.00000100	0.66803800
B	0.42898800	1.43877600	0.45560300
C	-1.55031700	-0.00000100	-0.75831800
H	1.14022600	0.00000200	-1.82745700
F	-2.27198800	1.64223600	1.18276700
F	-0.81350000	2.10743000	-1.95645700
F	-2.27198500	-1.64224100	1.18276500
F	-0.81349700	-2.10742800	-1.95646000
F	0.79193800	-2.65264400	0.92524700
F	2.32532000	-1.76877100	-1.40257500
F	2.65138100	0.00000000	1.44990900
F	2.32531700	1.76877600	-1.40257300
F	0.79193300	2.65264500	0.92525000
F	-0.00137900	-0.00000200	2.85059500
F	-2.72003200	-0.00000100	-1.41913400

H/[CB₁₁F₁₂]

Lowest normal mode frequency: 119.36 cm⁻¹

B	-1.13712736	1.30266171	0.00000000
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B	-0.15617917	0.89477138	-1.47299370
B	-0.15617917	0.89477138	1.47299370
B	1.44403330	0.21369558	0.91704301
B	1.44403330	0.21369558	-0.91704301
B	1.08901816	-1.24567183	0.00000000
B	0.12718994	-0.84152349	1.48316972
B	-1.48453264	-0.18302603	0.92574898
B	0.12718994	-0.84152349	-1.48316972
B	-1.48453264	-0.18302603	-0.92574898
B	-0.64496580	-1.41379719	0.00000000
C	0.59796661	1.41858107	0.00000000
H	0.06558059	-3.30078404	0.00000000
F	-1.86394060	2.42954356	0.00000000
F	-2.61874857	-0.37756100	1.63414989
F	-2.61874857	-0.37756100	-1.63414989
F	-0.84203748	-2.96534523	0.00000000
F	0.22454341	-1.65615994	-2.56597871
F	1.66682043	-2.52003971	0.00000000
F	2.56302018	0.54934591	-1.57354499
F	2.56302018	0.54934591	1.57354499
F	-0.18227442	1.72984299	-2.52154208
F	-0.18227442	1.72984299	2.52154208
F	0.22454341	-1.65615994	2.56597871
F	1.12257036	2.64624718	0.00000000

H/[CB₁₂F₁₃]

Lowest normal mode frequency: 22.39 cm⁻¹

B	-1.89713800	0.67184300	0.00687700
B	-1.38687100	-0.95040300	-0.00853300
B	-1.05370300	1.98802600	0.00649000
B	-0.80542600	0.05245900	-1.44106300
B	-0.02283800	-1.59070200	-0.92170600
B	0.47558600	1.39570400	-0.88422200
B	0.46793500	1.37929600	0.90935100
B	-0.02535500	-1.60780800	0.89556400
B	0.97801000	-0.24252800	-1.44046400
B	0.97270100	-0.26661700	1.44017000
B	1.44919100	-1.24975600	-0.00785100
B	-0.80961700	0.02312300	1.44190900
C	1.60825900	0.47918900	0.00753700
H	-3.44416900	-0.58805400	-0.00479700
F	-0.20960800	-2.73942500	1.61341200
F	-2.61552000	-1.69027200	-0.01727300
F	-3.42291400	0.42817500	0.00570800
F	-1.42681400	0.06554200	2.64547000

F	-1.21955300	3.29708800	0.00701800
F	0.92357300	2.35419400	1.71384600
F	0.94078300	2.38237100	-1.66890100
F	1.71243700	-0.26076600	2.55623100
F	1.72161100	-0.21879500	-2.55367000
F	2.58096600	-1.96227100	-0.01201700
F	-0.20744400	-2.70818100	-1.66121500
F	-1.42006400	0.11330700	-2.64493000
F	2.87390800	0.90567000	0.01376300

H/[CB₁₃F₁₄]

Lowest normal mode frequency: 57.48 cm⁻¹

B	-0.09766800	-0.02172700	1.59579100
B	-0.30237600	-1.74084100	-0.84677400
B	1.38994400	-1.29361200	-0.61397200
B	1.72214300	0.46631400	-0.57125000
B	-1.17018800	-1.20126800	0.54049500
B	-1.69273600	0.44502500	0.57761800
B	1.64494800	-0.48795400	0.92388000
B	0.43422600	-1.78935800	0.76920200
B	-1.48550900	-0.37787100	-0.97330900
B	-0.54378900	1.73882500	0.80635700
B	1.16167300	1.23236500	0.93191600
B	-1.20740200	1.37957300	-0.78790600
B	0.50694300	1.78742700	-0.60671600
C	0.17419600	0.06862800	-1.44235400
H	-2.93324900	-1.05580800	1.41215800
F	-2.44750400	-0.67134900	-1.87123600
F	-1.93258000	2.12317900	-1.62500700
F	0.90830300	2.82750000	-1.34744200
F	2.80051400	0.78447100	-1.30748200
F	-0.91895700	2.82303900	1.52067900
F	-2.96261600	0.36779100	1.22534700
F	-0.32566300	-0.11661100	2.92390600
F	-2.36599700	-1.87229100	1.22496200
F	0.61152800	-2.93590100	1.46300800
F	2.26599500	-1.98883900	-1.34586200
F	-0.58458300	-2.71559800	-1.71379000
F	2.70549900	-0.74837000	1.72161600
F	1.93827300	1.99905300	1.73095900
F	0.31745800	0.11943200	-2.76462400

H/[CB₅Cl₆]

Lowest normal mode frequency: 79.51 cm⁻¹

B	1.40247200	-0.34399100	0.00000000
B	-0.30848400	-0.87807300	0.91260600

B	0.44433500	0.70394600	-0.87329100
B	-0.30848400	-0.87807300	-0.91260600
B	0.44433500	0.70394600	0.87329100
C	-0.88629900	0.32751200	0.00000000
Cl	2.97561500	-1.07634200	0.00000000
Cl	0.62269000	1.83980300	2.19436300
Cl	0.62269000	1.83980300	-2.19436300
Cl	-0.97344200	-1.71866400	-2.29587400
Cl	-0.97344200	-1.71866400	2.29587400
H	0.08447500	-1.78093200	0.00000000
Cl	-2.45867200	1.02683500	0.00000000

H/[CB₆Cl₇]

Lowest normal mode frequency: 60.08 cm⁻¹

B	0.89470700	1.12617400	0.55281500
B	-0.89334600	1.12733300	0.55284400
B	1.32610000	-0.45432100	0.20954600
B	-0.00085700	-1.28373300	-0.41678600
B	-1.32668500	-0.45261500	0.20970100
C	0.00021500	0.35512900	-0.71063000
B	-0.00047600	-0.93458600	1.26895100
Cl	-0.00085900	-1.58896500	2.86609100
Cl	2.97965400	-0.84019900	-0.26675500
Cl	-0.00183300	-2.68999200	-1.45562500
Cl	1.96024400	2.51762900	0.45730600
Cl	-1.95702900	2.52020200	0.45729800
Cl	-2.98072100	-0.83653600	-0.26652500
H	0.00083800	1.33278200	1.48730900
Cl	0.00058200	0.97051900	-2.32760700

H/[CB₇Cl₈]

Lowest normal mode frequency: 63.11 cm⁻¹

B	-0.12067174	-0.32710096	1.26255621
B	-0.34587828	1.37511997	-0.86785847
B	-1.44105493	-0.22049087	0.00000000
B	-0.43090908	-1.54226698	0.00000000
B	-0.12067174	-0.32710096	-1.26255621
B	-0.34587828	1.37511997	0.86785847
B	1.08246317	0.70018685	0.00000000
C	0.95495699	-0.87741213	0.00000000
Cl	-0.46932939	2.57500793	-2.15038430
Cl	-0.46932939	2.57500793	2.15038430
Cl	-3.19170892	-0.13050067	0.00000000
Cl	2.64565026	1.51025068	0.00000000
Cl	0.08254218	-0.77456391	2.95352188
Cl	0.08254218	-0.77456391	-2.95352188

Cl	-0.82721227	-3.24569494	0.00000000
H	-1.20701271	1.81611211	0.00000000
Cl	2.38744489	-1.83614429	0.00000000

H/[CB₈Cl₉]

Lowest normal mode frequency:65.15 cm⁻¹

B	-0.10895600	-1.35401300	-0.91659000
B	-0.07378500	-1.03276600	0.89705100
B	-1.48554500	-0.82209300	-0.09563800
B	0.89092700	0.51483700	0.83824600
B	-0.92844200	0.58189200	0.83870100
B	-1.38933100	0.66147700	-0.86392800
B	1.38363700	0.60942200	-0.87130300
B	0.04615500	1.62873600	-0.27251100
C	1.22816400	-0.79845600	-0.19805200
Cl	-3.01367800	-1.71569200	0.05344700
Cl	-1.80751400	1.34533400	2.17461800
Cl	-2.55889500	1.36060000	-1.94163900
Cl	0.11938200	3.39276800	-0.28395900
Cl	0.08265700	-2.15971200	2.23716900
Cl	-0.04932500	-2.62393000	-2.09973500
Cl	2.66424400	1.13231300	-1.90465000
Cl	1.96916100	1.05400500	2.11739900
H	0.01207800	1.04266500	-1.44411100
Cl	2.64959400	-1.79682800	-0.06663300

H/[CB₉Cl₁₀]

Lowest normal mode frequency:91.56 cm⁻¹

B	-0.50037934	-1.72625382	0.00000000
B	-1.53106407	-0.40769461	0.00000000
B	-0.23475101	-0.70805958	1.33218910
B	0.99202481	-0.97466412	0.00000000
B	-0.23475101	-0.70805958	-1.33218910
B	-0.75185541	0.98817744	0.93928739
B	1.06523849	0.53933507	0.94781568
B	1.06523849	0.53933507	-0.94781568
B	-0.75185541	0.98817744	-0.93928739
C	0.39332034	1.64987900	0.00000000
Cl	-0.54877671	-3.52694281	0.00000000
Cl	-0.32676930	-1.35710050	-2.98821582
Cl	-3.30011211	-0.57668125	0.00000000

Cl	2.33431855	-2.28049439	0.00000000
Cl	-0.32676930	-1.35710050	2.98821582
Cl	-1.67182623	1.98097297	-2.06547943
Cl	2.36553556	0.92711215	-2.07564054
Cl	-1.67182623	1.98097297	2.06547943
Cl	2.36553556	0.92711215	2.07564054
H	1.30672735	-3.23584018	0.00000000
Cl	0.81260268	3.32195392	0.00000000

H/[CB₁₀Cl₁₁]

Lowest normal mode frequency: 75.97 cm⁻¹

B	-0.03702600	0.00002500	1.48816500
B	1.47547700	-0.87313100	-0.88307700
B	-0.54379600	1.25903900	-1.02524500
B	-0.54377200	-1.25900800	-1.02523400
B	1.47556300	0.87309500	-0.88305800
B	0.42381200	-1.43749900	0.44802700
B	-1.30893600	0.88638100	0.58851000
B	-1.30894600	-0.88638400	0.58851800
B	1.53728600	-0.00003100	0.66003200
B	0.42385200	1.43747500	0.44795300
C	-1.53540900	0.00001200	-0.81759600
Cl	3.02194900	-0.00000300	1.62934900
Cl	0.84783500	-3.03083000	1.11177000
Cl	-0.06138100	0.00005000	3.25385500
Cl	2.64984000	-1.93113200	-1.63850400
Cl	2.64993900	1.93102800	-1.63852000
Cl	0.84786400	3.03081600	1.11171700
Cl	-2.57685200	-1.87982500	1.28992700
Cl	-0.86072100	-2.44875300	-2.25008100
Cl	-0.86065500	2.44872000	-2.25016500
Cl	-2.57678000	1.87993500	1.28987600
H	1.08277700	-0.00002300	-1.79987900
Cl	-3.07150200	0.00000300	-1.63378300

H/[CB₁₁Cl₁₂]

Lowest normal mode frequency: 108.95 cm⁻¹

B	-1.12326519	1.31710793	0.00000000
B	-0.14627854	0.89928218	-1.46316549
B	-0.14627854	0.89928218	1.46316549
B	1.43287279	0.20768735	0.90842118
B	1.43287279	0.20768735	-0.90842118
B	1.07547722	-1.26793502	0.00000000
B	0.11813059	-0.85294724	1.46800064
B	-1.46156685	-0.17910135	0.90903100
B	0.11813059	-0.85294724	-1.46800064

B	-1.46156685	-0.17910135	-0.90903100
B	-0.66547761	-1.45347564	0.00000000
C	0.61850669	1.44572255	0.00000000
Cl	-1.18192592	-3.26108312	0.00000000
Cl	2.04993864	-2.78828111	0.00000000
Cl	0.24680916	-1.82510316	-2.95541267
Cl	-2.95761851	-0.43261087	-1.83727887
Cl	-2.95761851	-0.43261087	1.83727887
Cl	0.24680916	-1.82510316	2.95541267
Cl	-0.21690732	1.90863208	2.90645759
Cl	2.92292438	0.51906575	1.79838199
Cl	2.92292438	0.51906575	-1.79838199
Cl	-0.21690732	1.90863208	-2.90645759
Cl	-2.15487452	2.74601297	0.00000000
H	0.13099439	-3.60021590	0.00000000
Cl	1.31368521	3.03386520	0.00000000

H/[CB₁₂Cl₁₃]

Lowest normal mode frequency:26.91 cm⁻¹

B	1.95317500	0.71863700	-0.00245900
B	1.56579900	-0.84716900	0.00391400
B	0.79922700	1.82392900	-0.00428600
B	0.78569800	0.26688600	1.42203600
B	0.21207200	-1.52258200	0.90698500
B	-0.69965800	1.36439100	0.89601700
B	-0.69454200	1.35301300	-0.91326900
B	0.21341000	-1.53448500	-0.88953100
B	-0.94333700	-0.31376600	1.44938500
B	-0.93989300	-0.33015000	-1.44825500
B	-1.28500700	-1.36968000	0.00633800
B	0.78965600	0.24622500	-1.42387500
C	-1.69972700	0.31407400	-0.00420300
Cl	3.71647500	1.10269200	-0.00318600
Cl	3.13831900	-1.89047800	0.00873100
Cl	1.25374700	3.54093700	-0.00908400
Cl	1.56714200	0.48628100	3.00525800
Cl	0.55922300	-2.95213300	1.91292200
Cl	0.55968100	-2.97758700	-1.87646400
Cl	1.57459600	0.44998500	-3.00746200
Cl	-1.86671400	-0.55125200	2.93450700
Cl	-2.55692200	-2.58824700	0.01208300
Cl	-1.41947900	2.65579200	1.86237900
Cl	-1.40688200	2.63488600	-1.89746900
Cl	-1.85992400	-0.58388300	-2.93278400
H	3.85386500	-0.66931200	0.00393600

