

The Remarkable Ability of Anions to Bind Dihydrogen

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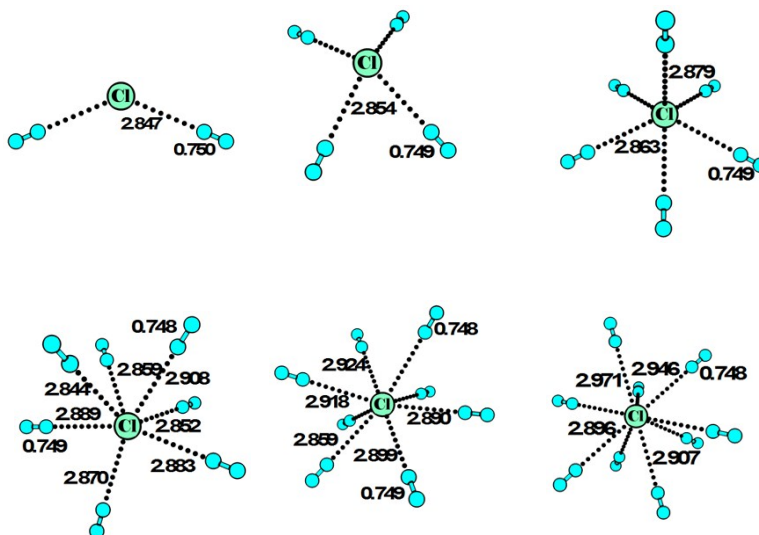
Supporting Information

Table of Contents

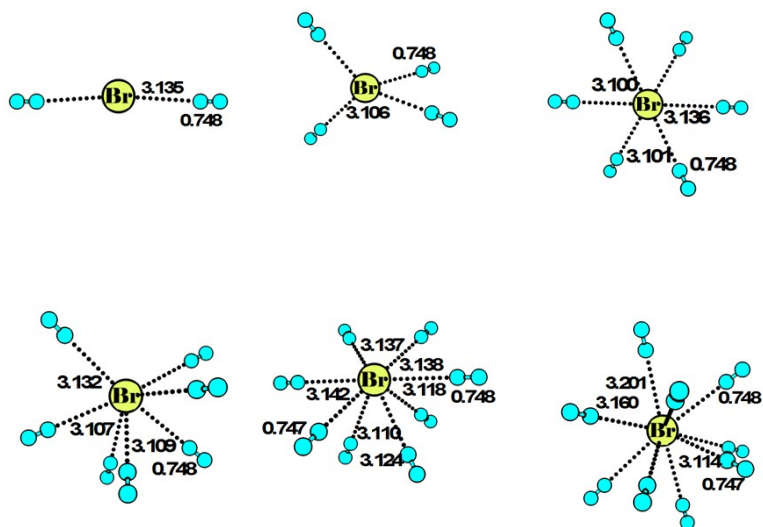
1. **Fig. S1** Optimized geometries of $\text{Cl}^-(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level.
2. **Fig. S2** Optimized geometries of $\text{Br}^-(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level.
3. **Fig. S3** Optimized geometries of $\text{OH}^-(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level.
4. **Fig. S4** Optimized geometries of $\text{NH}_2^-(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level.
5. **Fig. S5** Optimized geometries of $\text{NO}_2^-(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level.
6. **Fig. S6** Optimized geometries of $\text{CN}^-(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level.
7. **Fig. S7** Optimized geometries of $\text{ClO}^-(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level.
8. **Fig. S8** Correlation between E_{int} and No. of H_2 molecules of $\text{X}^-(\text{H}_2)_n$ complexes at CCSD(T)/6-311++G(d,p)// CCSD/6-311++G(d,p) level.
9. **Fig. S9** Optimized geometries of $\text{F}^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level.
10. **Fig. S10** Optimized geometries of $\text{Cl}^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level.
11. **Fig. S11** Optimized geometries of $\text{Br}^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level.
12. **Fig. S12** Optimized geometries of $\text{OH}^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level.
13. **Fig. S13** Optimized geometries of $\text{NH}_2^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level.
14. **Fig. S14** Optimized geometries of $\text{NO}_2^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level.

15. **Fig. S15** Optimized geometries of $\text{CN}^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level.
16. **Fig. S16** Optimized geometries of $\text{CN}^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level.
17. **Fig. S17** Extrapolation of $E_{\text{int}/\text{H}_2}$ of $\text{F}^-(\text{H}_2)$ to CBS limit
18. **Fig. S18** QTAIM features of $\text{X}^-(\text{H}_2)_{n_{\text{max}}+1}$ complexes optimized at M06L/6-311++G(d,p) level.
19. **Fig. S19** Variation of $\Sigma\rho_b$ values of $\text{X}^-(\text{H}_2)_n$ complexes with number of H_2 molecules.
20. **Fig. S20** Correlation between E_{int} and $\Sigma\rho_b$ values of $\text{X}^-(\text{H}_2)_n$ complexes at M06L/6-311++G(d,p) level.
21. **Fig. S21** MESP of $\text{X}^-(\text{H}_2)_{n_{\text{max}}}$ and $\text{X}^-(\text{H}_2)_{n_{\text{max}}+1}$ complexes at M06L/6-311++G(d,p) level (isosurface value of each complex is given in brackets).
22. **Fig. S22** Correlation between E_{int} and $\Sigma V_{\text{max-surface}}$ of $\text{X}^-(\text{H}_2)_n$ complexes at M06L/6-311++G(d,p) level.
23. **Table S1** BSSE corrected $E_{\text{int}/\text{H}_2}$ (kcal/mol) of anion complexes with $n = 1-3$ at aug-cc-pVnZ basis set ($n = \text{T, Q}$) and extrapolation to CBS.
24. **Table S2** BSSE correction of E_{int} (kcal/mol) of anion complexes with $n = 1-3$.
25. **Table S3** Average $\nabla^2(\rho_b)$ values (a. u.) of $\text{X}\cdots\text{H}$ bond in complexes optimized at M06L/6-311++G(d,p) level.
26. **Table S4** $\Sigma V_{\text{max-surface}}$ values (a. u.) of $\text{X}^-(\text{H}_2)_n$ complexes at M06L/6-311++G(d,p) level.
27. Cartesian coordinates of optimized geometry of complexes at M06L/6-311++G(d,p) level.
28. Cartesian coordinates of optimized geometry of complexes at CCSD/6-311++G(d,p) level.

