Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Constructing organic superacid from superhalogen is a rational route as verified by DFT calculations

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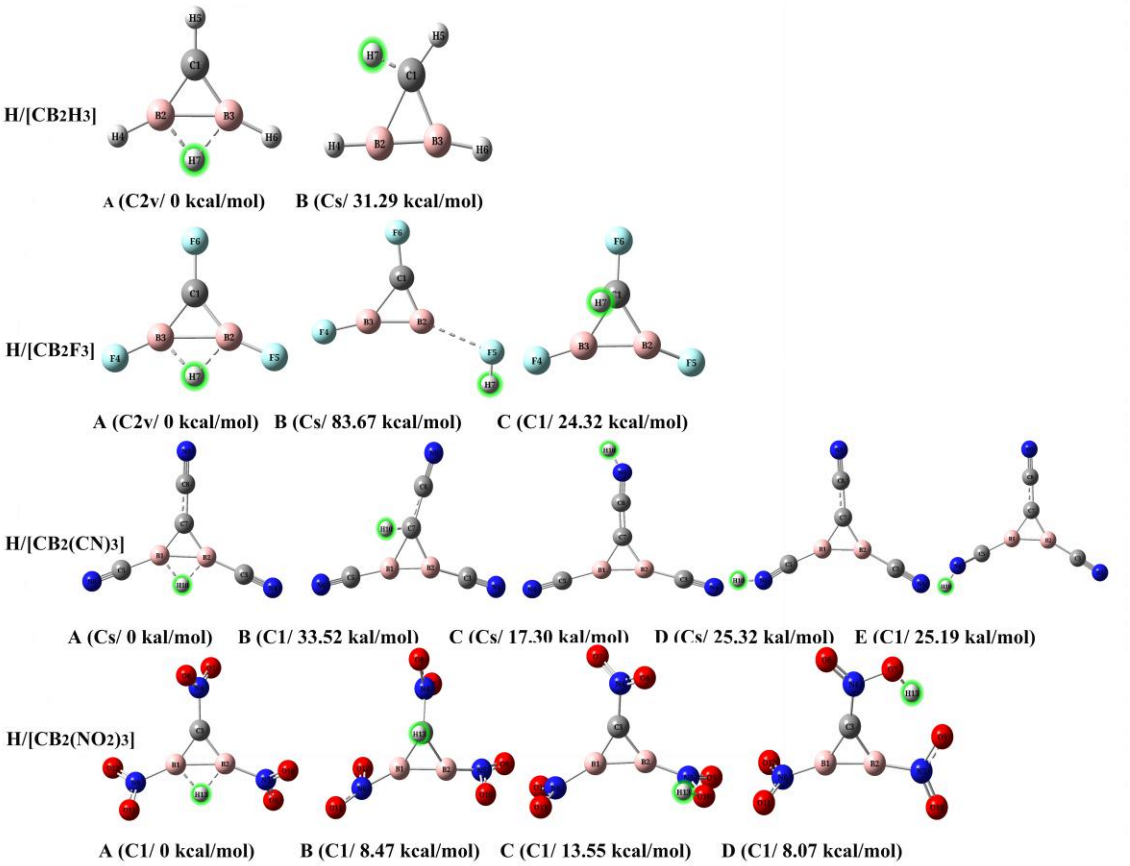

Fig. S1 Equilibrium structures of the composites H/[CB_2X_3] (X= H, F, Cl, CN).

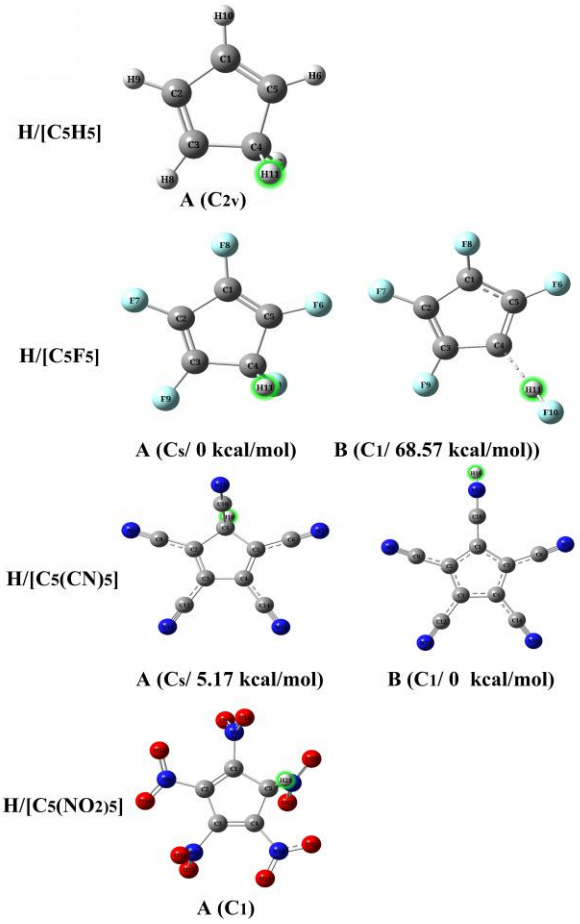

Fig. S2 Equilibrium structures of the composites H/[C_5X_5] (X= H, F, Cl, CN).

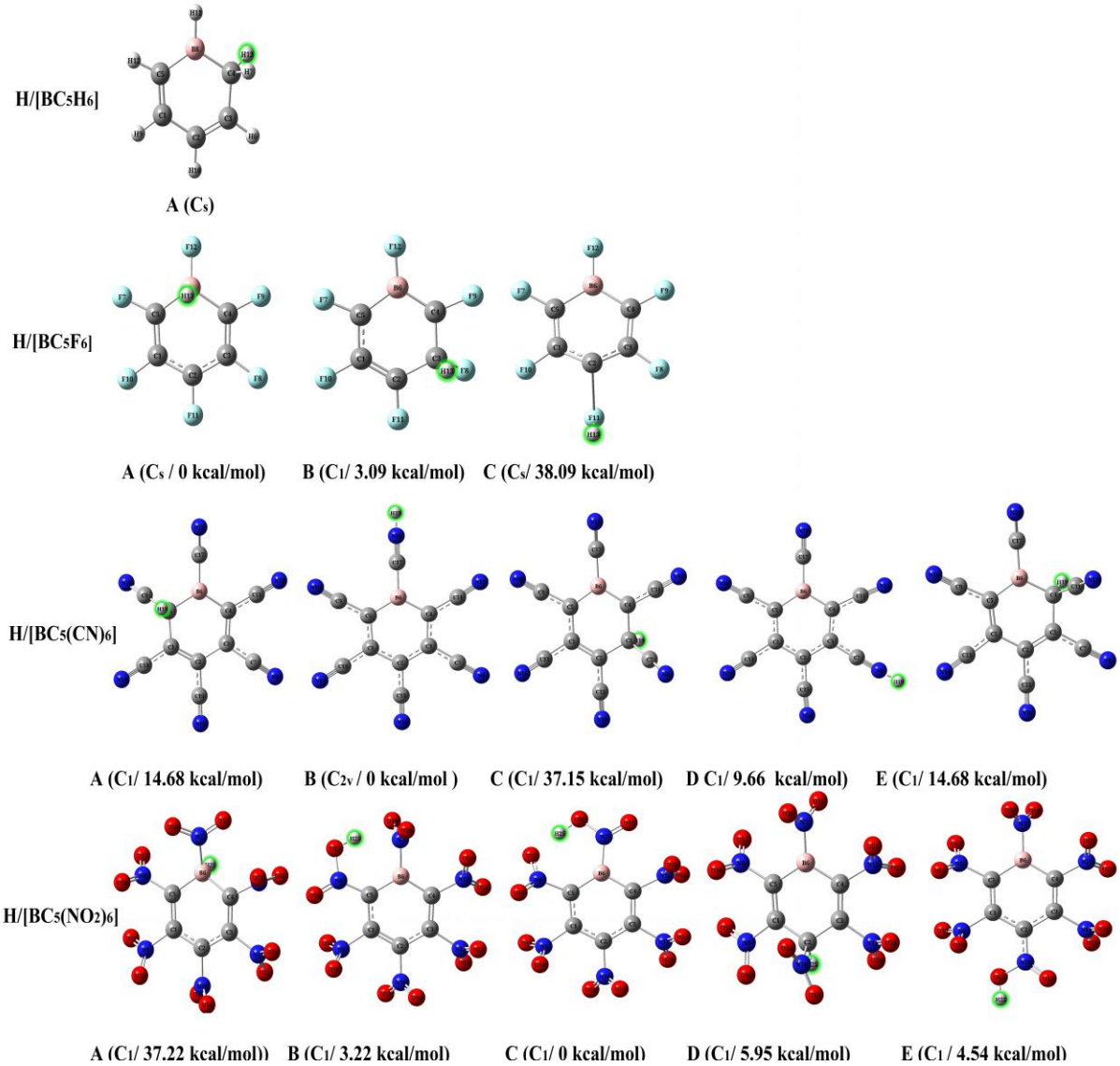

Fig. S3 Equilibrium structures of the composites H/[BC_5X_6] (X= H, F, Cl, CN).

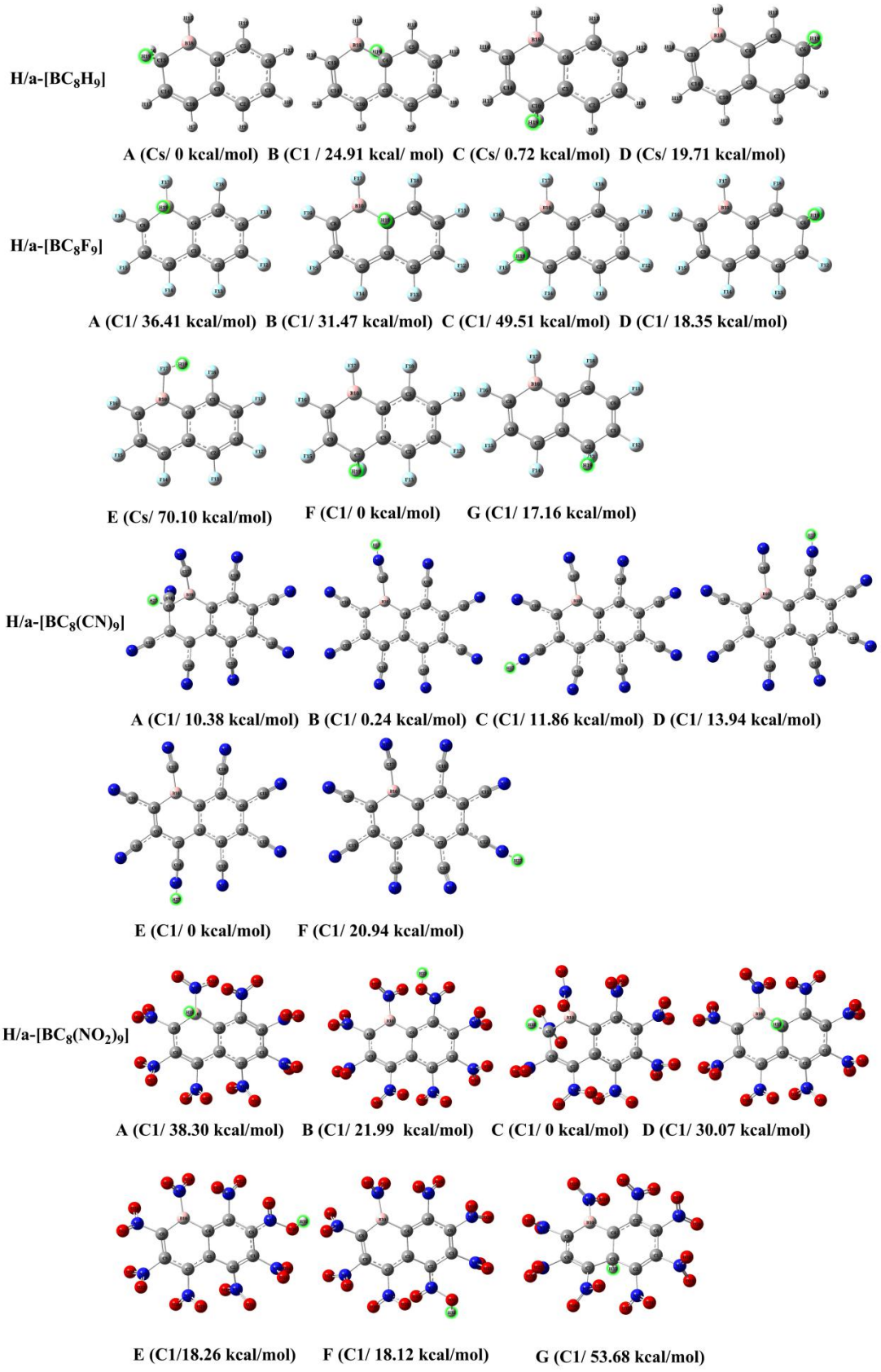

Fig. S4 Equilibrium structures of the composites H/a-[BC_8X_9] (X= H, F, Cl, CN).

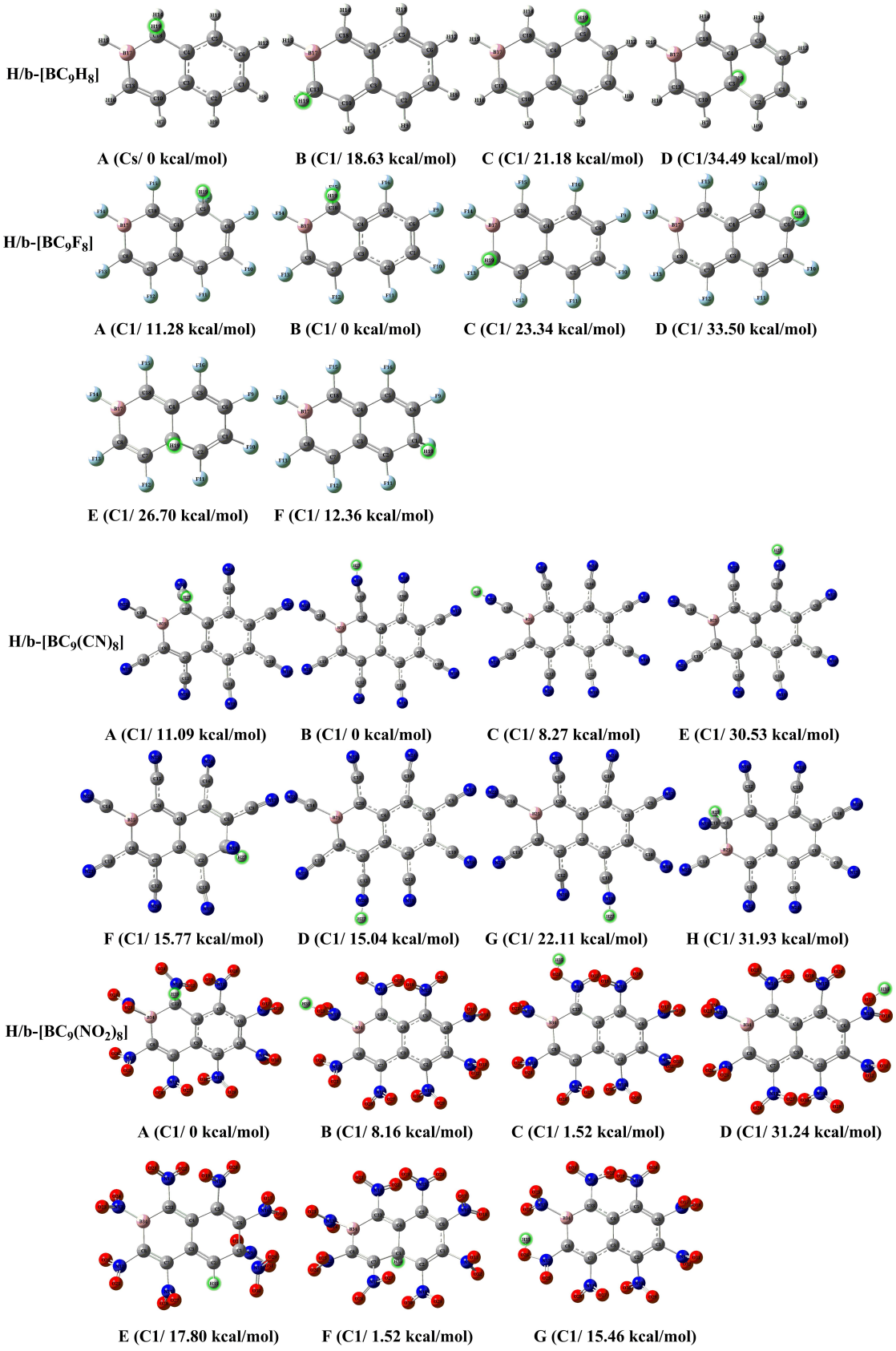

Fig. S5 Equilibrium structures of the composites H/b-[BC_8X_9] (X= H, F, Cl, CN).

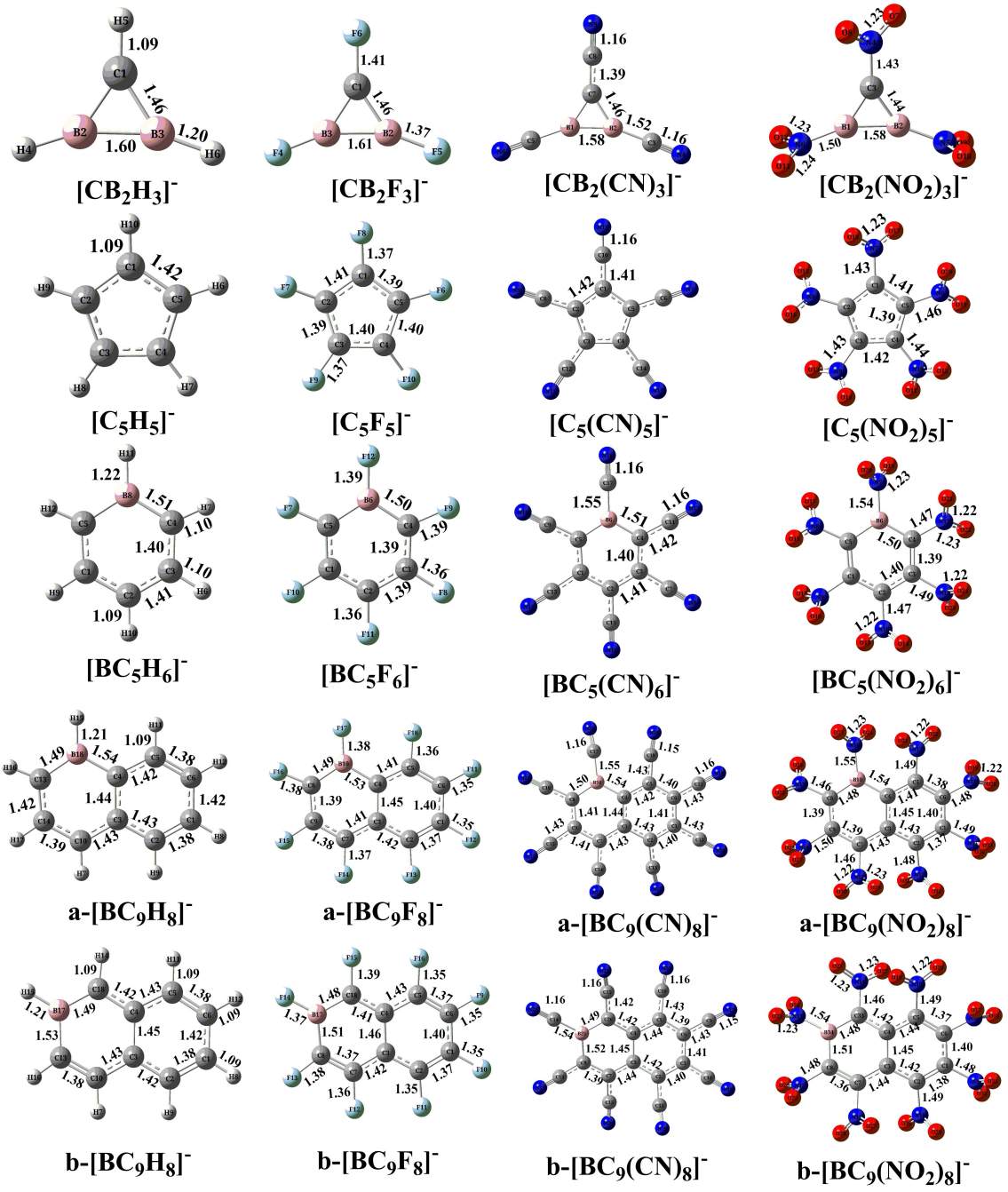

Fig. S6 Equilibrium structures of the composites $[CB_2X_3]^-$, $[C_5X_5]^-$, $[BC_5X_6]^-$, a-$[BC_9X_8]^-$ and b-$[BC_9X_8]^-$ (X= H, F, Cl, CN) in DMSO solvent

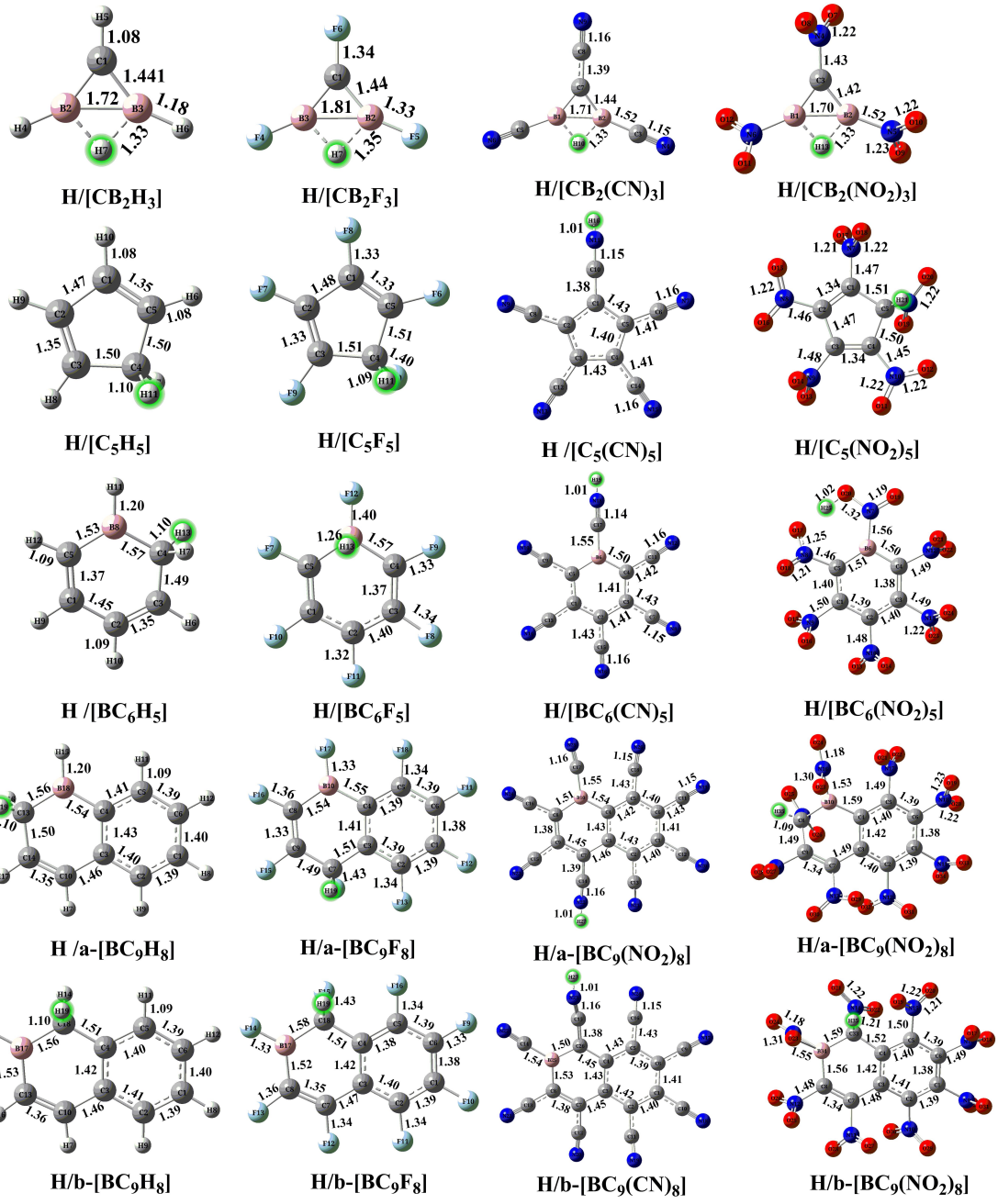

Fig. S7 Equilibrium structures of the composites H/[CB_2X_3], H/[C_5X_5], H/[BC_5X_6], H/a-[BC_9X_8], H/b-[BC_9X_8] (X= H, F, Cl, CN) in H_2O solvent.