Cl	-3.40270300	0.64410100	-0.00906200
H/[CB₁₃Cl₁₄]			
Lowest normal mode frequency: 57.23 cm⁻¹			
B	-0.15479200	-0.00454700	1.57788700
B	-1.38163400	-0.93244200	-0.93741200
B	0.16654000	-1.77666700	-0.75083000
B	1.66761700	-0.84760200	-0.54574800
B	-1.70856400	-0.04436400	0.52450500
B	-0.96874200	1.52027200	0.64009200
B	0.85030600	-1.51829300	0.86720500
B	-0.88857000	-1.56849200	0.63979100
B	-1.42865100	0.86010900	-0.93694100
B	0.77038300	1.56030200	0.86727300
B	1.67627000	0.04353100	0.98429600
B	0.07383200	1.78313500	-0.75052000
B	1.62096400	0.93271600	-0.54593900
C	0.16994200	0.00436200	-1.49032700
Cl	-0.55177300	-0.01483700	3.33946100
Cl	1.54381400	-2.86436300	1.79991400
Cl	3.11764500	0.08103000	2.02484700
Cl	-1.78145100	-2.91837700	1.39671500
Cl	-3.39164500	-0.08788300	1.41447700
Cl	-1.93003500	2.82202700	1.39755600
Cl	1.39334500	2.94029200	1.80008700
Cl	0.30088400	-3.25415400	-1.70714300
Cl	-2.58683500	-1.69629800	-1.98357700
Cl	-2.67219400	1.56059500	-1.98255400
Cl	3.07368000	-1.55246100	-1.34340700
Cl	2.98867100	1.70918400	-1.34383400
Cl	0.13169400	3.26554000	-1.70693500
H	-2.75357700	-0.07389600	2.58210800
Cl	0.37944200	0.01026000	-3.21198600
H/[CB₅(CN)₆]			
Lowest normal mode frequency: 59.20 cm⁻¹			
B	1.18873500	-0.00603000	-0.01394100
B	-0.01014900	-0.89784600	-0.82990000
B	0.01825800	0.89780600	0.82974000
B	-0.00258900	0.82983200	-0.89789400
B	0.01004700	-0.82991700	0.89776400
C	-1.08167800	0.00543800	0.01265000
C	-0.12546800	1.85873800	-2.00859300
N	-0.17571600	2.64005100	-2.85279200
C	-0.07869200	2.01077100	1.85893000
N	-0.10905300	2.85600900	2.64013800

C	-0.09708300	-1.85761100	2.01120600
N	-0.13533600	-2.63841400	2.85650600
C	-0.14251600	-2.00966900	-1.85639800
N	-0.19997900	-2.85449300	-2.63656100
C	2.70658300	-0.01351400	-0.03153300
N	3.85152300	-0.01943000	-0.04506400
H	4.85510700	-0.02475800	-0.05717200
C	-2.50289500	0.01260400	0.02928500
N	-3.65231500	0.01841900	0.04278000

H/[CB₆(CN)₇]

Lowest normal mode frequency: 51.93 cm⁻¹

B	-0.17784796	-0.34586402	-1.34413386
B	-0.19170676	-1.26192805	0.00000000
B	-0.12162324	1.20804198	-0.82639882
B	-0.12162324	1.20804198	0.82639882
B	-0.17784796	-0.34586402	1.34413386
C	0.91018599	0.05834715	0.00000000
B	-1.34551503	0.15476673	0.00000000
C	-2.87371003	0.14302345	0.00000000
N	-4.02413402	0.10168123	0.00000000
C	0.15518159	2.41500698	1.70931420
N	0.36364443	3.32319700	2.38526321
C	0.04443523	-0.90903606	2.74117013
N	0.21430134	-1.40163005	3.76820911
C	0.02383652	-2.76665101	0.00000000
N	0.18787573	-3.89838798	0.00000000
C	0.04443523	-0.90903606	-2.74117013
N	0.21430134	-1.40163005	-3.76820911
C	0.15518159	2.41500698	-1.70931420
N	0.36364443	3.32319700	-2.38526321
H	0.33652391	-4.89208995	0.00000000
C	2.33359901	-0.03239058	0.00000000
N	3.47853903	-0.13948837	0.00000000

H/[CB₇(CN)₈]

Lowest normal mode frequency: 45.35 cm⁻¹

B	0.18257900	-1.20790000	0.46131400
B	-1.18114300	0.94957300	-0.36558400
B	-0.32275900	-0.44805500	-1.22117600
B	1.30318400	-0.44858900	-0.74786700
B	0.48203500	1.18238000	-0.50849000
B	-1.33745300	-0.53662200	0.25159200
B	-0.25281600	0.56128000	1.14657800
C	1.22474800	0.15036900	0.66636300
C	-2.65705400	-1.22413600	0.54970700

N	-3.66433200	-1.72460300	0.75918800
C	-2.29458600	1.91320800	-0.74734800
N	-3.17361200	2.60635400	-1.01849800
C	-0.52925100	1.14031900	2.53327900
N	-0.79746200	1.54771700	3.57578900
C	1.18164800	2.44696600	-0.99627200
N	1.70470500	3.40272100	-1.36729100
C	-0.80094200	-1.00382100	-2.56436700
N	-1.20955400	-1.44409700	-3.54673300
C	0.45547300	-2.58105400	1.07147400
N	0.59693300	-3.62582700	1.53379000
C	2.54831900	-0.90811500	-1.48351400
N	3.48334700	-1.26854000	-2.04972900
H	-4.55348500	-2.15696900	0.93617600
C	2.34775500	0.36061000	1.51925500
N	3.24978900	0.52492500	2.21213100

H/[CB₈(CN)₉]

Lowest normal mode frequency: 54.08 cm⁻¹

B	-0.94194213	-0.41961187	0.98873878
B	0.82503981	-0.77758408	1.04192211
B	0.23354293	0.75353502	1.43402990
B	0.82503981	-0.77758408	-1.04192211
B	1.15319020	0.94230081	0.00000000
B	-0.61058177	1.16527303	0.00000000
B	-0.94194213	-0.41961187	-0.98873878
B	0.23354293	0.75353502	-1.43402990
C	-0.19708110	-1.48755002	0.00000000
C	-1.47940062	2.43208913	0.00000000
N	-2.10944950	3.38469321	0.00000000
C	0.29799282	1.57269609	2.71544786
N	0.29122874	2.23907016	3.65447782
C	2.37739531	1.85226166	0.00000000
N	3.29121740	2.55272455	0.00000000
C	0.29799282	1.57269609	-2.71544786
N	0.29122874	2.23907016	-3.65447782
C	-2.18549331	-0.78061266	1.79462159
N	-3.14585144	-0.99424951	2.39161845
C	-2.18549331	-0.78061266	-1.79462159
N	-3.14585144	-0.99424951	-2.39161845
C	1.78036757	-1.60204014	1.89128032
N	2.51422738	-2.21317219	2.53360449
C	1.78036757	-1.60204014	-1.89128032
N	2.51422738	-2.21317219	-2.53360449
H	-2.65708740	4.22813628	0.00000000

C	-0.47083527	-2.89023399	0.00000000
N	-0.69689640	-4.01640296	0.00000000

H/[CB₉(CN)₁₀]

Lowest normal mode frequency: cm⁻¹

B	-1.76445500	0.00033700	0.00036700
B	-0.71882900	-1.04931200	-0.79959500
B	-0.71857400	0.79990200	-1.04931000
B	-0.71819600	1.04961900	0.79992600
B	-0.71845000	-0.79961700	1.04962300
B	0.79522900	-0.17682600	-1.30853100
B	0.79568500	1.30828100	-0.17683500
B	0.79577000	0.17658200	1.30827500
B	0.79531600	-1.30852400	0.17657400
C	1.72638800	-0.00027800	-0.00030100
C	1.41362400	-2.68940200	0.36283400
N	1.86446200	-3.73831500	0.50423600
C	-1.30564200	-1.65689700	2.17460000
N	-1.81222800	-2.28341900	2.99659200
C	-1.30651100	-2.17410200	-1.65678700
N	-1.81347200	-2.99592900	-2.28322200
C	-3.28886400	0.00036700	0.00055700
N	-4.43003100	0.00045700	0.00046500
C	-1.30499700	2.17464500	1.65740600
N	-1.81125100	2.99669900	2.28411500
C	-1.30587100	1.65731500	-2.17413000
N	-1.81250600	2.28395400	-2.99600200
C	1.41440500	2.68894600	-0.36331100
N	1.86556600	3.73769900	-0.50487200
C	1.41458100	0.36285100	2.68892700
N	1.86580900	0.50425700	3.73767200
C	1.41345000	-0.36329800	-2.68941900
N	1.86422300	-0.50486000	-3.73833900
H	-5.43597000	0.00100100	-0.00048100
C	3.15334300	-0.00050800	-0.00056100
N	4.30157800	-0.00069200	-0.00077100

H/[CB₁₀(CN)₁₁]

Lowest normal mode frequency: 53.20c m⁻¹

B	-0.44378292	0.83133279	-1.36088253
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B	-0.44378292	0.83133279	1.36088253
B	1.08271424	-1.33883081	0.00000000
B	-0.05989897	-1.00790181	1.35664803
B	1.17716622	0.18174332	0.92839694
B	-1.25413717	1.40466784	0.00000000
B	-0.05989897	-1.00790181	-1.35664803
B	-1.51904591	-0.31510120	0.00000000
B	0.46725881	1.51528210	0.00000000
B	1.17716622	0.18174332	-0.92839694
C	-0.56926571	-1.67476506	0.00000000
C	1.19167860	2.88285421	0.00000000
N	1.73477045	3.88484829	0.00000000
C	-0.70666053	1.43095426	2.74134717
N	-0.88565748	1.92640036	3.76493596
C	-2.29405534	2.51492368	0.00000000
N	-3.02245947	3.40643357	0.00000000
C	-0.70666053	1.43095426	-2.74134717
N	-0.88565748	1.92640036	-3.76493596
C	2.40026242	0.50172261	1.79517495
N	3.32159785	0.82923483	2.40214971
C	2.40026242	0.50172261	-1.79517495
N	3.32159785	0.82923483	-2.40214971
C	-0.19267501	-1.72779267	2.69042300
N	-0.29742580	-2.26507956	3.70270898
C	-3.01287486	-0.63284643	0.00000000
N	-4.14030583	-0.86439960	0.00000000
C	2.12321841	-2.45202965	0.00000000
N	2.91600854	-3.28533953	0.00000000
C	-0.19267501	-1.72779267	-2.69042300
N	-0.29742580	-2.26507956	-3.70270898
H	2.22504732	4.76439837	0.00000000
C	-1.13278251	-2.99089514	0.00000000
N	-1.57693935	-4.04981021	0.00000000

H/[CB₁₁(CN)₁₂]

Lowest normal mode frequency: 61.35 cm⁻¹

B	-0.90121260	-1.24041272	-0.77502444
B	0.90121260	-1.24041272	-0.77502444
B	-1.45819261	0.47379550	-0.77502444
B	0.00000000	1.53323445	-0.77502444
B	1.45819261	0.47379550	-0.77502444
B	0.90169514	1.24107689	0.72915130
B	-0.90169514	1.24107689	0.72915130
B	-1.45897338	-0.47404919	0.72915130
B	1.45897338	-0.47404919	0.72915130

B	0.00000000	-1.53405540	0.72915130
B	-0.00000000	-0.00000000	1.61453593
C	0.00000000	0.00000000	-1.58298507
C	0.00000000	-0.00000000	3.16523293
N	0.00000000	-0.00000000	4.30386093
C	-1.68678632	2.32166220	1.47686538
N	-2.25082849	3.09799964	2.11150019
C	1.68678632	2.32166220	1.47686538
N	2.25082849	3.09799964	2.11150019
C	-2.72927760	-0.88679605	1.47686538
N	-3.64191700	-1.18333057	2.11150019
C	0.00000000	-2.86973230	1.47686538
N	0.00000000	-3.82933815	2.11150019
C	2.72927760	-0.88679605	1.47686538
N	3.64191700	-1.18333057	2.11150019
C	1.66514517	-2.29187571	-1.57143052
N	2.24571212	-3.09095756	-2.16054933
C	-1.66514517	-2.29187571	-1.57143052
N	-2.24571212	-3.09095756	-2.16054933
C	-2.69426149	0.87541862	-1.57143052
N	-3.63363854	1.18064073	-2.16054933
C	-0.00000000	2.83291418	-1.57143052
N	-0.00000000	3.82063366	-2.16054933
C	2.69426149	0.87541862	-1.57143052
N	3.63363854	1.18064073	-2.16054933
H	0.00000000	-0.00000000	5.31153493
C	0.00000000	0.00000000	-3.02082907
N	-0.00000000	0.00000000	-4.16870307

H/[CB₁₂(CN)₁₃]

Lowest normal mode frequency: 24.48 cm⁻¹

B	2.00762400	0.27675300	-0.00027100
B	1.45604900	-1.23867500	0.00055300
B	1.04814800	1.57095800	-0.00090600
B	0.80923200	0.10008400	1.39585000
B	-0.06326600	-1.56979800	0.89089900
B	-0.48706000	1.42932200	0.89400100
B	-0.48650400	1.42676700	-0.89750900
B	-0.06351100	-1.57240500	-0.88715100
B	-0.98952900	-0.18059900	1.43893900
B	-0.98944900	-0.18408500	-1.43855400
B	-1.51312600	-1.15288600	0.00137300
B	0.80946300	0.09566000	-1.39607200
C	-1.64012100	0.57280000	-0.00076300
C	2.53490500	-2.32823700	0.00122900