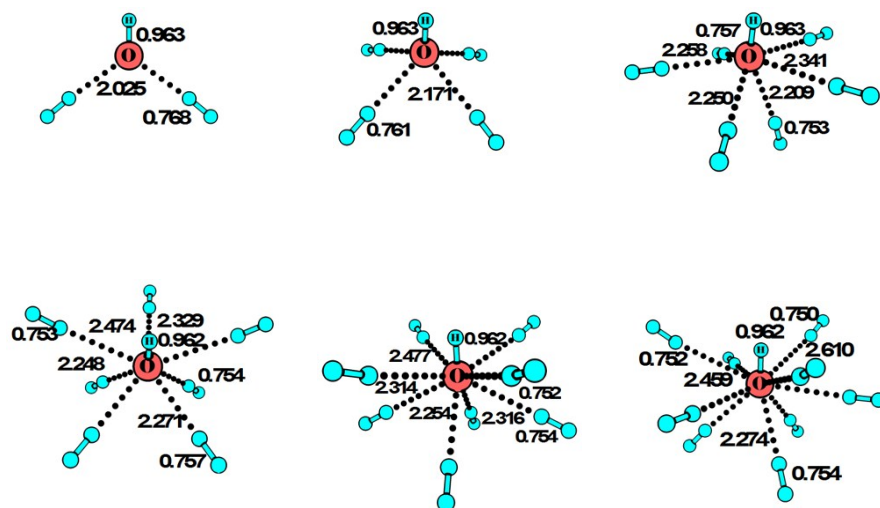
1. **Fig. S1** Optimized geometries of $\text{Cl}(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level



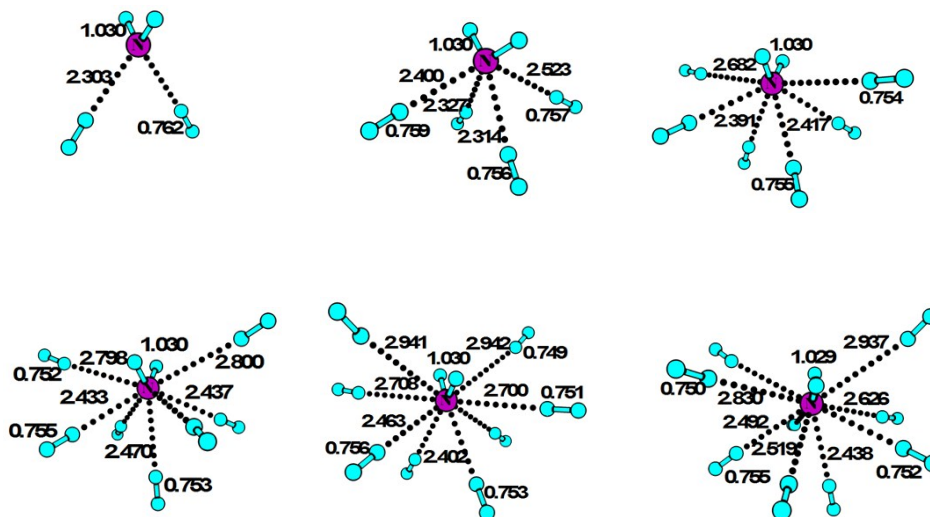
2. **Fig. S2** Optimized geometries of $\text{Br}(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level



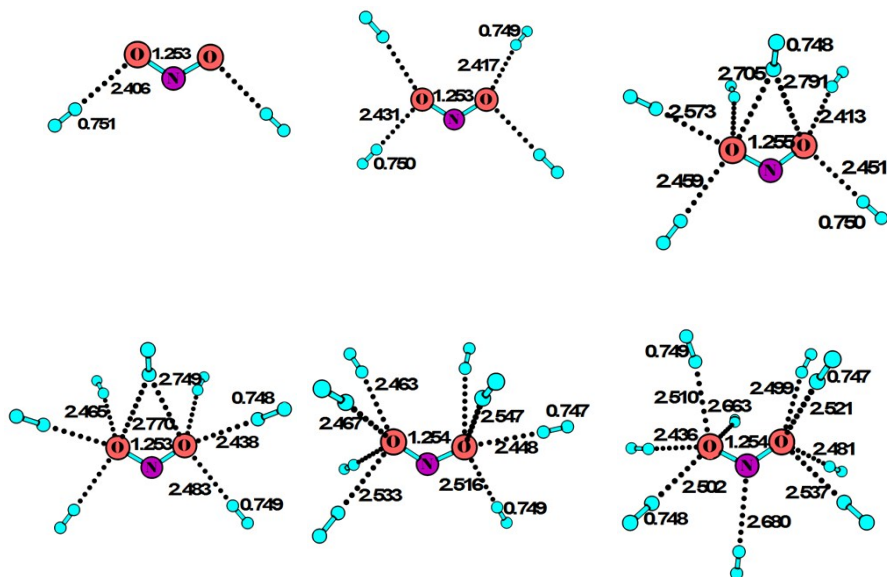
3. Fig. S3 Optimized geometries of $\text{OH}^-(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level



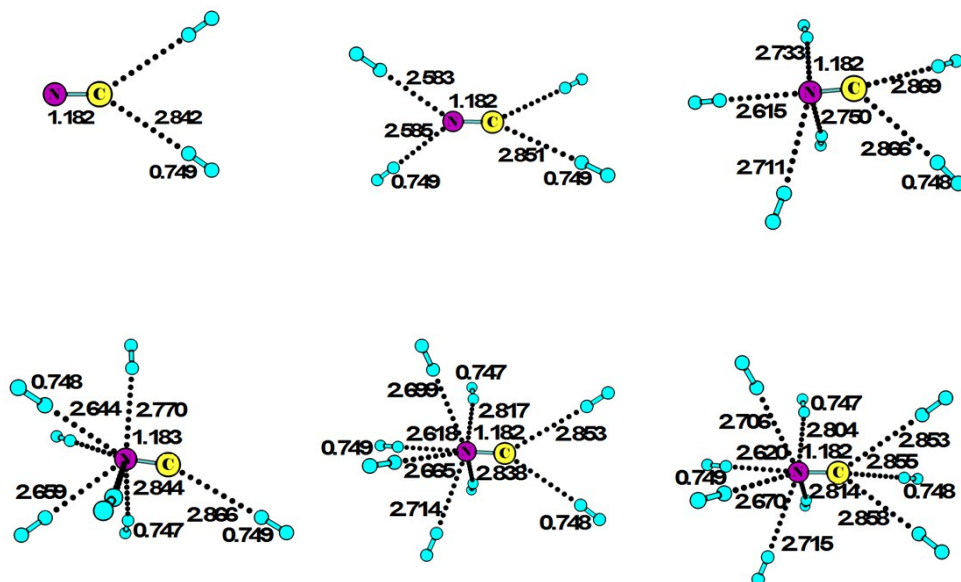
4. Fig. S4 Optimized geometries of $\text{NH}_2^-(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level



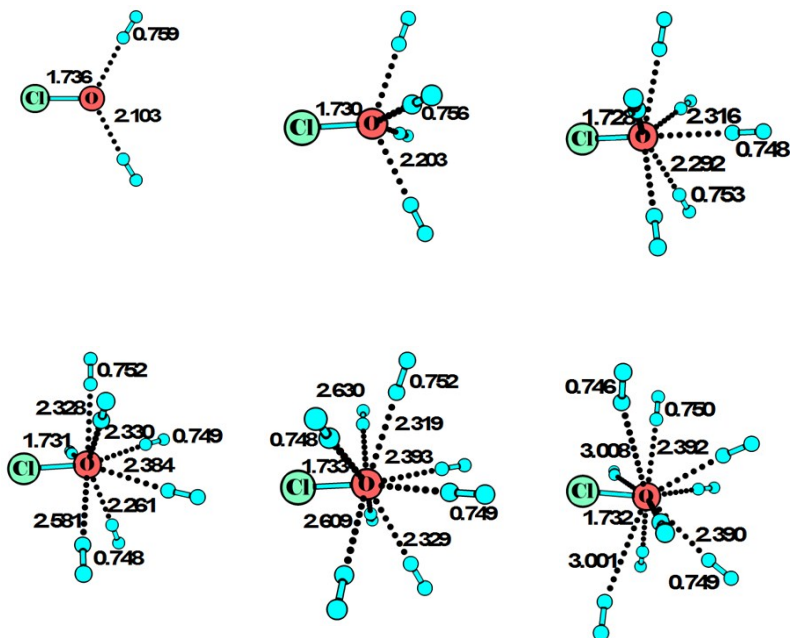
5. Fig. S5 Optimized geometries of $\text{NO}_2^-(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level