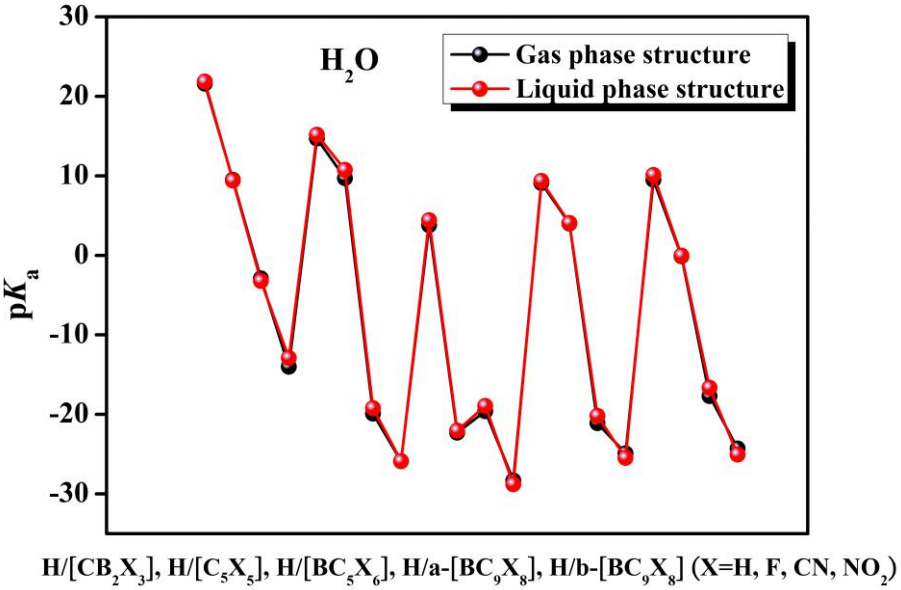

Fig. S8 The comparison of pK_a of composites under both Gas-phase and-liquid phase structure .

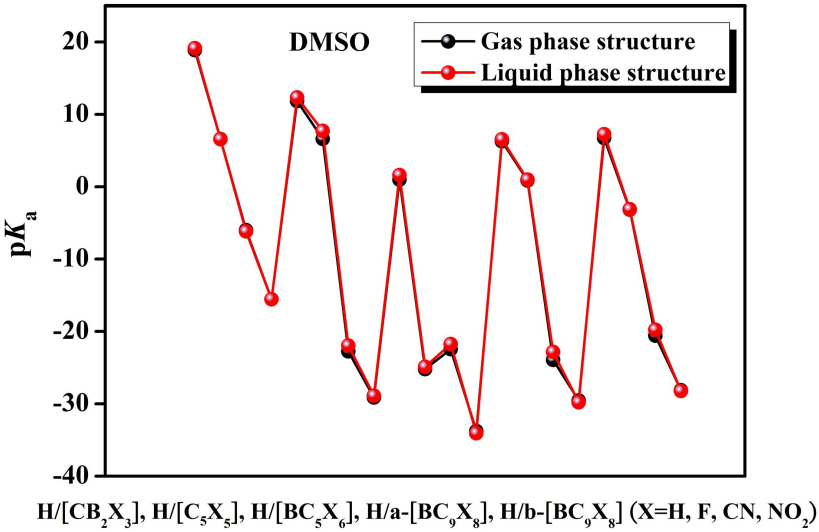

Fig. S9 The comparison of pK_a of composites under both Gas-phase and-liquid phase structure .

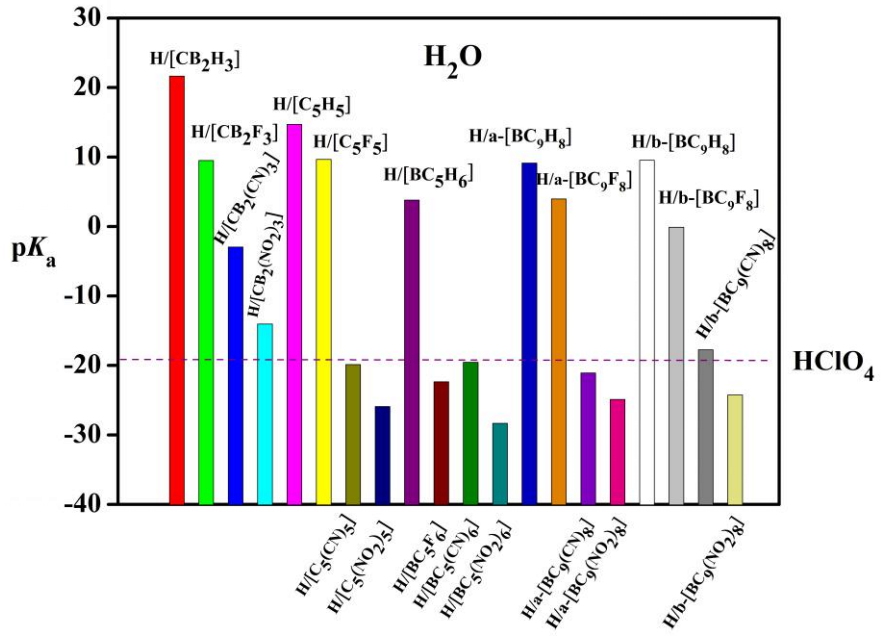

Fig. S10 Theoretical pK_a values of the composites here in H_2O solvents (dotted purple lines indicate the reference of perchloric acid $HClO_4$)

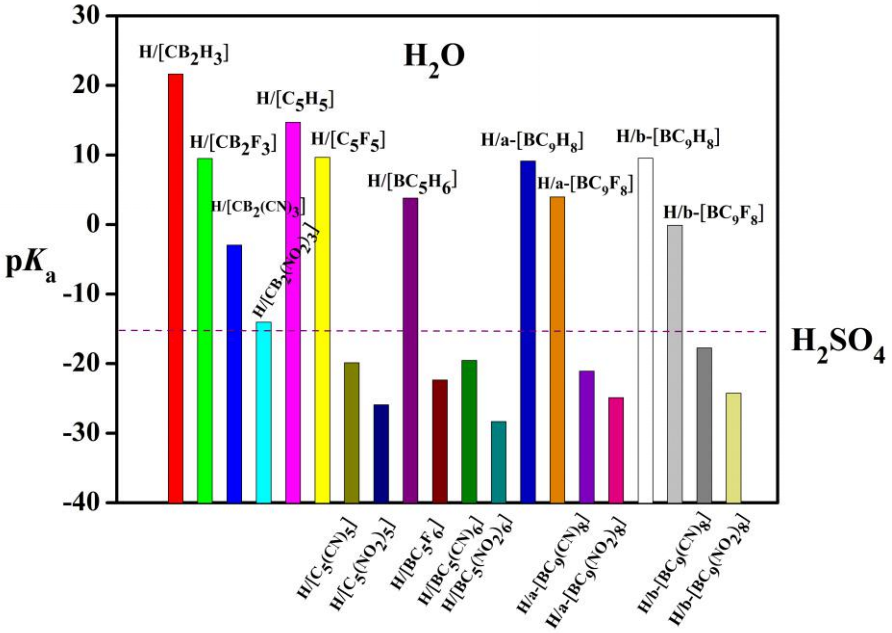

Fig. S11 Theoretical pK_a values of the composites here in H_2O solvents (dotted purple lines indicate the reference of sulfuric acid H_2SO_4)

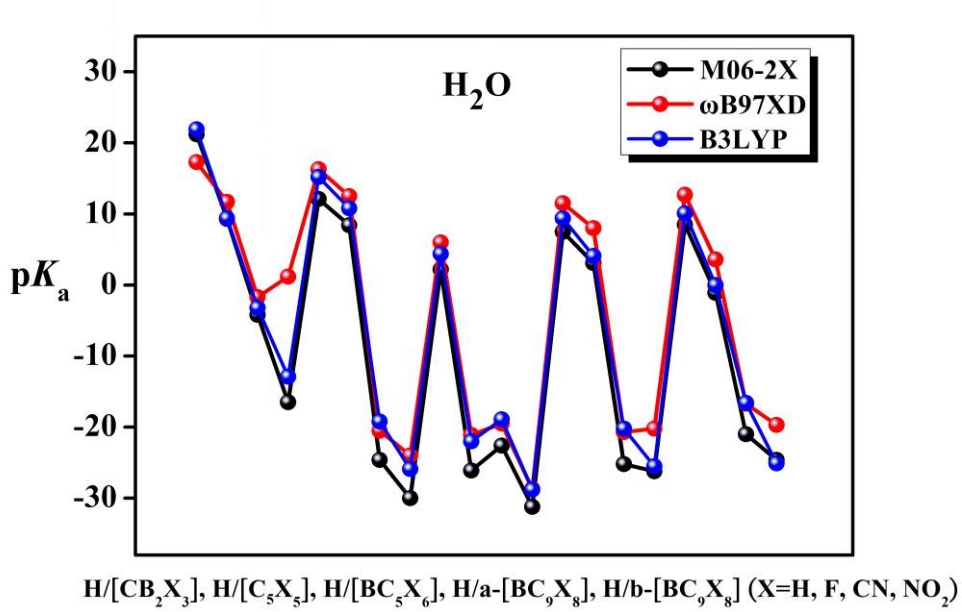

Fig. S12 The comparison among M06-2X, ωB97XD and B3LYP.

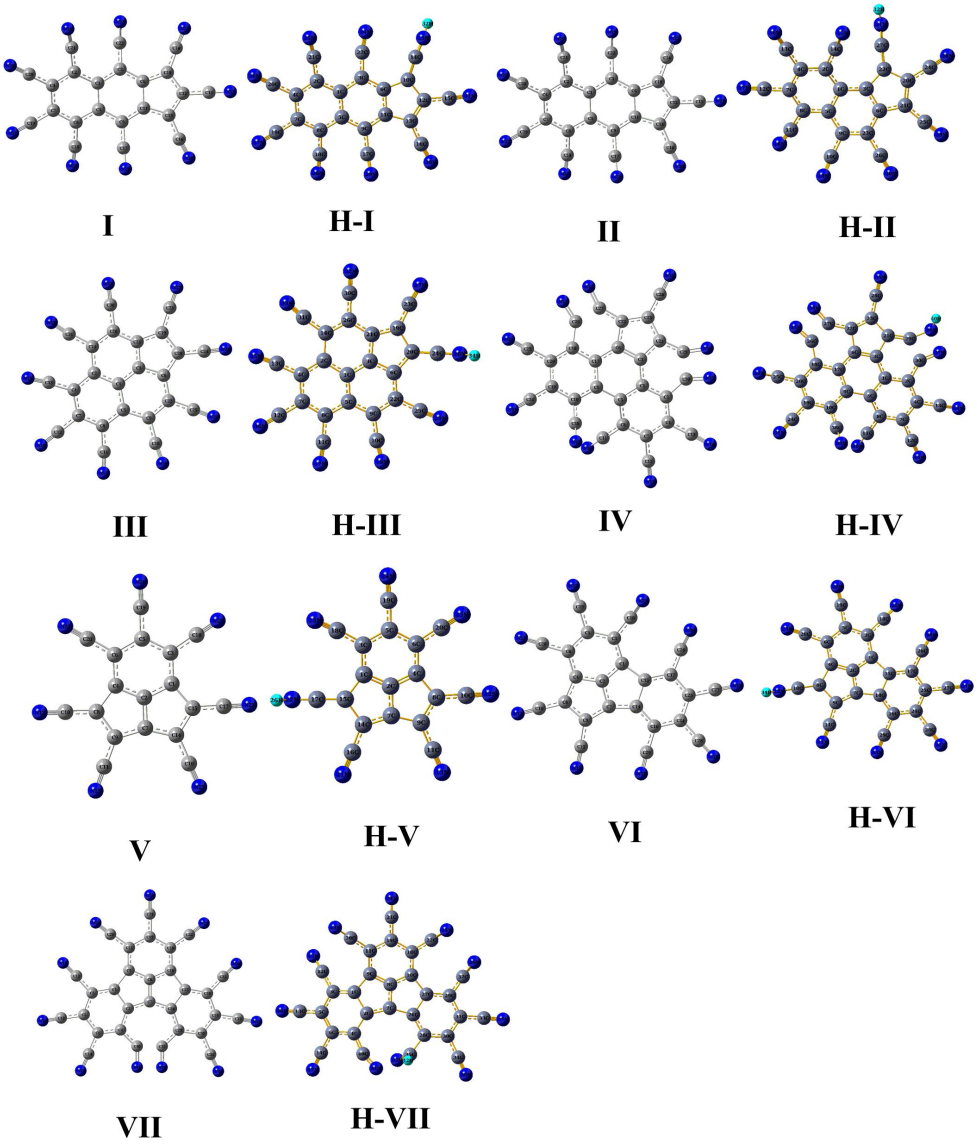

Fig. S13 Equilibrium structures of the Polycyclic Aromatic Compounds

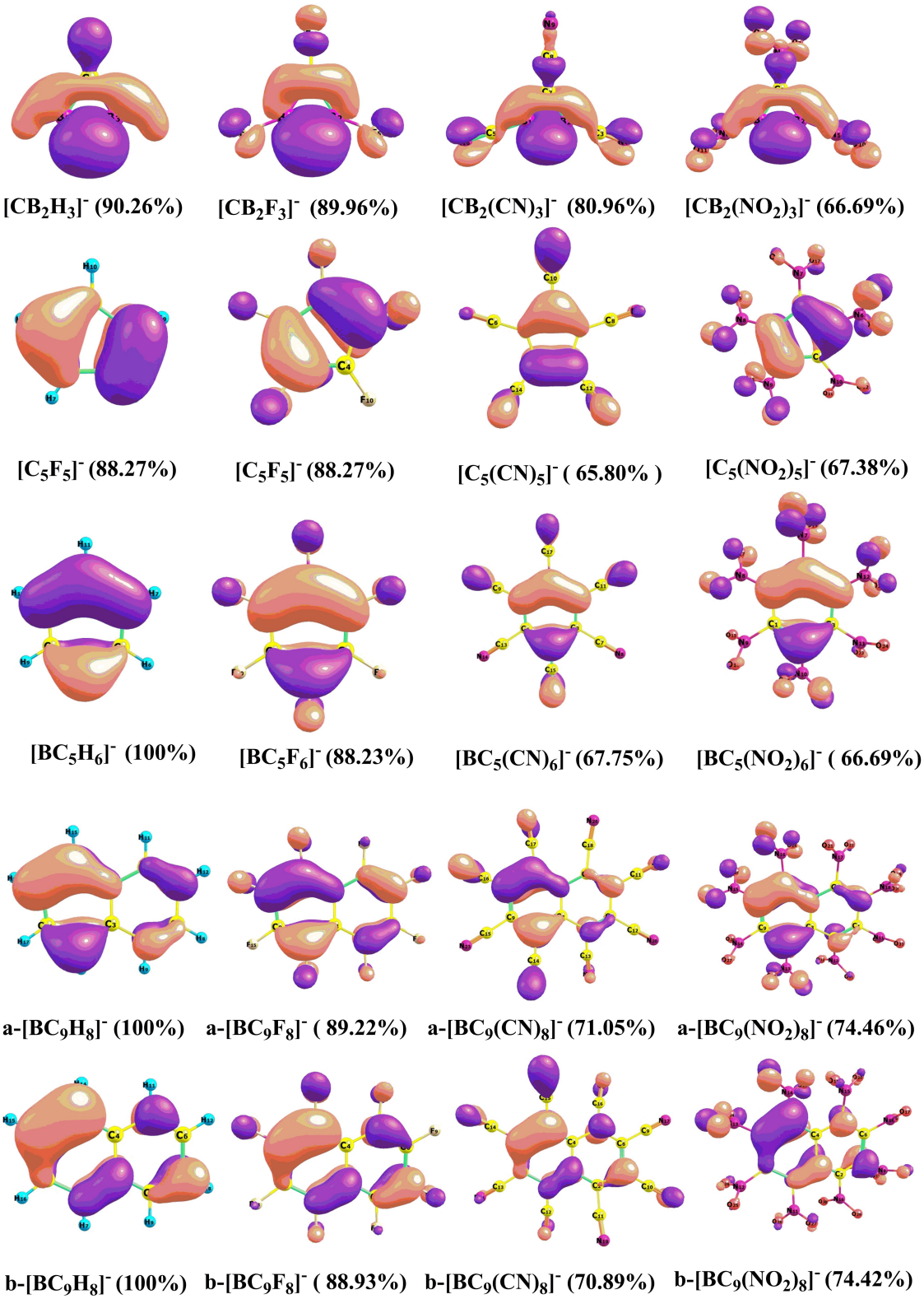

Fig. S14 The distribution HOMO (isovalue set to be 0.004 a.u.) orbital of anion of $[CB_2X_3]^-$, $[C_5X_5]^-$, $[BC_5X_6]^-$, a-$[BC_9X_8]^-$ and b-$[BC_9X_8]^-$ (X= H, F, Cl, CN)

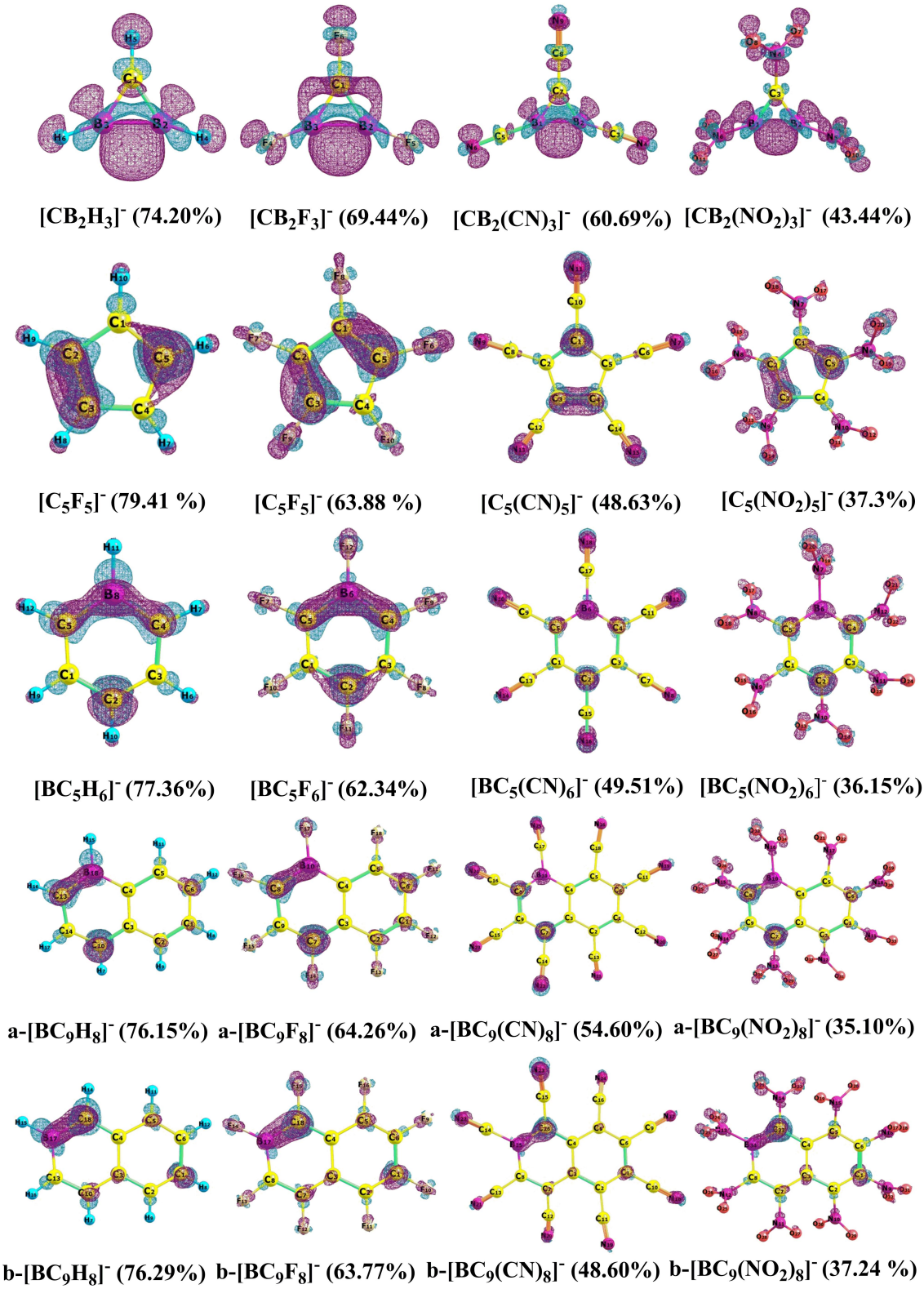

Fig. S15 The density of extra electron (isovalue set to be 0.005 a.u.) of anions of$[CB_2X_3]^-$, $[C_5X_5]^-$, $[BC_5X_6]^-$, a-$[BC_9X_8]^-$ and b-$[BC_9X_8]^-$ (X= H, F, Cl, CN).

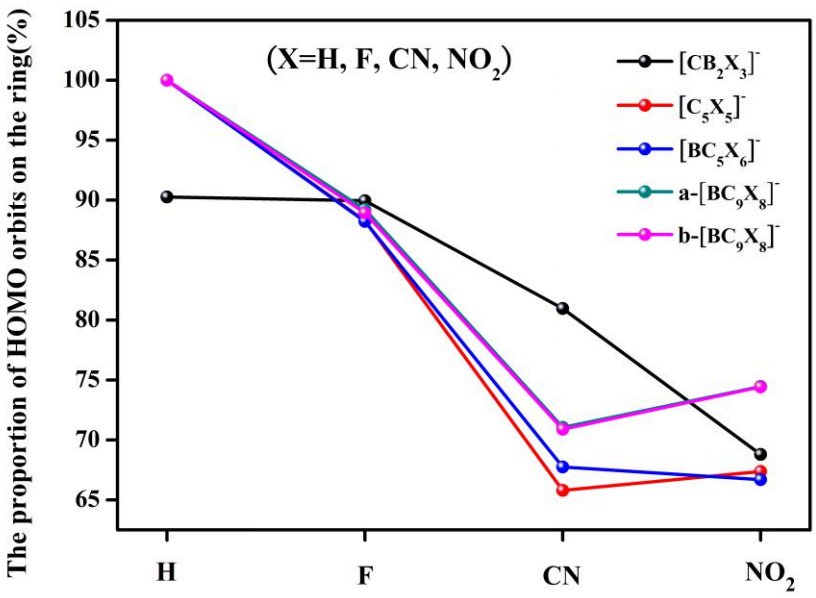

Fig. S16 The percentage contributions to HOMO from the ring for anions and their derivatives of $[CB_2X_3]^-$, $[C_5X_5]^-$, $[BC_5X_6]^-$, a-$[BC_9X_8]^-$ and b-$[BC_9X_8]^-$ (X= H, F, Cl, CN).

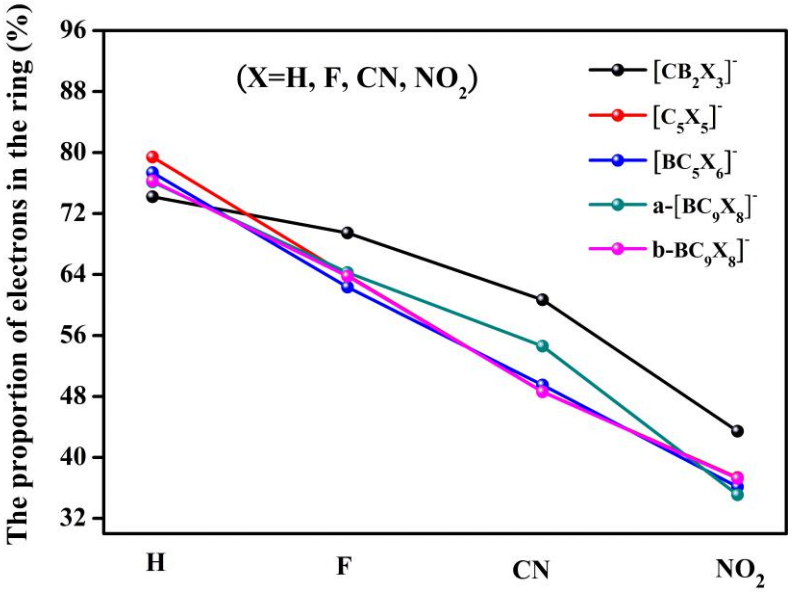

Fig. S17 The percentage contributions to electrons from the ring for anions and their derivatives of $[CB_2X_3]^-$, $[C_5X_5]^-$, $[BC_5X_6]^-$, a-$[BC_9X_8]^-$ and b-$[BC_9X_8]^-$ (X= H, F, Cl, CN).

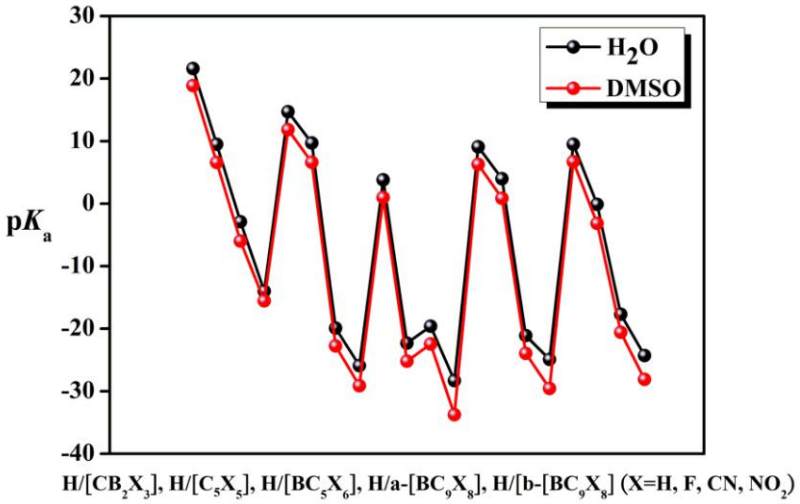

Fig. S18 The comparison of pK_a in H_2O and DMSO solvent.