N	3.43375600	-3.04811300	0.00170400
C	3.52857000	0.49257800	-0.00047700
N	4.65839100	0.64459300	-0.00063400
C	1.73704300	2.93954900	-0.00176800
N	2.36065400	3.90760500	-0.00244200
C	1.51802300	0.22264600	2.75014000
N	2.13460800	0.32910300	3.71621100
C	-0.00450200	-2.81301800	1.77847700
N	0.05852400	-3.73900000	2.45856700
C	-0.00579100	-2.81818800	-1.77122500
N	0.05629900	-3.74611800	-2.44873600
C	1.51825600	0.21562600	-2.75059400
N	2.13483700	0.32029700	-3.71686300
C	-0.89943700	2.64670600	1.71462500
N	-1.18352000	3.57026400	2.33895200
C	-0.89789700	2.64216300	-1.72154700
N	-1.18111900	3.56427600	-2.34839800
C	-1.80265000	-0.21679600	2.72847600
N	-2.41352100	-0.24565200	3.70262000
C	-2.80416500	-1.96258800	0.00237800
N	-3.77597800	-2.57753500	0.00318800
C	-1.80251700	-0.22328900	-2.72803700
N	-2.41335400	-0.25445400	-3.70213300
H	5.65734100	0.77168500	-0.00069100
C	-2.98518900	1.08132600	-0.00154400
N	-4.05741300	1.49118700	-0.00222100

H/[CB₁₃(CN)₁₄]

Lowest normal mode frequency: 54.87 cm⁻¹

B	0.00000000	0.00000000	1.50047001
B	-1.77004381	0.00000000	-0.76356891
B	-0.88502190	-1.53290290	-0.76356891
B	0.88502190	-1.53290290	-0.76356891
B	-1.52585051	0.88095020	0.73773136
B	0.00000000	1.76190040	0.73773136
B	0.00000000	-1.76190040	0.73773136
B	-1.52585051	-0.88095020	0.73773136
B	-0.88502190	1.53290290	-0.76356891
B	1.52585051	0.88095020	0.73773136
B	1.52585051	-0.88095020	0.73773136
B	0.88502190	1.53290290	-0.76356891
B	1.77004381	0.00000000	-0.76356891
C	0.00000000	-0.00000000	-1.49093700
C	0.00000000	0.00000000	3.06287601
N	0.00000000	0.00000000	4.20109502

C	0.00000000	-3.06012807	1.54811800
N	0.00000000	-3.99379084	2.22072843
C	2.65014865	-1.53006404	1.54811800
N	3.45872432	-1.99689542	2.22072843
C	2.65014865	1.53006404	1.54811800
N	3.45872432	1.99689542	2.22072843
C	-0.00000000	3.06012807	1.54811800
N	-0.00000000	3.99379084	2.22072843
C	-2.65014865	1.53006404	1.54811800
N	-3.45872432	1.99689542	2.22072843
C	-2.65014865	-1.53006404	1.54811800
N	-3.45872432	-1.99689542	2.22072843
C	-1.51301995	2.62062742	-1.62498627
N	-1.99031142	3.44732051	-2.26753326
C	1.51301995	2.62062742	-1.62498627
N	1.99031142	3.44732051	-2.26753326
C	3.02603990	0.00000000	-1.62498627
N	3.98062285	0.00000000	-2.26753326
C	1.51301995	-2.62062742	-1.62498627
N	1.99031142	-3.44732051	-2.26753326
C	-1.51301995	-2.62062742	-1.62498627
N	-1.99031142	-3.44732051	-2.26753326
C	-3.02603990	0.00000000	-1.62498627
N	-3.98062285	0.00000000	-2.26753326
H	0.00000000	0.00000000	5.20995903
C	0.00000000	-0.00000000	-2.92815200
N	-0.00000000	-0.00000000	-4.07694200

Lowest normal mode frequencies and optimized coordinates at ω B97XD/6-311+G(d, p) level of the superhalogens of $[\text{CB}_n\text{H}_m\text{X}_{n-m+1}]^-$ ($m=1$ and 0 ; $n=5-13$; $\text{X}=\text{H}, \text{F}, \text{Cl}, \text{CN}$).

$[\text{CB}_5\text{H}_6]^-$

Lowest normal mode frequency: 463.76 cm^{-1}

B	0.00000000	0.00000000	-1.24505700
B	0.00000000	1.21546500	-0.02105600
B	0.00000000	-1.21546500	-0.02105600
B	1.21546500	0.00000000	-0.02105600
B	-1.21546500	0.00000000	-0.02105600
H	0.00000000	0.00000000	-2.44269500
H	0.00000000	2.39930300	0.14023900
H	2.39930300	0.00000000	0.14023900
H	0.00000000	-2.39930300	0.14023900
H	-2.39930300	0.00000000	0.14023900
C	0.00000000	0.00000000	1.06374100
H	0.00000000	0.00000000	2.14569600

$[\text{CB}_6\text{H}_7]^-$

Lowest normal mode frequency: 446.66 cm^{-1}

B	0.00000000	1.39492400	-0.02377800
B	1.32665200	0.43105500	-0.02377800
B	-1.32665200	0.43105500	-0.02377800
B	-0.81991600	-1.12851700	-0.02377800
B	0.81991600	-1.12851700	-0.02377800
H	-1.51329600	-2.08287300	0.16963700
H	-2.44856400	0.79558700	0.16963700
H	0.00000000	2.57457300	0.16963700
H	2.44856400	0.79558700	0.16963700
H	1.51329600	-2.08287300	0.16963700
C	0.00000000	0.00000000	1.01286200
H	0.00000000	0.00000000	2.09934900
B	0.00000000	0.00000000	-1.20508000
H	0.00000000	0.00000000	-2.40484800

$[\text{CB}_7\text{H}_8]^-$

Lowest normal mode frequency: 301.56 cm^{-1}

B	-0.00305800	-0.28548900	1.28032400
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B	-0.00305800	1.34195900	-0.80909000
B	-1.28137100	0.32020300	0.00000000
B	-0.80795800	-1.30805500	0.00000000
B	-0.00305800	-0.28548900	-1.28032400
B	-0.00305800	1.34195900	0.80909000
B	1.25216100	0.32377300	0.00000000
C	0.70433500	-1.18133800	0.00000000
H	1.40422700	-2.00636100	0.00000000
H	-1.43098100	-2.32447900	0.00000000
H	0.04480500	-0.70533300	-2.40015600
H	-2.44820600	0.59656500	0.00000000
H	-0.01609000	2.25006700	-1.58682500
H	-0.01609000	2.25006700	1.58682500
H	2.43852200	0.48852900	0.00000000
H	0.04480500	-0.70533300	2.40015600

[CB₈H₉]⁻

Lowest normal mode frequency: 41.12 cm⁻¹

B	1.01108200	0.55773000	-0.88763900
B	0.99499500	0.54826800	0.89407900
B	1.42597100	-0.82995200	-0.00691600
B	-0.99498700	0.54828200	0.89407900
B	-0.00001000	-1.14099100	0.89484000
B	-0.00000800	-1.15880100	-0.88870700
B	-1.01107300	0.55774500	-0.88763800
B	-1.42598400	-0.82993100	-0.00691600
H	1.67367600	1.09238800	-1.72461400
H	1.65294200	1.08150400	1.73563800
H	0.00001900	2.52605700	-0.00513600
H	-1.65292600	1.08152800	1.73563700
H	-0.00001500	-1.97389900	1.75359500
H	-0.00001500	-1.99751000	-1.74158700
H	-1.67366100	1.09241400	-1.72461100
H	-2.46130600	-1.42127900	-0.00622600
C	0.00001100	1.44639300	-0.00706500
H	2.46128500	-1.42131600	-0.00622500

[CB₉H₁₀]⁻

Lowest normal mode frequency: 427.23 cm⁻¹

B	0.00000000	0.00000000	-1.87048400
B	0.91827700	0.91827700	-0.77050900
B	-0.91827700	0.91827700	-0.77050900

B	-0.91827700	-0.91827700	-0.77050900
B	0.91827700	-0.91827700	-0.77050900
B	0.00000000	1.30207900	0.73716600
B	-1.30207900	0.00000000	0.73716600
B	0.00000000	-1.30207900	0.73716600
B	1.30207900	0.00000000	0.73716600
H	0.00000000	0.00000000	-3.06116100
H	0.00000000	0.00000000	2.74907900
H	1.71649800	1.71649800	-1.16627000
H	-1.71649800	1.71649800	-1.16627000
H	-1.71649800	-1.71649800	-1.16627000
H	1.71649800	-1.71649800	-1.16627000
H	0.00000000	2.38175500	1.24231600
H	-2.38175500	0.00000000	1.24231600
H	0.00000000	-2.38175500	1.24231600
H	2.38175500	0.00000000	1.24231600
C	0.00000000	0.00000000	1.67119700

[CB₁₀H₁₁]⁻

Lowest normal mode frequency: 235.70 cm⁻¹

B	0.21287400	0.94190900	1.33832500
B	0.21287400	0.94190900	-1.33832500
B	-0.84202400	-1.47004400	0.00000000
B	0.21287400	-0.91633700	-1.33299700
B	-1.23905900	0.00062800	-0.91265300
B	0.88844400	1.68106900	0.00000000
B	0.21287400	-0.91633700	1.33299700
B	1.43900100	0.03600000	0.00000000
B	-0.84833600	1.48016600	0.00000000
B	-1.23905900	0.00062800	0.91265300
H	0.38082500	1.35549100	-2.44743200
H	-1.44635100	-2.49578300	0.00000000
H	0.45432900	-1.44194800	-2.37440500
H	-2.19062400	-0.01541400	-1.63438000
H	1.62130000	2.61974300	0.00000000
H	0.45432900	-1.44194800	2.37440500
H	2.63325000	0.00823700	0.00000000
H	-1.59367400	2.41482900	0.00000000
H	-2.19062400	-0.01541400	1.63438000
H	1.46494400	-2.35418500	0.00000000
H	0.38082500	1.35549100	2.44743200

C	0.82985800	-1.48117400	0.00000000
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[CB₁₁H₁₂]⁻

Lowest normal mode frequency: 526.90 cm⁻¹

B	0.00000000	1.51137600	0.73463300
B	1.43740400	0.46704100	0.73463300
B	-1.43740400	0.46704100	0.73463300
B	-0.88836500	-1.22272900	0.73463300
B	0.88836500	-1.22272900	0.73463300
B	0.00000000	-1.51789200	-0.77014400
B	-1.44360100	-0.46905400	-0.77014400
B	-0.89219500	1.22800000	-0.77014400
B	1.44360100	-0.46905400	-0.77014400
B	0.89219500	1.22800000	-0.77014400
H	1.47135600	-2.02514800	1.39267600
H	0.00000000	-2.59796600	-1.27731700
H	-2.47081200	-0.80281600	-1.27731700
H	-1.52704600	2.10179800	-1.27731700
H	1.52704600	2.10179800	-1.27731700
H	2.47081200	-0.80281600	-1.27731700
H	2.38070400	0.77353800	1.39267600
H	0.00000000	2.50322000	1.39267600
H	-2.38070400	0.77353800	1.39267600
H	-1.47135600	-2.02514800	1.39267600
B	0.00000000	0.00000000	-1.70248600
H	0.00000000	0.00000000	-2.89649600
C	0.00000000	0.00000000	1.51984200
H	0.00000000	0.00000000	2.60086900

[CB₁₂H₁₃]⁻

Lowest normal mode frequency: 150.16 cm⁻¹

B	-1.71658300	-1.25300200	0.00000000
B	-1.86084800	0.35943600	0.00000000
B	-0.22609900	-1.88419700	0.00000000
B	-0.68375400	-0.49450900	1.35719600
B	-0.68375400	1.36981200	0.87825500

B	1.06892500	-1.05209400	0.87981100
B	1.06892500	-1.05209400	-0.87981100
B	-0.68375400	1.36981200	-0.87825500
B	0.77432300	0.58427700	1.42328700
B	0.77432300	0.58427700	-1.42328700
B	0.78596200	1.67846500	0.00000000
H	-2.96455600	0.82402200	0.00000000
H	-0.09136300	-3.07461800	0.00000000
H	-1.07201500	-0.79675100	2.44649200
H	-1.07201500	-0.79675100	-2.44649200
H	1.41094500	2.69058600	0.00000000
H	2.74587000	0.36044800	0.00000000
H	1.83248900	-1.72266200	1.49872400
H	-1.17590600	2.22016000	1.55397100
H	-1.17590600	2.22016000	-1.55397100
H	1.83248900	-1.72266200	-1.49872400
H	1.35000000	0.89955200	-2.41502600
H	1.35000000	0.89955200	2.41502600
H	-2.67689500	-1.95924100	0.00000000
B	-0.68375400	-0.49450900	-1.35719600
C	1.67288400	0.22997400	0.00000000

[CB₁₃H₁₄]⁻

Lowest normal mode frequency: 211.47 cm⁻¹

B	0.00000000	0.00000000	-1.57840700
B	0.00000000	1.73715100	0.73212900
B	1.50441700	0.86857600	0.73212900
B	1.50441700	-0.86857600	0.73212900
B	-0.87186300	1.51011100	-0.76646900
B	-1.74372600	0.00000000	-0.76646900
B	1.74372600	0.00000000	-0.76646900
B	0.87186300	1.51011100	-0.76646900
H	0.00000000	0.00000000	2.49642800
H	0.00000000	0.00000000	-2.77197300
H	0.00000000	2.68905700	1.44702300
H	2.32879100	1.34452800	1.44702300
H	2.32879100	-1.34452800	1.44702300
H	-2.32879100	1.34452800	1.44702300
H	-1.39792500	2.42127700	-1.32730700

H	-2.79585000	0.00000000	-1.32730700
H	2.79585000	0.00000000	-1.32730700
H	1.39792500	2.42127700	-1.32730700
B	-1.50441700	0.86857600	0.73212900
B	-0.87186300	-1.51011100	-0.76646900
B	0.87186300	-1.51011100	-0.76646900
B	-1.50441700	-0.86857600	0.73212900
B	0.00000000	-1.73715100	0.73212900
H	0.00000000	-2.68905700	1.44702300
H	1.39792500	-2.42127700	-1.32730700
H	-1.39792500	-2.42127700	-1.32730700
H	-2.32879100	-1.34452800	1.44702300
C	0.00000000	0.00000000	1.41324500