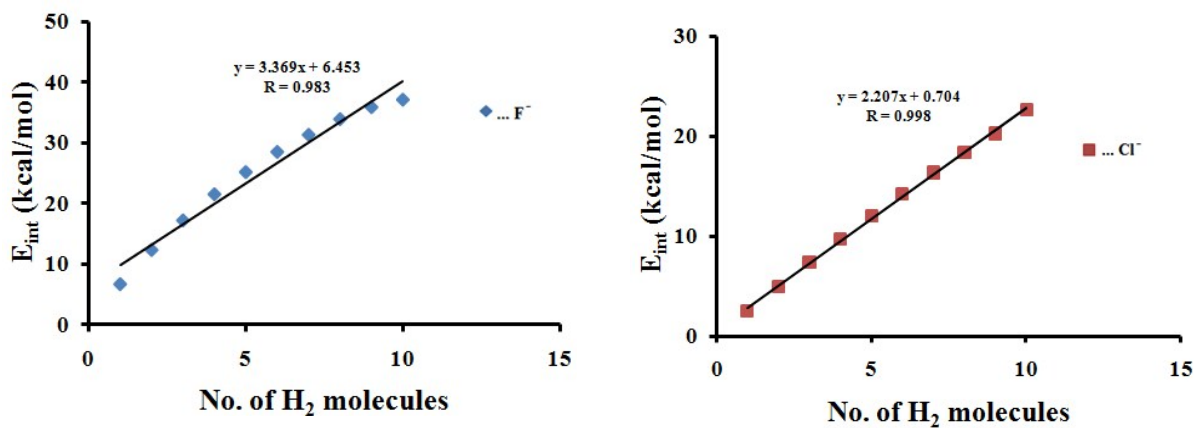
6. Fig. S6 Optimized geometries of $\text{CN}^-(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level

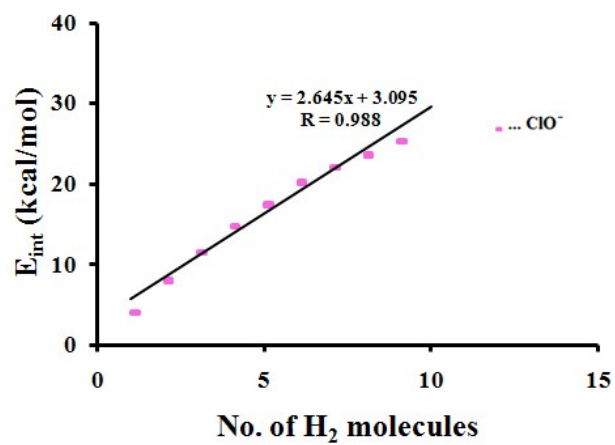
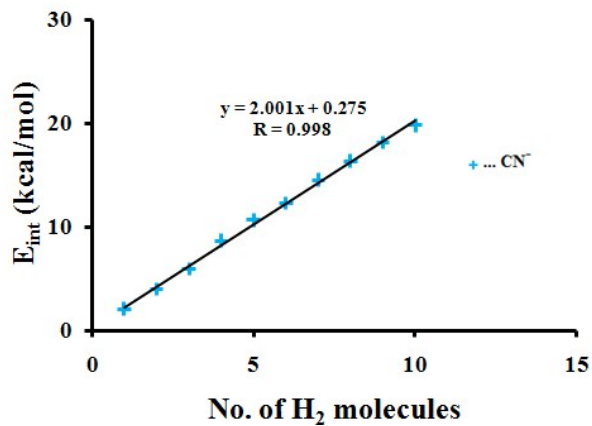
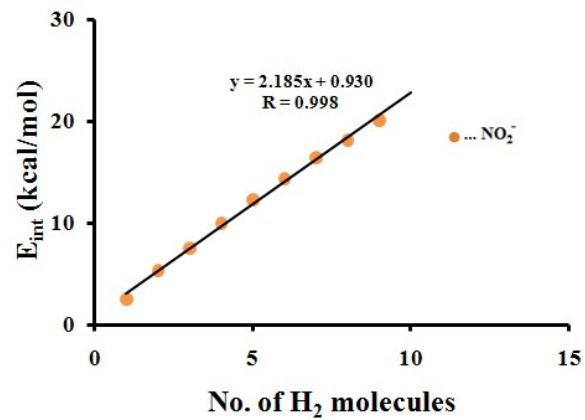
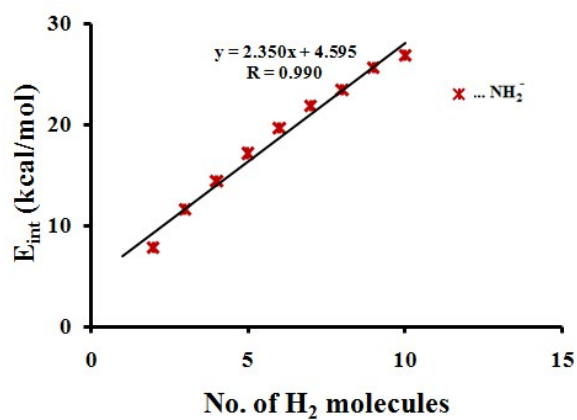
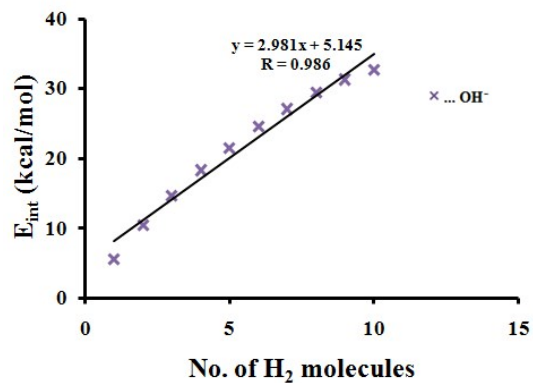
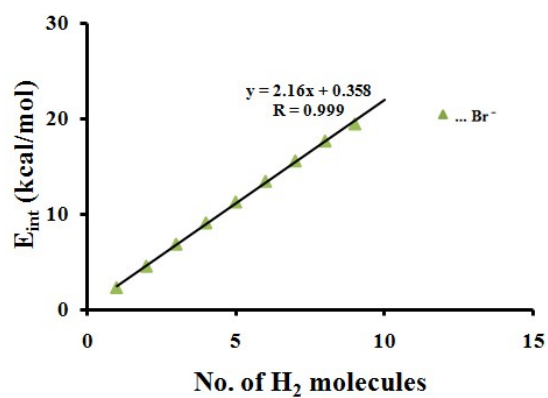


7. **Fig. S7** Optimized geometries of $\text{ClO}^-(\text{H}_2)_n$ complexes at CCSD/6-311++G(d,p) level