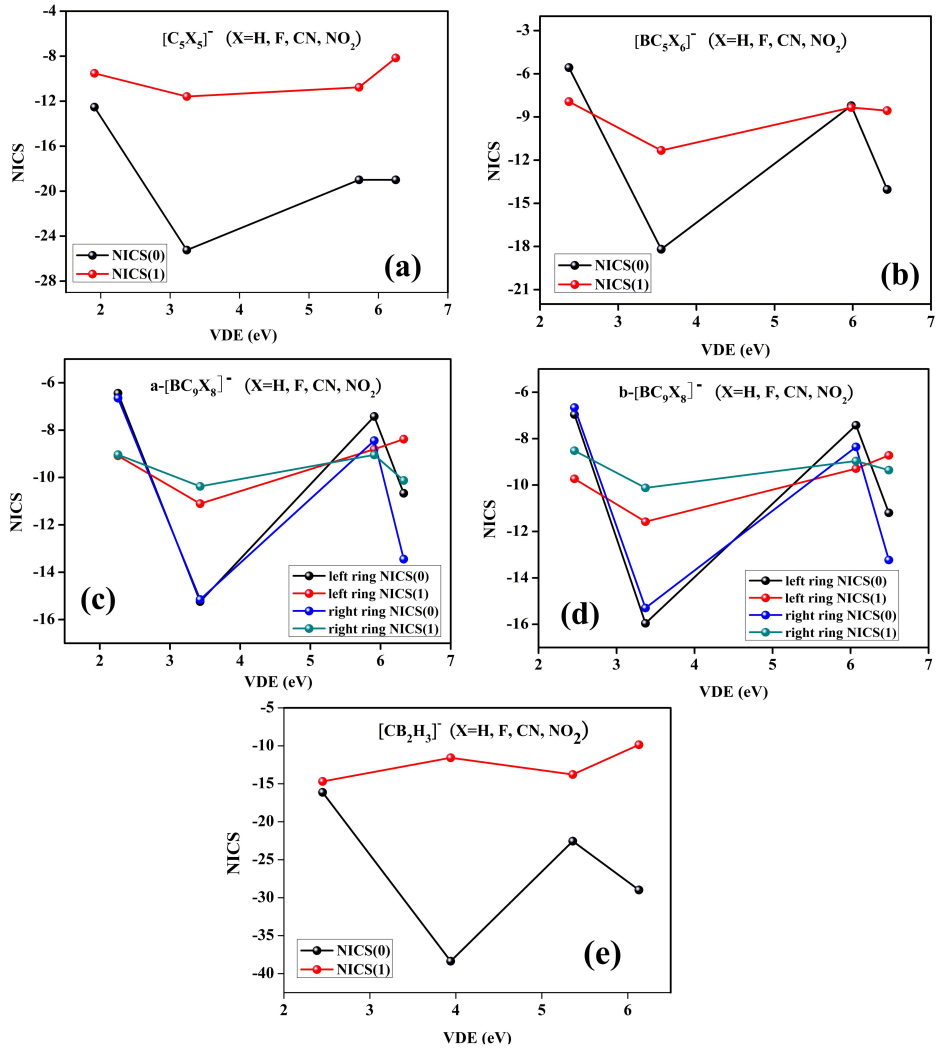

Fig. S19 The relationship between the NICS and the VDE of the superhalogen (a)H/[C_5X_5], (b)H/[BC_5H_6], (c)H/a-[BC_9H_8], (d)H/b-[BC_9H_8], (e)H/CB_2X_3, (X=H, F, CN, NO_2).

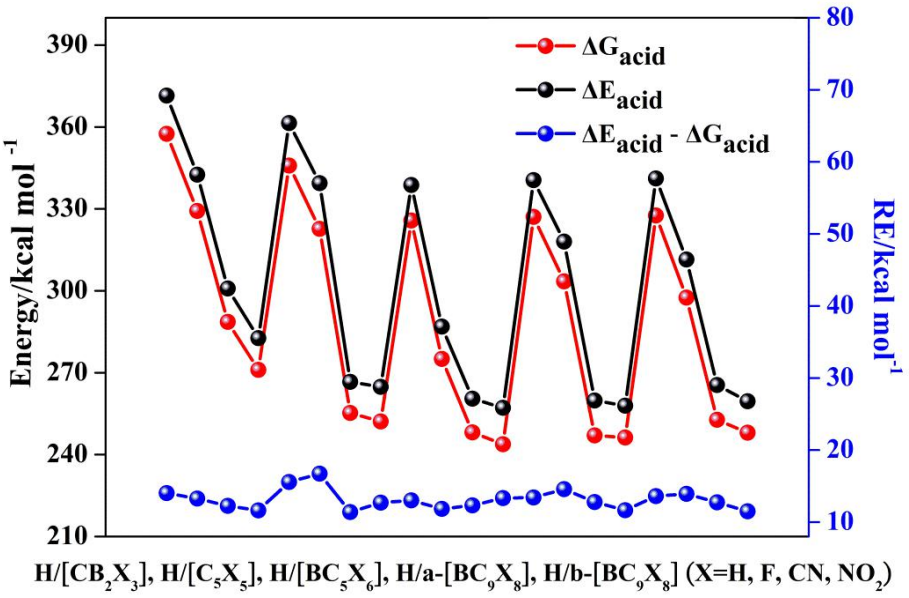

Fig. S20 The comparison between ΔG_{acid} and ΔE_{acid}

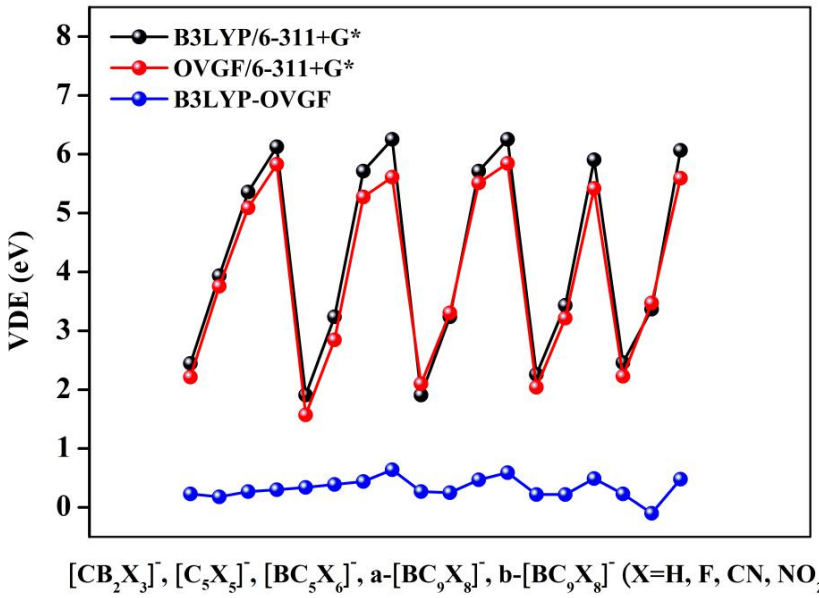

Fig. S21 The comparison between B3LYP and OVGF methods

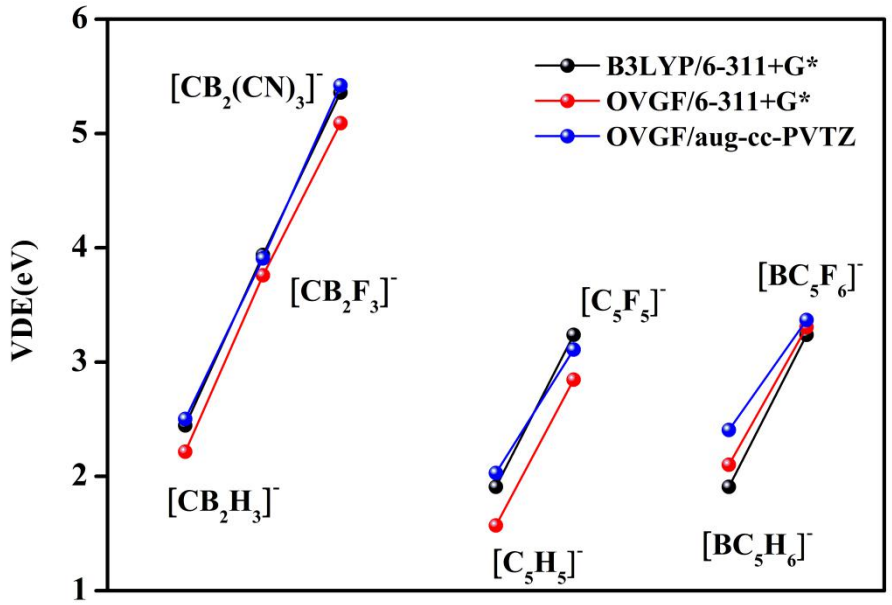

Fig. S22 The comparison among B3LYP/6-311+G*, OVGF/6-311+G* and OVGF/aug-cc-PVTZ methods

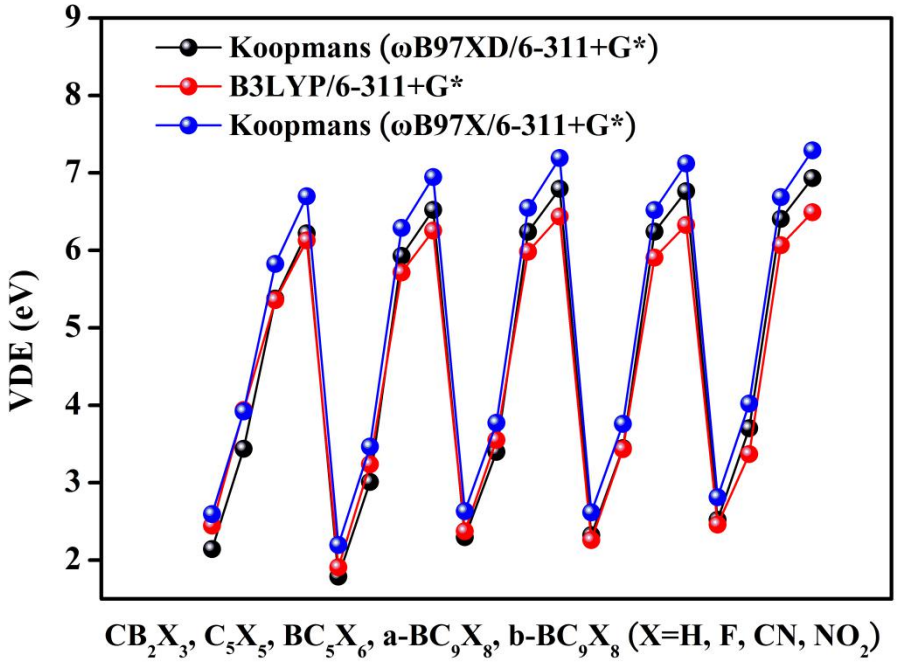

Fig. S23 The comparison between Koopmans energies and VDE values

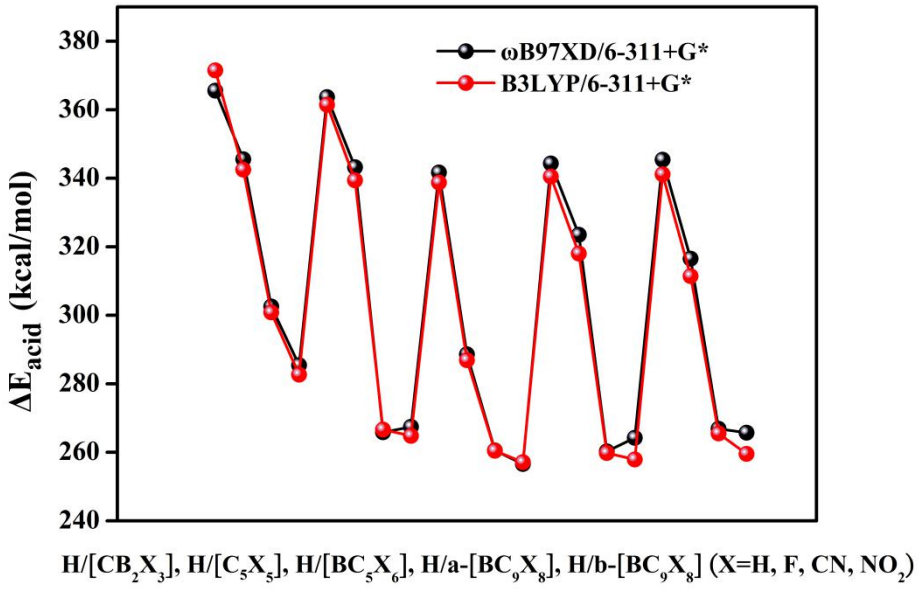

Fig. S24 The comparison between ωB97XD and B3LYP methods

Table. S1 The calculated ΔG_{acid} values of the composites of H/[CB_2X_3], H/[C_5X_5], H/[BC_5X_6], H/a-[BC_9X_8], H/b-[BC_9X_8] (X= H, F, CN, NO_2) (kcal/mol)

	ΔG_{acid}		ΔG_{acid}
H/[CB_2H_3]-A	357.409	H/a-[BC_9F_8]-E	234.774
H/[CB_2H_3]-B	328.323	H/a-[BC_9F_8]-F	303.399
H/[CB_2F_3]-A	329.199	H/a-[BC_9F_8]-G	286.452
H/[CB_2F_3]-B	250.267	H/a-[$BC_9(CN)_8$]-A	237.021
H/[CB_2F_3]-C	306.466	H/a-[$BC_9(CN)_8$]-B	246.835
H/[$CB_2(CN)_3$]-A	288.540	H/a-[$BC_9(CN)_8$]-C	236.309
H/[$CB_2(CN)_3$]-B	256.428	H/a-[$BC_9(CN)_8$]-D	233.783
H/[$CB_2(CN)_3$]-C	272.472	H/a-[$BC_9(CN)_8$]-E	246.965
H/[$CB_2(CN)_3$]-D	263.923	H/a-[$BC_9(CN)_8$]-F	227.998
H/[$CB_2(CN)_3$]-E	263.990	H/a-[$BC_9(NO_2)_8$]-A	209.474
H/[$CB_2(NO_2)_3$]-A	270.983	H/a-[$BC_9(NO_2)_8$]-B	222.823
H/[$CB_2(NO_2)_3$]-B	261.063	H/a-[$BC_9(NO_2)_8$]-C	246.218
C_H/[$CB_2(NO_2)_3$]-C	256.805	H/a-[$BC_9(NO_2)_8$]-D	213.639
H/[$CB_2(NO_2)_3$]-D	260.909	H/a-[$BC_9(NO_2)_8$]-E	227.218
H/[C_5H_5]-A	345.828	H/a-[$BC_9(NO_2)_8$]-F	227.257
H/[C_5F_5]-A	322.639	H/a-[$BC_9(NO_2)_8$]-G	193.261
H/[C_5F_5]-B	259.790	H/b-[BC_9H_8]-A	327.518
H/[$C_5(CN)_5$]-A	250.078	H/b-[BC_9H_8]-B	309.590
H/[$C_5(CN)_5$]-B	255.221	H/b-[BC_9H_8]-C	306.119
H/[$C_5(NO_2)_5$]-A	252.070	H/b-[BC_9H_8]-D	294.829
H/[BC_5H_6]-A	325.707	H/b-[BC_9F_8]-A	285.661
H/[BC_5F_6]-A	274.989	H/b-[BC_9F_8]-B	297.481
H/[BC_5F_6]-B	270.397	H/b-[BC_9F_8]-C	274.711
H/[BC_5F_6]-C	241.702	H/b-[BC_9F_8]-D	262.354
H/[$BC_5(CN)_6$]-A	234.678	H/b-[BC_9F_8]-E	270.676
H/[$BC_5(CN)_6$]-B	248.106	H/b-[BC_9F_8]-F	284.976
H/[$BC_5(CN)_6$]-C	212.345	H/b-[$BC_9(CN)_8$]-A	241.984
H/[$BC_5(CN)_6$]-D	240.188	H/b-[$BC_9(CN)_8$]-B	252.700
H/[$BC_5(CN)_6$]-E	234.680	H/b-[$BC_9(CN)_8$]-C	244.879
H/[$BC_5(NO_2)_6$]-A	209.717	H/b-[$BC_9(CN)_8$]-D	237.822
H/[$BC_5(NO_2)_6$]-B	240.782	H/b-[$BC_9(CN)_8$]-E	222.585
H/[$BC_5(NO_2)_6$]-C	243.737	H/b-[$BC_9(CN)_8$]-F	237.478
H/[$BC_5(NO_2)_6$]-D	240.488	H/b-[$BC_9(CN)_8$]-G	231.229
H/[$BC_5(NO_2)_6$]-E	239.585	H/b-[$BC_9(CN)_8$]-H	221.972
H/a-[BC_9H_8]-A	327.051	H/b-[$BC_9(NO_2)_8$]-A	247.990

H/a-[BC_9H_8]-B	302.561	H/b-[$BC_9(NO_2)_8$]-B	237.701
H/a-[BC_9H_8]-C	325.783	H/b-[$BC_9(NO_2)_8$]-C	244.856
H/a-[BC_9H_8]-D	307.112	H/b-[$BC_9(NO_2)_8$]-D	216.052
H/a-[BC_9F_8]-A	269.370	H/b-[$BC_9(NO_2)_8$]-E	231.212
H/a-[BC_9F_8]-B	273.176	H/b-[$BC_9(NO_2)_8$]-F	212.259
H/a-[BC_9F_8]-C	255.196	H/b-[$BC_9(NO_2)_8$]-G	230.757
H/a-[BC_9F_8]-D	285.510		

Table. S2 The calculated acid dissociation constants(pK_a) of the composites of H/[CB_2X_3], H/[C_5X_5], H/[BC_5X_6], H/a-[BC_9X_8], H/b-[BC_9X_8] (X= H, F, CN, NO_2) in DMSO solvent.

DMSO			
	Gas phase structure	Liquid phase structure	
	pK_a(1)	pK_a(2)	pK_a(2)-pK_a(1)
H/[CB_2H_3]	18.87	19.141	0.271
H/[CB_2F_3]	6.59	6.573	-0.017
H/[$CB_2(CN)_3$]	-5.99	-6.166	-0.176
H/[$CB_2(NO_2)_3$]	-15.54	-15.537	0.003
H/[C_5H_5]	11.84	12.331	0.491
H/[C_5F_5]	6.62	7.715	1.095
H/[$C_5(CN)_5$]	-22.76	-21.946	0.814
H/[$C_5(NO2)_5$]	-29.13	-28.866	0.264
H/[BC_5H_6]	0.98	1.602	0.622
H/[BC_5F_6]	-25.2	-24.878	0.322
H/[$BC_5(CN)_6$]	-22.44	-21.751	0.689
H/[$BC_5(NO_2)_6$]	-33.76	-34.076	-0.316
H/a-[BC_9H_8]	6.28	6.554	0.274
H/a-[BC_9F_8]	0.86	0.987	0.127
H/a-[$BC_9(CN)_8$]	-23.94	-22.821	1.119
H/a-[$BC_9(NO_2)_8$	-29.55	-29.794	-0.244
H/b-[BC_9H_8]	6.72	7.256	0.536
H/b-[BC_9F_8]	-3.16	-3.101	0.059
H/b-[$BC_9(CN)_8$]	-20.59	-19.761	0.829
H/b-[$BC_9(NO_2)_8$]	-28.11	-28.224	-0.114
		MAE	0.3324

Table. S3 The calculated acid dissociation constants(pK_a) of the composites of H/[CB_2X_3], H/[C_5X_5], H/[BC_5X_6], H/a-[BC_9X_8], H/b-[BC_9X_8] (X= H, F, CN, NO_2) in H_2O solvent.

H_2O			
	Gas phase structure	Liquid phase structure	
	pK_a(1)	pK_a(2)	pK_a(2)-pK_a(1)
H/[CB_2H_3]	21.6	21.86	0.26
H/[CB_2F_3]	9.5	9.41	-0.09
H/[$CB_2(CN)_3$]	-2.9	-3.23	-0.33
H/[$CB_2(NO_2)_3$]	-14	-12.9	1.1
H/[C_5H_5]	14.7	15.17	0.47
H/[C_5F_5]	9.7	10.76	1.06
H/[$C_5(CN)_5$]	-19.9	-19.21	0.69
H/[$C_5(NO2)_5$]	-25.9	-25.88	0.02
H/[BC_5H_6]	3.8	4.43	0.63
H/[BC_5F_6]	-22.3	-22.03	0.27
H/[$BC_5(CN)_6$]	-19.6	-18.94	0.66
H/[$BC_5(NO_2)_6$]	-28.3	-28.78	-0.48
H/a-[BC_9H_8]	9.1	9.37	0.27
H/a-[BC_9F_8]	4	4.08	0.08
H/a-[$BC_9(CN)_8$]	-21.1	-20.18	0.92
H/a-[$BC_9(NO_2)_8$	-24.9	-25.47	-0.57
H/b-[BC_9H_8]	9.5	10.1	0.6
H/b-[BC_9F_8]	-0.1	-0.03	0.07
H/b-[$BC_9(CN)_8$]	-17.7	-16.65	1.05
H/b-[$BC_9(NO_2)_8$]	-24.3	-25.06	-0.76
		MAE	0.296

Table. S4 The calculated acid dissociation constants(pK_a) of the composites of H/[CB_2X_3], H/[C_5X_5], H/[BC_5X_6], H/a-[BC_9X_8], H/b-[BC_9X_8] (X= H, F, CN, NO_2) at various theoretical levels in DMSO and H_2O solvent.

	DMSO		H_2O	
	M06-2X	ωB97XD	M06-2X	ωB97XD
H/[CB_2H_3]	18.41	14.53	21.17	17.29
H/[CB_2F_3]	6.42	8.84	9.32	11.74
H/[$CB_2(CN)_3$]	-7.27	-4.72	-4.22	-1.67
H/[$CB_2(NO_2)_3$]	-18.05	-0.30	-16.54	1.21
H/[C_5H_5]	9.25	13.47	12.11	16.34
H/[C_5F_5]	5.39	9.42	8.43	12.46
H/[$C_5(CN)_5$]	-27.48	-23.37	-24.59	-20.48
H/[$C_5(NO2)_5$]	-33.25	-27.19	-30.03	-23.97
H/[BC_5H_6]	-0.60	3.12	2.23	5.95
H/[BC_5F_6]	-29.01	-23.94	-26.15	-21.08
H/[$BC_5(CN)_6$]	-25.44	-22.37	-22.55	-19.49
H/[$BC_5(NO_2)_6$]	-36.65	-34.14	-31.22	-28.71
H/a-[BC_9H_8]	4.63	8.61	7.48	11.47
H/a-[BC_9F_8]	0.00	4.88	3.12	8.00
H/a-[$BC_9(CN)_8$]	-28.05	-23.58	-25.18	-20.70
H/a-[$BC_9(NO_2)_8$	-30.82	-24.90	-26.16	-20.24
H/b-[BC_9H_8]	5.70	9.85	8.52	12.67
H/b-[BC_9F_8]	-4.15	0.56	-1.10	3.61
H/b-[$BC_9(CN)_8$]	-23.90	-19.58	-21.04	-16.72
H/b-[$BC_9(NO_2)_8$]	-28.48	-23.57	-24.64	-19.73

Table. S5 The calculated VDE and ΔG_{acid} of Polycyclic Aromatic Compounds at B3LYP/6-311+G* level.