[CB₅HF₅]⁻

Lowest normal mode frequency: 113.86 cm⁻¹

B	0.00000000	0.00000000	1.04188700
B	0.00000000	1.21104200	-0.19081200
B	0.00000000	-1.21104200	-0.19081200
B	-1.21104200	0.00000000	-0.19081200
B	1.21104200	0.00000000	-0.19081200
C	0.00000000	0.00000000	-1.28443200
H	0.00000000	0.00000000	-2.36248100
F	0.00000000	2.57927600	-0.36332300
F	0.00000000	0.00000000	2.41728200
F	2.57927600	0.00000000	-0.36332300
F	0.00000000	-2.57927600	-0.36332300
F	-2.57927600	0.00000000	-0.36332300

[CB₇HF₇]⁻

Lowest normal mode frequency: 51.43 cm⁻¹

B	-1.16808600	1.00920100	-0.33905900
B	1.36241900	-0.00747300	0.10630000
B	0.36749200	-1.00376800	-0.89914400
B	-1.17963500	-0.99658000	-0.33971600
B	0.21015000	-0.92307500	0.98534200
B	0.37974600	1.00214700	-0.89679200
B	0.21980200	0.91924200	0.98698400
C	-1.14630600	0.00542900	0.91471400
H	-1.91310700	0.00929900	1.67919900

F	-2.27884300	1.78349000	-0.52538300
F	-2.29841900	-1.75925500	-0.52595600
F	0.99770000	1.81648800	-1.81665600
F	0.97644700	-1.82227300	-1.82124000
F	2.74179700	-0.01556900	0.14749200
F	0.37544400	1.84221500	1.98441100
F	0.35604000	-1.84957900	1.98099400

[CB₈HF₈]⁻

Lowest normal mode frequency: 71.63 cm⁻¹

B	-0.97924600	0.97975600	-0.59457400
B	-1.07350800	-0.79234200	-0.87346300
B	-1.43653100	-0.13285500	0.62848200
B	1.07350400	-0.79233900	-0.87346400
B	0.00000600	-1.00395000	0.94645500
B	0.00000000	0.77467500	1.05074300
B	0.97924200	0.97976100	-0.59458200
B	1.43653600	-0.13284200	0.62847600
H	-0.00000700	0.28605500	-2.68209900
C	-0.00000400	0.14282300	-1.60882800
F	1.66795400	2.06154400	-1.06001400
F	1.79639700	-1.68897400	-1.59746600
F	-1.66797000	2.06153500	-1.05999900
F	-1.79640000	-1.68897800	-1.59746500
F	-2.62281400	-0.20091500	1.32866800
F	-0.00000400	1.69354900	2.07625000
F	0.00001600	-2.09712000	1.77522600
F	2.62282200	-0.20090000	1.32865700

[CB₉HF₉]⁻

Lowest normal mode frequency: 155.31 cm⁻¹

B	0.00000000	0.00000000	1.68440200
B	0.00000000	1.32126800	0.61169200
B	1.32126800	0.00000000	0.61169200
B	0.00000000	-1.32126800	0.61169200
B	-1.32126800	0.00000000	0.61169200
B	0.92427500	0.92427500	-0.92261500
B	0.92427500	-0.92427500	-0.92261500
B	-0.92427500	-0.92427500	-0.92261500
B	-0.92427500	0.92427500	-0.92261500
H	0.00000000	0.00000000	-2.92914400

C	0.00000000	0.00000000	-1.85096300
F	1.80520100	1.80520100	-1.47453800
F	1.80520100	-1.80520100	-1.47453800
F	-1.80520100	1.80520100	-1.47453800
F	-1.80520100	-1.80520100	-1.47453800
F	-2.62804800	0.00000000	1.03909600
F	0.00000000	0.00000000	3.05636900
F	0.00000000	2.62804800	1.03909600
F	2.62804800	0.00000000	1.03909600
F	0.00000000	-2.62804800	1.03909600

[CB₁₀HF₁₀]⁻

Lowest normal mode frequency: 63.85 cm⁻¹

B	-0.14606000	0.87549800	1.36189200
B	-0.14606000	0.87549800	-1.36189200
B	0.16160600	-1.77143900	0.00000000
B	0.78698800	-0.77964800	-1.34973400
B	-0.92299100	-0.68375800	-0.94396400
B	0.09472800	1.82203200	0.00000000
B	0.78698800	-0.77964800	1.34973400
B	1.44173100	0.70116000	0.00000000
B	-1.32368600	0.81345200	0.00000000
B	-0.92299100	-0.68375800	0.94396400
H	2.58526200	-1.36713100	0.00000000
C	1.59571100	-0.93194200	0.00000000
F	1.31103100	-1.18985400	2.53162200
F	-1.90169700	-1.24061800	1.72445600
F	-0.25268900	1.38581700	2.63081200
F	-2.61612400	1.27104800	0.00000000
F	0.28410800	3.18022300	0.00000000
F	-0.25268900	1.38581700	-2.63081200
F	2.64797200	1.33010600	0.00000000
F	1.31103100	-1.18985400	-2.53162200
F	-1.90169700	-1.24061800	-1.72445600
F	0.12510900	-3.13519400	0.00000000

[CB₁₁HF₁₁]⁻

Lowest normal mode frequency: 129.56 cm⁻¹

B	0.00000000	-1.52419300	-0.86175700
B	1.44959400	-0.47100200	-0.86175700
B	-1.44959400	-0.47100200	-0.86175700

B	-0.89589800	1.23309800	-0.86175700
B	0.89589800	1.23309800	-0.86175700
B	0.00000000	1.53879000	0.64351900
B	-1.46347600	0.47551200	0.64351900
B	-0.90447800	-1.24490700	0.64351900
B	1.46347600	0.47551200	0.64351900
B	0.90447800	-1.24490700	0.64351900
B	0.00000000	0.00000000	1.57266500
C	0.00000000	0.00000000	-1.63899200
H	0.00000000	0.00000000	-2.72226200
F	0.00000000	-2.65866700	-1.61530600
F	-2.52854200	-0.82157300	-1.61530600
F	2.52854200	-0.82157300	-1.61530600
F	1.56272500	2.15090600	-1.61530600
F	-1.56272500	2.15090600	-1.61530600
F	0.00000000	2.76558400	1.25244800
F	2.63022700	0.85461200	1.25244800
F	0.00000000	0.00000000	2.94193400
F	1.62556900	-2.23740400	1.25244800
F	-1.62556900	-2.23740400	1.25244800
F	-2.63022700	0.85461200	1.25244800

[CB₁₂HF₁₂]⁻

Lowest normal mode frequency: 33.29 cm⁻¹

B	1.37571000	-1.36403900	-0.63684200
B	-0.31515400	-1.09162100	-1.16034600
B	2.14427600	-0.13997600	0.01250700
B	-0.11876300	-1.56630100	0.54877700
B	-1.64851900	-0.79174200	-0.03191600
B	0.89945100	-0.21607500	1.43146300
B	1.23136200	1.26942100	0.41290400
B	-1.14265200	0.48750600	-1.20757200
B	-0.91195000	-0.31542000	1.51365500
B	-0.31052100	1.75353200	-0.34890800
B	-1.66577100	0.91574900	0.43163500
H	-0.26908400	1.91275600	2.06750600
B	0.74937500	0.53393800	-1.27883500
C	-0.21360000	1.19379800	1.25797800
F	2.00998100	2.34546400	0.73243400
F	1.46195600	-0.38835800	2.65683300
F	3.46558900	0.16208300	0.13343200

F	-0.12888800	-2.83470000	1.06414200
F	1.83164700	-2.48643000	-1.24034600
F	-0.58159500	-1.89867000	-2.23571700
F	-2.82945600	-1.47612700	-0.13472400
F	-1.86252300	0.77914900	-2.32988600
F	-2.77472200	1.60329600	0.80819600
F	-1.43979500	-0.57612700	2.73940100
F	-0.39489000	3.08150500	-0.62052800
F	1.25563600	0.97220300	-2.46745700

[CB₁₃HF₁₃]⁻

Lowest normal mode frequency: 94.76 cm⁻¹

B	0.00000000	0.00000000	1.49224400
B	-0.87875600	1.52205100	-0.83145100
B	-1.75751300	0.00000000	-0.83145100
B	-0.87875600	-1.52205100	-0.83145100
B	0.00000000	1.76926100	0.66879000
B	1.53222500	0.88463100	0.66879000
B	-1.53222500	-0.88463100	0.66879000
B	-1.53222500	0.88463100	0.66879000
H	0.00000000	0.00000000	-2.58056700
B	0.87875600	1.52205100	-0.83145100
B	1.53222500	-0.88463100	0.66879000
B	0.00000000	-1.76926100	0.66879000
B	1.75751300	0.00000000	-0.83145100
B	0.87875600	-1.52205100	-0.83145100
C	0.00000000	0.00000000	-1.49379500
F	-1.41459100	-2.45014300	-1.66609300
F	-2.82918200	0.00000000	-1.66609300
F	-2.55456000	-1.47487600	1.35647000
F	0.00000000	-2.94975200	1.35647000
F	0.00000000	0.00000000	2.85350800
F	2.55456000	-1.47487600	1.35647000
F	2.55456000	1.47487600	1.35647000
F	2.82918200	0.00000000	-1.66609300
F	1.41459100	2.45014300	-1.66609300
F	1.41459100	-2.45014300	-1.66609300
F	-1.41459100	2.45014300	-1.66609300
F	0.00000000	2.94975200	1.35647000
F	-2.55456000	1.47487600	1.35647000

[CB₅HCl₅]⁻

Lowest normal mode frequency: 76.20 cm⁻¹

B	0.00000200	-0.00000100	0.92974800
B	0.84379000	0.86264600	-0.29559300
B	-0.84379300	-0.86264500	-0.29559000
B	-0.86264700	0.84379200	-0.29559100
B	0.86264500	-0.84379200	-0.29559700
C	-0.00000400	0.00000100	-1.38566200
H	-0.00000800	0.00000300	-2.46348200
Cl	0.00001000	-0.00000300	2.72418100
Cl	2.13526500	-2.08856500	-0.50398300
Cl	-2.08857100	-2.13526200	-0.50397500
Cl	-2.13526700	2.08856500	-0.50397300
Cl	2.08856600	2.13526300	-0.50398100

[CB₆HCl₆]⁻**Lowest normal mode frequency: 80.73 cm⁻¹**

B	0.00000000	1.38692800	-0.19496700
B	-1.31904700	0.42858400	-0.19496700
B	1.31904700	0.42858400	-0.19496700
B	0.81521600	-1.12204900	-0.19496700
B	-0.81521600	-1.12204900	-0.19496700
C	0.00000000	0.00000000	-1.25072800
H	0.00000000	0.00000000	-2.33246600
B	0.00000000	0.00000000	1.00182900
Cl	0.00000000	0.00000000	2.79388000
Cl	3.00958700	0.97787400	-0.44463600
Cl	1.86002700	-2.56010800	-0.44463600
Cl	0.00000000	3.16446700	-0.44463600
Cl	-3.00958700	0.97787400	-0.44463600
Cl	-1.86002700	-2.56010800	-0.44463600

[CB₇HCl₇]⁻**Lowest normal mode frequency: 53.07 cm⁻¹**

B	-0.42032200	0.35311300	1.29684000
B	0.42057800	-1.01809000	-0.81542100
B	1.05166700	0.50746200	0.00000000
B	-0.17837500	1.63419900	0.00000000
B	-0.42032200	0.35311300	-1.29684000
B	0.42057800	-1.01809000	0.81542100
B	-1.16934200	-0.82149500	0.00000000

C	-1.43787500	0.75250000	0.00000000
Cl	1.15972600	-2.21129000	-1.92917700
Cl	1.15972600	-2.21129000	1.92917700
Cl	2.79469300	0.94323900	0.00000000
Cl	-2.54225600	-1.97638400	0.00000000
Cl	-0.83250400	0.85530000	2.96896900
Cl	-0.83250400	0.85530000	-2.96896900
Cl	-0.16858600	3.41519400	0.00000000
H	-2.44606200	1.14274100	0.00000000

[CB₈HCl₈]⁻

Lowest normal mode frequency: 46.78 cm⁻¹

B	-0.90797600	-0.77803600	0.97981200
B	0.87787000	-0.85341600	1.04339400
B	0.05291200	0.56301100	1.42350100
B	0.87787000	-0.85341600	-1.04339400
B	0.90764700	0.93624600	0.00000000
B	-0.87819300	0.88880200	0.00000000
B	-0.90797600	-0.77803600	-0.97981200
B	0.05291200	0.56301100	-1.42350100
H	-0.02075600	-2.78148700	0.00000000
C	0.00846700	-1.70125700	0.00000000
Cl	0.05624100	1.44495700	2.97964400
Cl	2.23012300	2.14484400	0.00000000
Cl	-2.19691600	2.11006100	0.00000000
Cl	0.05624100	1.44495700	-2.97964400
Cl	2.14110000	-1.63955900	2.02377500
Cl	-2.22586800	-1.50496200	1.94218200
Cl	-2.22586800	-1.50496200	-1.94218200
Cl	2.14110000	-1.63955900	-2.02377500

[CB₉HCl₉]⁻

Lowest normal mode frequency: 96.85 cm⁻¹

B	0.00000000	0.00000000	1.60075700
B	0.00000000	1.31417900	0.52669000
B	1.31417900	0.00000000	0.52669000
B	0.00000000	-1.31417900	0.52669000
B	-1.31417900	0.00000000	0.52669000
B	0.92677300	0.92677300	-0.99949000
B	0.92677300	-0.92677300	-0.99949000
B	-0.92677300	-0.92677300	-0.99949000
B	-0.92677300	0.92677300	-0.99949000

H	0.00000000	0.00000000	-2.99355400
C	0.00000000	0.00000000	-1.91588200
Cl	0.00000000	0.00000000	3.37911800
Cl	-3.00160000	0.00000000	1.14284900
Cl	0.00000000	3.00160000	1.14284900
Cl	0.00000000	-3.00160000	1.14284900
Cl	3.00160000	0.00000000	1.14284900
Cl	-2.07026500	2.07026500	-1.75320100
Cl	-2.07026500	-2.07026500	-1.75320100
Cl	2.07026500	2.07026500	-1.75320100
Cl	2.07026500	-2.07026500	-1.75320100