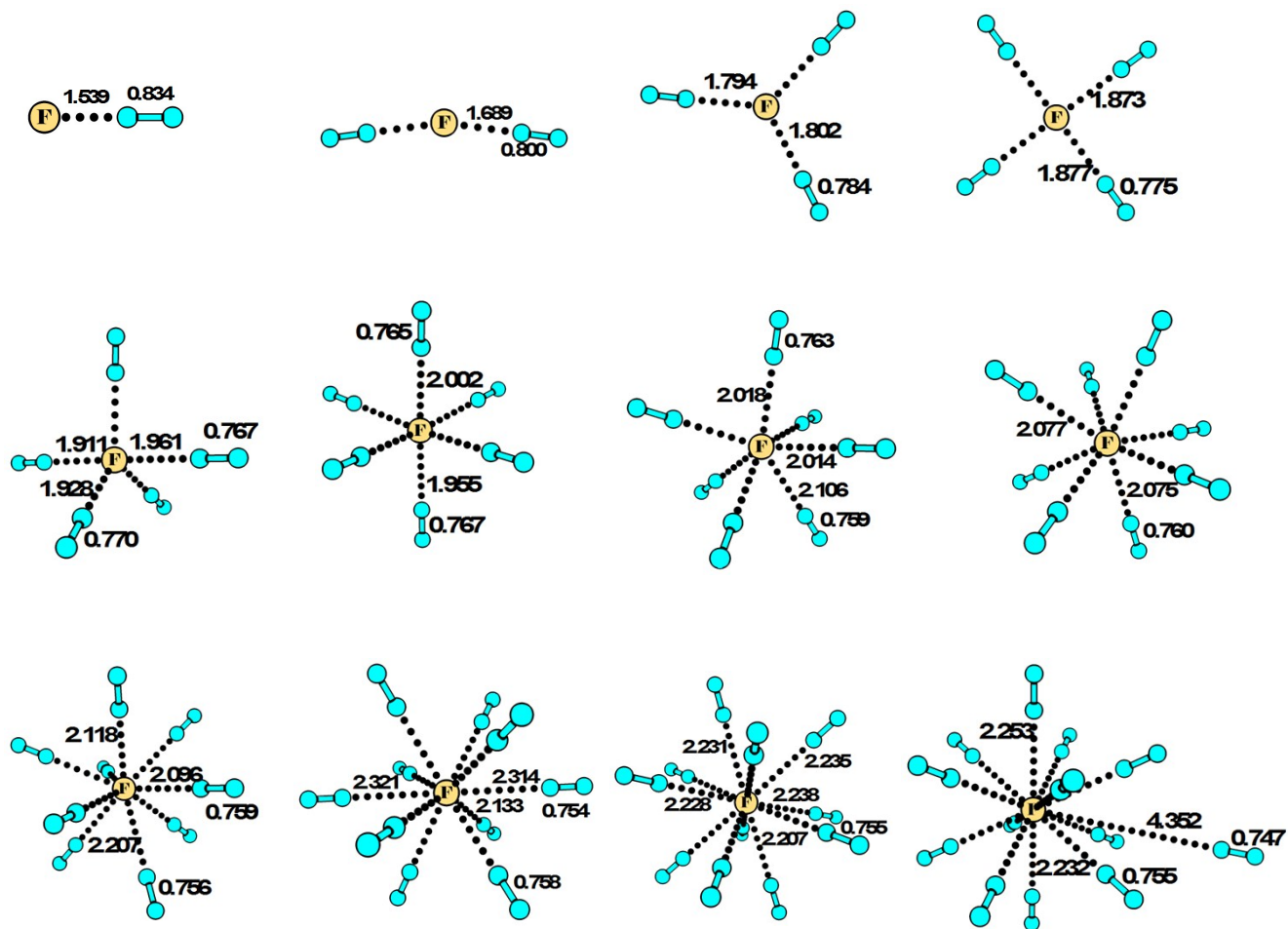


8. **Fig. S8** Correlation between E_{int} and No. of H_2 molecules of $\text{X}^-(\text{H}_2)_n$ complexes at CCSD(T)/aug-cc-pVTZ// CCSD/6-311++G(d,p)level