	VDE (eV)		ΔG_{acid} (kcal/mol)
I	5.57	H-I	251.09
II	5.83	H-II	247.90
III	5.82	H-III	242.00
IV	5.06	H-IV	277.98
V	5.59	H-V	251.82
VI	5.80	H-VI	248.31
VII	5.86	H-VII	234.58

Table. S6 The calculated NICS (0/1) of organic anion at the B3LYP/6-311+G* level of theory (ppm)

	NICS(0)	NICS(1)
$[CB_2H_3]^-$	-16.1218	-14.6903
$[CB_2F_3]^-$	-38.3658	-11.5692
$[CB_2(CN)_3]^-$	-22.5534	-13.7728
$[CB_2(NO_2)_3]^-$	-28.9883	-9.8652
$[C_5H_5]^-$	-12.5288	-9.524
$[C_5F_5]^-$	-25.2403	-11.5868
$[C_5(CN)_5]^-$	-18.9934	-10.7654
$[C_5(NO_2)_5]^-$	-18.9954	-8.1514
$[BC_5H_6]^-$	-5.5705	-7.9342
$[BC_5F_6]^-$	-18.1917	-11.3276
$[BC_5(CN)_6]^-$	-8.2214	-8.3441
$[BC_5(NO_2)_6]^-$	-14.0387	-8.5618

Table. S7 The calculated NICS (0/1) of organic anion at the B3LYP/6-311+G* level of theory (ppm)

	left ring		right ring	
	NICS(0)	NICS(1)	NICS(0)	NICS(1)
a-[BC_9H_8]$^-$	-6.4437	-9.0825	-6.6496	-9.0391
a-[BC_9F_8]$^-$	-15.2418	-11.105	-15.1527	-10.3754
a-[$BC_9(CN)_8$]$^-$	-7.4231	-8.8073	-8.4441	-9.0452
a-[$BC_9(NO_2)_8$]$^-$	-10.6656	-8.3803	-13.4472	-10.1272
b-[BC_9H_8]$^-$	-6.9627	-9.7331	-6.6595	-8.5204
b-[BC_9F_8]$^-$	-15.9588	-11.578	-15.2981	-10.122
b-[$BC_9(CN)_8$]$^-$	-7.4217	-9.2948	-8.3563	-8.9648
b-[$BC_9(NO_2)_8$]$^-$	-11.197	-8.7217	-13.231	-9.356

Table. S8 The calculated VDE values of organic anions under study here with various methods (in eV)

	VDE		
	B3LYP/6-311+G*	**OVGF/6-311+G***	**OVGF/aug-cc-PVQZ**
[CB_2H_3]$^-$	2.446	2.216	2.503
[CB_2F_3]$^-$	3.937	3.759	3.906
[$CB_2(CN)_3$]$^-$	5.358	5.090	5.421
[$CB_2(NO_2)_3$]$^-$	6.127	5.830	
[C_5H_5]$^-$	1.909	1.571	2.030
[C_5F_5]$^-$	3.238	2.846	3.110
[$C_5(CN)_5$]$^-$	5.715	5.275	
[$C_5(NO_2)_5$]$^-$	6.254	5.612	
[BC_5H_6]$^-$	2.374	2.101	2.406
[BC_5F_6]$^-$	3.552	3.305	3.369
[$BC_5(CN)_6$]$^-$	5.983	5.513	
[$BC_5(NO_2)_6$]$^-$	6.437	5.847	
a-[BC_9H_8]$^-$	2.260	2.041	
a-[BC_9F_8]$^-$	3.434	3.216	
a-[$BC_9(CN)_8$]$^-$	5.907	5.418	
a-[$BC_9(NO_2)_8$]$^-$	6.328		
b-[BC_9H_8]$^-$	2.459	2.228	
b-[BC_9F_8]$^-$	3.369	3.473	

b-[$BC_9(CN)_8$]$^-$	6.067	5.592
b-[$BC_9(NO_2)_8$]$^-$	6.491	

Table. S9 The calculated Koopmans energies of organic anions under study here with various methods (in eV)

	ωB97XD/6-311+G*		ωB97X/6-311+G*	
	Koopmans Ⅰ	Koopmans Ⅰ-B3LYP	Koopmans Ⅱ	Koopmans Ⅱ-B3LYP
[CB_2H_3]$^-$	2.142	-0.304	2.595	0.149
[CB_2F_3]$^-$	3.438	-0.498	3.920	-0.017
[$CB_2(CN)_3$]$^-$	5.378	0.020	5.824	0.466
[$CB_2(NO_2)_3$]$^-$	6.220	0.094	6.699	0.573
[C_5H_5]$^-$	1.788	-0.120	2.195	0.286
[C_5F_5]$^-$	3.010	-0.227	3.465	0.227
[$C_5(CN)_5$]$^-$	5.929	0.213	6.291	0.576
[$C_5(NO_2)_5$]$^-$	6.523	0.269	6.946	0.692
[BC_5H_6]$^-$	2.297	-0.077	2.632	0.258
[BC_5F_6]$^-$	3.398	-0.154	3.774	0.222
[$BC_5(CN)_6$]$^-$	6.239	0.256	6.548	0.565
[$BC_5(NO_2)_6$]$^-$	6.794	0.357	7.193	0.756
a-[BC_9H_8]$^-$	2.322	0.062	2.616	0.356
a-[BC_9F_8]$^-$	3.447	0.014	3.761	0.328
a-[$BC_9(CN)_8$]$^-$	6.241	0.334	6.520	0.613
a-[$BC_9(NO_2)_8$]$^-$	6.763	0.434	7.121	0.793
b-[BC_9H_8]$^-$	2.521	0.062	2.813	0.354
b-[BC_9F_8]$^-$	3.702	0.333	4.022	0.654
b-[$BC_9(CN)_8$]$^-$	6.407	0.340	6.687	0.620
b-[$BC_9(NO_2)_8$]$^-$	6.932	0.441	7.290	0.799

Lowest normal mode frequencies and optimized coordinates at B3LYP/6-311+G* level.

$[CB_2H_3]^-$

Lowest normal mode frequency: 571.74 cm^{-1}
Energy -89.6018483 a.u

C	0.00000000	0.00000000	0.75944100
B	0.00000000	0.80154500	-0.46992900
B	0.00000000	-0.80154500	-0.46992900
H	0.00000000	1.94566900	-0.85551300
H	0.00000000	0.00000000	1.85366800
H	0.00000000	-1.94566900	-0.85551300

$[CB_2F_3]^-$

Lowest normal mode frequency: 179.24 cm^{-1}
Energy -387.559558 a.u

C	0.00000000	0.00000000	0.70578000
B	0.00000000	0.80528900	-0.51250800
B	0.00000000	-0.80528900	-0.51250800
F	0.00000000	-2.09195800	-1.00884300
F	0.00000000	2.09195800	-1.00884300
F	0.00000000	0.00000000	2.11661900

$[CB_2(CN)_3]^-$

Lowest normal mode frequency: 82.31 cm^{-1}
Energy -366.5403133 a.u

B	0.00000000	0.78837500	-0.55122300
B	0.00000000	-0.78837500	-0.55122300
C	0.00000000	-2.21452200	-1.07085600
N	0.00000000	-3.29537100	-1.49253800
C	0.00000000	2.21452200	-1.07085600
N	0.00000000	3.29537100	-1.49253800
C	0.00000000	0.00000000	0.68409800
C	0.00000000	0.00000000	2.07765700
N	0.00000000	0.00000000	3.24107300

$[CB_2(NO_2)_3]^-$

Lowest normal mode frequency: 18.09 cm^{-1}
Energy -703.4348707 a.u

B	0.00000000	0.78988400	-0.52836500
B	0.00000000	-0.78988400	-0.52836500
C	0.00000000	0.00000000	0.68017100
N	0.00000000	0.00000000	2.11352000
N	-0.05004800	-2.18787500	-1.07838600
N	0.05004800	2.18787500	-1.07838600
O	0.80329200	-0.73112900	2.69330500
O	-0.80329200	0.73112900	2.69330500
O	1.01103900	-2.71768100	-1.42090900
O	-1.14979500	-2.74089400	-1.17830900
O	-1.01103900	2.71768100	-1.42090900
O	1.14979500	2.74089400	-1.17830900

$[C_5H_5]^-$

Lowest normal mode frequency: 598.7 cm^{-1}
Energy -193.5699266 a.u

C	0.82246400	0.87915500	0.00000000
C	1.09028400	-0.51053400	0.00000000
C	-0.14863100	-1.19468300	0.00000000
C	-1.18214300	-0.22782100	0.00000000
C	-0.58197200	1.05388300	0.00000000
H	-1.10764000	2.00580100	0.00000100
H	-2.24990900	-0.43359900	-0.00000100
H	-0.28288400	-2.27378000	0.00000100
H	2.07507800	-0.97167500	0.00000000
H	1.56534800	1.67325400	0.00000000

$[C_5F_5]^-$

Lowest normal mode frequency: 20.22 cm^{-1}
Energy -689.9105567 a.u

C	-0.15622700	-0.94471600	0.70810700
C	-0.15622700	-0.94471600	-0.70810700
C	0.06262300	0.35883600	-1.13842500
C	0.18898300	1.17337100	0.00000000

C	0.06262300	0.35883600	1.13842500
F	0.00809500	0.81666800	2.43076800
F	0.00809500	-2.08227800	-1.46061500
F	0.00809500	-2.08227800	1.46061500
F	0.00809500	0.81666800	-2.43076800
F	-0.03356400	2.53014700	0.00000000

$[C_5(CN)_5]^-$

Lowest normal mode frequency: 72.95 cm^{-1}
Energy -655.0277154 a.u

C	0.00000000	1.20600000	0.00000000
C	1.14697400	0.37267500	0.00000000
C	0.70886900	-0.97567500	0.00000000
C	-0.70886900	-0.97567500	0.00000000
C	-1.14697400	0.37267500	0.00000000
C	-2.49120600	0.80944200	0.00000000
N	-3.59252100	1.16728100	0.00000000
C	2.49120600	0.80944200	0.00000000
N	3.59252100	1.16728100	0.00000000
C	0.00000000	2.61940900	0.00000000
N	0.00000000	3.77740000	0.00000000
C	1.53965000	-2.11914600	0.00000000
N	2.22030000	-3.05598100	0.00000000
C	-1.53965000	-2.11914600	0.00000000
N	-2.22030000	-3.05598100	0.00000000

$[C_5(NO_2)_5]^-$

Lowest normal mode frequency: 9.43 cm^{-1}
Energy -1216.458059 a.u

C	-0.62921500	1.01608200	-0.00001800
C	-1.16078900	-0.28443300	-0.00001800
C	-0.08819200	-1.19187100	-0.00001800
C	1.10628400	-0.45218400	-0.00001800
C	0.77191300	0.91240600	-0.00001800
N	1.70627500	2.01701200	-0.00002800
N	-1.39102400	2.24605500	-0.00002800
N	-2.56597600	-0.62887300	-0.00002800
N	-0.19483600	-2.63472000	-0.00002800

N	2.44556000	-0.99947300	-0.00002800
O	2.67006300	-1.93991400	-0.75268600
O	3.26437500	-0.48525100	0.75272400
O	-1.01987300	-3.13884700	-0.75268600
O	0.54724600	-3.25455600	0.75272400
O	-3.30037900	0.00000000	-0.75268600
O	-2.92615800	-1.52617500	0.75272400
O	-1.01987300	3.13884700	-0.75268600
O	-2.35571100	2.31132800	0.75272400
O	2.67006300	1.93991400	-0.75268600
O	1.47024900	2.95465400	0.75272400

$[BC_5H_6]^-$

Lowest normal mode frequency: 364.31 cm^{-1}
Energy -219.0788864 a.u

C	0.00000000	1.22012900	0.67713400
C	0.00000000	0.00000000	1.37390600
C	0.00000000	-1.22012900	0.67713400
C	0.00000000	-1.27918800	-0.72009700
C	0.00000000	1.27918800	-0.72009700
H	0.00000000	-2.14168200	1.26865000
H	0.00000000	-2.27958800	-1.16564700
B	0.00000000	0.00000000	-1.52990600
H	0.00000000	2.14168200	1.26865000
H	0.00000000	0.00000000	2.46404700
H	0.00000000	0.00000000	-2.74840400
H	0.00000000	2.27958800	-1.16564700

$[BC_5F_6]^-$

Lowest normal mode frequency: 109.65 cm^{-1}
Energy -814.7813598 a.u

C	0.00000000	1.20953900	-0.66533900
C	0.00000000	0.00000000	-1.35798600
C	0.00000000	-1.20953900	-0.66533900
C	0.00000000	-1.25887300	0.72149900
C	0.00000000	1.25887300	0.72149900
B	0.00000000	0.00000000	1.54411000
F	0.00000000	2.52384900	1.28420000
F	0.00000000	-2.36115800	-1.39800900

F	0.00000000	-2.52384900	1.28420000
F	0.00000000	2.36115800	-1.39800900
F	0.00000000	0.00000000	-2.72675800
F	0.00000000	0.00000000	2.92698400

$[BC_5(CN)_6]^-$

Lowest normal mode frequency: 50.58 cm^{-1}
Energy -772.7957979 a.u

C	0.00000000	1.23198000	-0.68361600
C	0.00000000	0.00000000	-1.38290900
C	0.00000000	-1.23198000	-0.68361600
C	0.00000000	-1.28679200	0.72149900
C	0.00000000	1.28679200	0.72149900
B	0.00000000	0.00000000	1.52026100
C	0.00000000	-2.44471000	-1.44921500
N	0.00000000	-3.42647500	-2.05797400
C	0.00000000	2.55914700	1.36276000
N	0.00000000	3.57772600	1.91272600
C	0.00000000	-2.55914700	1.36276000
N	0.00000000	-3.57772600	1.91272600
C	0.00000000	2.44471000	-1.44921500
N	0.00000000	3.42647500	-2.05797400
C	0.00000000	0.00000000	-2.80874800
N	0.00000000	0.00000000	-3.96535100
C	0.00000000	0.00000000	3.06352700
N	0.00000000	0.00000000	4.22018100

$[BC_5(NO_2)_6]^-$

Lowest normal mode frequency: 39.99 cm^{-1}
Energy -1446.540428 a.u

C	1.21094400	-0.68447100	0.02234800
C	-0.01242100	-1.36820200	-0.00016700
C	-1.22323600	-0.66257800	-0.02276800
C	-1.26513600	0.72130400	-0.02691000
C	1.27772000	0.69837000	0.02649800
B	0.01345400	1.50598100	-0.00012400
N	0.02780700	3.04418700	-0.00002400
N	2.59506200	1.35442400	-0.00902900
N	2.47150500	-1.48969700	0.00836300

N	-0.02567200	-2.83780900	0.00007100
N	-2.49802300	-1.44490600	-0.00850000
N	-2.57042600	1.40093900	0.00906800
O	0.72890500	-3.40522700	0.77758700
O	-0.79042500	-3.39185300	-0.77712400
O	3.19605300	-1.38479800	0.97946600
O	2.66975400	-2.17469500	-0.97790800
O	2.75187500	2.30600100	0.74197600
O	3.43198400	0.93103100	-0.79651500
O	-0.41826300	3.61996300	0.98896100
O	0.48471100	3.61164000	-0.98887500
O	-2.71036100	2.35524600	-0.74184200
O	-3.41461100	0.99260500	0.79678300
O	-2.70843200	-2.12612200	0.97788300
O	-3.22072500	-1.32709300	-0.97951900

a-[BC_9H_8]$^-$

Lowest normal mode frequency: 156.76 cm^{-1}
Energy -372.7651566 a.u

C	-2.44004900	-0.71623300	0.00000000
C	-1.23262400	-1.38081100	0.00000000
C	0.00848300	-0.67928000	0.00000000
C	-0.00749000	0.76615300	0.00000000
C	-1.27653500	1.39883200	0.00000000
C	-2.46981400	0.69832600	0.00000000
H	1.23164700	-2.46534200	0.00000000
H	-3.37199200	-1.27942200	0.00000000
H	-1.21615300	-2.47074500	0.00000000
C	1.24714700	-1.37562400	0.00000000
H	-1.29948500	2.48823500	0.00000000
H	-3.42312200	1.22342100	0.00000000
C	2.56907600	0.70380000	0.00000000
C	2.46392900	-0.70147900	0.00000000
H	1.32806400	2.74868200	0.00000000
H	3.58095600	1.11751800	0.00000000
H	3.37181800	-1.31259400	0.00000000
B	1.32510600	1.53362800	0.00000000

a-[BC_9F_8]$^-$

Lowest normal mode frequency: 61.22 cm^{-1}
Energy -1166.992097 a.u

C	2.44180500	-0.70416400	0.00000000
C	1.24968600	-1.37688900	0.00000000
C	0.00125100	-0.69256500	0.00000000
C	0.01906400	0.76427600	0.00000000
C	1.28173000	1.38868600	0.00000000
C	2.46912600	0.70093000	0.00000000
C	-1.23684000	-1.35789700	0.00000000
C	-2.53861300	0.71008400	0.00000000
C	-2.44652800	-0.67664100	0.00000000
B	-1.30244800	1.54491300	0.00000100
F	3.66666800	1.33751400	0.00000000
F	3.61358500	-1.37942300	0.00000000
F	1.30812000	-2.73174000	0.00000000
F	-1.29808800	-2.72686400	0.00000000
F	-3.58329100	-1.42165100	0.00000000
F	-3.81393800	1.23394500	0.00000000
F	-1.36374700	2.91876700	0.00000000
F	1.36715200	2.74061900	0.00000000

a-$[BC_9(CN)_8]^-$

Lowest normal mode frequency: 23.89 cm^{-1}
Energy -1110.97219 a.u

C	-2.47228000	0.69460900	-0.05707400
C	-1.25904000	1.38073000	-0.13358600
C	-0.00843300	0.68548300	0.00359500
C	-0.01781400	-0.75781600	0.00516200
C	-1.27639900	-1.41364500	0.10329500
C	-2.48953700	-0.71187600	0.11352700
C	1.23116200	1.39191000	0.12257300
C	2.57593100	-0.67502600	-0.09502100
C	2.47087500	0.72024400	0.06901500
B	1.32450100	-1.50739600	-0.10884600
C	-3.73773200	-1.38806800	0.25412000
C	-3.71236700	1.39685200	-0.16962000
C	-1.34720400	2.76857700	-0.46964300
C	1.27427600	2.78289400	0.43445700
C	3.66987400	1.50119400	0.18694500
C	3.86984800	-1.26016000	-0.20381900
C	1.47529900	-3.03155500	-0.28567400

C	-1.38734300	-2.83617000	0.24656100
N	-4.75729100	-1.91847300	0.37222400
N	-4.72441100	1.94631900	-0.25314600
N	-1.51786800	3.85538900	-0.82200500
N	1.37345900	3.88951700	0.75672400
N	4.64779500	2.10874100	0.27655500
N	4.91164200	-1.75553400	-0.29785200
N	1.68299300	-4.15576300	-0.46057600
N	-1.58449000	-3.96335100	0.39884200

a-[$BC_9(NO_2)_8$]$^-$

Lowest normal mode frequency: 25.96 cm^{-1}
Energy -2009.287409 a.u

C	-2.46027000	-0.69257600	0.06482000
C	-1.26629400	-1.36975400	0.12141800
C	-0.00943500	-0.69686200	-0.03537900
C	-0.02649800	0.74934900	-0.04012500
C	-1.28591400	1.37895800	-0.14635600
C	-2.48052400	0.69392400	-0.12945500
C	1.24157400	-1.37757800	-0.14207900
C	2.55348000	0.66372000	0.13217900
C	2.46000800	-0.70787800	-0.06374000
B	1.31627100	1.48400900	0.12276100
N	-3.76327000	-1.40375900	0.21749100
N	-1.35465000	-2.81208500	0.48263700
N	1.28094900	-2.81140400	-0.45849100
N	3.72878400	-1.49270600	-0.21927000
N	3.88412200	1.28327200	0.25669700
N	1.44533500	3.00719800	0.31964800
N	-1.38398400	2.86033200	-0.30531400
N	-3.77865200	1.39366500	-0.27708100
O	-3.91417500	2.09477000	-1.26379300
O	-4.60768600	1.19885900	0.59484900
O	-0.80806100	3.33538800	-1.26624500
O	-2.05402600	3.45998300	0.51479600
O	2.08937300	3.66053400	-0.49210300
O	0.90557900	3.47751300	1.32270500
O	4.73532200	0.99717500	-0.57485700
O	4.03710600	2.06378800	1.18425900
O	3.96220700	-1.93239900	-1.32796600
O	4.42412600	-1.59411300	0.77209800
O	0.49129900	-3.20633900	-1.31297500

O	2.10021400	-3.51244100	0.11236300
O	-2.14043600	-3.50364200	-0.13634600
O	-0.65753900	-3.17020100	1.41788800
O	-4.48380700	-1.40973000	-0.76246200
O	-3.99806500	-1.88907900	1.30582500

b-[BC_9H_8]$^-$

Lowest normal mode frequency: 165.05 cm^{-1}
Energy -372.7641688 a.u

C	-2.44899900	0.59501900	0.00000000
C	-1.27125500	1.31707900	0.00000000
C	0.00000000	0.69367000	0.00000000
C	0.07663900	-0.75369100	0.00000000
C	-1.16780300	-1.46093100	0.00000000
C	-2.38654100	-0.82010800	0.00000000
H	1.08151200	2.55291500	0.00000000
H	-3.41061600	1.10293500	0.00000000
H	-1.30738900	2.40647200	0.00000000
C	1.20133400	1.46530200	0.00000000
H	-1.13135200	-2.54950100	0.00000000
H	-3.30699400	-1.40171400	0.00000000
C	2.45389500	0.89213300	0.00000000
H	1.28912300	-2.50097800	0.00000000
H	3.70266700	-1.15997600	0.00000000
H	3.30434000	1.58103200	0.00000000
B	2.60850100	-0.63188700	0.00000000
C	1.33209800	-1.40709800	0.00000000

b-[BC_9F_8]$^-$

Lowest normal mode frequency: 53.77 cm^{-1}
Energy -1166.989716 a.u

C	2.40367000	-0.73990900	0.00000000
C	1.19671200	-1.38945100	0.00000000
C	-0.03836400	-0.69851800	0.00000000
C	-0.02164700	0.76398700	0.00000000
C	1.26643800	1.38237700	0.00000000
C	2.43066400	0.66445900	0.00000000
C	-1.29392700	-1.36517900	0.00000000
C	-2.49479400	-0.70687800	0.00000000
F	3.62907800	1.29158700	0.00000000

F	3.57161400	-1.42741000	0.00000000
F	1.23931600	-2.74242400	0.00000000
F	-1.31252600	-2.72864800	0.00000000
F	-3.62391500	-1.48764600	0.00000000
F	-3.76858200	1.47605400	0.00000000
F	-1.17045500	2.85340900	0.00000000
F	1.38869800	2.73066400	0.00000000
B	-2.56899900	0.80571900	0.00000000
C	-1.23776300	1.46930000	0.00000000

b-[$BC_9(CN)_8$]$^-$

Lowest normal mode frequency: 32.15 cm^{-1}
Energy -1110.969488 a.u

C	-2.43164600	-0.71363900	-0.13621500
C	-1.20334600	-1.38575000	-0.15740400
C	0.03114700	-0.69427500	0.01486700
C	0.02192100	0.75637200	-0.00293900
C	-1.25739900	1.40003300	0.16627000
C	-2.45184500	0.68451300	0.09654000
C	1.27978800	-1.39810300	0.16733400
C	2.50586700	-0.74186200	0.10149400
C	-3.70926200	1.34468600	0.25608800
C	-3.65772200	-1.41475000	-0.33014500
C	-1.26883900	-2.77953600	-0.48088000
C	1.29960500	-2.78754100	0.52022800
C	3.70925500	-1.48359800	0.28496500
C	3.89831000	1.48826300	-0.35533700
C	1.24625600	2.87548100	-0.43075000
C	-1.37173500	2.78094700	0.51973300
N	-4.73541400	1.85883000	0.38233300
N	-4.66136300	-1.96615700	-0.48427600
N	-1.42142400	-3.87224100	-0.82191400
N	1.40214500	-3.88034400	0.88129100
N	4.71028600	-2.04482900	0.43069100
N	4.91498500	2.01772400	-0.50811600
N	1.35199700	3.99197500	-0.71910000
N	-1.56448200	3.85829700	0.88957600
B	2.55361600	0.76250400	-0.15411200
C	1.23544400	1.47620900	-0.16432400

b-[$BC_9(NO_2)_8$]$^-$

Lowest normal mode frequency: 28.27 cm^{-1}
Energy -2009.284615 a.u

C	-2.41548000	-0.71280200	0.15001300
C	-1.20403200	-1.36700900	0.17519900
C	0.03109800	-0.69134400	-0.00395000
C	0.01135900	0.76162400	0.01903300
C	-1.27479400	1.37698600	-0.17406700
C	-2.44416100	0.66387800	-0.10931900
C	1.29656000	-1.36117300	-0.16152200
C	2.49148200	-0.70558800	-0.10356000
N	-3.69121500	-1.42586800	0.40434700
N	-1.25801500	-2.82520200	0.48789500
N	1.32739800	-2.80898500	-0.52399500
N	3.75609300	-1.43577700	-0.35609500
N	3.89046600	1.47778600	0.37047800
N	1.20290200	2.89892800	0.52052100
N	-1.39257500	2.80187900	-0.58818000
N	-3.77087100	1.31539000	-0.31388600
O	-4.01398300	1.71730600	-1.43418800
O	-4.50147300	1.35671100	0.65752700
O	-0.65133500	3.16000000	-1.48862700
O	-2.24571400	3.47927300	-0.04690000
O	2.08857400	3.60361800	0.06267600
O	0.33080200	3.29180900	1.29629500
O	4.64057400	1.54061100	-0.60136100
O	4.16228400	1.89594400	1.49071200
O	3.92295300	-1.90189100	-1.47088500
O	4.55286200	-1.46229600	0.56458300
O	0.58951700	-3.14732600	-1.43920800
O	2.09990600	-3.53053300	0.07541400
O	-2.02627700	-3.51074900	-0.15813500
O	-0.54387900	-3.20152300	1.40256500
O	-4.53465500	-1.36274600	-0.47239000
O	-3.79818800	-1.99380500	1.47633000
C	1.22436200	1.47099100	0.18759900
B	2.53532500	0.78486800	0.16011600

H/[CB_2H_3]

Lowest normal mode frequency: 533.60 cm^{-1}
Energy -90.1938118 a.u

C	0.00000000	0.00000000	0.79035100

B	0.00000000	0.86286900	-0.35536300
B	0.00000000	-0.86286900	-0.35536300
H	0.00000000	1.94141200	-0.83986800
H	0.00000000	0.00000000	1.86535300
H	0.00000000	-1.94141200	-0.83986800
H	0.00000000	0.00000000	-1.37409100

H/[CB_2F_3]

Lowest normal mode frequency: 153.03 cm^{-1}
Energy -388.1053579 a.u

C	0.00000000	0.00000000	0.69768500
B	0.00000000	0.91216200	-0.41594300
B	0.00000000	-0.91216200	-0.41594300
F	0.00000000	-2.12475600	-0.93793700
F	0.00000000	2.12475600	-0.93793700
F	0.00000000	0.00000000	2.02987500
H	0.00000000	0.00000000	-1.41269500

H/[$CB_2(CN)_3$]

Lowest normal mode frequency: 81.05 cm^{-1}
Energy -367.0197321 a.u

B	0.86399100	-0.46931800	0.00000000
B	-0.86122800	-0.47180400	0.00000000
C	-2.26025600	-1.03845300	0.00000000
N	-3.33094800	-1.47219900	0.00000000
C	2.26335400	-1.03515300	0.00000000
N	3.33414200	-1.46867300	0.00000000
C	0.00000000	0.68388700	0.00000000
C	-0.00304900	2.07859900	0.00000000
N	-0.00553700	3.23492700	0.00000000
H	0.00228200	-1.48605500	0.00000000