[CB₁₀HCl₁₀]⁻

Lowest normal mode frequency: 57.68 cm⁻¹

B	-0.15165500	0.82871200	1.36274800
B	-0.15165500	0.82871200	-1.36274800
B	0.38507400	-1.75795100	0.00000000
B	0.92432300	-0.72109800	-1.35253200
B	-0.79561600	-0.78674300	-0.93763400
B	0.01538600	1.78843700	0.00000000
B	0.92432300	-0.72109800	1.35253200
B	1.45390600	0.80762200	0.00000000
B	-1.31012000	0.66086700	0.00000000
B	-0.79561600	-0.78674300	0.93763400
H	2.75304600	-1.17032500	0.00000000
C	1.73980400	-0.79697800	0.00000000
Cl	-3.01702100	1.20855600	0.00000000
Cl	0.00439500	3.57194100	0.00000000
Cl	-0.39436900	1.55240800	2.98214000
Cl	-0.39436900	1.55240800	-2.98214000
Cl	-1.98033900	-1.64787200	-1.96905100
Cl	-1.98033900	-1.64787200	1.96905100
Cl	2.97524300	1.75070100	0.00000000
Cl	1.67361300	-1.24723100	-2.87684700
Cl	0.51700800	-3.53706600	0.00000000
Cl	1.67361300	-1.24723100	2.87684700

[CB₁₁HCl₁₁]⁻

Lowest normal mode frequency: 109.70 cm⁻¹

B	-0.89391331	-1.23036612	-0.92148028
B	0.89391331	-1.23036612	-0.92148028
B	-1.44638211	0.46995804	-0.92148028

B	0.00000000	1.52081616	-0.92148028
B	1.44638211	0.46995804	-0.92148028
B	0.89940954	1.23793104	0.58989726
B	-0.89940954	1.23793104	0.58989726
B	-1.45527521	-0.47284758	0.58989726
B	1.45527521	-0.47284758	0.58989726
B	0.00000000	-1.53016691	0.58989726
B	0.00000000	0.00000000	1.52642588
C	0.00000000	-0.00000000	-1.70744512
H	-0.00000000	-0.00000000	-2.78965712
Cl	-0.00000000	0.00000000	3.31550188
Cl	1.84812002	2.54371898	1.36128564
Cl	2.99032100	-0.97161419	1.36128564
Cl	0.00000000	-3.14420957	1.36128564
Cl	-2.99032100	-0.97161419	1.36128564
Cl	-1.84812002	2.54371898	1.36128564
Cl	-2.88587299	0.93767698	-1.86333241
Cl	0.00000000	3.03438644	-1.86333241
Cl	2.88587299	0.93767698	-1.86333241
Cl	1.78356760	-2.45487019	-1.86333241
Cl	-1.78356760	-2.45487019	-1.86333241

[CB₁₂HCl₁₂]⁻

Lowest normal mode frequency: 13.63 cm⁻¹

B	1.59332300	1.17141200	0.00000000
B	1.69864800	-0.45158200	0.00000000
B	0.14149200	1.89564700	0.00000000
B	0.54306600	0.46308200	1.40468200
B	0.46611000	-1.42428800	0.89147800
B	-1.19293000	1.10076000	0.89653200
B	-1.19293000	1.10076000	-0.89653200
B	0.46611000	-1.42428800	-0.89147800
B	-0.96893300	-0.56453500	1.43584900
B	-0.96893300	-0.56453500	-1.43584900
B	-1.02603400	-1.65487700	0.00000000
H	-2.92030800	-0.25354000	0.00000000
B	0.54306600	0.46308200	-1.40468200
C	-1.84137200	-0.16326000	0.00000000
Cl	3.07031300	2.16383700	0.00000000
Cl	3.35289400	-1.15083900	0.00000000

Cl	0.09243600	3.68969000	0.00000000
Cl	1.18199400	0.89878600	3.01850100
Cl	1.08919500	-2.74131400	1.93002300
Cl	1.08919500	-2.74131400	-1.93002300
Cl	1.18199400	0.89878600	-3.01850100
Cl	-1.83372900	-1.05606200	2.91576900
Cl	-2.00744600	-3.14194200	0.00000000
Cl	-2.29572700	2.13821500	1.84146300
Cl	-2.29572700	2.13821500	-1.84146300
Cl	-1.83372900	-1.05606200	-2.91576900

[CB₁₃HCl₁₃]⁻

Lowest normal mode frequency: 58.52 cm⁻¹

B	-0.00000000	-0.00000000	1.46518411
B	1.76142603	-0.01265952	-0.88991169
B	0.88998940	1.51349912	-0.89262904
B	-0.86768255	1.52543545	-0.89274924
B	1.51933419	-0.89203526	0.62387743
B	-0.01280844	-1.76227087	0.62206140
B	0.01280844	1.76227087	0.62206140
B	1.53206554	0.87024969	0.62383914
H	-0.00000000	-0.00000000	-2.67225489
B	0.86768255	-1.52543545	-0.89274924
B	-1.53206554	-0.87024969	0.62383914
B	-1.51933419	0.89203526	0.62387743
B	-0.88998940	-1.51349912	-0.89262904
B	-1.76142603	0.01265952	-0.88991169
C	-0.00000000	0.00000000	-1.58675189
Cl	0.00000000	0.00000000	3.25492211
Cl	0.02429179	3.34902111	1.44822056
Cl	-2.88603611	1.69586725	1.45275251
Cl	2.91045772	1.65356207	1.45258217
Cl	2.88603611	-1.69586725	1.45275251
Cl	-0.02429179	-3.34902111	1.44822056
Cl	-2.91045772	-1.65356207	1.45258217
Cl	1.64540488	2.80157380	-1.86946616
Cl	3.25740610	-0.02335792	-1.86144551
Cl	1.60491141	-2.82546903	-1.86927424
Cl	-1.60491141	2.82546903	-1.86927424

Cl	-3.25740610	0.02335792	-1.86144551
Cl	-1.64540488	-2.80157380	-1.86946616

[CB₅H(CN)₅]⁻

Lowest normal mode frequency: 68.33 cm⁻¹

B	0.00000000	0.00000000	0.93894500
B	0.00000000	1.20757900	-0.28517200
B	0.00000000	-1.20757900	-0.28517200
B	-1.20757900	0.00000000	-0.28517200
B	1.20757900	0.00000000	-0.28517200
C	0.00000000	0.00000000	-1.37382800
C	-2.72618600	0.00000000	-0.47037800
N	-3.86988300	0.00000000	-0.61490500
C	0.00000000	-2.72618600	-0.47037800
N	0.00000000	-3.86988300	-0.61490500
C	2.72618600	0.00000000	-0.47037800
N	3.86988300	0.00000000	-0.61490500
C	0.00000000	2.72618600	-0.47037800
N	0.00000000	3.86988300	-0.61490500
C	0.00000000	0.00000000	2.47236200
N	0.00000000	0.00000000	3.62509900
H	0.00000000	0.00000000	-2.45176600

[CB₆H(CN)₆]⁻

Lowest normal mode frequency: 66.86 cm⁻¹

B	0.00000000	1.38766300	-0.17227900
B	-1.31974600	0.42881200	-0.17227900
B	1.31974600	0.42881200	-0.17227900
B	0.81564800	-1.12264300	-0.17227900
B	-0.81564800	-1.12264300	-0.17227900
C	0.00000000	0.00000000	-1.22187200
H	0.00000000	0.00000000	-2.30403400
B	0.00000000	0.00000000	1.01441100
C	0.00000000	0.00000000	2.55405800
N	0.00000000	0.00000000	3.70602800
C	1.70440700	-2.34591500	-0.40238900
N	2.37360000	-3.26698000	-0.58070500
C	-1.70440700	-2.34591500	-0.40238900
N	-2.37360000	-3.26698000	-0.58070500
C	-2.75778800	0.89606000	-0.40238900
N	-3.84056500	1.24787500	-0.58070500

C	0.00000000	2.89971000	-0.40238900
N	0.00000000	4.03820900	-0.58070500
C	2.75778800	0.89606000	-0.40238900
N	3.84056500	1.24787500	-0.58070500

[CB₇H(CN)₇]⁻

Lowest normal mode frequency: 62.66 cm⁻¹

B	-0.40458700	0.33886800	1.28159700
B	0.46295500	-1.03251600	-0.80992600
B	1.02233700	0.50569900	0.00000000
B	-0.24687300	1.62105600	0.00000000
B	-0.40458700	0.33886800	-1.28159700
B	0.46295500	-1.03251600	0.80992600
B	-1.14101800	-0.84871200	0.00000000
C	-1.46978100	0.71231200	0.00000000
C	1.09410100	-2.02585300	1.78448800
N	1.56310500	-2.77464200	2.52448200
C	1.09410100	-2.02585300	-1.78448800
N	1.56310500	-2.77464200	-2.52448200
C	-2.29677800	-1.86492700	0.00000000
N	-3.16802200	-2.61789100	0.00000000
C	-0.74481100	0.74774900	-2.72282600
N	-1.01240100	1.05784800	-3.79928700
C	2.48707800	0.97129700	0.00000000
N	3.58352000	1.32482800	0.00000000
C	-0.74481100	0.74774900	2.72282600
N	-1.01240100	1.05784800	3.79928700
H	-2.49305700	1.05775100	0.00000000
C	-0.25470200	3.14911800	0.00000000
N	-0.26679600	4.30078900	0.00000000

[CB₈H(CN)₈]⁻

Lowest normal mode frequency: 7.14 cm⁻¹

B	1.00090505	-0.89260777	-0.80286111
B	1.00090505	0.89260777	-0.80286111
B	1.42270580	-0.00000000	0.58096736
B	-1.00090505	0.89260777	-0.80286111
B	0.00000000	0.89448962	0.91099437

B	0.00000000	-0.89448962	0.91099437
B	-1.00090505	-0.89260777	-0.80286111
B	-1.42270580	-0.00000000	0.58096736
C	0.00000000	0.00000000	-1.69561499
C	0.00000000	-2.01233181	1.96267319
N	0.00000000	-2.86298612	2.73911484
C	2.75319161	-0.00000000	1.33100468
N	3.76083748	-0.00000000	1.88873893
C	-0.00000000	2.01233181	1.96267319
N	-0.00000000	2.86298612	2.73911484
C	-2.75319161	-0.00000000	1.33100468
N	-3.76083748	-0.00000000	1.88873893
C	1.85418612	-1.98121658	-1.46417335
N	2.48881916	-2.79741044	-1.97069752
C	-1.85418612	-1.98121658	-1.46417335
N	-2.48881916	-2.79741044	-1.97069752
C	1.85418612	1.98121658	-1.46417335
N	2.48881916	2.79741044	-1.97069752
C	-1.85418612	1.98121658	-1.46417335
N	-2.48881916	2.79741044	-1.97069752
H	0.00000000	0.00000000	-2.77509999

[CB₉H(CN)₉]⁻

Lowest normal mode frequency: 74.37 cm⁻¹

B	0.00000000	0.00000000	1.62463600
B	0.00000000	1.30532900	0.53454000
B	1.30532900	0.00000000	0.53454000
B	0.00000000	-1.30532900	0.53454000
B	-1.30532900	0.00000000	0.53454000
B	0.92258200	0.92258200	-0.98675900
B	0.92258200	-0.92258200	-0.98675900
B	-0.92258200	-0.92258200	-0.98675900
B	-0.92258200	0.92258200	-0.98675900
H	0.00000000	0.00000000	-2.99263300
C	0.00000000	0.00000000	-1.91471100
C	-1.90649000	1.90649000	-1.63160300
N	-2.63818000	2.63818000	-2.13494300
C	-2.75197400	0.00000000	1.05077700
N	-3.83784000	0.00000000	1.43300800
C	0.00000000	2.75197400	1.05077700
N	0.00000000	3.83784000	1.43300800

C	0.00000000	0.00000000	3.14901400
N	0.00000000	0.00000000	4.30028900
C	0.00000000	-2.75197400	1.05077700
N	0.00000000	-3.83784000	1.43300800
C	2.75197400	0.00000000	1.05077700
N	3.83784000	0.00000000	1.43300800
C	1.90649000	-1.90649000	-1.63160300
N	2.63818000	-2.63818000	-2.13494300
C	-1.90649000	-1.90649000	-1.63160300
N	-2.63818000	-2.63818000	-2.13494300
C	1.90649000	1.90649000	-1.63160300
N	2.63818000	2.63818000	-2.13494300

[CB₁₀H(CN)₁₀]⁻

Lowest normal mode frequency: 54.30 cm⁻¹

B	0.81195000	-1.35281900	0.21390500
B	0.81558800	1.35060000	0.21385900
B	-1.73461300	0.00234500	-0.47141500
B	-0.65203000	1.34210400	-0.95546800
B	-0.82946800	0.92343600	0.76286800
B	1.79753400	-0.00246000	0.12195000
B	-0.65581400	-1.34050100	-0.95539400
B	0.87097100	-0.00114300	-1.35824600
B	0.57979800	-0.00076900	1.37018300
B	-0.83196400	-0.92121100	0.76287700
H	-1.01341100	0.00128600	-2.81888000
C	-0.70926100	0.00083600	-1.78253700
C	0.95114900	-0.00121300	2.86070100
N	1.24050500	-0.00136100	3.97446200
C	1.40762100	2.75111500	0.41243800
N	1.86258200	3.79994000	0.54883400
C	3.32258800	-0.00449500	0.18203400
N	4.47284500	-0.00602400	0.23051700
C	1.40018400	-2.75494300	0.41236800
N	1.85227900	-3.80502200	0.54864700
C	-1.61889000	1.83088600	1.71883500
N	-2.22014300	2.50865200	2.42835300
C	-1.62377200	-1.82651700	1.71890800
N	-2.22681700	-2.50265900	2.42845500
C	-1.02809500	2.66924300	-1.62072200
N	-1.31579600	3.64876600	-2.15199500