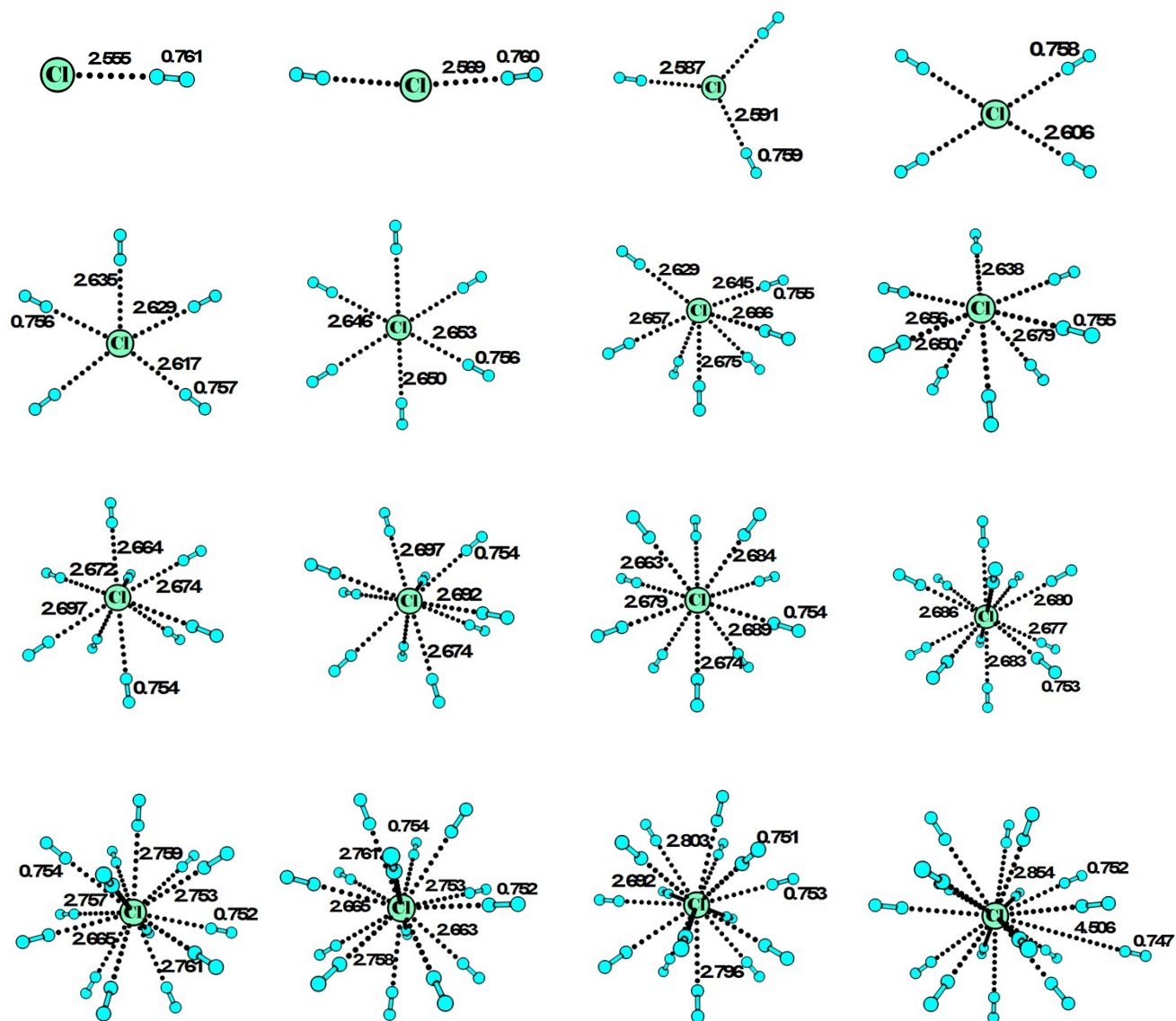




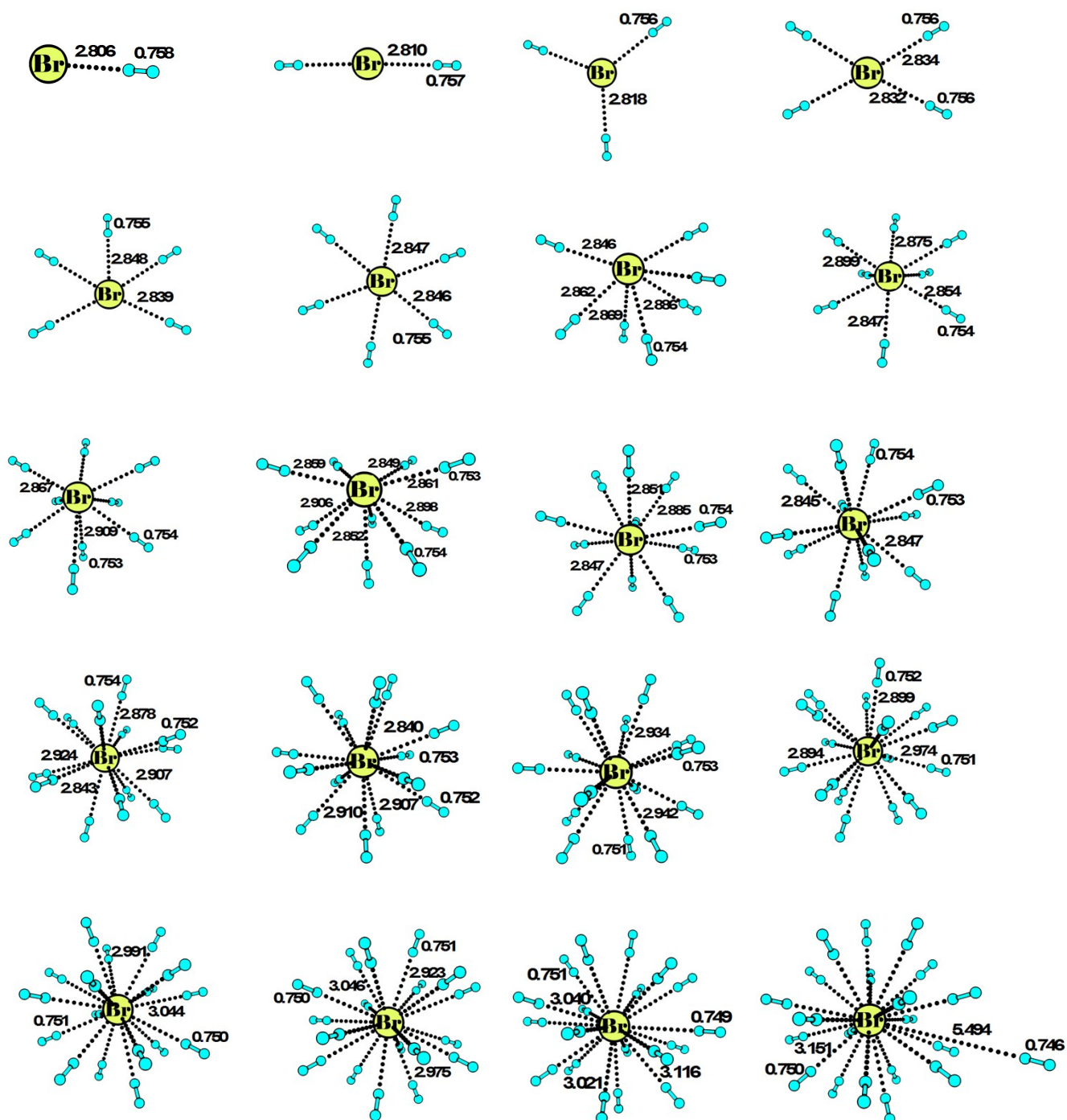
9. Fig. S9 Optimized geometries of $\text{F}^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level



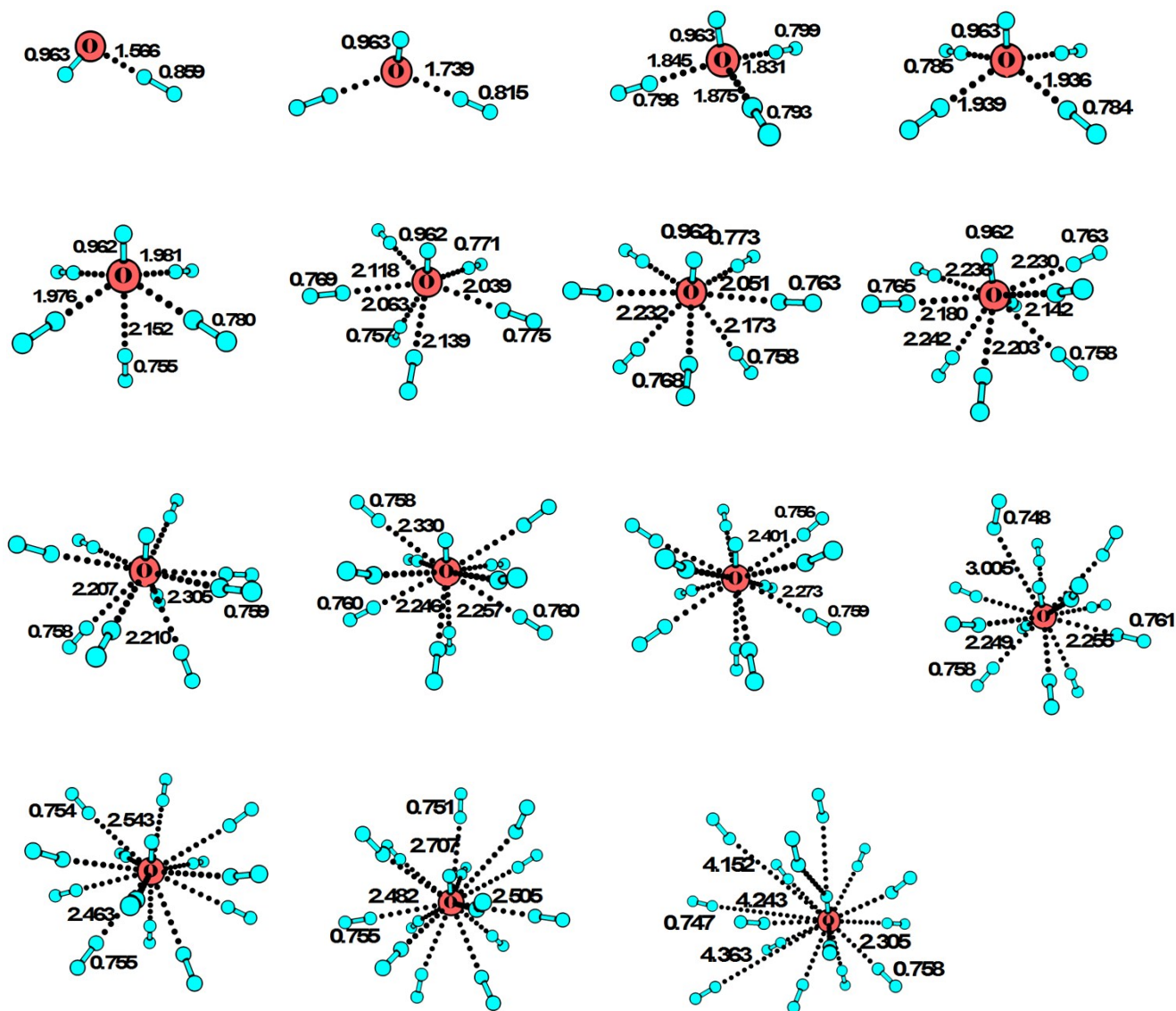
10. Fig. S10 Optimized geometries of $\text{Cl}^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level