H/[$CB_2(NO_2)_3$]

Lowest normal mode frequency: 22.81 cm^{-1}
Energy -703.8852892 a.u

B	0.85927500	-0.47451800	0.02179500
B	-0.85757800	-0.47634900	-0.02232700
C	0.00001800	0.66468800	-0.00066600

N	-0.00099200	2.10446700	-0.00092900
N	-2.26127400	-1.04769800	-0.00589800
N	2.26215300	-1.04768200	0.00675500
O	-0.43085000	2.64562500	1.00197500
O	0.42823000	2.64580500	-1.00401300
O	-2.50771700	-1.85011100	0.88936200
O	-3.03693700	-0.65766900	-0.86637500
O	2.50311100	-1.86600700	-0.87567500
O	3.04312200	-0.64308000	0.85569700
H	0.00051900	-1.49392000	-0.00060400

H/[C_5H_5]

Lowest normal mode frequency: 347.35 cm^{-1}
Energy -194.1458952 a.u

C	0.00000000	0.73433900	-0.99032600
C	0.00000000	-0.73433900	-0.99032600
C	0.00000000	-1.17949700	0.28157700
C	0.00000000	0.00000000	1.21628300
C	0.00000000	1.17949700	0.28157700
H	0.00000000	2.21180400	0.60785600
H	0.87646200	0.00000000	1.87906500
H	0.00000000	-2.21180400	0.60785600
H	0.00000000	-1.34855600	-1.88327600
H	0.00000000	1.34855600	-1.88327600
H	-0.87646200	0.00000000	1.87906500

H/[C_5F_5]

Lowest normal mode frequency: 112.32 cm^{-1}
Energy -690.4514362 a.u

C	0.91824200	-0.01579800	0.74332800
C	0.91824200	-0.01579800	-0.74332800
C	-0.32947900	0.14171300	-1.18019900
C	-1.26182200	0.30078300	0.00000000
C	-0.32947900	0.14171300	1.18019900
F	-0.77692700	0.20459800	2.43043500
F	2.04109400	-0.13856600	-1.43501800
F	2.04109400	-0.13856600	1.43501800
F	-0.77692700	0.20459800	-2.43043500

F	-2.27910400	-0.64362600	0.00000000
H	-1.73729200	1.28838500	0.00000000

H/[$C_5(CN)_5$]

Lowest normal mode frequency: 67.98 cm^{-1}
Energy -655.4526638 a.u

C	-1.15633400	0.00561800	-0.00636300
C	-0.29899600	1.16979100	-0.00105300
C	1.01353400	0.71812900	-0.00173900
C	1.00684400	-0.72697800	-0.00180000
C	-0.30980200	-1.16649400	-0.00108600
C	-0.77908600	-2.49914600	0.00582700
N	-1.20427000	-3.57420800	0.01654400
C	-0.75593700	2.50673700	0.00584300
N	-1.17117600	3.58567800	0.01646800
C	-2.50406400	0.01145600	0.00942300
N	-3.68130900	0.01481800	-0.11563900
C	2.17311700	1.53117900	-0.00160000
N	3.12095200	2.19145200	-0.00072800
C	2.15884900	-1.55073900	-0.00165700
N	3.10051800	-2.21977600	-0.00078100
H	-4.44175600	0.01693900	0.55418200

H/[$C_5(NO_2)_5$]

Lowest normal mode frequency: 22.9 cm^{-1}
Energy -1216.88004 a.u

C	1.20936600	-0.08036100	-0.26313100
C	0.33967500	-1.08028100	-0.04808100
C	-1.02639200	-0.53516800	-0.06306300
C	-0.95987100	0.78480600	-0.30203600
C	0.46513800	1.21512200	-0.44413900
N	0.91665700	2.22317900	0.66718300
N	2.67227800	-0.14586300	-0.36495300
N	0.67380900	-2.48770200	0.17133800
N	-2.23759600	-1.36434500	0.08083700
N	-2.05543000	1.71525400	-0.47098900
O	-3.18798600	1.27170200	-0.38595900
O	-1.73521600	2.87612600	-0.69692500
O	-2.77955900	-1.35383800	1.16085300
O	-2.54526500	-1.98682900	-0.91753800

O	1.76489600	-2.85754200	-0.22208600
O	-0.17442400	-3.15257700	0.74177200
O	3.28707200	-0.35722200	0.65892100
O	3.11501300	0.06144300	-1.47903200
O	0.27327300	2.23870700	1.69110400
O	1.90080600	2.87042700	0.38987400
H	0.69558900	1.70845600	-1.38909200

H/[BC_5H_6]

Lowest normal mode frequency: 128.95 cm^{-1}
Energy -219.6187276 a.u

C	1.26176100	0.67175700	0.00000000
C	0.00000000	1.39360600	0.00000000
C	-1.18987000	0.75967700	0.00000000
C	-1.28409400	-0.73003900	0.00000000
C	1.36031800	-0.68927300	0.00000000
H	-2.10789500	1.34387500	0.00000000
H	-1.89751300	-1.06389100	0.85519200
B	0.07673400	-1.51543600	0.00000000
H	2.16334800	1.28440100	0.00000000
H	0.03801400	2.47933100	0.00000000
H	0.07142100	-2.71292600	0.00000000
H	2.35777600	-1.12408800	0.00000000
H	-1.89751300	-1.06389100	-0.85519200

H/[BC_5F_6]

Lowest normal mode frequency: 11.46 cm^{-1}
Energy -815.2384962 a.u

C	-0.68304000	0.00139600	1.24446600
C	-1.33158300	0.02243500	0.00000000
C	-0.68304000	0.00139600	-1.24446600
C	0.69315700	-0.01476400	-1.29811200
C	0.69315700	-0.01476400	1.29811200
B	1.56512300	-0.20767400	0.00000000
F	1.25304400	0.00257400	2.49697700
F	-1.44405700	0.02402600	-2.34615400
F	1.25304400	0.00257400	-2.49697700
F	-1.44405700	0.02402600	2.34615400
F	-2.65155600	0.02664300	0.00000000
F	2.88086200	0.20123200	0.00000000

H	1.41697200	-1.46550500	0.00000000

H/[$BC_5(CN)_6$]

Lowest normal mode frequency: 54.5 cm^{-1}
Energy -773.2108731 a.u

C	0.00000000	1.23921700	-0.74569400
C	0.00000000	0.00000000	-1.43216500
C	0.00000000	-1.23921700	-0.74569400
C	0.00000000	-1.29546200	0.66073100
C	0.00000000	1.29546200	0.66073100
B	0.00000000	0.00000000	1.41355400
C	0.00000000	-2.45190500	-1.50620300
N	0.00000000	-3.44195400	-2.09981000
C	0.00000000	2.54538000	1.34204700
N	0.00000000	3.51246700	1.97669400
C	0.00000000	-2.54538000	1.34204700
N	0.00000000	-3.51246700	1.97669400
C	0.00000000	2.45190500	-1.50620300
N	0.00000000	3.44195400	-2.09981000
C	0.00000000	0.00000000	-2.86011100
N	0.00000000	0.00000000	-4.01490800
C	0.00000000	0.00000000	2.94915600
N	0.00000000	0.00000000	4.10067200
H	0.00000000	0.00000000	5.10363100

H/[$BC_5(NO_2)_6$]

Lowest normal mode frequency: 31.69 cm^{-1}
Energy -1446.950166 a.u

C	-1.39479200	-0.16231400	0.03107100
C	-0.53365900	-1.24813700	-0.01654200
C	0.85536200	-1.08153300	0.01878000
C	1.43595400	0.17007300	0.07038500
C	-0.92467600	1.15600200	0.05051000
B	0.56274700	1.39216500	0.00826100
N	1.28365300	2.75724800	-0.15540500
N	-1.93914200	2.20289300	0.25342000
N	-2.86893700	-0.44425700	0.00796600

N	-1.09386900	-2.62704600	-0.09269500
N	1.72308200	-2.29800000	-0.08518100
N	2.92306400	0.22713800	0.13630500
O	-1.87368200	-2.84501600	-0.99870800
O	-0.71471100	-3.40439100	0.76136300
O	-3.48467100	0.02868600	-0.92622200
O	-3.30170300	-1.12155900	0.91680500
O	-1.79429200	3.27945000	-0.36089600
O	-2.85621800	1.99565800	1.00784300
O	2.46162800	2.86468100	-0.01361000
O	0.65006800	3.85731900	-0.53490600
O	3.40270400	0.47884300	1.22103000
O	3.52084900	0.02704500	-0.90663700
O	1.54414900	-2.98960100	-1.06884500
O	2.53423100	-2.46405000	0.80179500
H	-0.34462800	3.65226800	-0.60951200

H/a-[BC_9H_8]

Lowest normal mode frequency: 111.17 cm^{-1}
Energy -373.3077847 a.u

C	2.41764800	0.89705200	0.00000000
C	1.15198200	1.47292000	0.00000000
C	0.00000000	0.67144600	0.00000000
C	0.13725500	-0.74704200	0.00000000
C	1.43257300	-1.29744400	0.00000000
C	2.56599700	-0.49352400	0.00000000
H	-1.35161800	2.38174900	0.00000000
H	3.29716400	1.53405800	0.00000000
H	1.05288500	2.55489600	0.00000000
C	-1.32443100	1.29443600	0.00000000
H	1.53958700	-2.37859100	0.00000000
H	3.55699500	-0.93590000	0.00000000
C	-2.52411900	-0.89323700	0.00000000
C	-2.47712400	0.60465700	0.00000000
H	-1.06417700	-2.80618000	0.00000000
H	-3.11763300	-1.25419000	0.85774600
H	-3.41781700	1.15158000	0.00000000
B	-1.13128700	-1.60976500	0.00000000
H	-3.11763300	-1.25419000	-0.85774600

H/a-[BC_9F_8]

Lowest normal mode frequency: 46.69 cm^{-1}
Energy -1167.4988914 a.u

C	2.47562800	-0.70898300	0.10697700
C	1.24835800	-1.36838100	0.14796300
C	0.05452300	-0.66725600	0.07807900
C	0.07393400	0.74234400	-0.02278000
C	1.31139800	1.38230300	-0.05789100
C	2.50857300	0.67412300	-0.00001900
C	-1.22827900	-1.46707700	0.06468200
C	-2.56798900	0.65834500	0.12743400
C	-2.49400700	-0.67721700	0.17509300
B	-1.28300900	1.49974100	-0.02476900
F	3.67860900	1.30890200	-0.03618000
F	3.61048900	-1.39827300	0.17601200
F	1.25784600	-2.70317500	0.26464200
F	-1.29279900	-2.19385100	-1.14338000
F	-3.58268700	-1.44065200	0.29714800
F	-3.76926000	1.26156700	0.21507400
F	-1.37193700	2.81990400	-0.12460900
F	1.39620300	2.71389300	-0.14303800
H	-1.21597000	-2.22273500	0.85558800

H/a-[$BC_9(CN)_8$]

Lowest normal mode frequency: 17.22 cm^{-1}
Energy -1111.3861755 a.u

C	-2.48187200	-0.75161400	-0.08152400
C	-1.23582800	-1.38948200	-0.10852800
C	-0.03114200	-0.64249800	0.03183700
C	-0.08511800	0.78232700	0.05865800
C	-1.36625700	1.40021600	0.09126800
C	-2.55405600	0.65037700	0.05154400
C	1.26163000	-1.30972000	0.12533200
C	2.54801000	0.78332900	-0.12414600
C	2.50800200	-0.59311100	-0.02145400
B	1.24598400	1.57840300	-0.01275900
C	-3.83075200	1.28559300	0.11154900
C	-3.67988500	-1.51924500	-0.20502900

C	-1.21434100	-2.79421000	-0.36466200
C	1.37165600	-2.61808100	0.48680300
C	3.71136900	-1.36962500	-0.03664300
C	3.80768600	1.43047700	-0.28652700
C	1.36309200	3.10362200	-0.00932500
C	-1.52881500	2.81915300	0.17913000
N	-4.87128500	1.78224700	0.16387700
N	-4.64414000	-2.14605000	-0.30106000
N	-1.18077600	-3.92246200	-0.61022000
N	1.53331300	-3.68060700	0.97786000
N	4.65702800	-2.03196500	-0.05047000
N	4.82025100	1.96984700	-0.42432300
N	1.56311800	4.24241100	-0.00815400
N	-1.75903900	3.94688800	0.26400300
H	1.56050500	-4.61923000	0.59348800

H/a-[$BC_9(NO_2)_8$]

Lowest normal mode frequency: 25.87 cm^{-1}
Energy -2009.6983849 a.u

C	-2.21197800	-0.96769600	0.07492100
C	-0.91030900	-1.45292100	0.00607500
C	0.17537200	-0.59639300	-0.21998700
C	-0.05771000	0.80166600	-0.32917300
C	-1.37489500	1.24714500	-0.26320100
C	-2.45062300	0.38718800	-0.07084700
C	1.57511000	-1.07927500	-0.34886500
C	2.47582700	1.08668800	0.45964900
C	2.62273100	-0.31479500	-0.02138500
B	1.24727300	1.70503600	-0.36377200
N	-3.36331100	-1.88779400	0.32855500
N	-0.70216300	-2.91268200	0.22182600
N	1.81561600	-2.39061000	-1.01664500
N	4.03687000	-0.74419300	-0.19132800
N	2.18134700	1.18271400	1.97910000
N	1.32032800	3.20190000	-0.65982000
N	-1.65712200	2.70681500	-0.33509700
N	-3.84243600	0.91636600	-0.01685800
O	-4.17760800	1.61767800	-0.95154800
O	-4.50428000	0.59717500	0.94912500
O	-1.25995800	3.28480300	-1.33221500
O	-2.23350200	3.19803100	0.61522700
O	1.69841000	2.47899800	-1.68378600

O	1.33470900	4.37198500	-0.55931000
O	2.52056000	2.23006700	2.49392900
O	1.59935800	0.25996900	2.50893200
O	4.45237700	-0.86070900	-1.32707600
O	4.66547800	-0.84455200	0.84424600
O	1.03811800	-2.65555100	-1.92205500
O	2.75622900	-3.05629800	-0.64519600
O	-1.44022900	-3.66954800	-0.37235400
O	0.19756700	-3.20907000	0.98947200
O	-4.19443700	-1.94872800	-0.55295000
O	-3.35510600	-2.46348500	1.39546100
H	3.39709600	1.65146700	0.32838000

H/b-[BC_9H_8]

Lowest normal mode frequency: 57.74 cm^{-1}
Energy -373.3078383 a.u

C	2.43203300	0.75562900	0.00000000
C	1.20790900	1.40802000	0.00000000
C	0.00000000	0.68605500	0.00000000
C	0.03392100	-0.72780400	0.00000000
C	1.27733400	-1.36596400	0.00000000
C	2.46566600	-0.64078600	0.00000000
H	-1.17867400	2.49525300	0.00000000
H	3.35522300	1.32582800	0.00000000
H	1.17303900	2.49397400	0.00000000
C	-1.26712800	1.40797200	0.00000000
H	1.31195600	-2.45229600	0.00000000
H	3.41775200	-1.16221400	0.00000000
C	-2.49606300	0.82587400	0.00000000
H	-1.26625700	-2.20682600	0.85783700
H	-3.63687900	-1.28057000	0.00000000
H	-3.36437100	1.48155000	0.00000000
B	-2.59044700	-0.69823300	0.00000000
C	-1.25255500	-1.51511400	0.00000000
H	-1.26625700	-2.20682600	-0.85783700

H/b-[BC_9F_8]

Lowest normal mode frequency: 34.01 cm^{-1}
Energy -1167.4860237 a.u

C	2.42491600	0.72399200	0.01588400

C	1.19412000	1.37747900	0.03941400
C	-0.00869400	0.66289800	-0.01392600
C	0.05041400	-0.75066900	-0.10535300
C	1.28658800	-1.37438800	-0.14458100
C	2.47844900	-0.65606700	-0.07911300
C	-1.31099800	1.34129500	-0.00758500
C	-2.50852000	0.71747100	-0.11118800
F	3.65162400	-1.28190000	-0.11525200
F	3.55113200	1.43150300	0.07409500
F	1.23396900	2.71062400	0.11300400
F	-1.29234900	2.66800100	0.10266900
F	-3.62473900	1.47472000	-0.09693500
F	-3.71089300	-1.46788300	-0.24331700
F	-1.23207400	-2.42243000	1.01068300
F	1.36653000	-2.70471400	-0.26077200
B	-2.56547800	-0.80131800	-0.18362600
C	-1.19490500	-1.60344700	-0.15044700
H	-1.12963200	-2.29608900	-0.99808600

H/b-[$BC_9(CN)_8$]

Lowest normal mode frequency: 29.53 cm^{-1}
Energy -1111.3925686 a.u

C	-2.50719100	-0.61485700	-0.08724600
C	-1.31365400	-1.35212700	-0.15649500
C	-0.04341100	-0.72084600	-0.01864400
C	0.00581400	0.70935600	0.00577000
C	-1.21530800	1.42573000	0.15454900
C	-2.45517000	0.77779300	0.12125600
C	1.18840000	-1.49605300	0.11255000
C	2.44523200	-0.91934600	0.08611400
C	-3.66127700	1.52498600	0.27768000
C	-3.77371900	-1.25878300	-0.22042500
C	-1.46261600	-2.73949100	-0.47012500
C	1.13387900	-2.89798100	0.40405900
C	3.60828800	-1.72484100	0.24979900
C	3.94565800	1.29548600	-0.20780200
C	1.43437900	2.70478900	-0.36435000
C	-1.20328100	2.83145700	0.40362600
N	-4.63269000	2.13495900	0.40584200
N	-4.80784500	-1.76041100	-0.32543700
N	-1.68582200	-3.82186100	-0.80389800
N	1.19177900	-4.00779600	0.71751300

N	4.58553100	-2.32919200	0.37566700
N	4.94765200	1.86376000	-0.30283600
N	1.68994400	3.78461200	-0.75138900
N	-1.17930100	3.96191500	0.63926800
B	2.58788900	0.59612700	-0.08256000
C	1.28861000	1.37417900	-0.10330700
H	1.80802000	4.72074200	-0.39236700

H/b-[$BC_9(NO_2)_8$]

Lowest normal mode frequency: 10.97 cm^{-1}
Energy -2009.6981983 a.u

C	2.40437000	-0.71785200	-0.10859400
C	1.16452200	-1.33162400	-0.21573700
C	-0.03200500	-0.63291500	0.04196500
C	0.05081700	0.76750200	0.24823500
C	1.31437400	1.34646700	0.40049800
C	2.48416100	0.61705800	0.25073500
C	-1.34840300	-1.30426600	0.18130800
C	-2.51451500	-0.64858300	0.24714900
N	3.66735200	-1.46920300	-0.38920500
N	1.14359000	-2.74455900	-0.69311500
N	-1.36889800	-2.77197900	0.49467500
N	-3.79576700	-1.35145900	0.50806100
N	-3.83009100	1.58674000	-0.42452800
N	-1.10780100	2.58271800	-1.04199300
N	1.44212100	2.80888400	0.68281400
N	3.81437200	1.25908700	0.45476500
O	3.98195000	1.78544900	1.53717600
O	4.59693200	1.18555600	-0.46894400
O	0.80099400	3.24024700	1.62677000
O	2.16907900	3.44240800	-0.05404700
O	-1.93254200	3.47582300	-1.05670200
O	-0.28270200	2.34615500	-1.90021300
O	-3.81493600	1.59239400	0.89115000
O	-4.66352300	2.01210300	-1.13026000
O	-3.93466500	-1.90041800	1.58177200
O	-4.63055800	-1.22994700	-0.37227100
O	-0.58238000	-3.12081500	1.36045100
O	-2.17495600	-3.46228600	-0.08609800
O	1.92777000	-3.51980500	-0.19105700
O	0.33688100	-2.97897100	-1.57859700
O	4.42371900	-1.59912100	0.55006800

O	3.81312100	-1.85043500	-1.53070300
C	-1.17732000	1.65127100	0.20692600
B	-2.58435200	0.90277800	0.17542900
H	-1.18186400	2.35546500	1.03968500

H/[CB_2H_3]-B

Lowest normal mode frequency: 146.50 cm^{-1}
Energy -90.1439433 a.u

C	0.00000000	0.78844700	0.00000000
B	-0.71018300	-0.69636400	0.00000000
B	0.77637100	-0.52124600	0.00000000
H	-1.87934900	-0.82862600	0.00000000
H	0.63467700	1.66986000	0.00000000
H	1.94883900	-0.61253400	0.00000000
H	-1.03510600	1.12866700	0.00000000

H/[CB_2F_3]-B

Lowest normal mode frequency: 48.37 cm^{-1}
Energy -387.9720271 a.u

C	-0.61700300	-0.57854100	0.00000000
B	0.00000000	0.66226600	0.00000000
B	0.96333200	-0.53851300	0.00000000
F	1.99170400	-1.35427400	0.00000000
F	-0.57629800	2.79822500	0.00000000
F	-1.55994300	-1.49753300	0.00000000
H	0.18618500	3.33472500	0.00000000

H/[CB_2F_3]-C

Lowest normal mode frequency: 125.01 cm^{-1}
Energy -388.0666069 a.u

C	0.08207800	0.74717400	0.23917400
B	0.77800200	-0.59836000	0.23369400
B	-0.86945400	-0.50430200	0.10578800
F	-2.11467700	-0.81442300	-0.14682900
F	1.89238700	-1.18412900	-0.14462200

F	0.25588600	2.03221500	-0.20038000
H	-0.33757400	0.72729300	1.29402800

H/[$CB_2(CN)_3$]-B

Lowest normal mode frequency: 54.9 cm^{-1}
Energy -366.966308 a.u

B	-1.04875300	-0.47640200	0.06514500
B	0.45370100	-0.76672500	0.31660400
C	1.72060000	-1.50910300	0.00729600
N	2.68917400	-2.10448200	-0.20437300
C	-2.54002400	-0.42740500	-0.08053300
N	-3.68997900	-0.42039700	-0.20794400
C	0.07558000	0.69029800	0.36776300
C	0.83315000	1.83993600	0.02460000
N	1.47008600	2.76014600	-0.26438600
H	-0.84553900	1.00641400	0.91341800

H/[$CB_2(CN)_3$]-C

Lowest normal mode frequency: 46.51 cm^{-1}
Energy -366.992158 a.u

B	-0.76822600	-0.71229100	0.00000000
B	0.80407600	-0.68744200	0.00000000
C	2.25810600	-1.08020800	0.00000000
N	3.37320500	-1.38983200	0.00000000
C	-2.21355800	-1.13675800	0.00000000
N	-3.32369400	-1.46404300	0.00000000
C	0.00000000	0.57007200	0.00000000
C	-0.04982100	1.89852800	0.00000000
N	-0.00058300	3.07388000	0.00000000
H	-0.49010100	3.94882900	0.00000000

H/[$CB_2(CN)_3$]-D

Lowest normal mode frequency: 48.34 cm^{-1}
Energy -366.9793905 a.u

B	0.00000000	0.80395200	0.00000000
B	0.81528400	-0.56917900	0.00000000
C	2.09128100	-1.36523100	0.00000000
N	3.08765800	-1.95388500	0.00000000
C	-0.16973800	2.26163100	0.00000000
N	-0.14113200	3.43250400	0.00000000
C	-0.63275700	-0.50790000	0.00000000
C	-1.88385200	-1.12476400	0.00000000
N	-2.92695600	-1.63005900	0.00000000
H	-0.64301100	4.30379300	0.00000000

H/[$CB_2(CN)_3$]-E

Lowest normal mode frequency: 46.49 cm^{-1}
Energy -366.9795956 a.u

B	0.72437900	-0.34504800	-0.00357200
B	-0.87443300	-0.42336800	-0.00072700
C	-2.16838700	-1.18897200	0.00035100
N	-3.14737900	-1.80623900	0.00126700
C	2.05238300	-0.96180000	-0.00339200
N	3.11472000	-1.45808400	0.00271900
C	-0.13945400	0.82466600	-0.00116100
C	-0.10464100	2.21948400	0.00004700
N	-0.07243100	3.37785200	0.00168100
H	3.64649400	-2.31289300	0.00675400

H/[$CB_2(NO_2)_3$]-B

Lowest normal mode frequency: 42.09 cm^{-1}
Energy -703.8717876 a.u

B	0.94372100	-0.41273500	0.02618100
B	-0.58794500	-0.76614500	-0.39784400
C	0.02920500	0.64557900	-0.75830700
N	-0.46432700	1.84592200	-0.07592200
N	-1.88532200	-1.21226600	0.10642400
N	2.38364500	-0.68349200	0.00966400
O	-0.92880200	1.68837500	1.05268900

O	-0.37221600	2.91685400	-0.65391300
O	-2.82879700	-1.36540700	0.79231300
O	-1.65261500	-1.75329400	-1.08052300
O	3.47138600	-0.96886200	-0.34424400
O	1.99534800	-0.32824500	1.22221000
H	0.33346800	0.85441900	-1.78126600