C	1.77569100	-0.00226700	-2.60171200
N	2.42670300	-0.00306000	-3.55104700
C	-3.25387200	0.00444800	-0.66920800
N	-4.39112800	0.00602400	-0.84320500
C	-1.03547600	-2.66669100	-1.62048100
N	-1.32582400	-3.64548600	-2.15165700

[CB₁₁H(CN)₁₁]⁻

Lowest normal mode frequency: 78.41 cm⁻¹

B	0.06318900	-1.51414800	-0.90475100
B	1.45969200	-0.40779700	-0.90464500
B	-1.42063400	-0.52799200	-0.90464700
B	-0.94118300	1.18794500	-0.90467200
B	0.83894700	1.26222900	-0.90467000
B	-0.06356700	1.52338900	0.60892700
B	-1.46848000	0.41029400	0.60895400
B	-0.84400300	-1.26982500	0.60887800
B	1.42919700	0.53121200	0.60895600
B	0.94686900	-1.19509300	0.60888000
B	0.00000300	-0.00002800	1.54539100
C	0.00000200	0.00006900	-1.69570300
H	0.00000200	0.00007700	-2.77852600
C	0.00000200	-0.00002100	3.08103100
N	-0.00000700	0.00009100	4.23145300
C	-2.80551000	0.78385400	1.26354600
N	-3.81198700	1.06502100	1.74452800
C	-0.12144800	2.91043500	1.26350000
N	-0.16501700	3.95447900	1.74463300
C	-1.61243600	-2.42600500	1.26343100
N	-2.19082200	-3.29623700	1.74463200
C	1.80895400	-2.28323200	1.26343400
N	2.45783100	-3.10225100	1.74463600
C	2.73045500	1.01486600	1.26355100
N	3.71000900	1.37890900	1.74453400
C	2.70525600	-0.75583100	-1.72741600
N	3.63003300	-1.01439000	-2.36055200
C	0.11710700	-2.80622200	-1.72763100
N	0.15709800	-3.76551900	-2.36094100
C	-2.63287000	-0.97858800	-1.72742100
N	-3.53291400	-1.31320400	-2.36057100

C	-1.74432900	2.20159800	-1.72748200
N	-2.34060500	2.95401700	-2.36093400
C	1.55485100	2.33927100	-1.72748000
N	2.08632800	3.13877200	-2.36093800

[CB₁₂H(CN)₁₂]⁻

Lowest normal mode frequency: 33.31 cm⁻¹

B	-1.67024098	1.08602207	0.00000000
B	-1.68078305	-0.53988793	0.00000000
B	-0.24643695	1.86735101	0.00000000
B	-0.57886729	0.42929012	-1.38112346
B	-0.40504790	-1.43881692	-0.88584375
B	1.12764519	1.15004902	-0.88692799
B	1.12764519	1.15004902	0.88692799
B	-0.40504790	-1.43881692	0.88584375
B	0.98648963	-0.51638294	-1.42789897
B	0.98648963	-0.51638294	1.42789897
B	1.09761491	-1.60233104	0.00000000
H	2.93260197	-0.11064711	0.00000000
B	-0.57886729	0.42929012	1.38112346
C	1.85001397	-0.07649107	0.00000000
C	-3.05614707	-1.22551588	0.00000000
N	-4.09664909	-1.71811984	0.00000000
C	-2.97422595	1.87306112	0.00000000
N	-3.95803693	2.47184816	0.00000000
C	-0.25993189	3.40365201	0.00000000
N	-0.28353785	4.55463902	0.00000000
C	-1.12983657	0.77613424	-2.77374592
N	-1.54721052	1.04427633	-3.81201552
C	-0.90093377	-2.58800084	-1.77280436
N	-1.25490144	-3.44677078	-2.45181610
C	-0.90093377	-2.58800084	1.77280436
N	-1.25490144	-3.44677078	2.45181610
C	-1.12983657	0.77613424	2.77374592
N	-1.54721052	1.04427633	3.81201552
C	2.01817148	2.09582204	-1.70101575
N	2.70050794	2.79251206	-2.31112534
C	2.01817148	2.09582204	1.70101575
N	2.70050794	2.79251206	2.31112534
C	1.75024943	-0.88036488	-2.70606371

N	2.34269954	-1.15872584	-3.65178428
C	2.00385286	-2.83775507	0.00000000
N	2.70503683	-3.74941210	0.00000000
C	1.75024943	-0.88036488	2.70606371
N	2.34269954	-1.15872584	3.65178428

[CB₁₃H(CN)₁₃]⁻

Lowest normal mode frequency: 56.84 cm⁻¹

B	-0.00000000	0.00000000	-1.47468600
B	0.00000000	-1.74799198	0.86603693
B	-1.51380546	-0.87399599	0.86603693
B	-1.51380546	0.87399599	0.86603693
B	0.87747991	-1.51983978	-0.64424706
B	1.75495981	-0.00000000	-0.64424706
B	-1.75495981	-0.00000000	-0.64424706
B	-0.87747991	-1.51983978	-0.64424706
H	0.00000000	0.00000000	2.64783900
B	1.51380546	-0.87399599	0.86603693
B	0.87747991	1.51983978	-0.64424706
B	-0.87747991	1.51983978	-0.64424706
B	1.51380546	0.87399599	0.86603693
B	-0.00000000	1.74799198	0.86603693
C	0.00000000	-0.00000000	1.56182000
C	0.00000000	-0.00000000	-3.01303100
N	0.00000000	-0.00000000	-4.16337900
C	-3.11052900	0.00000000	-1.36180100
N	-4.13248800	0.00000000	-1.89023200
C	-1.55526450	2.69379713	-1.36180100
N	-2.06624400	3.57883959	-1.89023200
C	1.55526450	2.69379713	-1.36180100
N	2.06624400	3.57883959	-1.89023200
C	3.11052900	0.00000000	-1.36180100
N	4.13248800	0.00000000	-1.89023200
C	1.55526450	-2.69379713	-1.36180100
N	2.06624400	-3.57883959	-1.89023200
C	-1.55526450	-2.69379713	-1.36180100
N	-2.06624400	-3.57883959	-1.89023200
C	2.59857424	-1.50028754	1.74668894
N	3.40792603	-1.96756701	2.41774692
C	2.59857424	1.50028754	1.74668894
N	3.40792603	1.96756701	2.41774692

C	-0.00000000	3.00057508	1.74668894
N	-0.00000000	3.93513403	2.41774692
C	-2.59857424	1.50028754	1.74668894
N	-3.40792603	1.96756701	2.41774692
C	-2.59857424	-1.50028754	1.74668894
N	-3.40792603	-1.96756701	2.41774692
C	0.00000000	-3.00057508	1.74668894
N	0.00000000	-3.93513403	2.41774692

[CB₅F₆]⁻

Lowest normal mode frequency: 101.30 cm⁻¹

B	-0.00000300	0.00000100	1.28310000
B	-0.86266700	-0.86086900	0.06452700
B	0.86266700	0.86086900	0.06453000
B	0.86086800	-0.86266700	0.06453200
B	-0.86086900	0.86266700	0.06452600
C	0.00000300	-0.00000100	-1.01694300
F	-1.82660600	-1.82280800	-0.11596700
F	-0.00000700	0.00000200	2.65928100
F	-1.82280900	1.82660500	-0.11597000
F	1.82660700	1.82280800	-0.11596000
F	1.82280900	-1.82660600	-0.11595800
F	0.00000700	-0.00000200	-2.37369500

[CB₆F₇]⁻

Lowest normal mode frequency: 71.63 cm⁻¹

B	0.02658300	1.44469600	0.09499000
B	-1.28297000	0.47309000	0.08476100
B	1.29856500	0.41969000	0.08544400
B	0.78237400	-1.18069700	0.08207900
B	-0.82570100	-1.14743500	0.08130500
C	0.00015900	-0.00171000	-0.97181400
B	-0.00062600	-0.01289600	1.27772800
F	0.06103000	2.80546100	-0.11046000
F	-0.00121800	-0.01869600	2.64114900
F	2.62973800	0.70404200	-0.12545100
F	1.70330800	-2.17987100	-0.12718600
F	-1.78804400	-2.10671400	-0.12821500
F	-2.60483200	0.79723800	-0.12625300
F	0.00089800	0.00165200	-2.32365600

[CB₇F₈]⁻

Lowest normal mode frequency: 71.63 cm⁻¹

B	0.82565607	0.77500031	1.01074481
B	-0.52597500	-1.42068300	0.00000000
B	0.76871601	-0.86881136	-1.00078859
B	0.82565607	0.77500031	-1.01074481
B	-0.92600590	-0.03405030	-0.92836116
B	0.76871601	-0.86881136	1.00078859
B	-0.92600590	-0.03405030	0.92836116
C	-0.34987294	1.21188800	0.00000000
F	1.39711486	1.73980755	1.77939891
F	1.39711486	1.73980755	-1.77939891
F	1.39809083	-1.76935943	1.82777508
F	1.39809083	-1.76935943	-1.82777508
F	-1.08677303	-2.67989499	0.00000000
F	-1.91158611	0.19816464	1.83714675
F	-1.91158611	0.19816464	-1.83714675
F	-0.89832291	2.45591101	0.00000000

[CB₈F₉]⁻

Lowest normal mode frequency: 71.63 cm⁻¹

B	0.54054200	1.03523700	0.90080800
B	0.55224500	1.05362900	-0.89785800
B	-0.82961800	1.44495600	-0.00914400
B	0.55224600	-1.05362800	-0.89785700
B	-1.19323600	-0.00000200	-0.88475400
B	-1.17446900	0.00000000	0.88723900
B	0.54054400	-1.03523600	0.90080900
B	-0.82961600	-1.44495800	-0.00914100
C	1.40692600	0.00000100	-0.01018500
F	1.14328400	-1.69393000	1.92067600
F	1.15768600	-1.72110700	-1.90956700
F	1.14328000	1.69393300	1.92067400
F	1.15768400	1.72110700	-1.90956900
F	-1.55688600	2.61482200	-0.00696400
F	-2.07436000	0.00000000	1.92308500
F	-2.10022300	-0.00000300	-1.91293100
F	-1.55688200	-2.61482400	-0.00696100
F	2.77144800	0.00000200	-0.00615400

[CB₉F₁₀]⁻

Lowest normal mode frequency: 71.63 cm⁻¹

B	0.00000000	0.00000000	1.86878000
B	-0.93500600	0.93500600	0.79859400
B	0.93500600	0.93500600	0.79859400

B	0.93500600	-0.93500600	0.79859400
B	-0.93500600	-0.93500600	0.79859400
B	0.00000000	1.31701700	-0.73245200
B	1.31701700	0.00000000	-0.73245200
B	0.00000000	-1.31701700	-0.73245200
B	-1.31701700	0.00000000	-0.73245200
C	0.00000000	0.00000000	-1.65594700
F	0.00000000	2.54883200	-1.30085000
F	2.54883200	0.00000000	-1.30085000
F	-2.54883200	0.00000000	-1.30085000
F	0.00000000	-2.54883200	-1.30085000
F	-1.85869300	-1.85869300	1.22202700
F	0.00000000	0.00000000	3.24055300
F	-1.85869300	1.85869300	1.22202700
F	1.85869300	1.85869300	1.22202700
F	1.85869300	-1.85869300	1.22202700
F	0.00000000	0.00000000	-3.00648700

[CB₁₀F₁₁]⁻

Lowest normal mode frequency: 71.63 cm⁻¹

B	0.22248100	0.97436500	1.35930800
B	0.22248100	0.97436500	-1.35930800
B	-0.84895900	-1.48062000	0.00000000
B	0.20170800	-0.92913500	-1.35340200
B	-1.22874800	0.00695900	-0.94058200
B	0.89826600	1.68551800	0.00000000
B	0.20170800	-0.92913500	1.35340200
B	1.51668800	0.05691500	0.00000000
B	-0.83171300	1.50806500	0.00000000
B	-1.22874800	0.00695900	0.94058200
C	0.82926000	-1.45976300	0.00000000
F	0.46111300	-1.55176200	2.52307000
F	-2.34738000	0.00934000	1.73032100
F	0.38056600	1.46033700	2.63019700
F	-1.72953200	2.54301600	0.00000000
F	1.73028800	2.77440700	0.00000000
F	0.38056600	1.46033700	-2.63019700
F	2.86617300	-0.03165600	0.00000000
F	0.46111300	-1.55176200	-2.52307000
F	-2.34738000	0.00934000	-1.73032100
F	-1.55427400	-2.64085900	0.00000000
F	1.63192600	-2.54881400	0.00000000

[CB₁₁F₁₂]⁻

Lowest normal mode frequency: 71.63 cm⁻¹

B	1.45744949	-0.47355405	0.71500566
B	0.00000000	-1.53245309	0.71500566
B	0.90075332	1.23978059	0.71500566
B	-0.90075332	1.23978059	0.71500566
B	-1.45744949	-0.47355405	0.71500566
B	-1.46242922	0.47517206	-0.78799773
B	0.00000000	1.53768908	-0.78799773
B	1.46242922	0.47517206	-0.78799773
B	-0.90383096	-1.24401660	-0.78799773
B	0.90383096	-1.24401660	-0.78799773
B	-0.00000000	-0.00000000	-1.71877003
C	0.00000000	0.00000000	1.50957797
F	2.52870972	-0.82162760	1.47026664
F	1.56282856	2.15104897	1.47026664
F	0.00000000	-2.65884275	1.47026664
F	-2.52870972	-0.82162760	1.47026664
F	-1.56282856	2.15104897	1.47026664
F	-2.62977644	0.85446616	-1.39354088
F	-1.62529122	-2.23702145	-1.39354088
F	0.00000000	-0.00000000	-3.08721203
F	1.62529122	-2.23702145	-1.39354088
F	2.62977644	0.85446616	-1.39354088
F	0.00000000	2.76511058	-1.39354088
F	0.00000000	0.00000000	2.85529197

[CB₁₂F₁₃]⁻

Lowest normal mode frequency: 71.63 cm⁻¹

B	-2.12328200	0.39560500	0.12102900
B	-0.83303700	1.50069800	-0.39490200
B	-1.83726500	-1.16349800	0.09853800
B	-0.65928800	0.90468600	1.28577000
B	0.74625900	1.65256500	0.40440000
B	-0.37700100	-0.98552000	1.27692600
B	-0.24363200	-1.66667800	-0.40676000
B	0.64048700	1.03860800	-1.29310600
B	0.97081500	0.22195100	1.41892900
B	0.94876100	-0.67048900	-1.30514500
B	1.83474000	0.38156000	-0.16550600
B	-0.83175300	-0.15087800	-1.39664200
C	1.15359400	-1.10004400	0.35569700