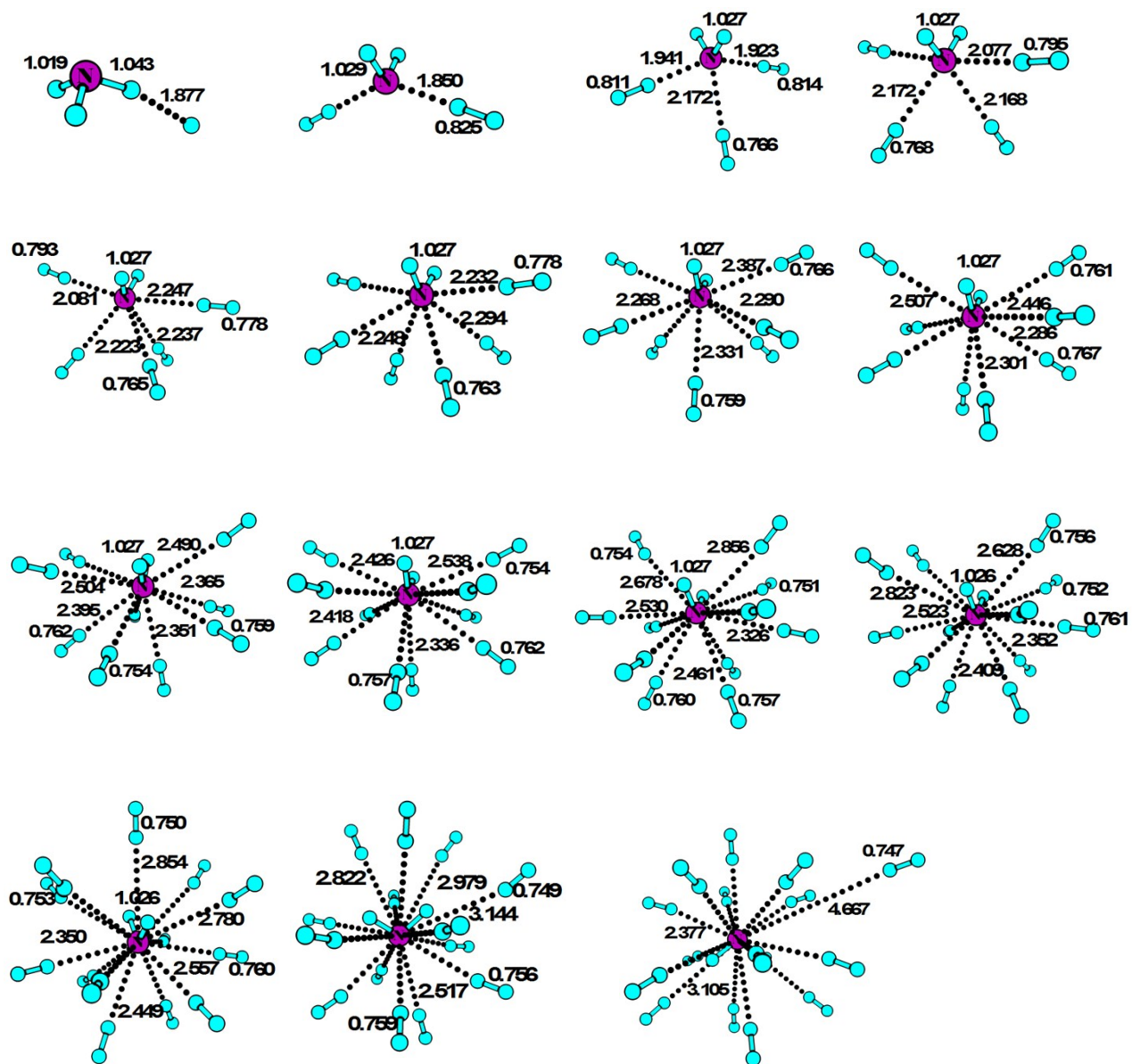
11. Fig. S11 Optimized geometries of $\text{Br}(\text{H}_2)_n$ at M06L/6-311++G(d,p) level



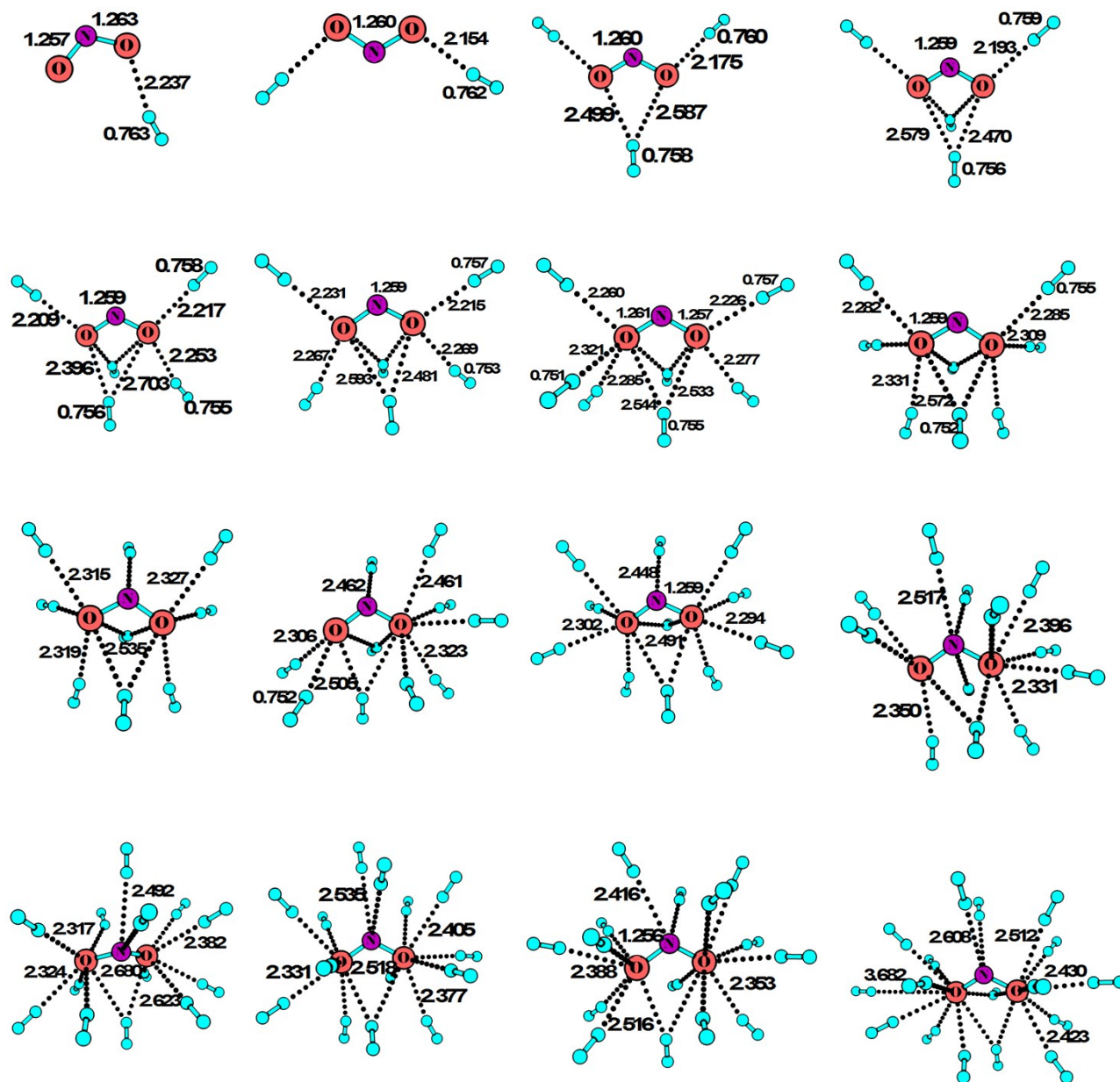
12. Fig. S12 Optimized geometries of $\text{OH}\cdot(\text{H}_2)_n$ at M06L/6-311++G(d,p) level