H/[$CB_2(NO_2)_3$]-C

Lowest normal mode frequency: 21.7 cm^{-1}
Energy -703.8636947 a.u

B	-0.96687200	-0.29806500	-0.07319000
B	0.61338600	-0.54450400	-0.20204900
C	0.00171800	0.75041800	-0.09291200
N	0.36482800	2.15337600	-0.00262100
N	1.86498900	-1.28828600	-0.22372900
N	-2.37115300	-0.80785800	0.07625100
O	-0.28649900	2.93957200	-0.66684800
O	1.29915300	2.43141100	0.73911500
O	2.43712100	-1.70795700	-1.17731700
O	2.43931500	-1.60375300	0.98885200
O	-2.77265300	-0.98586000	1.22426700
O	-3.01484600	-1.01716300	-0.94555600
H	1.93374200	-1.14029100	1.68426100

H/[$CB_2(NO_2)_3$]-D

Lowest normal mode frequency: 13.57 cm^{-1}
Energy -703.8724275 a.u

B	1.09512700	-0.41451900	-0.01971900
B	-0.45389000	-0.82259900	-0.02127900
C	-0.01619200	0.55458300	-0.05283500
N	-0.52108000	1.84259400	-0.04189300
N	-1.85069000	-1.45101000	-0.00121400
N	2.58369200	-0.54021700	0.02824100
O	-1.86176000	1.95088000	0.04857200
O	0.09985600	2.85680000	-0.09750200
O	-2.78581000	-0.62555400	0.15449100

O	-2.03082500	-2.64267600	-0.12979400
O	3.17282800	-0.61866400	-1.04609000
O	3.11213500	-0.56079400	1.13614400
H	-2.24387700	1.01857200	0.09948100

H/[C_5F_5]-B

Lowest normal mode frequency: 24.49 cm^{-1}
Energy -690.342165 a.u

C	-0.92479500	0.85181900	-0.01753900
C	-1.29662200	-0.56925000	0.07281800
C	-0.15766200	-1.19266700	-0.23210900
C	0.92465800	-0.15791200	-0.29772700
C	0.35204700	1.04916400	-0.58678600
F	0.93459100	2.24484600	-0.63781600
F	-2.53142000	-0.98158000	0.32781900
F	-1.54770800	1.75844700	0.67952600
F	0.08252900	-2.45649600	-0.49181100
F	3.50453400	-0.51011900	0.78289000
H	2.63149600	-0.38281000	0.42259100

H/[$C_5(CN)_5$]-A

Lowest normal mode frequency: 55.27 cm^{-1}
Energy -655.444425 a.u

C	-1.29262400	-0.43938000	0.00000000
C	-0.36081700	-0.24825400	1.18812900
C	0.90312100	-0.02693400	0.73672900
C	0.90312100	-0.02693400	-0.73672900
C	-0.36081700	-0.24825400	-1.18812900
C	-0.79086800	-0.33576800	-2.52869900
N	-1.16760900	-0.42107800	-3.61825400
C	-0.79086800	-0.33576800	2.52869900
N	-1.16760900	-0.42107800	3.61825400

C	-2.44613300	0.46069700	0.00000000
N	-3.35588800	1.16637000	0.00000000
C	2.06195000	0.16334800	1.53309200
N	3.01241900	0.31781000	2.16960700
C	2.06195000	0.16334800	-1.53309200
N	3.01241900	0.31781000	-2.16960700
H	-1.66422300	-1.47545500	0.00000000

H/[BC_5F_6]-B

Lowest normal mode frequency: 76.94 cm^{-1}
Energy -815.2335755 a.u

C	-1.32664400	0.48267600	0.02147800
C	-1.11721000	-0.84520400	0.09962600
C	0.25418100	-1.41771700	0.27330700
C	1.39550300	-0.46235600	0.08850300
C	-0.21494100	1.39412100	-0.01978900
B	1.24507400	1.00621300	0.01028600
F	-0.58238300	2.66695500	-0.08824100
F	0.39541000	-2.55677200	-0.50035200
F	2.57106100	-1.09501300	0.11123700
F	-2.56239900	0.98418800	-0.04128000
F	-2.11758200	-1.71577700	0.10596000
F	2.24310000	1.91629500	-0.04964200
H	0.30442800	-1.73907300	1.33067000

H/[BC_5F_6]-C

Lowest normal mode frequency: 33.5 cm^{-1}
Energy -815.1778006 a.u

C	-0.23985500	0.56325500	1.24128500
C	-0.62927400	1.10629600	0.00000000
C	-0.23985500	0.56325500	-1.24128500
C	0.02454400	-0.76447800	-1.32739100
C	0.02454400	-0.76447800	1.32739100
B	0.17469300	-1.57185700	0.00000000
F	0.01931700	-1.39772500	2.50771200

F	-0.33467300	1.33221900	-2.33852600
F	0.01931700	-1.39772500	-2.50771200
F	-0.33467300	1.33221900	2.33852600
F	0.88685900	3.01909400	0.00000000
F	0.33658200	-2.88295000	0.00000000
H	0.15133900	3.59001300	0.00000000

H/[$BC_5(CN)_6$]-A

Lowest normal mode frequency: 20.39 cm^{-1}
Energy -773.1874744 a.u

C	-1.26649400	-0.73263900	-0.21369700
C	-1.23114900	0.62473900	-0.07052300
C	0.02773000	1.37732700	0.01280500
C	1.26872800	0.77812700	-0.04866000
C	-0.00271500	-1.55517900	-0.35429800
B	1.35354700	-0.74648300	-0.20994400
C	-0.07568300	2.79429300	0.16644500
N	-0.15082000	3.94019700	0.28844600
C	-0.02881900	-2.76096600	0.47430700
N	-0.03363500	-3.69195100	1.15276700
C	2.44991700	1.56657700	0.05116100
N	3.43199200	2.17131400	0.12478600
C	-2.50837800	-1.42120400	-0.29270200
N	-3.49658200	-2.01463400	-0.37668800
C	-2.45365000	1.36399600	0.00417000
N	-3.43833600	1.96279400	0.06229300
C	2.68460000	-1.47890200	-0.30695400
N	3.69107800	-2.03976500	-0.40511300
H	0.02187300	-1.90028500	-1.40803500

H/[$BC_5(CN)_6$]-C

Lowest normal mode frequency: 31.68 cm^{-1}
Energy -773.1516687 a.u

C	-1.22053300	0.72763500	-0.05411500
C	-1.27105300	-0.64515100	-0.19083700
C	-0.02471400	-1.47807100	-0.33800800
C	1.29740100	-0.77504900	-0.19570200
C	0.03248800	1.42730700	0.01685900

B	1.37405000	0.71618200	-0.05491700
C	-0.10637300	-2.72173300	0.43965200
N	-0.16181800	-3.68918800	1.06071800
C	-0.01396500	2.83520000	0.15941100
N	-0.01870300	3.98783800	0.27397100
C	2.44505300	-1.58504900	-0.26628300
N	3.40023700	-2.24048100	-0.33246200
C	-2.44831600	1.46414000	0.01987600
N	-3.43167200	2.06448100	0.07722800
C	-2.51196200	-1.32514600	-0.27438400
N	-3.51241700	-1.89971400	-0.35648500
C	2.70359200	1.47107000	0.02596800
N	3.70844900	2.03853500	0.08104600
H	-0.04848800	-1.78211700	-1.40814400

H/[$BC_5(CN)_6$]-D

Lowest normal mode frequency: 41.97 cm^{-1}
Energy -773.1954794 a.u

C	0.84418200	-1.18266100	0.00003800
C	-0.56463500	-1.24684800	0.00053900
C	-1.32304300	-0.04452500	0.00018600
C	-0.75165100	1.25238100	0.00052000
C	1.52203400	0.05304100	-0.00051500
B	0.75753800	1.36817400	-0.00019400
C	-2.71715900	-0.15824100	0.00018100
N	-3.86584600	-0.22026900	-0.01399100
C	2.94527600	0.04357100	-0.00105200
N	4.10153300	0.06783300	-0.00154700
C	-1.63118100	2.36739900	0.00194100
N	-2.38229900	3.24834900	0.00385700
C	1.57070800	-2.41740200	0.00024700
N	2.14911700	-3.41612900	0.00049300
C	-1.25903000	-2.48876300	0.00173900
N	-1.89165300	-3.45687700	0.00326400
C	1.45472200	2.73430200	-0.00019000
N	1.96596600	3.77080800	-0.00003300
H	-4.86675200	-0.27039600	0.03487000

H/[$BC_5(CN)_6$]-E

Lowest normal mode frequency: 20.36 cm^{-1}
Energy -773.1874743 a.u

C	0.02760100	1.37743500	0.01273300
C	-1.23118400	0.62461300	-0.07041300
C	-1.26638500	-0.73277000	-0.21352800
C	-0.00255100	-1.55519500	-0.35440600
C	1.26866300	0.77835800	-0.04856200
B	1.35359400	-0.74623100	-0.20984300
C	-2.50825100	-1.42140900	-0.29228700
N	-3.49639200	-2.01489700	-0.37656000
C	2.44980300	1.56685500	0.05133600
N	3.43183100	2.17163500	0.12521600
C	-0.02837200	-2.76119900	0.47378700
N	-0.03326500	-3.69232100	1.15205300
C	-0.07602000	2.79440000	0.16612700
N	-0.15129100	3.94035400	0.28756800
C	-2.45378300	1.36370900	0.00445300
N	-3.43853100	1.96239000	0.06272200
C	2.68469900	-1.47858400	-0.30692000
N	3.69118400	-2.03948700	-0.40476800
H	0.02196300	-1.89983600	-1.40832600

H/[$BC_5(NO_2)_6$]-A

Lowest normal mode frequency: 38.61cm^{-1}
Energy -1446.8908449 a.u

C	1.30589600	-0.53680400	0.01442100
C	0.13814100	-1.31867300	0.00379800
C	-1.15972500	-0.79019700	0.04702200
C	-1.35853700	0.57461200	0.08936900
C	1.22473600	0.83075700	0.11438900
B	-0.15594500	1.53873300	0.32622100
N	-0.32895300	3.04571700	-0.11675800
N	2.47359400	1.61907000	0.13045000

N	2.63184100	-1.22659500	-0.11688300
N	0.29036100	-2.80686700	-0.04871100
N	-2.32117500	-1.73997300	0.08096400
N	-2.74316200	1.08565200	0.02198600
O	0.84422800	-3.30508200	0.90618900
O	-0.15773700	-3.34421900	-1.03619100
O	3.48710100	-0.89786100	0.67718800
O	2.71870200	-2.03921500	-1.01635600
O	2.74714800	2.18975300	1.16018900
O	3.07681300	1.62321400	-0.92453300
O	-1.41426600	3.56206200	0.10475200
O	0.63023500	3.60360500	-0.63147200
O	-3.08656700	1.47856100	-1.06907100
O	-3.37359100	1.06743300	1.05848900
O	-2.25295800	-2.62310500	0.91410700
O	-3.22087700	-1.52247800	-0.70139400
H	-0.12671900	1.56779200	1.56239200

H/[$BC_5(NO_2)_6$]-B

Lowest normal mode frequency: 17.67cm^{-1}
Energy -1446.9450667 a.u

C	-0.24225700	1.37174600	0.03437800
C	-1.27538100	0.47102000	0.05769500
C	-1.05186100	-0.93085600	0.01676100
C	0.20766300	-1.46731300	-0.01397800
C	1.11712600	0.94287100	0.00430200
B	1.40013500	-0.54847000	0.05276000
N	2.84370200	-1.07239500	0.17328800
N	2.10821000	1.93854200	0.04319100
N	-0.58411200	2.83080400	-0.03390700
N	-2.68125900	0.96188000	0.12753100
N	-2.25897000	-1.81877000	-0.04180000
N	0.36829000	-2.93408200	-0.18072200
O	-3.01905000	1.79689100	-0.68692500
O	-3.36063000	0.47463600	1.01184200
O	-0.30922900	3.38653300	-1.07697000
O	-1.09461200	3.30973200	0.95623700
O	3.33825100	1.68166500	-0.43729700
O	1.95150300	3.04291900	0.46924800
O	3.52576200	-0.91607600	-0.86840000

O	3.26911100	-1.53878200	1.20053700
O	1.22328200	-3.46419800	0.50596200
O	-0.33505700	-3.47905800	-1.01315400
O	-2.97687100	-1.65790500	-1.00801400
O	-2.39728200	-2.60021400	0.87296400
H	3.37514800	0.78655000	-0.88007000

H/[$BC_5(NO_2)_6$]-D

Lowest normal mode frequency: 23.93cm^{-1}
Energy -1446.9406869 a.u

C	-1.15209900	-0.91197700	-0.35174900
C	0.20756600	-1.50709300	-0.26903000
C	1.34031200	-0.54469700	-0.31796600
C	1.20184300	0.77545900	-0.12264700
C	-1.39954700	0.38895200	-0.14212600
B	-0.20825800	1.35263600	0.05647900
N	-0.43598000	2.82266900	0.33564200
N	-2.77675000	0.94739200	-0.14243000
N	-2.22868800	-1.90618000	-0.61283500
N	0.36201400	-2.25267800	1.18177300
N	2.66571400	-1.18582800	-0.57086300
N	2.38737300	1.67180200	-0.10564500
O	0.99918800	-3.27261000	1.14801500
O	-0.13448100	-1.69023600	2.12404700
O	-3.21012400	-1.51967600	-1.21290000
O	-2.00521600	-3.03913900	-0.21613800
O	-2.99505300	1.74623200	-1.03469100
O	-3.51695600	0.61139300	0.75539000
O	-0.14413300	3.59904300	-0.56449800
O	-0.90125200	3.11293200	1.42919600
O	2.46710000	2.38685000	0.87544400
O	3.14103700	1.62761100	-1.05662000
O	2.72927100	-1.84151100	-1.59364800
O	3.53133000	-1.01094900	0.26003100
H	0.35135900	-2.32680300	-0.96980700

H/[$BC_5(NO_2)_6$]-E

Lowest normal mode frequency: 30.12cm^{-1}

Energy -1446.9429268 a.u

C	-1.30468800	-0.51593800	-0.04034900
C	-0.14179300	-1.36814500	-0.00937400
C	1.17640600	-0.78900800	0.04964900
C	1.36615600	0.55692900	0.06374000
C	-1.19157100	0.83817800	-0.07511400
B	0.17648900	1.49566400	-0.02280000
N	0.34105000	3.00684700	-0.04571300
N	-2.41433800	1.68115900	-0.08032300
N	-2.66555100	-1.12587200	0.12715500
N	-0.25072500	-2.73056000	-0.01615300
N	2.36816500	-1.69787800	-0.03486200
N	2.74386100	1.10815100	0.10738900
O	-1.39742700	-3.20772000	-0.59183400
O	0.56491800	-3.52877000	0.38192400
O	-3.43229100	-1.00677800	-0.80307900
O	-2.86581100	-1.67347800	1.19350200
O	-2.45419700	2.51752600	-0.96362200
O	-3.24432600	1.48942600	0.78814100
O	0.88835600	3.48916100	-1.02974200
O	-0.08738600	3.62846500	0.91861200
O	2.92596800	1.96095900	0.95719700
O	3.55341900	0.69199200	-0.69971000
O	2.51893300	-2.27199900	-1.09340600
O	3.06496100	-1.75856000	0.95493600
H	-1.44769400	-4.14514600	-0.32310800

H/a-[BC_9H_8]-B

Lowest normal mode frequency: 148.89 cm^{-1}
Energy -373.2680812 a.u

C	-2.42693300	-0.74127100	-0.08832000
C	-1.24376700	-1.41321900	-0.01016000
C	0.00627800	-0.71667400	0.06598300
C	-0.01535600	0.75879100	0.12262200
C	-1.32396400	1.41252200	0.05411100
C	-2.46612200	0.69498600	-0.07109600
H	1.21654600	-2.47186000	0.07730000
H	-3.35878500	-1.29279200	-0.16314700
H	-1.22826000	-2.49922300	-0.02791800

C	1.22201600	-1.38541500	0.06091400
H	-1.35013900	2.49720600	0.09204400
H	-3.42374700	1.19915600	-0.15250800
C	2.57220500	0.66371800	-0.12349200
C	2.45981200	-0.71277600	-0.01615200
H	1.31911200	2.72709900	-0.09981800
H	3.56996900	1.07213100	-0.26913500
H	3.35663900	-1.33019600	-0.02865600
B	1.34261900	1.53362400	-0.10533700
H	0.48055900	1.06638500	1.13206200

H/a-[BC_9H_8]-C

Lowest normal mode frequency: 100.61 cm^{-1}
Energy -373.3066402 a.u

C	2.41448700	0.86052300	0.00000000
C	1.15131400	1.44192100	0.00000000
C	0.00000000	0.64641100	0.00000000
C	0.11721200	-0.76275200	0.00000000
C	1.41112800	-1.32498100	0.00000000
C	2.54918600	-0.53140100	0.00000000
H	-1.42727800	1.98976000	0.86486000
H	3.29818200	1.49155200	0.00000000
H	1.05975800	2.52547600	0.00000000
C	-1.35489500	1.31278600	0.00000000
H	1.50878100	-2.40681900	0.00000000
H	3.53637300	-0.98275400	0.00000000
C	-2.51614100	-0.92048300	0.00000000
C	-2.55991500	0.42753700	0.00000000
H	-1.06619800	-2.82937200	0.00000000
H	-3.46362900	-1.45692500	0.00000000
H	-3.51395300	0.95635400	0.00000000
B	-1.15580400	-1.63487900	0.00000000
H	-1.42727800	1.98976000	-0.86486000

H/a-[BC_9H_8]-D

Lowest normal mode frequency: 112.23 cm^{-1}
Energy -373.2763769 a.u

C	2.44689700	0.62444300	0.00000000
C	1.31153700	1.34157300	0.00000000

C	0.00000000	0.71436300	0.00000000
C	-0.08480100	-0.75314200	0.00000000
C	1.06787200	-1.47147700	0.00000000
C	2.43329100	-0.87176000	0.00000000
H	-1.09661300	2.53314900	0.00000000
H	3.41341800	1.11973000	0.00000000
H	1.35474800	2.42793500	0.00000000
C	-1.15621100	1.44782200	0.00000000
H	1.01209600	-2.55826500	0.00000000
H	2.99548700	-1.26270500	0.86445200
C	-2.67844600	-0.51187100	0.00000000
C	-2.46044400	0.84287200	0.00000000
H	-1.55024100	-2.63795800	0.00000000
H	-3.71087400	-0.85507000	0.00000000
H	-3.30622400	1.53034400	0.00000000
B	-1.47709100	-1.44227900	0.00000000
H	2.99548700	-1.26270500	-0.86445200

H/a-[BC_9F_8]-A

Lowest normal mode frequency: 57.59 cm^{-1}
Energy -1167.4408636 a.u

C	2.46542600	-0.71456800	-0.03354600
C	1.26094400	-1.38408200	-0.01869800
C	0.04240300	-0.66361800	0.02234400
C	0.05447300	0.76603800	0.06275200
C	1.29341300	1.39478900	0.06195200
C	2.48319400	0.68246000	0.00132500
C	-1.22028100	-1.33394600	0.01921500
C	-2.55801700	0.66529100	-0.02132800
C	-2.46453600	-0.72129000	0.02039100
B	-1.31190000	1.58435500	0.21553100
F	3.65138500	1.31195700	-0.02468700
F	3.61506800	-1.38660100	-0.08176900
F	1.29603900	-2.71904200	-0.04098100
F	-1.24102400	-2.65589500	0.03506200
F	-3.55720900	-1.49525800	0.01696200
F	-3.77333600	1.16374600	-0.10950900
F	-1.38812100	2.87661000	-0.27678300
F	1.38669500	2.72777700	0.12265200
H	-1.48808600	1.52213100	1.46737000

H/a-[BC_9F_8]-B

Lowest normal mode frequency: 39.93 cm^{-1}
Energy -1167.4487409 a.u

C	2.43652900	-0.71399200	-0.01629900
C	1.27817400	-1.40632800	0.10540200
C	0.00960500	-0.73269100	0.14662200
C	0.01829300	0.77044000	0.37680800
C	1.32250100	1.42667400	0.07421200
C	2.45577900	0.72793500	-0.08283500
C	-1.19267300	-1.36375100	0.03129000
C	-2.58112700	0.67668600	-0.02662600
C	-2.45585200	-0.68003000	-0.04050700
B	-1.33670400	1.54073000	0.07003100
F	3.63349200	1.31611300	-0.31253600
F	3.60747500	-1.34241700	-0.09427100
F	1.32800900	-2.74428200	0.12325200
F	-1.28539100	-2.69946500	-0.04964600
F	-3.52909300	-1.45744400	-0.15489000
F	-3.81162700	1.20638000	-0.17833200
F	-1.39525300	2.86901500	0.03907400
F	1.34589200	2.76242900	0.04445000
H	-0.10537900	0.87372400	1.48753000

H/a-[BC_9F_8]-C

Lowest normal mode frequency: 50.95 cm^{-1}
Energy -1167.4200004 a.u

C	2.47098700	-0.69545700	-0.01428200
C	1.30346400	-1.38945200	0.02721200
C	0.03518700	-0.70318300	0.04979100
C	0.00407400	0.76597900	0.02678200
C	1.25805600	1.40961600	0.00239600
C	2.44857300	0.72355800	-0.02449900
C	-1.15303700	-1.38776000	0.05264600
C	-2.53305900	0.73869900	0.04115600

C	-2.47704700	-0.73141300	0.24588400
B	-1.30721900	1.56993000	0.00969300
F	3.60858500	1.36518700	-0.05873700
F	3.64915900	-1.31521900	-0.02762100
F	1.35021000	-2.72194600	0.06180200
F	-1.21775600	-2.70804600	-0.02460500
F	-3.48134100	-1.43536500	-0.38104300
F	-3.78414100	1.21808400	0.06450300
F	-1.34254000	2.92182500	-0.05573800
F	1.33141300	2.74424500	-0.00451700
H	-2.62938400	-0.85206100	1.34262000

H/a-[BC_9F_8]-D

Lowest normal mode frequency: 42.63 cm^{-1}
Energy -1167.4696418 a.u

C	2.49165900	-0.63609900	0.16803600
C	1.35153300	-1.33678400	0.11317400
C	0.05020000	-0.68983500	0.05171500
C	-0.00249900	0.77632200	0.11684600
C	1.16955400	1.44387700	0.16994600
C	2.54323500	0.84353900	0.13331400
C	-1.12436600	-1.36935600	-0.04644700
C	-2.61481300	0.59811200	-0.01643100
C	-2.43549400	-0.74205300	-0.08100800
B	-1.38256200	1.50134400	0.09760900
F	3.17948400	1.28352900	-1.04808800
F	3.67974900	-1.24739000	0.26487000
F	1.40521200	-2.67261500	0.15027300
F	-1.17214900	-2.70116200	-0.11787600
F	-3.46638000	-1.57782700	-0.17717300
F	-3.86585400	1.09025700	-0.04526100
F	-1.50699400	2.82334100	0.17258300
F	1.21180900	2.77179100	0.23447000
H	3.15486200	1.23762900	0.95290000

H/a-[BC_9F_8]-E

Lowest normal mode frequency: 72.14 cm^{-1}
Energy -1167.3871822 a.u

C	-2.46971600	-0.64321600	0.00000000

C	-1.30475200	-1.37195500	0.00000000
C	-0.02658800	-0.74629700	0.00000000
C	0.00000000	0.69692000	0.00000000
C	-1.22523300	1.37339400	0.00000000
C	-2.44611200	0.77051700	0.00000000
C	1.20339500	-1.44221600	0.00000000
C	2.58076800	0.59772200	0.00000000
C	2.43368300	-0.80407900	0.00000000
B	1.33756300	1.34291300	0.00000000
F	-3.59031900	1.45765200	0.00000000
F	-3.65633600	-1.25763800	0.00000000
F	-1.41369800	-2.70505700	0.00000000
F	1.21423700	-2.79066800	0.00000000
F	3.53821300	-1.56206500	0.00000000
F	3.83645600	1.09945900	0.00000000
F	1.29252600	2.92939100	0.00000000
F	-1.16574000	2.77694400	0.00000000
H	0.34147300	3.16854400	0.00000000

H/a-[BC_9F_8]-G

Lowest normal mode frequency: 48.87 cm^{-1}
Energy -1167.471552 a.u

C	2.48134900	-0.69764700	0.20002400
C	1.25606200	-1.51649900	-0.02096700
C	-0.00718200	-0.70305400	0.05899800
C	0.00140500	0.74483500	-0.05875700
C	1.22026200	1.35403300	-0.01157000
C	2.46967100	0.64307500	0.16328900
C	-1.19861600	-1.34326800	0.16360400
C	-2.60818200	0.65519700	0.00213900
C	-2.48936000	-0.68751000	0.14274200
B	-1.33951800	1.51518000	-0.11737900
F	3.58161500	1.36479600	0.30373300
F	3.61468200	-1.37197500	0.37572100
F	1.37194300	-2.09012300	-1.31715400
F	-1.24919400	-2.67584700	0.28602900
F	-3.55349500	-1.48069200	0.26499500
F	-3.83878200	1.19700400	-0.01968300
F	-1.42291400	2.84113900	-0.23373000
F	1.35198400	2.67076700	-0.09480800