F	-0.18462000	-2.97738000	-0.76164900
F	-0.46498300	-1.76278600	2.38389800
F	-2.63879700	-2.25804300	0.08080700
F	-1.15940900	1.47334600	2.42469600
F	-3.27775600	1.09779600	0.16369900
F	-1.39742300	2.67245900	-0.82726900
F	1.25218100	2.88434800	0.71469100
F	0.97732400	1.80759500	-2.36866600
F	3.18281400	0.47101700	-0.22120900
F	1.65702500	0.18565600	2.58502000
F	1.61465600	-1.35817100	-2.26095300
F	-1.39666100	-0.25963000	-2.63359700
F	2.04669500	-2.05318300	0.68143900

[CB₁₃F₁₄]⁻

Lowest normal mode frequency: 71.63 cm⁻¹

B	0.00000000	-0.00000000	1.61102948
B	0.00000000	1.76868311	-0.71244364
B	-1.53172450	0.88434155	-0.71244364
B	-1.53172450	-0.88434155	-0.71244364
B	0.88385739	1.53088590	0.78498569
B	1.76771477	0.00000000	0.78498569
B	-1.76771477	-0.00000000	0.78498569
B	-0.88385739	1.53088590	0.78498569
B	1.53172450	0.88434155	-0.71244364
B	0.88385739	-1.53088590	0.78498569
B	-0.88385739	-1.53088590	0.78498569
B	1.53172450	-0.88434155	-0.71244364
B	0.00000000	-1.76868311	-0.71244364
C	-0.00000000	-0.00000000	-1.41383252
F	-2.45652419	-1.41827490	-1.54285451
F	-2.45652419	1.41827490	-1.54285451
F	-2.94596978	0.00000000	1.47460566
F	-1.47298489	-2.55128467	1.47460566
F	0.00000000	-0.00000000	2.97103148
F	1.47298489	-2.55128467	1.47460566
F	2.94596978	0.00000000	1.47460566
F	2.45652419	-1.41827490	-1.54285451
F	2.45652419	1.41827490	-1.54285451
F	-0.00000000	-2.83654980	-1.54285451
F	0.00000000	2.83654980	-1.54285451
F	1.47298489	2.55128467	1.47460566

F	-1.47298489	2.55128467	1.47460566
F	0.00000000	-0.00000000	-2.75580652

[CB₅Cl₆]⁻

Lowest normal mode frequency: 75.36 cm⁻¹

B	0.00000000	0.00000000	1.30709200
B	0.00000000	1.21345300	0.09346700
B	0.00000000	-1.21345300	0.09346700
B	-1.21345300	0.00000000	0.09346700
B	1.21345300	0.00000000	0.09346700
C	0.00000000	0.00000000	-0.99110500
Cl	0.00000000	0.00000000	3.09906200
Cl	2.98331600	0.00000000	-0.13019900
Cl	0.00000000	-2.98331600	-0.13019900
Cl	-2.98331600	0.00000000	-0.13019900
Cl	0.00000000	2.98331600	-0.13019900
Cl	0.00000000	0.00000000	-2.72286500

[CB₆Cl₇]⁻

Lowest normal mode frequency: 80.22 cm⁻¹

B	0.00000000	1.39205600	0.12663400
B	-1.32392400	0.43016900	0.12663400
B	1.32392400	0.43016900	0.12663400
B	0.81823000	-1.12619700	0.12663400
B	-0.81823000	-1.12619700	0.12663400
C	0.00000000	0.00000000	-0.93108200
B	0.00000000	0.00000000	1.30844800
Cl	0.00000000	0.00000000	3.09808600
Cl	3.00617300	0.97676500	-0.13416600
Cl	1.85791700	-2.55720300	-0.13416600
Cl	0.00000000	3.16087700	-0.13416600
Cl	-3.00617300	0.97676500	-0.13416600
Cl	-1.85791700	-2.55720300	-0.13416600
Cl	0.00000000	0.00000000	-2.66970300

[CB₇Cl₈]⁻

Lowest normal mode frequency: 65.03 cm⁻¹

B	0.03470800	-0.26060700	-1.31023800
B	0.00396500	1.33989000	0.81683500
B	1.30743300	0.35371000	0.00000000
B	0.81839300	-1.25835800	0.00000000
B	0.03470800	-0.26060700	1.31023800
B	0.00396500	1.33989000	-0.81683500

B	-1.26791300	0.35940000	0.00000000
C	-0.70985700	-1.13245400	0.00000000
Cl	0.00396500	2.75122500	1.91870200
Cl	0.00396500	2.75122500	-1.91870200
Cl	3.04558600	0.80533400	0.00000000
Cl	-3.01952000	0.69483900	0.00000000
Cl	-0.01867700	-0.90429900	-2.97516900
Cl	-0.01867700	-0.90429900	2.97516900
Cl	1.75375500	-2.76274600	0.00000000
Cl	-1.77493500	-2.50609400	0.00000000

[CB₈Cl₉]⁻

Lowest normal mode frequency: 42.32 cm⁻¹

B	0.55505000	-1.05219700	-0.89731000
B	0.52110900	-0.98888300	0.89982400
B	-0.83712400	-1.42508000	-0.03205600
B	0.52184000	0.98858200	0.89980000
B	-1.14124000	0.00035500	0.90112100
B	-1.21981900	0.00041100	-0.88420200
B	0.55575600	1.05184300	-0.89730400
B	-0.83616500	1.42561500	-0.03200800
C	1.43064100	-0.00049000	-0.04555900
Cl	-1.72851000	-2.97472500	-0.01866100
Cl	-2.32239000	0.00074000	2.25307200
Cl	-2.44092700	0.00086200	-2.19238200
Cl	-1.72657400	2.97582400	-0.01860400
Cl	1.25986000	-1.93304600	2.21211100
Cl	1.28531100	-2.01905200	-2.19161000
Cl	1.28665800	2.01820500	-2.19161000
Cl	1.26126700	1.93228100	2.21203200
Cl	3.17348900	-0.00110600	-0.03587400

[CB₉Cl₁₀]⁻

Lowest normal mode frequency: 95.92 cm⁻¹

B	0.00000000	0.00000000	1.86141500
B	-0.92978200	0.92978200	0.78943800
B	0.92978200	0.92978200	0.78943800
B	0.92978200	-0.92978200	0.78943800
B	-0.92978200	-0.92978200	0.78943800
B	0.00000000	1.31795600	-0.73158700
B	1.31795600	0.00000000	-0.73158700
B	0.00000000	-1.31795600	-0.73158700
B	-1.31795600	0.00000000	-0.73158700

C	0.00000000	0.00000000	-1.65874600
Cl	0.00000000	0.00000000	3.63850700
Cl	-2.12180800	-2.12180800	1.40575600
Cl	-2.12180800	2.12180800	1.40575600
Cl	2.12180800	-2.12180800	1.40575600
Cl	2.12180800	2.12180800	1.40575600
Cl	-2.93031500	0.00000000	-1.47585600
Cl	0.00000000	-2.93031500	-1.47585600
Cl	0.00000000	2.93031500	-1.47585600
Cl	2.93031500	0.00000000	-1.47585600
Cl	0.00000000	0.00000000	-3.38820200

[CB₁₀Cl₁₁]⁻

Lowest normal mode frequency: 55.31 cm⁻¹

B	0.21205800	0.96719200	1.35900100
B	0.21205800	0.96719200	-1.35900100
B	-0.79346800	-1.48289700	0.00000000
B	0.23853500	-0.91893600	-1.35703900
B	-1.22343300	-0.01766100	-0.93451200
B	0.87108100	1.68741500	0.00000000
B	0.23853500	-0.91893600	1.35703900
B	1.53846400	0.07781900	0.00000000
B	-0.85271200	1.47158600	0.00000000
B	-1.22343300	-0.01766100	0.93451200
C	0.88828400	-1.44788600	0.00000000
Cl	-1.97387500	2.86827600	0.00000000
Cl	1.82912900	3.18962500	0.00000000
Cl	0.41194700	1.70216000	2.97866600
Cl	0.41194700	1.70216000	-2.97866600
Cl	-2.68058400	-0.07715100	-1.97337600
Cl	-2.68058400	-0.07715100	1.97337600
Cl	3.31763000	0.07253400	0.00000000
Cl	0.54386600	-1.75145700	-2.88848900
Cl	-1.68281100	-3.02069200	0.00000000
Cl	0.54386600	-1.75145700	2.88848900
Cl	1.87604900	-2.87968400	0.00000000

[CB₁₁Cl₁₂]⁻

Lowest normal mode frequency: 114.33 cm⁻¹

B	0.00000000	1.52922954	-0.71689281
B	-1.45438371	0.47255791	-0.71689281
B	1.45438371	0.47255791	-0.71689281
B	0.89885857	-1.23717268	-0.71689281

B	-0.89885857	-1.23717268	-0.71689281
B	0.00000000	-1.52762740	0.79206576
B	1.45285999	-0.47206283	0.79206576
B	0.89791686	1.23587653	0.79206576
B	-1.45285999	-0.47206283	0.79206576
B	-0.89791686	1.23587653	0.79206576
B	0.00000000	-0.00000000	1.72954506
C	-0.00000000	-0.00000000	-1.53539875
Cl	0.00000000	-0.00000000	3.51759531
Cl	0.00000000	-3.14147023	1.56257496
Cl	-2.98771573	-0.97076769	1.56257496
Cl	-1.84650987	2.54150280	1.56257496
Cl	1.84650987	2.54150280	1.56257496
Cl	2.98771573	-0.97076769	1.56257496
Cl	2.90459133	0.94375893	-1.62663236
Cl	1.79513616	-2.47079296	-1.62663236
Cl	-1.79513616	-2.47079296	-1.62663236
Cl	-2.90459133	0.94375893	-1.62663236
Cl	-0.00000000	3.05406806	-1.62663236
Cl	0.00000000	-0.00000000	-3.27501675

[CB₁₂Cl₁₃]⁻

Lowest normal mode frequency: 27.68 cm⁻¹

B	-0.06611500	2.14513300	0.00000000
B	1.36518100	1.36744600	0.00000000
B	-1.44910000	1.30433700	0.00000000
B	-0.00249900	0.87659000	1.40108900
B	1.53680800	-0.19033700	0.89237300
B	-1.48005500	-0.24698900	0.90260400
B	-1.48005500	-0.24698900	-0.90260400
B	1.53680800	-0.19033700	-0.89237300
B	0.05375500	-0.95160100	1.44403800
B	0.05375500	-0.95160100	-1.44403800
B	0.95160500	-1.58239200	0.00000000
B	-0.00249900	0.87659000	-1.40108900
C	-0.77392600	-1.50576200	0.00000000
Cl	-0.11245700	3.92309200	0.00000000
Cl	2.83535100	2.39896000	0.00000000
Cl	-2.99402000	2.21591800	0.00000000
Cl	-0.03342500	1.64812200	3.01507800
Cl	2.98863300	-0.36312800	1.92447500
Cl	2.98863300	-0.36312800	-1.92447500

Cl	-0.03342500	1.64812200	-3.01507800
Cl	0.01536000	-1.92488800	2.93012000
Cl	1.74686200	-3.16814400	0.00000000
Cl	-2.93157700	-0.57984600	1.87366100
Cl	-2.93157700	-0.57984600	-1.87366100
Cl	0.01536000	-1.92488800	-2.93012000
Cl	-1.57985800	-3.04885600	0.00000000

[CB₁₃Cl₁₄]⁻

Lowest normal mode frequency: 62.19 cm⁻¹

B	0.00000000	-0.00000000	1.63618929
B	0.00000000	1.77412803	-0.71499170
B	-1.53643995	0.88706402	-0.71499170
B	-1.53643995	-0.88706402	-0.71499170
B	0.88014001	1.52444722	0.79438292
B	1.76028003	0.00000000	0.79438292
B	-1.76028003	-0.00000000	0.79438292
B	-0.88014001	1.52444722	0.79438292
B	1.53643995	0.88706402	-0.71499170
B	0.88014001	-1.52444722	0.79438292
B	-0.88014001	-1.52444722	0.79438292
B	1.53643995	-0.88706402	-0.71499170
B	0.00000000	-1.77412803	-0.71499170
C	0.00000000	-0.00000000	-1.46452071
Cl	0.00000000	-0.00000000	3.42548628
Cl	-3.34445823	0.00000000	1.62323463
Cl	-1.67222912	-2.89638579	1.62323463
Cl	-1.67222912	2.89638579	1.62323463
Cl	1.67222912	2.89638579	1.62323463
Cl	3.34445823	0.00000000	1.62323463
Cl	1.67222912	-2.89638579	1.62323463
Cl	-2.82718356	1.63227519	-1.67728351
Cl	0.00000000	3.26455037	-1.67728351
Cl	2.82718356	1.63227519	-1.67728351
Cl	-2.82718356	-1.63227519	-1.67728351
Cl	0.00000000	-3.26455037	-1.67728351
Cl	2.82718356	-1.63227519	-1.67728351
Cl	0.00000000	-0.00000000	-3.20563770

[CB₅(CN)₆]⁻

Lowest normal mode frequency: 66.88 cm⁻¹

B	0.00000000	0.00000000	1.31174200
B	1.21314100	0.00000000	0.09645800

B	-1.21314100	0.00000000	0.09645800
B	0.00000000	1.21314100	0.09645800
B	0.00000000	-1.21314100	0.09645800
C	0.00000000	0.00000000	-0.99910800
C	0.00000000	2.72857400	-0.08550400
N	0.00000000	3.87367100	-0.21280400
C	-2.72857400	0.00000000	-0.08550400
N	-3.87367100	0.00000000	-0.21280400
C	0.00000000	-2.72857400	-0.08550400
N	0.00000000	-3.87367100	-0.21280400
C	2.72857400	0.00000000	-0.08550400
N	3.87367100	0.00000000	-0.21280400
C	0.00000000	0.00000000	2.84216000
N	0.00000000	0.00000000	3.99446000
C	0.00000000	0.00000000	-2.41847400
N	0.00000000	0.00000000	-3.56942000