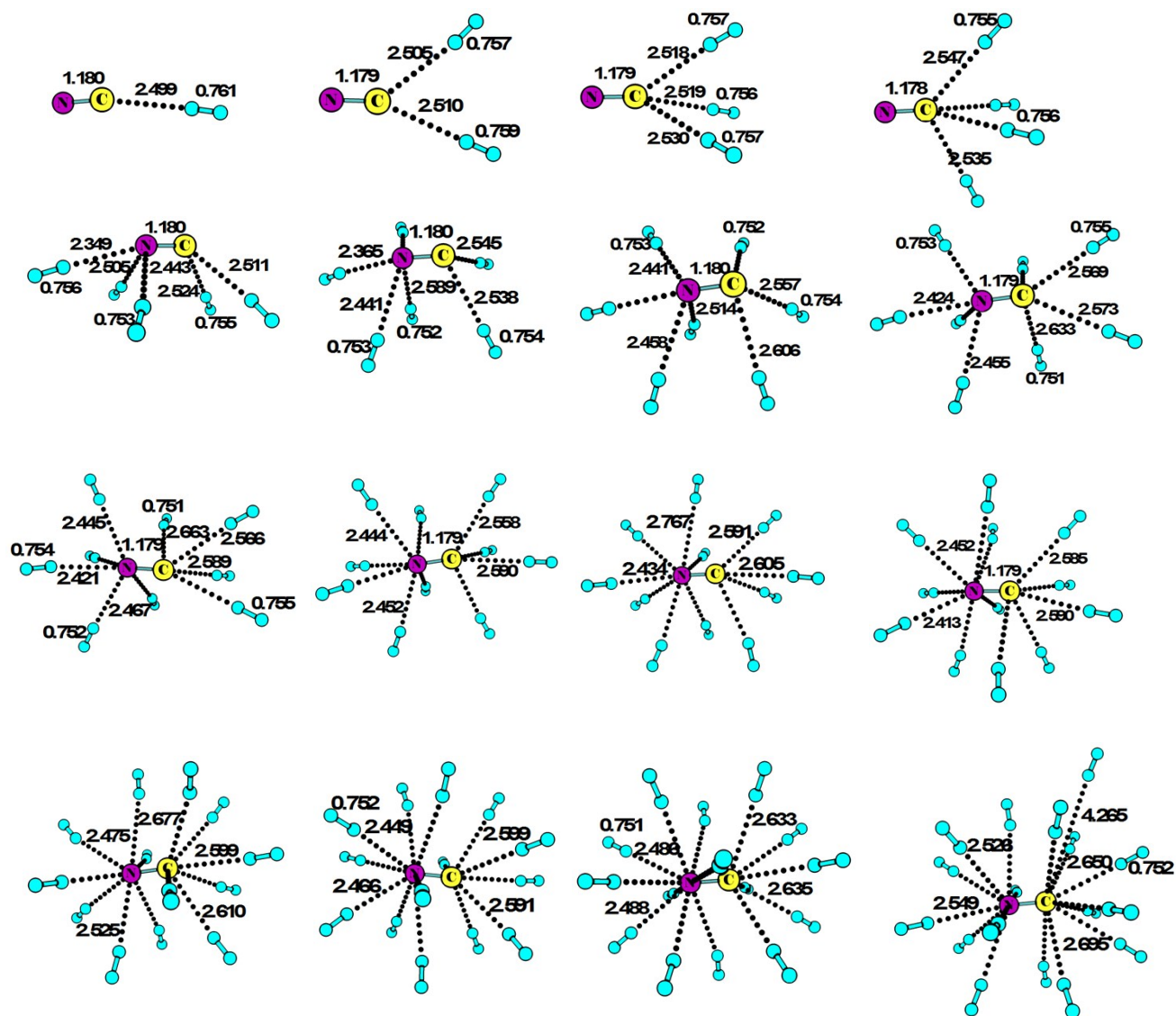
13. Fig. S13 Optimized geometries of $\text{NH}_2^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level



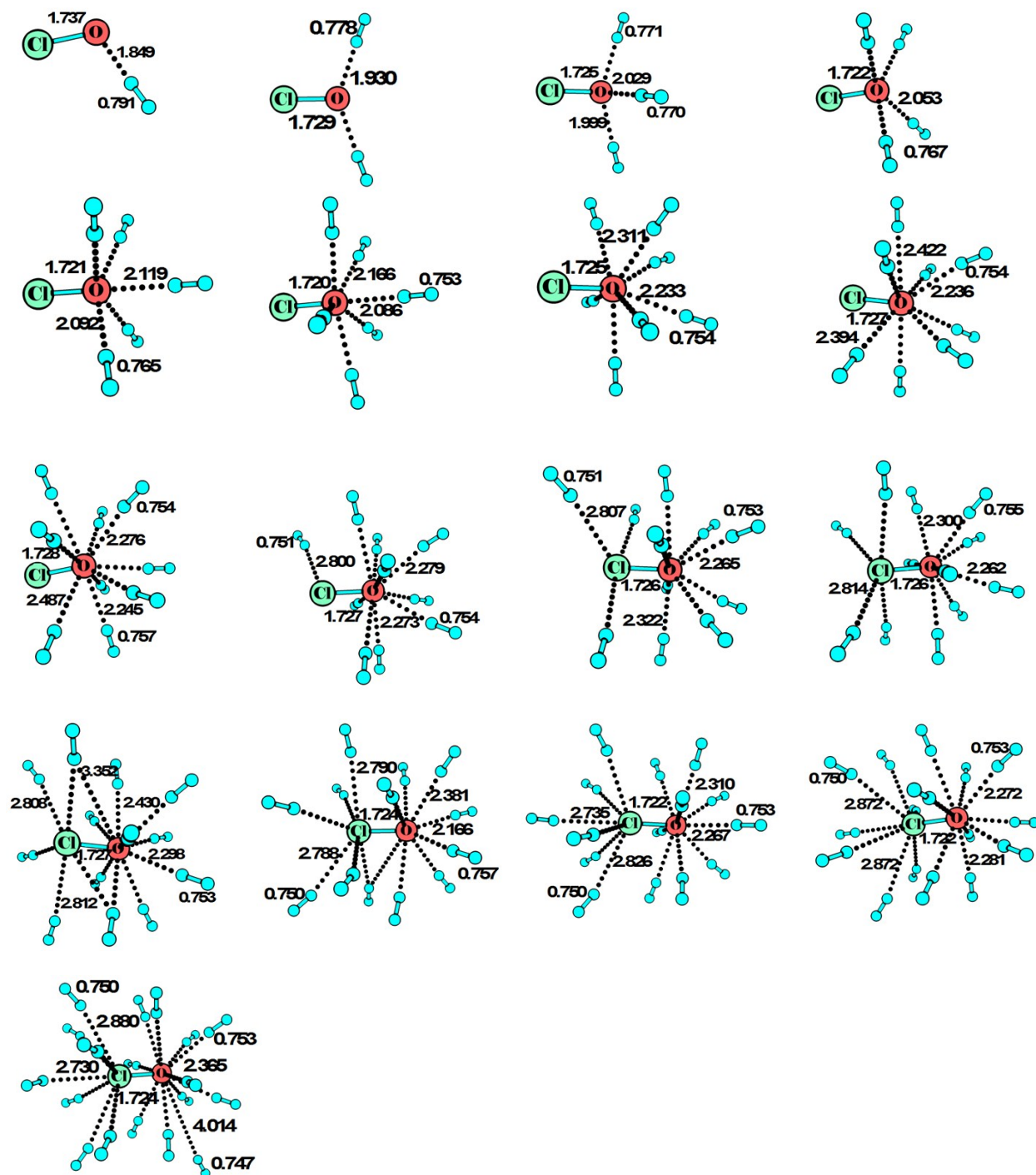
14. Fig. S14 Optimized geometries of $\text{NO}_2^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level