H	1.24260000	-2.36649300	0.66395900

H/a-[BC$_9$(CN)$_8$]-A

Lowest normal mode frequency: 20.45 cm^{-1}
Energy -1111.3696416 a.u

C	-2.23068200	-1.02346100	0.10403100
C	-0.90081400	-1.49769000	0.08478300
C	0.16742700	-0.60560800	-0.15843500
C	-0.08890600	0.79258800	-0.24242800
C	-1.42884100	1.24372100	-0.23513500
C	-2.50257500	0.34100500	-0.09016500
C	1.54721900	-1.11526500	-0.36027300
C	2.53691000	1.12966600	0.18719100
C	2.64739300	-0.33693400	-0.18133700
B	1.12625900	1.75308800	-0.21419000
C	-3.85222500	0.80386600	-0.10580800
C	-3.30946800	-1.93151900	0.32517000
C	-0.70051000	-2.87476800	0.41069400
C	1.74054200	-2.43528900	-0.87802000
C	3.96220800	-0.84157100	-0.37802900
C	2.64226500	1.32785400	1.63800900
C	1.11740100	3.25105400	-0.48030100
C	-1.76374300	2.62795900	-0.36186400
N	-4.94567500	1.17252800	-0.12339700
N	-4.18829900	-2.65867900	0.50059700
N	-0.60151000	-3.97260800	0.75318400
N	1.93788900	-3.45818200	-1.37542300
N	5.05590900	-1.18433700	-0.52712000
N	2.66144700	1.48919800	2.78007900
N	1.25150000	4.37273300	-0.72986700
N	-2.09840200	3.72756900	-0.46600900
H	3.35708900	1.68336600	-0.28186100

H/a-[BC$_9$(CN)$_8$]-B

Lowest normal mode frequency: 22.21 cm^{-1}
Energy -1111.3858015 a.u

C	2.55078600	-0.58193900	0.02056500
C	1.38194700	-1.34682700	0.07808200

C	0.08818900	-0.72659500	-0.00465300
C	0.01718700	0.70921200	-0.01076100
C	1.23361500	1.44950500	-0.06082000
C	2.48181900	0.83115700	-0.07623100
C	-1.12584700	-1.49902900	-0.07619500
C	-2.57563600	0.49622400	0.07094600
C	-2.39807600	-0.90819300	-0.02352900
B	-1.36269500	1.35292500	0.04688600
C	3.67784900	1.60525200	-0.15646700
C	3.83396700	-1.20641200	0.08049700
C	1.57418100	-2.74512800	0.30665800
C	-1.11386200	-2.91030600	-0.29736100
C	-3.56021200	-1.74332000	-0.08185600
C	-3.88459900	1.04954300	0.14965300
C	-1.66189000	2.86328300	0.09647300
C	1.19351000	2.87817900	-0.10495000
N	4.63905800	2.24090100	-0.22522700
N	4.88248700	-1.68678200	0.12288200
N	1.84373100	-3.83991200	0.55534900
N	-1.20102500	-4.03730200	-0.53566900
N	-4.52178400	-2.38069400	-0.12220100
N	-4.90942300	1.58173300	0.21854300
N	-2.03266600	3.95184900	0.14496500
N	1.13065500	4.03084600	-0.13938100
H	-2.28133000	4.92326600	0.17044700

H/a-[$BC_9(CN)_8$]-C

Lowest normal mode frequency: 14.55cm^{-1}
Energy -1111.3672781 a.u

C	-2.50063100	-0.77821500	0.03053700
C	-1.26699300	-1.42470300	0.07241100
C	-0.04286500	-0.67390900	0.00491600
C	-0.09694100	0.76767300	-0.00138800
C	-1.38422300	1.38281500	-0.05725900
C	-2.56583200	0.63537800	-0.06138700
C	1.22371700	-1.33635800	-0.05665300
C	2.50167700	0.82340900	0.05561700
C	2.42266300	-0.58577600	-0.02871600
B	1.20588900	1.59358400	0.06363500
C	-3.84068700	1.27175500	-0.13753400
C	-3.71385900	-1.53083700	0.08756300

C	-1.30205300	-2.84266400	0.24272900
C	1.41340500	-2.73886000	-0.22275400
C	3.63334700	-1.29921500	-0.09278400
C	3.78922100	1.41869400	0.10835000
C	1.31654600	3.12057400	0.16480100
C	-1.54704300	2.80292800	-0.13869700
N	-4.87962900	1.77098000	-0.20148400
N	-4.70001200	-2.12862200	0.13038700
N	-1.41657700	-3.97763500	0.42252500
N	1.76021300	-3.82995900	-0.39292600
N	4.65083900	-1.82995100	-0.13734600
N	4.86294300	1.85009000	0.14766100
N	1.53040100	4.25220800	0.26532200
N	-1.77971200	3.92990700	-0.22674900
H	5.53460000	-2.30317900	-0.18841900

H/a-[$BC_9(CN)_8$]-D

Lowest normal mode frequency: 22.92cm^{-1}
Energy -1111.3639567 a.u

C	-2.42436800	-0.84241900	0.03682000
C	-1.16960900	-1.47133900	0.09813000
C	0.05610000	-0.73177500	-0.01004900
C	-0.01083000	0.71489400	0.00048700
C	-1.31021500	1.30001300	-0.06647300
C	-2.50881700	0.56023600	-0.07923400
C	1.32856800	-1.37522800	-0.09867800
C	2.56892000	0.76411200	0.08898800
C	2.53321600	-0.64136700	-0.04465600
B	1.28672600	1.52625800	0.09381800
C	-3.76775800	1.21827900	-0.17773900
C	-3.63295700	-1.59874400	0.11016600
C	-1.21504600	-2.87545800	0.36105500
C	1.45027900	-2.77478500	-0.34785000
C	3.77015800	-1.35997400	-0.13228700
C	3.82545600	1.42743200	0.18112000
C	1.27834200	3.06440300	0.20456500
C	-1.48126600	2.69420800	-0.16216600
N	-4.75973300	1.80465500	-0.26202400
N	-4.62959400	-2.17848500	0.16182900
N	-1.37889700	-3.98169000	0.64952400

N	1.61927400	-3.88729800	-0.61084400
N	4.78051500	-1.91426700	-0.19894600
N	4.82328500	2.00644500	0.26115500
N	1.20870900	4.21571200	0.29150200
N	-1.72428700	3.80912300	-0.29014100
H	-1.74956600	4.81443200	-0.25667000

H/a-[$BC_9(CN)_8$]-F

Lowest normal mode frequency: 16.85cm^{-1}
Energy -1111.3528036 a.u

C	2.43016900	-0.56516200	0.03376600
C	1.24369200	-1.32582700	0.07675800
C	-0.01918400	-0.67777400	-0.01490300
C	-0.05603800	0.78132400	-0.00944900
C	1.17318700	1.49579100	-0.08363100
C	2.41557900	0.85511700	-0.08442000
C	-1.23164100	-1.43031700	-0.08650200
C	-2.64061200	0.59552600	0.06566600
C	-2.49406900	-0.80015000	-0.04874300
B	-1.42090500	1.48212500	0.08031400
C	3.65576000	1.54408600	-0.17401400
C	3.65852100	-1.22016100	0.11950900
C	1.45785700	-2.72518300	0.28437300
C	-1.22340300	-2.84234100	-0.27532200
C	-3.66331400	-1.62646300	-0.12516000
C	-3.95287000	1.14027300	0.13960600
C	-1.62559700	2.99770600	0.21495600
C	1.23704500	2.92324300	-0.19451900
N	4.70914700	2.01571700	-0.24233000
N	4.68445400	-1.73259200	0.21813700
N	1.84712700	-3.79200000	0.49964700
N	-1.26825000	-3.98097800	-0.47155300
N	-4.61326600	-2.27937500	-0.18446900
N	-5.00986900	1.60556500	0.20358300
N	-1.86802800	4.11981800	0.35052900
N	1.42553000	4.05543400	-0.31406600
H	5.56611500	-2.20987600	0.15425500

H/a-[$BC_9(NO_2)_8$]-A

Lowest normal mode frequency: 25.98cm^{-1}
Energy -2009.637354 a.u

C	-2.46044800	-0.70277300	0.10779600
C	-1.25405400	-1.35538300	0.18765500
C	-0.03024500	-0.65101500	-0.00954900
C	-0.05944000	0.76812700	-0.15375100
C	-1.31799400	1.37941500	-0.27962000
C	-2.49688700	0.66655200	-0.17325000
C	1.25124900	-1.30311200	-0.16006000
C	2.56047300	0.71040600	0.02193700
C	2.47996200	-0.66605500	-0.15699900
B	1.30495200	1.59248200	-0.18508900
N	-3.74921000	-1.42804800	0.33428900
N	-1.28335400	-2.79622100	0.57333300
N	1.29894100	-2.77413300	-0.44743900
N	3.73612900	-1.45622500	-0.40504800
N	3.89256900	1.29643500	0.24330100
N	1.36868400	2.93794800	0.67984800
N	-1.42615400	2.84668700	-0.55367800
N	-3.82799700	1.32505500	-0.33622000
O	-4.05822200	1.77539100	-1.43762600
O	-4.54443100	1.31633700	0.64171400
O	-0.68472500	3.28557600	-1.41402100
O	-2.25576300	3.46075200	0.08227500
O	2.36633100	3.62858400	0.56448800
O	0.42893700	3.17894500	1.43010900
O	4.56270500	1.51078900	-0.74408700
O	4.16313900	1.49670200	1.40611600
O	3.78687500	-2.04176100	-1.46790100
O	4.58439700	-1.39384600	0.45778500
O	0.64702000	-3.11883700	-1.41463200
O	1.98588000	-3.45668500	0.27640700
O	-2.01385500	-3.52869400	-0.05747800
O	-0.56871600	-3.08992500	1.51671300
O	-4.52415800	-1.42122700	-0.59940000
O	-3.89367300	-1.93068000	1.42794800
H	1.51835500	1.92876200	-1.34547500

H/a-[$BC_9(NO_2)_8$]-B

Lowest normal mode frequency: 27.43cm^{-1}

Energy -2009.6633501 a.u

C	-2.42596600	-0.74054500	0.13360200
C	-1.20445900	-1.39343500	0.09690700
C	0.02575200	-0.70483200	-0.10756000
C	-0.01983700	0.74237400	-0.09522300
C	-1.30799600	1.35041700	-0.17235300
C	-2.49847800	0.63318700	-0.04567400
C	1.29411200	-1.35926200	-0.20377200
C	2.53508100	0.70030500	0.17520900
C	2.48895000	-0.67085800	-0.07417900
B	1.28595900	1.49056400	0.14587800
N	-3.69946900	-1.49489000	0.35837300
N	-1.26405800	-2.86121900	0.39279500
N	1.36424200	-2.79764100	-0.54054200
N	3.78638100	-1.41078500	-0.21918200
N	3.84723400	1.34565500	0.39446000
N	1.32575900	3.01293200	0.39096200
N	-1.45972600	2.74064600	-0.42722700
N	-3.84132800	1.27389000	-0.17007600
O	-4.10454200	1.77151000	-1.24626400
O	-4.53705300	1.22671100	0.82208000
O	-0.61235500	3.21190500	-1.36450900
O	-2.31407400	3.44347200	0.01936400
O	2.13128900	3.70228800	-0.21535300
O	0.47863700	3.47429900	1.17058000
O	4.68858500	1.21564500	-0.47734900
O	3.96262100	1.97881800	1.42856300
O	4.03738200	-1.83453500	-1.32803900
O	4.46906700	-1.48141200	0.78085700
O	0.60855000	-3.16900700	-1.43119800
O	2.16435600	-3.48958200	0.05615300
O	-1.99908900	-3.52844700	-0.30173100
O	-0.59576200	-3.22561300	1.34010000
O	-4.52078600	-1.42694800	-0.53270900
O	-3.79035000	-2.07477800	1.41931300
H	-0.69780600	4.18835800	-1.34692500

H/a-[$BC_9(NO_2)_8$]-D

Lowest normal mode frequency: 24.18cm^{-1}

Energy -2009.6456869 a.u

C	-2.39884800	-0.75516300	0.08520500
C	-1.21776200	-1.42464400	0.03217800
C	0.03602300	-0.74757600	-0.20483400
C	-0.01820400	0.75793700	-0.39140400
C	-1.37174700	1.37929100	-0.32161800
C	-2.48980900	0.66117400	-0.13991200
C	1.27963700	-1.34216200	-0.26019600
C	2.54170100	0.73409600	0.13729800
C	2.50023800	-0.60055900	-0.14068400
B	1.25881300	1.52896100	0.14032700
N	-3.67371500	-1.47933000	0.37743800
N	-1.26271000	-2.87339700	0.41389300
N	1.42444900	-2.81488800	-0.42871800
N	3.79121700	-1.34326400	-0.33108300
N	3.83282900	1.40559900	0.42015200
N	1.24758200	3.00264800	0.51418300
N	-1.46313900	2.82344900	-0.64953000
N	-3.85497700	1.27880500	-0.14610900
O	-4.23714100	1.74097400	-1.19708800
O	-4.44483700	1.22135800	0.91373000
O	-0.68094400	3.20037700	-1.51197500
O	-2.28776000	3.49039100	-0.06590300
O	1.90259100	3.82647700	-0.09555000
O	0.54609200	3.21584200	1.50762000
O	4.70516500	1.32996500	-0.42214400
O	3.87461600	2.00640700	1.47785800
O	3.95050600	-1.78453800	-1.45219200
O	4.54003600	-1.39959800	0.61539800
O	0.73267200	-3.31979900	-1.29780700
O	2.22643600	-3.37947900	0.28691500
O	-2.00319800	-3.58879100	-0.22313200
O	-0.56792800	-3.17620400	1.36585100
O	-4.49066300	-1.45204400	-0.52059100
O	-3.76985100	-1.99595300	1.46811800
H	0.28147200	0.90038800	-1.46227800

H/a-[$BC_9(NO_2)_8$]-E

Lowest normal mode frequency:16.24 cm^{-1}
Energy -2009.6692871 a.u

C	-2.49714300	-0.61217600	0.03444900
C	-1.34482100	-1.30910100	0.20156300
C	-0.03808000	-0.69594300	0.04058400
C	0.00988000	0.76855900	0.05257100
C	-1.18101700	1.44299800	-0.11138200
C	-2.45208500	0.80198400	-0.21650200
C	1.14221500	-1.40577300	-0.11854000
C	2.61149800	0.54361400	0.06398100
C	2.43034100	-0.79240500	-0.13247100
B	1.40523700	1.43869200	0.19064300
N	-3.81318500	-1.33010500	0.08772800
N	-1.46690900	-2.70836300	0.72193100
N	1.12008900	-2.87665100	-0.31829700
N	3.62034600	-1.65765300	-0.42223800
N	3.98208400	1.10678500	0.09285500
N	1.64530000	2.92560700	0.44130900
N	-1.18432700	2.94039300	-0.09432500
N	-3.55214600	1.55581800	-0.53324100
O	-3.55123700	2.65704700	-1.03945700
O	-4.75320800	0.99963000	-0.19979600
O	-0.66126700	3.49260200	-1.03882700
O	-1.71522700	3.45019500	0.87129000
O	2.23238400	3.56994500	-0.41661000
O	1.26033600	3.35749100	1.52514900
O	4.70067100	0.89388700	-0.86569500
O	4.25445800	1.75995900	1.08357400
O	3.63003400	-2.16061100	-1.52861400
O	4.45599200	-1.74750000	0.44860000
O	0.31953400	-3.29785500	-1.13933800
O	1.90305900	-3.53693700	0.33536800
O	-2.27886900	-3.44485800	0.20629200
O	-0.74908200	-2.95730200	1.67527500
O	-4.30653900	-1.59238300	-0.98780500
O	-4.25928700	-1.55439000	1.19243600
H	-5.42369200	1.55380300	-0.64350800

H/a-[$BC_9(NO_2)_8$]-F

Lowest normal mode frequency: 21.24 cm^{-1}
Energy -2009.6695035 a.u

C	2.51045900	-0.58667500	-0.01019600
C	1.32724800	-1.33595200	-0.23851100

C	0.02171800	-0.70116200	-0.07614000
C	-0.01625100	0.75644200	-0.09134000
C	1.18316800	1.41416700	0.12059300
C	2.42727300	0.76027100	0.23067600
C	-1.16936700	-1.39697900	0.13072800
C	-2.60899900	0.56959600	-0.11228500
C	-2.44437900	-0.76203200	0.13841900
B	-1.39287100	1.44336900	-0.25259800
N	3.87641200	-1.19054900	-0.13384000
N	1.41058900	-2.61722800	-0.74110900
N	-1.16477900	-2.85221200	0.39693100
N	-3.64646800	-1.59419100	0.47365300
N	-3.97380900	1.14498700	-0.17044000
N	-1.58284900	2.92709200	-0.56548200
N	1.22829900	2.90524700	0.21780400
N	3.64762600	1.54087100	0.58139100
O	3.53916300	2.25063200	1.56332400
O	4.62864900	1.38978900	-0.11722600
O	0.58359900	3.41119000	1.11104500
O	1.92402600	3.45826800	-0.61137100
O	-2.23625000	3.61762500	0.20167600
O	-1.07811600	3.30987000	-1.62124100
O	-4.69441500	0.99106900	0.79784600
O	-4.23974300	1.74588800	-1.19514800
O	-3.66132300	-2.04689000	1.60157000
O	-4.48665400	-1.71202700	-0.39012600
O	-0.32919300	-3.26632800	1.18977200
O	-1.98340900	-3.53230400	-0.19080800
O	2.52893100	-3.30616500	-0.38327900
O	0.59571400	-3.17222600	-1.44359400
O	4.45307000	-1.40596300	0.90945000
O	4.26429700	-1.39228200	-1.26410600
H	2.54724500	-4.09217400	-0.96331000

H/a-[$BC_9(NO_2)_8$]-G

Lowest normal mode frequency: 24.44 cm^{-1}
Energy -2009.6128429 a.u

C	2.48496100	-0.64578200	-0.05842300
C	1.35975400	-1.36685800	-0.25916800

C	0.01593500	-0.70120300	-0.36673500
C	-0.00771300	0.80184500	-0.15362800
C	1.22971500	1.43693500	0.05500300
C	2.42299200	0.75966700	0.15316700
C	-1.22666900	-1.42462000	0.04907700
C	-2.56173200	0.59076700	-0.12482500
C	-2.43722700	-0.79154300	0.10022700
B	-1.36623000	1.47894200	-0.24237700
N	3.84686500	-1.28153700	-0.07040900
N	1.47442500	-2.78157100	-0.68524400
N	-1.15221500	-2.85712500	0.41175100
N	-3.67092600	-1.58483500	0.43511500
N	-3.92893200	1.15504900	-0.15907700
N	-1.57384800	2.97838800	-0.49115600
N	1.27437800	2.91801300	0.28387100
N	3.68848100	1.49046900	0.43690300
O	3.72981700	2.09789200	1.48556700
O	4.55246600	1.39347100	-0.41085200
O	0.58613200	3.32821500	1.19692500
O	2.00449600	3.55334400	-0.44649500
O	-2.34266500	3.60038600	0.22772600
O	-0.96332600	3.44587500	-1.45445500
O	-4.57435300	1.08829400	0.86872300
O	-4.26713400	1.64339100	-1.21823600
O	-3.71360500	-2.06440700	1.54769700
O	-4.50434500	-1.64528200	-0.44382600
O	-0.30336300	-3.10777800	1.25778500
O	-1.92451400	-3.63359600	-0.10186300
O	2.30124500	-3.47564400	-0.13995500
O	0.71057600	-3.10804300	-1.58514100
O	4.41426500	-1.28033400	1.00174300
O	4.24214800	-1.69258500	-1.13656500
H	-0.13925400	-0.75353400	-1.47875600

H/b-[BC_9H_8]-B

Lowest normal mode frequency: 65.68 cm^{-1}
Energy -373.2781538 a.u

C	2.42543800	-0.77201500	-0.00082700
C	1.23698600	-1.42118900	-0.00499800
C	-0.02238000	-0.70215500	-0.00298500
C	0.00650000	0.77765300	0.00003800

C	1.31218400	1.39825900	0.00562900
C	2.45738500	0.66814200	0.00530700
H	-1.17509300	-2.47053500	-0.01856500
H	3.35868900	-1.32520800	-0.00197700
H	1.20004000	-2.50677900	-0.00886200
C	-1.20562900	-1.38181200	-0.00802100
H	1.35416900	2.48315700	0.00927100
H	3.41958100	1.17145400	0.00884200
C	-2.52435400	-0.70536000	0.00961900
H	-1.02521300	2.61542600	-0.01399900
H	-3.54174400	1.47195800	-0.01751400
H	-3.16947000	-1.12018700	-0.78272700
B	-2.50863000	0.86640000	-0.01433100
C	-1.15423000	1.53379900	-0.00749500
H	-3.06920500	-1.02321600	0.91957900

H/b-[BC_9H_8]-C

Lowest normal mode frequency: 65.55 cm^{-1}
Energy -373.2740841 a.u

C	-2.35914500	0.86046200	0.00357300
C	-1.04009700	1.44351500	-0.00025500
C	0.11261000	0.70386900	-0.00192000
C	0.03531700	-0.75931400	-0.00087300
C	-1.33993700	-1.40133700	-0.00529800
C	-2.51196600	-0.47628100	0.00262100
H	1.36962900	2.46302600	-0.00306600
H	-3.22191400	1.51869700	0.00743100
H	-0.96227100	2.52783200	-0.00039700
C	1.39895500	1.37343700	-0.00190200
H	-1.42690300	-2.06513700	-0.87778600
H	-3.50352300	-0.92004900	0.00579600
C	2.57473700	0.69421100	0.00019200
H	1.05789200	-2.59240300	0.00422600
H	3.56361000	-1.49095200	0.00681500
H	3.49427000	1.27713200	0.00034800
B	2.55523600	-0.84402700	0.00270200
C	1.17596700	-1.50752500	0.00233400
H	-1.42561000	-2.08422900	0.85229100

H/b-[BC_9H_8]-D

Lowest normal mode frequency: 112.58 cm^{-1}
Energy -373.2560633 a.u

C	-2.34376400	-0.79147600	-0.23573600
C	-1.17191700	-1.43017100	-0.08978000
C	0.06262000	-0.69027800	0.36105100
C	0.01199400	0.80457100	0.12858200
C	-1.31218800	1.39887000	0.11240500
C	-2.42611400	0.64847800	-0.06086300
H	1.34962200	-2.45600500	0.14852200
H	-3.24147400	-1.34122500	-0.50034100
H	-1.09920100	-2.50663000	-0.21484700
C	1.37319900	-1.36707700	0.08757600
H	-1.38034400	2.48228000	0.15035900
H	-3.39823900	1.12714900	-0.12716500
C	2.51985300	-0.69792500	-0.14245300
H	1.04169200	2.61333700	-0.11083000
H	3.52042900	1.47152100	-0.35149900
H	3.42385000	-1.28746200	-0.28822000
B	2.51369900	0.84476100	-0.18687700
C	1.15699500	1.53177700	-0.03479000
H	-0.00890000	-0.76738200	1.47245200

H/b-[BC_9F_8]-A

Lowest normal mode frequency: 47.49 cm^{-1}
Energy -1167.4680545 a.u

C	2.39162800	0.69381100	-0.16266800
C	1.10552100	1.34799800	-0.01125100
C	-0.08161700	0.67302300	0.03482300
C	-0.02087300	-0.78140600	-0.07833500
C	1.29706500	-1.51433800	0.01528200
C	2.48394500	-0.64079400	-0.18665100
C	-1.36692300	1.34456600	0.10249200
C	-2.54905400	0.68504500	0.01785800
F	3.65488200	-1.25537200	-0.33241500

F	3.45706800	1.48301600	-0.29287800
F	1.18577200	2.66828800	0.05247600
F	-1.36446700	2.67502100	0.23508700
F	-3.68924900	1.40206600	0.07917700
F	-3.68706800	-1.53955100	-0.27476100
F	-1.08678500	-2.83532600	-0.30492100
F	1.41567200	-2.08547300	1.30604700
B	-2.56821100	-0.83010200	-0.15868600
C	-1.16924400	-1.49238900	-0.18784500
H	1.32595200	-2.35660900	-0.67911000

H/b-[BC_9F_8]-C

Lowest normal mode frequency: 41.9 cm^{-1}
Energy -1167.4488309 a.u

C	2.41142100	-0.74966100	-0.02724600
C	1.23918500	-1.41453400	0.02323100
C	-0.03448200	-0.71698700	0.05289600
C	-0.01892700	0.77863500	0.05175100
C	1.28014900	1.40567400	0.00477400
C	2.42653000	0.68445200	-0.03693700
C	-1.21840800	-1.39085400	0.06680700
C	-2.53852200	-0.74056200	0.27128700
F	3.61183200	1.28394300	-0.07739800
F	3.58244300	-1.38638700	-0.05114200
F	1.25918000	-2.74925600	0.05520700
F	-1.27066100	-2.71890800	0.00099900
F	-3.55578600	-1.43572900	-0.36923300
F	-3.70384300	1.47850600	-0.05149300
F	-1.15042300	2.85103200	-0.02043400
F	1.38009300	2.73881400	0.01127700
B	-2.55275000	0.82682600	0.05886900
C	-1.19456900	1.50050100	0.07039000
H	-2.72601400	-0.83225700	1.36389500

H/b-[BC_9F_8]-D

Lowest normal mode frequency: 39.22 cm^{-1}
Energy -1167.4294479 a.u

C	-2.45830800	-0.66510300	-0.13996000
C	-1.31108200	-1.35354800	-0.09591900
C	-0.00843500	-0.71237200	-0.04935700
C	0.06868100	0.75709600	-0.10819900
C	-1.11862400	1.42916500	-0.14207300
C	-2.49093800	0.81231000	-0.17492400
C	1.17273500	-1.40961800	0.04326200
C	2.44803500	-0.78115900	0.07503900
F	-3.21541800	1.32915900	0.90670200
F	-3.64973800	-1.27054300	-0.22212500
F	-1.36045900	-2.68792500	-0.11631400
F	1.18049900	-2.74420600	0.11092500
F	3.47602300	-1.62656300	0.16604900
F	3.86300500	1.30126000	0.03304100
F	1.31847800	2.76603600	-0.16634500
F	-1.18642700	2.74277600	-0.14474400
B	2.65245400	0.70576600	0.01084300
C	1.34976700	1.42584000	-0.08798200
H	-3.00690800	1.16555300	-1.07822800