[CB₆(CN)₇]⁻

Lowest normal mode frequency: 66.83 cm⁻¹

B	-1.32517285	0.43057476	0.14063099
B	-0.81900186	-1.12725936	0.14063099
B	0.00000000	1.39336920	0.14063099
B	1.32517285	0.43057476	0.14063099
B	0.81900186	-1.12725936	0.14063099
C	0.00000000	-0.00000000	-0.92394699
B	0.00000000	-0.00000000	1.31398600
C	0.00000000	0.00000000	2.85047099
N	0.00000000	-0.00000000	4.00216798
C	2.76145762	0.89725197	-0.08364036
N	3.84637469	1.24976290	-0.24405479
C	1.70667467	-2.34903616	-0.08364036
N	2.37719029	-3.27192174	-0.24405479
C	-1.70667467	-2.34903616	-0.08364036
N	-2.37719029	-3.27192174	-0.24405479
C	-2.76145762	0.89725197	-0.08364036
N	-3.84637469	1.24976290	-0.24405479
C	-0.00000000	2.90356837	-0.08364036
N	-0.00000000	4.04431769	-0.24405479
C	0.00000000	0.00000000	-2.35128298
N	-0.00000000	0.00000000	-3.50162197

[CB₇(CN)₈]⁻

Lowest normal mode frequency: 63.94 cm⁻¹

B	-0.02741200	-0.25193300	1.29057100
B	-0.00824400	1.36720300	-0.81113300
B	-1.29678000	0.37019100	0.00000000
B	-0.82733600	-1.25589700	0.00000000
B	-0.02741200	-0.25193300	-1.29057100
B	-0.00824400	1.36720300	0.81113300
B	1.25077500	0.36817600	0.00000000
C	0.70096300	-1.14372500	0.00000000
C	-0.01051400	2.54363700	1.78438600
N	-0.00917200	3.42765100	2.52341200
C	-0.01051400	2.54363700	-1.78438600
N	-0.00917200	3.42765100	-2.52341200
C	2.76315200	0.62849000	0.00000000
N	3.89442600	0.84150900	0.00000000
C	0.02245300	-0.78388700	-2.72695400
N	0.05838700	-1.18307100	-3.80636000
C	-2.78780000	0.73772000	0.00000000
N	-3.90617300	1.01295400	0.00000000
C	0.02245300	-0.78388700	2.72695400
N	0.05838700	-1.18307100	3.80636000
C	1.59151500	-2.25640600	0.00000000
N	2.30816100	-3.15561300	0.00000000
C	-1.64629800	-2.54120200	0.00000000
N	-2.27330300	-3.50676700	0.00000000

[CB₈(CN)₉]⁻

Lowest normal mode frequency: 71.63 cm⁻¹

B	-0.91222900	0.97026200	0.50464800
B	0.88634600	1.00452600	0.52546900
B	0.00444600	1.41004800	-0.86054600
B	0.89633500	-1.03370600	0.51793200
B	0.89394400	-0.00820000	-1.20073900
B	-0.89956500	-0.01706600	-1.17838600
B	-0.90247800	-1.01695000	0.49726000
B	0.01842500	-1.43756700	-0.87110300
C	0.00627300	-0.02227600	1.41913900
C	-2.02148100	-0.01868800	-2.22448800
N	-2.87322800	-0.01998200	-2.99931500
C	-0.00192700	2.74077600	-1.60711300
N	-0.00710700	3.74816500	-2.16497400
C	2.01080600	0.00119600	-2.25015000
N	2.86203100	0.00826300	-3.02574200

C	0.02507200	-2.76269900	-1.62755400
N	0.02972500	-3.76589900	-2.19291600
C	-2.02141700	1.80166100	1.15195200
N	-2.85990800	2.42771700	1.63114900
C	-2.00340100	-1.86399800	1.13835600
N	-2.83564600	-2.50184100	1.61287800
C	1.97562500	1.85507200	1.17920000
N	2.80263000	2.49349000	1.66230900
C	1.99392600	-1.87839100	1.16533600
N	2.82716200	-2.51226300	1.64370300
C	-0.00215100	-0.02760100	2.84772600
N	-0.00899200	-0.03187000	3.99677300

[CB₉(CN)₁₀]⁻

Lowest normal mode frequency: 74.12 cm⁻¹

B	0.00000000	0.00000000	1.88433300
B	-0.92380500	0.92380500	0.79430100
B	0.92380500	0.92380500	0.79430100
B	0.92380500	-0.92380500	0.79430100
B	-0.92380500	-0.92380500	0.79430100
B	0.00000000	1.31193200	-0.72070300
B	1.31193200	0.00000000	-0.72070300
B	0.00000000	-1.31193200	-0.72070300
B	-1.31193200	0.00000000	-0.72070300
C	0.00000000	0.00000000	-1.66198600
C	2.70333500	0.00000000	-1.35731900
N	3.74811800	0.00000000	-1.83897400
C	0.00000000	-2.70333500	-1.35731900
N	0.00000000	-3.74811800	-1.83897400
C	0.00000000	2.70333500	-1.35731900
N	0.00000000	3.74811800	-1.83897400
C	-2.70333500	0.00000000	-1.35731900
N	-3.74811800	0.00000000	-1.83897400
C	1.94588700	-1.94588700	1.31106700
N	2.71272700	-2.71272700	1.69676500
C	0.00000000	0.00000000	3.40725400
N	0.00000000	0.00000000	4.55844800
C	-1.94588700	1.94588700	1.31106700
N	-2.71272700	2.71272700	1.69676500
C	-1.94588700	-1.94588700	1.31106700
N	-2.71272700	-2.71272700	1.69676500
C	1.94588700	1.94588700	1.31106700

N	2.71272700	2.71272700	1.69676500
C	0.00000000	0.00000000	-3.08786700
N	0.00000000	0.00000000	-4.23647000

[CB₁₀(CN)₁₁]⁻

Lowest normal mode frequency: 55.43 cm⁻¹

B	0.19079900	0.97168500	1.35013600
B	0.19079900	0.97168500	-1.35013600
B	-0.79958700	-1.47913500	0.00000000
B	0.23556200	-0.89971400	-1.34824800
B	-1.23899400	-0.01398300	-0.92101400
B	0.84267300	1.71778900	0.00000000
B	0.23556200	-0.89971400	1.34824800
B	1.48568300	0.09457100	0.00000000
B	-0.88237800	1.47927500	0.00000000
B	-1.23899400	-0.01398300	0.92101400
C	0.88130300	-1.44854400	0.00000000
C	-1.85669900	2.66516200	0.00000000
N	-2.57764400	3.56201900	0.00000000
C	0.38555000	1.56231200	-2.75106000
N	0.54596000	2.01036100	-3.79933100
C	1.69839900	2.97960900	0.00000000
N	2.33792300	3.93682500	0.00000000
C	0.38555000	1.56231200	2.75106000
N	0.54596000	2.01036100	3.79933100
C	-2.47531000	-0.07489200	-1.82923600
N	-3.40387200	-0.12964300	-2.50662400
C	-2.47531000	-0.07489200	1.82923600
N	-3.40387200	-0.12964300	2.50662400
C	0.52947400	-1.59414600	-2.67676500
N	0.75989400	-2.12601800	-3.67076200
C	3.01929500	0.10580100	0.00000000
N	4.17019800	0.10809800	0.00000000
C	-1.55076600	-2.81067300	0.00000000
N	-2.10868800	-3.81657200	0.00000000
C	0.52947400	-1.59414600	2.67676500
N	0.75989400	-2.12601800	3.67076200
C	1.72394700	-2.60535300	0.00000000
N	2.39209400	-3.53943900	0.00000000

[CB₁₁(CN)₁₂]⁻

Lowest normal mode frequency: 78.14 cm⁻¹

B	0.00000000	1.52447133	-0.69677001
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B	-1.44985839	0.47108755	-0.69677001
B	1.44985839	0.47108755	-0.69677001
B	0.89606176	-1.23332321	-0.69677001
B	-0.89606176	-1.23332321	-0.69677001
B	0.00000000	-1.52367970	0.81484992
B	1.44910551	-0.47084292	0.81484992
B	0.89559646	1.23268277	0.81484992
B	-1.44910551	-0.47084292	0.81484992
B	-0.89559646	1.23268277	0.81484992
B	0.00000000	-0.00000000	1.75104795
C	0.00000000	0.00000000	-1.51085604
C	0.00000000	-0.00000000	3.28561395
N	0.00000000	-0.00000000	4.43597795
C	2.76964121	-0.89991098	1.46695480
N	3.76239902	-1.22247755	1.95027110
C	0.00000000	-2.91217311	1.46695480
N	-0.00000000	-3.95602044	1.95027110
C	1.71173241	2.35599754	1.46695480
N	2.32529047	3.20048777	1.95027110
C	-1.71173241	2.35599754	1.46695480
N	-2.32529047	3.20048777	1.95027110
C	-2.76964121	-0.89991098	1.46695480
N	-3.76239902	-1.22247755	1.95027110
C	-2.68351422	0.87192663	-1.50713686
N	-3.61099698	1.17328404	-2.11666615
C	-0.00000000	2.82161383	-1.50713686
N	0.00000000	3.79682692	-2.11666615
C	2.68351422	0.87192663	-1.50713686
N	3.61099698	1.17328404	-2.11666615
C	1.65850300	-2.28273354	-1.50713686
N	2.23171887	-3.07169750	-2.11666615
C	-1.65850300	-2.28273354	-1.50713686
N	-2.23171887	-3.07169750	-2.11666615
C	-0.00000000	0.00000000	-2.94895304
N	0.00000000	0.00000000	-4.09678304

[CB₁₂(CN)₁₃]⁻

Lowest normal mode frequency: 37.77 cm⁻¹

B	-2.05162800	0.68692400	-0.00000300
B	-1.72352000	-0.90786400	-0.00000400
B	-0.81720500	1.74537100	-0.00000100
B	-0.85031700	0.26637000	-1.37781200

B	-0.29233500	-1.52514300	-0.88612800
B	0.66847300	1.32680600	-0.89352200
B	0.66847300	1.32680600	0.89351700
B	-0.29233600	-1.52514200	0.88612400
B	0.87645000	-0.33915600	-1.43600800
B	0.87645000	-0.33915500	1.43600400
B	1.20924400	-1.38659100	-0.00000200
B	-0.85031800	0.26637200	1.37780700
C	1.65476700	0.27747600	-0.00000200
C	-2.93145300	-1.86277800	-0.00000600
N	-3.85660500	-2.56030900	0.00002800
C	-3.49223700	1.18978500	-0.00000300
N	-4.58523800	1.57563400	-0.00000400
C	-1.14711100	3.24872200	-0.00000100
N	-1.41592700	4.37573400	0.00000000
C	-1.45751100	0.49261500	-2.77509600
N	-1.92476600	0.66952500	-3.81991200
C	-0.54277200	-2.75272900	-1.77717500
N	-0.72068800	-3.66841500	-2.46336400
C	-0.54277500	-2.75272800	1.77717100
N	-0.72069200	-3.66841500	2.46335900
C	-1.45751300	0.49261500	2.77509000
N	-1.92476800	0.66952300	3.81990700
C	1.32905000	2.43854200	-1.71870400
N	1.82148700	3.27387700	-2.35127500
C	1.32905200	2.43854200	1.71869900
N	1.82149300	3.27387500	2.35127000
C	1.69407800	-0.53647200	-2.71867800
N	2.31614400	-0.69130400	-3.68260600
C	2.33557900	-2.42662800	-0.00000100
N	3.18353900	-3.21451400	0.00000600
C	1.69407700	-0.53647200	2.71867500
N	2.31614600	-0.69130100	3.68260200
C	3.07445200	0.53257700	-0.00000300
N	4.21198000	0.73660500	0.00003800

[CB₁₃(CN)₁₄]⁻

Lowest normal mode frequency: 57.92 cm⁻¹

B	0.00000000	0.00000000	1.64457595
B	1.52540112	-0.88069075	-0.69107946
B	1.52540112	0.88069075	-0.69107946
B	-0.00000000	1.76138150	-0.69107946

B	0.87673965	-1.51855761	0.81506388
B	-0.87673965	-1.51855761	0.81506388
B	0.87673965	1.51855761	0.81506388
B	1.75347930	-0.00000000	0.81506388
B	0.00000000	-1.76138150	-0.69107946
B	-1.75347930	-0.00000000	0.81506388
B	-0.87673965	1.51855761	0.81506388
B	-1.52540112	-0.88069075	-0.69107946
B	-1.52540112	0.88069075	-0.69107946
C	-0.00000000	-0.00000000	-1.42436105
C	0.00000000	0.00000000	3.18238895
N	0.00000000	0.00000000	4.33270895
C	1.55401767	2.69163757	1.53389978
N	2.06415256	3.57521711	2.06551019
C	-1.55401767	2.69163757	1.53389978
N	-2.06415256	3.57521711	2.06551019
C	-3.10803535	-0.00000000	1.53389978
N	-4.12830512	-0.00000000	2.06551019
C	-1.55401767	-2.69163757	1.53389978
N	-2.06415256	-3.57521711	2.06551019
C	1.55401767	-2.69163757	1.53389978
N	2.06415256	-3.57521711	2.06551019
C	3.10803535	0.00000000	1.53389978
N	4.12830512	0.00000000	2.06551019
C	0.00000000	-3.01653438	-1.56373402
N	0.00000000	-3.96190087	-2.21949559
C	-2.61239540	-1.50826719	-1.56373402
N	-3.43110680	-1.98095043	-2.21949559
C	-2.61239540	1.50826719	-1.56373402
N	-3.43110680	1.98095043	-2.21949559
C	-0.00000000	3.01653438	-1.56373402
N	-0.00000000	3.96190087	-2.21949559
C	2.61239540	1.50826719	-1.56373402
N	3.43110680	1.98095043	-2.21949559
C	2.61239540	-1.50826719	-1.56373402
N	3.43110680	-1.98095043	-2.21949559
C	-0.00000000	-0.00000000	-2.86267405
N	-0.00000000	-0.00000000	-4.01131105