H/b-[BC_9F_8]-E

Lowest normal mode frequency: 43.31 cm^{-1}
Energy -1167.4434759 a.u

C	2.27829200	-0.88202800	-0.23318200
C	1.07855800	-1.45399100	-0.09110700
C	-0.07040300	-0.67517800	0.53307900
C	0.05057100	0.81497000	0.22669900
C	1.40395900	1.33625200	0.28772500
C	2.46059800	0.52734300	0.06595100
C	-1.42871200	-1.28408600	0.33871900
C	-2.53067800	-0.60013200	-0.00807300
F	3.70944200	0.98856000	0.07139000
F	3.34447100	-1.55393400	-0.67540900
F	0.89224900	-2.74087800	-0.38716000
F	-1.50119700	-2.58089800	0.65301300
F	-3.70863700	-1.25167200	-0.08143700
F	-3.50967200	1.64133100	-0.56116000
F	-0.93970400	2.87767400	-0.25977500
F	1.60137500	2.64328400	0.48932100
B	-2.44626400	0.91311800	-0.24075500
C	-1.05233400	1.54682000	-0.06330100
H	0.09727700	-0.75661800	1.62567800

H/b-[BC_9F_8]-F

Lowest normal mode frequency: 37.57 cm^{-1}
Energy -1167.4663239 a.u

C	-2.44387800	-0.91747300	-0.13142700
C	-1.04274700	-1.44492600	-0.15855100
C	0.08912100	-0.70459700	-0.10281300
C	-0.04583100	0.76751700	-0.04226900
C	-1.39410000	1.32400700	-0.11519300
C	-2.48939300	0.56024000	-0.16914100
C	1.41657300	-1.32065300	-0.09276100
C	2.56283000	-0.61259600	0.00207800
F	-3.71193400	1.09396300	-0.26807400
F	-3.06447000	-1.39247500	1.04151600
F	-1.03082900	-2.77316400	-0.21485000
F	1.47495000	-2.65182600	-0.17648200
F	3.73509000	-1.27444700	0.00982300
F	3.58214500	1.67397000	0.19638800
F	0.99980400	2.86545900	0.12706900
F	-1.52732300	2.65189300	-0.16178600
B	2.50072600	0.91046200	0.09606200
C	1.08051100	1.52451900	0.05941800
H	-3.01904600	-1.34889100	-0.95878500

H/b-[$BC_9(CN)_8$]-A

Lowest normal mode frequency: 27.66 cm^{-1}
Energy -1111.3748998 a.u

C	-2.48193100	-0.67977400	-0.10239900
C	-1.23883000	-1.34670500	-0.08262700
C	-0.02490500	-0.61365200	-0.00676300
C	-0.08370000	0.79521400	-0.05506400
C	-1.32438200	1.45089400	-0.08410600
C	-2.52970200	0.72360800	-0.08650200
C	1.28713600	-1.29250000	0.10032200
C	2.48074000	-0.67058800	-0.19729900
C	-3.78278400	1.40436400	-0.10440000
C	-3.69895300	-1.42470800	-0.15982800

C	-1.28606800	-2.76634400	-0.23960900
C	1.35331100	-2.63442100	0.58860200
C	3.70321200	-1.39981200	-0.16665200
C	3.72880800	1.58824500	-0.95716700
C	1.47020600	2.18245200	1.24955800
C	-1.37070900	2.87917500	-0.12907100
N	-4.79397200	1.96066200	-0.11805800
N	-4.69037100	-2.01332700	-0.20376300
N	-1.41165500	-3.89664200	-0.43778700
N	1.49980100	-3.67841300	1.06095000
N	4.72132200	-1.94677100	-0.16521000
N	4.63642300	2.16808100	-1.37872100
N	1.73100900	2.55754400	2.30875800
N	-1.38189200	4.03209300	-0.18356200
B	2.49890400	0.84392500	-0.46148600
C	1.18087100	1.63889200	-0.08564100
H	1.03690000	2.49176700	-0.75892600

H/b-[$BC_9(CN)_8$]-C

Lowest normal mode frequency: 24.78 cm^{-1}
Energy -1111.3793943 a.u

C	-2.51248100	-0.61531900	-0.08373600
C	-1.32667800	-1.35088800	-0.12441800
C	-0.05000000	-0.71513200	0.00831900
C	0.00001200	0.73079400	0.00383100
C	-1.23885300	1.44943400	0.11627500
C	-2.46638400	0.79126500	0.08820400
C	1.15958000	-1.49434400	0.13014500
C	2.42068800	-0.90632200	0.07275300
C	-3.68741600	1.52138200	0.21229400
C	-3.77786700	-1.26173700	-0.21679400
C	-1.47193000	-2.74487400	-0.41029900
C	1.12973700	-2.89570900	0.42507400
C	3.60931300	-1.68148800	0.19556500
C	3.86732700	1.28404200	-0.23341600
C	1.42339300	2.80087400	-0.28101200
C	-1.28185400	2.86246000	0.32484100
N	-4.68112800	2.09955100	0.31336900
N	-4.80989400	-1.76806200	-0.32150800
N	-1.68936400	-3.83610500	-0.71827200

N	1.22864600	-4.00276700	0.73888100
N	4.63263200	-2.21400200	0.27770200
N	4.88841900	1.80477000	-0.33501600
N	1.74862100	3.89542400	-0.47227500
N	-1.40814600	3.98919500	0.54337700
B	2.50195500	0.58802400	-0.09912900
C	1.26065600	1.39638800	-0.10457300
H	5.77825800	2.25889900	-0.42648800

H/b-[$BC_9(CN)_8$]-D

Lowest normal mode frequency: 31.74 cm^{-1}
Energy -1111.3685978 a.u

C	-2.38382400	-0.84043100	-0.16019100
C	-1.09675300	-1.46242300	-0.13086200
C	0.09163200	-0.73159700	0.04720000
C	0.02019200	0.72347600	0.02282100
C	-1.30168800	1.30543200	0.17591600
C	-2.48707100	0.53114400	0.03804200
C	1.38835500	-1.37660400	0.18532000
C	2.56947900	-0.66454400	0.07628000
C	-3.76027900	1.16817300	0.11995700
C	-3.56422600	-1.61567200	-0.35744800
C	-1.11165700	-2.86892800	-0.38783300
C	1.47702000	-2.75991500	0.54430000
C	3.81646800	-1.33291100	0.23610900
C	3.81431500	1.65403000	-0.44687400
C	1.04302000	2.89384100	-0.39712900
C	-1.46472100	2.62167600	0.55279600
N	-4.76673900	1.72964700	0.19150500
N	-4.53427300	-2.22094600	-0.51657800
N	-1.23811000	-3.98004100	-0.67535700
N	1.63127200	-3.84468500	0.90896400
N	4.85262700	-1.83068600	0.35898800
N	4.77271200	2.27133900	-0.63925800
N	0.90651100	4.02381000	-0.61210300
N	-1.67162700	3.66004400	1.04978100
B	2.53631600	0.84909900	-0.19683800
C	1.17348600	1.49699300	-0.16716200
H	-1.69068300	4.64469800	0.81515900

H/b-[$BC_9(CN)_8$]-E

Lowest normal mode frequency: 28.35 cm^{-1}
Energy -1111.343919 a.u

C	-2.33830200	-1.20423400	-0.21883400
C	-0.89588300	-1.65253500	-0.00238400
C	0.11978500	-0.76312000	0.21269400
C	-0.19143600	0.67926300	0.16662800
C	-1.58216200	1.06774000	0.46745700
C	-2.60403000	0.19192800	0.30182100
C	1.51760200	-1.19595300	0.38219000
C	2.56198400	-0.34074100	0.13397900
C	-3.95558200	0.51202200	0.59651800
C	-2.68405500	-1.29577700	-1.64834500
C	-0.74588800	-3.05755200	-0.15983800
C	1.79635000	-2.51162000	0.86408900
C	3.90697100	-0.78281800	0.28228100
C	3.36499000	2.05207300	-0.75065800
C	0.51132000	2.95870100	-0.40896400
C	-1.85396900	2.34632600	1.04629300
N	-5.07007700	0.71225800	0.82720400
N	-2.94231300	-1.35159600	-2.76944500
N	-0.77440400	-4.19914600	-0.34039900
N	2.07730100	-3.53628000	1.31712200
N	5.01275000	-1.09992000	0.39251000
N	4.20965200	2.75402600	-1.11346200
N	0.36456500	4.07042800	-0.68935800
N	-2.10937100	3.33544800	1.58332200
B	2.25820900	1.11495000	-0.28749000
C	0.79287000	1.58529500	-0.15333700
H	-2.99116300	-1.90527000	0.31546500

H/b-[$BC_9(CN)_8$]-F

Lowest normal mode frequency: 26.72 cm^{-1}
Energy -1111.3674313 a.u

C	-2.43741000	-0.78876400	-0.12551400
C	-1.18542400	-1.40408200	-0.13794000
C	0.01742500	-0.65424800	0.00493100
C	-0.04841900	0.78560100	0.01293000

C	-1.35620300	1.38113700	0.13418800
C	-2.51935400	0.61395600	0.06156300
C	1.30646500	-1.29900300	0.10115700
C	2.53485800	-0.59498900	0.03748700
C	-3.80672300	1.22227900	0.17182900
C	-3.62359700	-1.56345500	-0.28499300
C	-1.14681400	-2.81227100	-0.37325500
C	1.43267300	-2.65222400	0.39707300
C	3.74878000	-1.32441300	0.13965800
C	3.82084500	1.70022200	-0.27107400
C	1.12523000	2.96206900	-0.29004200
C	-1.54363400	2.76998200	0.41180200
N	-4.85823600	1.68983700	0.25823700
N	-4.57894600	-2.19889800	-0.41403800
N	-1.09577700	-3.94593800	-0.58926200
N	1.67764000	-3.71507700	0.79661500
N	4.72698700	-1.93745900	0.22231800
N	4.82079000	2.26879000	-0.38233000
N	1.23183000	4.09526000	-0.50026100
N	-1.80764100	3.85509200	0.70543300
B	2.51435100	0.91147200	-0.12346100
C	1.15064200	1.55230000	-0.10571300
H	1.79568200	-4.70319800	0.63581100

H/b-[$BC_9(CN)_8$]-G

Lowest normal mode frequency: 29.63 cm^{-1}
Energy -1111.357332 a.u

C	-2.45736500	-0.57286300	-0.07710200
C	-1.23710600	-1.28970800	-0.10994000
C	0.04087800	-0.65720500	0.01853100
C	0.08651400	0.79708900	-0.02084100
C	-1.16996800	1.48504100	0.13066900
C	-2.40812800	0.82276100	0.09196400
C	1.24590400	-1.41337800	0.16550900
C	2.50436200	-0.81458000	0.12316000
C	-3.63437700	1.54292900	0.22166500
C	-3.69690800	-1.25772300	-0.20848500
C	-1.38119900	-2.64893800	-0.40433800
C	1.15413500	-2.81483000	0.43426700
C	3.65648800	-1.62916700	0.29972300
C	3.99728900	1.35341600	-0.27787100
C	1.40979600	2.86032100	-0.40438100

C	-1.23817600	2.88218700	0.41574300
N	-4.64332300	2.09429500	0.32083800
N	-4.67507600	-1.86320800	-0.31926700
N	-1.62045900	-3.71278900	-0.78736400
N	1.04194200	-3.93999000	0.67563500
N	4.60475300	-2.27677400	0.43945300
N	5.04201100	1.83192500	-0.40296200
N	1.57339100	3.97433000	-0.67031600
N	-1.41409300	3.98117400	0.72538100
B	2.62348800	0.69201000	-0.11719100
C	1.33004200	1.46006100	-0.15962000
H	-1.69456200	-4.71526300	-0.71574500

H/b-[$BC_9(CN)_8$]-G

Lowest normal mode frequency: 21.51 cm^{-1}
Energy -1111.341689 a.u

C	2.48229400	0.39979600	-0.13626800
C	1.42122800	1.26317900	-0.26802100
C	0.04017500	0.79245100	-0.13243100
C	-0.18270100	-0.67360400	-0.13471400
C	0.97290900	-1.51138200	0.16991100
C	2.24930600	-0.99412400	0.17740000
C	-1.01646500	1.66766100	-0.01977500
C	-2.45963800	1.20050300	-0.02066200
C	3.36950300	-1.81841900	0.48814300
C	3.82506000	0.85393000	-0.28957900
C	1.72077500	2.61059800	-0.62695500
C	-0.89136100	3.07237400	0.14841000
C	-3.05991300	1.38541200	1.30640500
C	-4.07070900	-0.81602600	-0.74134200
C	-1.63629100	-2.59286100	-0.70682000
C	0.81399900	-2.87219700	0.57006100
N	4.28860900	-2.47096200	0.73848100
N	4.91783900	1.20442300	-0.41435500
N	2.03314600	3.66470900	-0.98064400
N	-0.94888400	4.21296900	0.33397500
N	-3.51511200	1.48727700	2.36070600
N	-5.14121000	-1.15747000	-1.01484700
N	-1.89733000	-3.66870800	-1.04275100
N	0.76378300	-3.95562300	0.96631100
B	-2.66820900	-0.31440100	-0.42459600

C	-1.43580300	-1.21526200	-0.41518500
H	-3.01906300	1.84352000	-0.71660600

H/b-[$BC_9(NO_2)_8$]-B

Lowest normal mode frequency: 28.14 cm^{-1}
Energy -2009.685201 a.u

C	2.48376800	-0.59936200	-0.12880200
C	1.32170000	-1.32241900	-0.19415200
C	0.03857100	-0.70959100	-0.04697600
C	-0.00596000	0.73695600	-0.06815900
C	1.23026600	1.42914100	0.15076300
C	2.43470100	0.77929600	0.13137000
C	-1.18505500	-1.44447700	0.12960700
C	-2.41614200	-0.84237100	0.15474800
N	3.81522500	-1.24432500	-0.32642300
N	1.46275600	-2.76950100	-0.53917900
N	-1.14527300	-2.92037000	0.38624300
N	-3.65078300	-1.59059400	0.47169800
N	-3.90137400	1.29356000	-0.34707800
N	-1.36128500	2.78655000	-0.66337000
N	1.23711600	2.86247200	0.56534300
N	3.71859600	1.49941000	0.39084700
O	3.87865900	1.92200000	1.51599100
O	4.48246200	1.56468100	-0.55023500
O	0.42390800	3.16529800	1.42380900
O	2.06307800	3.59017900	0.05808200
O	-2.41009300	3.36827500	-0.38043200
O	-0.46262100	3.26913400	-1.33312100
O	-4.56446500	1.50584400	0.79301500
O	-4.39341700	1.56299300	-1.38186900
O	-3.63589900	-2.37911600	1.39346000
O	-4.63451700	-1.28441400	-0.19800400
O	-0.44705400	-3.26944100	1.32247300
O	-1.82129200	-3.62675500	-0.32973200
O	2.24051900	-3.42916300	0.11616500
O	0.79734900	-3.14236200	-1.49054300
O	4.58054000	-1.17982800	0.61438600
O	4.01200800	-1.74845500	-1.41316900
C	-1.26037600	1.38606500	-0.24993500
B	-2.50071900	0.62217900	-0.13671100

H	-5.44338800	1.87831500	0.56400100

H/b-[$BC_9(NO_2)_8$]-C

Lowest normal mode frequency: 24.67 cm^{-1}
Energy -2009.6957696 a.u

C	2.44764100	-0.66917300	-0.16371700
C	1.24297000	-1.33650300	-0.25521800
C	0.00708600	-0.67200100	-0.07501400
C	0.01995600	0.75827800	-0.02735000
C	1.26911500	1.38603400	0.21121100
C	2.45807000	0.68435800	0.15628800
C	-1.25861000	-1.37830900	0.13274600
C	-2.45934300	-0.76068100	0.17883700
N	3.74672100	-1.36506100	-0.40985900
N	1.29295100	-2.77635500	-0.64861800
N	-1.22125500	-2.82883600	0.51767700
N	-3.69439200	-1.52052600	0.51100600
N	-3.94469900	1.34025900	-0.30719800
N	-1.21108400	2.73844800	-0.69442400
N	1.34549600	2.81336900	0.64243600
N	3.76883600	1.34584500	0.43873900
O	3.93386800	1.72726500	1.57798400
O	4.54144500	1.40960800	-0.49428500
O	0.53496100	3.15838700	1.48580300
O	2.21196400	3.50043700	0.14380000
O	-2.38427500	3.42585300	-0.57218000
O	-0.28915800	3.30418900	-1.24430400
O	-4.56860500	1.56367500	0.72594800
O	-4.34384900	1.53726900	-1.44408500
O	-3.77072700	-1.98569100	1.63134900
O	-4.53633400	-1.55460800	-0.36457000
O	-0.43708500	-3.10340200	1.41123000
O	-1.98552900	-3.57857800	-0.04585500
O	2.10089000	-3.48366600	-0.08754900
O	0.52046000	-3.09731200	-1.53706500
O	4.51587300	-1.40458000	0.52735900
O	3.91027200	-1.79585700	-1.53251800
C	-1.24457900	1.47318500	-0.19051200
B	-2.56407400	0.73371000	-0.09013800
H	-2.28486800	4.20640000	-1.14974300

H/b-[$BC_9(NO_2)_8$]-D

Lowest normal mode frequency: 16.08 cm^{-1}
Energy -2009.6484114 a.u

C	-2.39980800	-0.73141000	0.22545900
C	-1.18954800	-1.37540200	0.24651700
C	0.04383200	-0.70150200	0.01685300
C	0.03822400	0.76563700	0.05961500
C	-1.22576700	1.37240100	-0.17739800
C	-2.41410300	0.64306700	-0.11633900
C	1.28539900	-1.37156400	-0.19580800
C	2.48782900	-0.71430200	-0.15272400
N	-3.68038400	-1.45808100	0.44219100
N	-1.22039900	-2.82979300	0.61199900
N	1.28642800	-2.81396500	-0.59400400
N	3.73997800	-1.44421000	-0.45559700
N	3.91781700	1.43684700	0.37499100
N	1.22803800	2.88639800	0.61925500
N	-1.35327400	2.82475700	-0.49505100
N	-3.66482900	1.25407900	-0.37888200
O	-3.68799900	1.96213300	-1.52179600
O	-4.64966300	1.11755900	0.27257000
O	-0.62898600	3.24332900	-1.37466800
O	-2.21151500	3.45018700	0.10592600
O	2.11193900	3.59881400	0.18325700
O	0.34078300	3.24840200	1.39301000
O	4.63641600	1.51026600	-0.61830200
O	4.21284500	1.82323000	1.49786200
O	3.89019200	-1.81352400	-1.60470700
O	4.52131900	-1.55571200	0.46650000
O	0.46742800	-3.12338600	-1.44775200
O	2.10540600	-3.54144900	-0.07653900
O	-2.02692600	-3.53217900	0.04154700
O	-0.44402700	-3.15764800	1.49033200
O	-4.45889800	-1.46948100	-0.49536100
O	-3.84256300	-1.94107300	1.54239100
C	1.25133300	1.46440700	0.25089300
B	2.55746800	0.76999300	0.17213000
H	-4.51131400	2.49408100	-1.51154100

H/b-[$BC_9(NO_2)_8$]-E

Lowest normal mode frequency: 17.2 cm^{-1}
Energy -2009.6698329 a.u

C	2.26347600	-0.96448000	-0.08587300
C	0.93078200	-1.56275300	0.06895100
C	-0.20528700	-0.83176600	0.15998900
C	-0.15330600	0.64313900	0.11880700
C	1.19429200	1.21910800	0.25650800
C	2.31555800	0.48222300	0.20309600
C	-1.49116200	-1.52286300	0.22132000
C	-2.67856600	-0.89814400	0.10299100
N	2.69749200	-1.18098700	-1.71199700
N	3.28725100	-1.83311400	0.71001500
N	-1.42486800	-3.00776500	0.38172400
N	-3.93930700	-1.67830500	0.10549500
N	-3.97725100	1.38216700	-0.25821300
N	-1.35981900	2.79989400	-0.22991000
N	1.33718900	2.67575700	0.58517200
N	3.66613500	1.11311600	0.28965400
O	3.91567300	1.78182100	1.26441100
O	4.38782000	0.87282700	-0.66153700
O	0.72845000	3.02509000	1.58032400
O	2.03973000	3.34804700	-0.13270700
O	-2.11291700	3.40666600	0.50722600
O	-0.67865200	3.26183700	-1.12910600
O	-4.74512300	1.43970600	0.69098400
O	-4.15116300	1.87636700	-1.36590600
O	-4.07988900	-2.52236100	0.97067800
O	-4.72934000	-1.38416800	-0.77238000
O	-1.02070000	-3.40729700	1.45606900
O	-1.74264500	-3.67060200	-0.58597700
O	4.08845900	-1.24356400	1.39846100
O	3.16481000	-3.02876600	0.56806300
O	3.64930800	-1.86655800	-1.93202200
O	1.95784900	-0.60089300	-2.46082500
C	-1.32433800	1.32991700	-0.04459200
B	-2.68261700	0.61563200	-0.07037400
H	0.92326300	-2.64500100	0.07506300

H/b-[$BC_9(NO_2)_8$]-F

Lowest normal mode frequency: 17.48 cm^{-1}
Energy -2009.6957696 a.u

C	2.41856700	-0.64835700	-0.22228700
C	1.29624700	-1.35239800	-0.41485300
C	-0.05931900	-0.70027200	-0.49248200
C	-0.07948800	0.82202300	-0.23880200
C	1.18946600	1.45081400	0.07085600
C	2.34980900	0.75510600	0.10975600
C	-1.24128900	-1.42269300	0.14456500
C	-2.45197400	-0.85212700	0.17029200
N	3.78725500	-1.25312400	-0.33342000
N	1.36553200	-2.76625900	-0.86326100
N	-1.01869100	-2.75964700	0.75637400
N	-3.64356700	-1.56813600	0.70538400
N	-3.94969600	1.18513700	-0.61933300
N	-1.43370300	2.89922500	-0.47676900
N	1.23039900	2.86208500	0.57540800
N	3.62853400	1.42067400	0.50810300
O	3.70676600	1.80256000	1.65430700
O	4.46415400	1.48590300	-0.36988000
O	0.46599900	3.10509600	1.49027600
O	2.03433800	3.60750000	0.06204600
O	-2.36200100	3.40693600	0.12523700
O	-0.64712500	3.47037400	-1.21705800
O	-4.81481700	1.42462400	0.19515500
O	-4.03903000	1.29870400	-1.84679900
O	-3.65463700	-1.82247300	1.89228700
O	-4.51314700	-1.78652100	-0.11411000
O	-0.03834000	-2.81176000	1.48893900
O	-1.80739500	-3.64430800	0.52247000
O	2.30019000	-3.43907100	-0.49170100
O	0.44560100	-3.12358600	-1.59030600
O	4.38397100	-1.35540200	0.71830600
O	4.16593100	-1.53364800	-1.44730800
C	-1.29743000	1.43119500	-0.35150300
B	-2.59039300	0.61169400	-0.28495100
H	-0.28168300	-0.77733100	-1.57080200

H/b-[$BC_9(NO_2)_8$]-G

Lowest normal mode frequency: 22.05 cm^{-1}
Energy -2009.6735669 a.u

C	2.43872400	-0.65904100	-0.10540600
C	1.27022700	-1.35178800	-0.17450700
C	-0.01052000	-0.70022800	-0.01867800
C	-0.01318900	0.75446400	-0.09200200
C	1.25056900	1.41948600	0.13851100
C	2.42416400	0.73344700	0.15941500
C	-1.23301800	-1.37766100	0.16076300
C	-2.47130300	-0.72006500	0.17921100
N	3.75865800	-1.33150700	-0.29657300
N	1.37858900	-2.79471200	-0.55063600
N	-1.24182900	-2.86742800	0.32383200
N	-3.61890900	-1.48394300	0.55222900
N	-3.88561400	1.50572300	-0.04880700
N	-1.18886000	2.79070900	-0.92029200
N	1.28107400	2.85160100	0.56794500
N	3.72766000	1.40050000	0.46249800
O	3.88544300	1.77884000	1.60241600
O	4.50538400	1.46299600	-0.46678900
O	0.41713400	3.18023300	1.36354200
O	2.17482300	3.54479600	0.13447100
O	-2.21347600	3.44905300	-0.86358800
O	-0.17283300	3.12363900	-1.51958000
O	-4.17133500	2.26614000	0.84037600
O	-4.67855500	1.17212800	-0.96739500
O	-3.60193500	-2.37076700	1.34541700
O	-4.79855400	-1.21455400	0.00040800
O	-0.57054400	-3.29847900	1.24356700
O	-1.93072100	-3.50540100	-0.44556500
O	2.12672400	-3.49105200	0.10000100
O	0.71971300	-3.12281500	-1.52268500
O	4.50549100	-1.30092600	0.66043800
O	3.96268100	-1.81973400	-1.38825900
C	-1.21813200	1.43826800	-0.32604600
B	-2.52745000	0.77524000	-0.09220500
H	-4.73877700	-0.42687300	-0.63212100