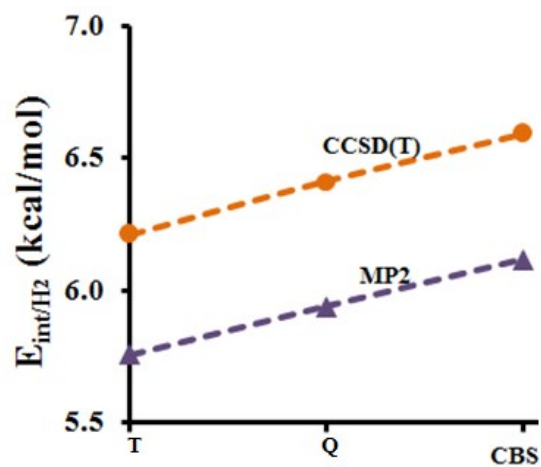
15. Fig. S15 Optimized geometries of $\text{CN}^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level



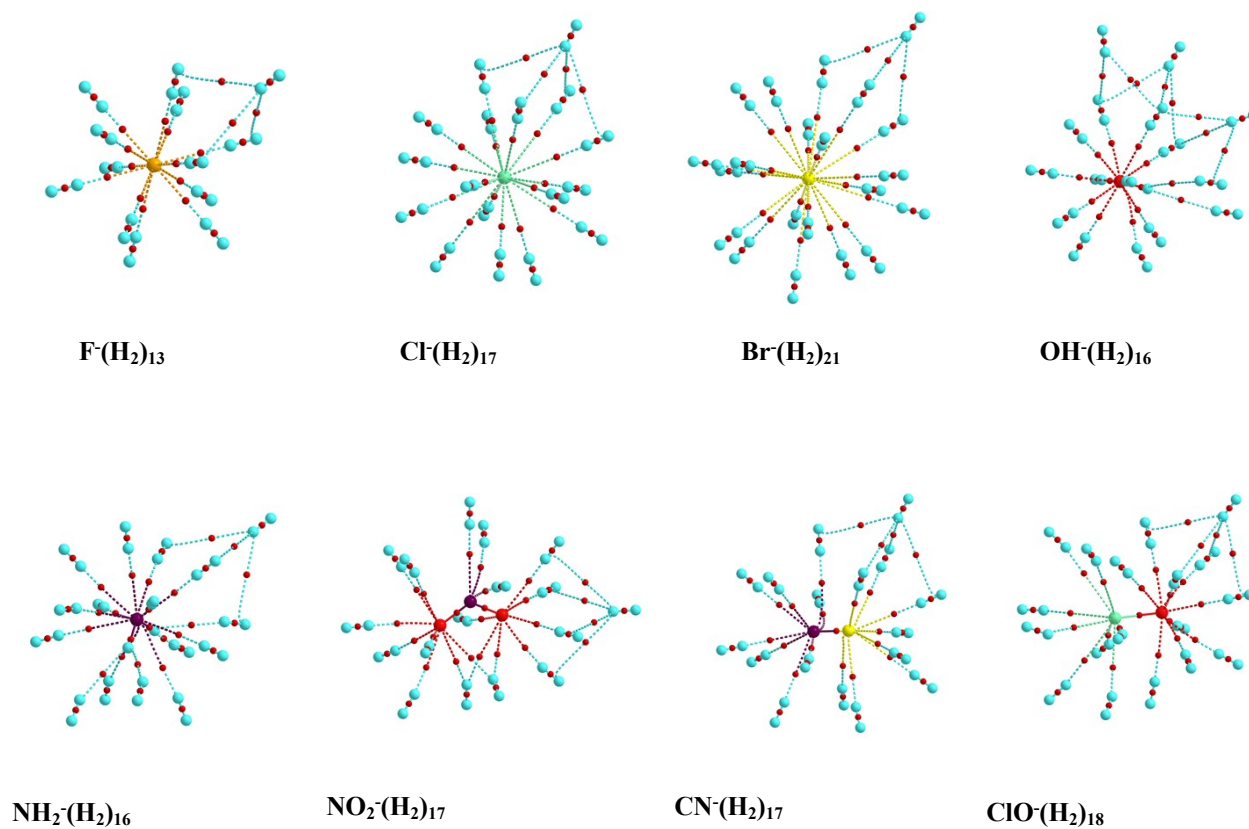
16. Fig. S16 Optimized geometries of $\text{CN}^-(\text{H}_2)_n$ at M06L/6-311++G(d,p) level



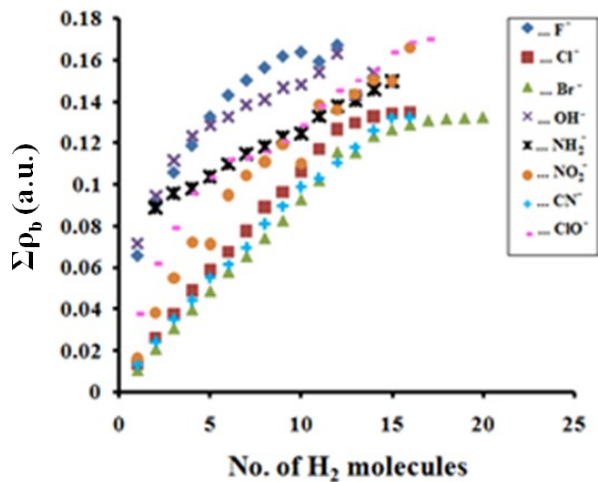
17. **Fig. S17** Extrapolation of $E_{\text{int}/\text{H}_2}$ of $\text{F}^-(\text{H}_2)$ to CBS limit



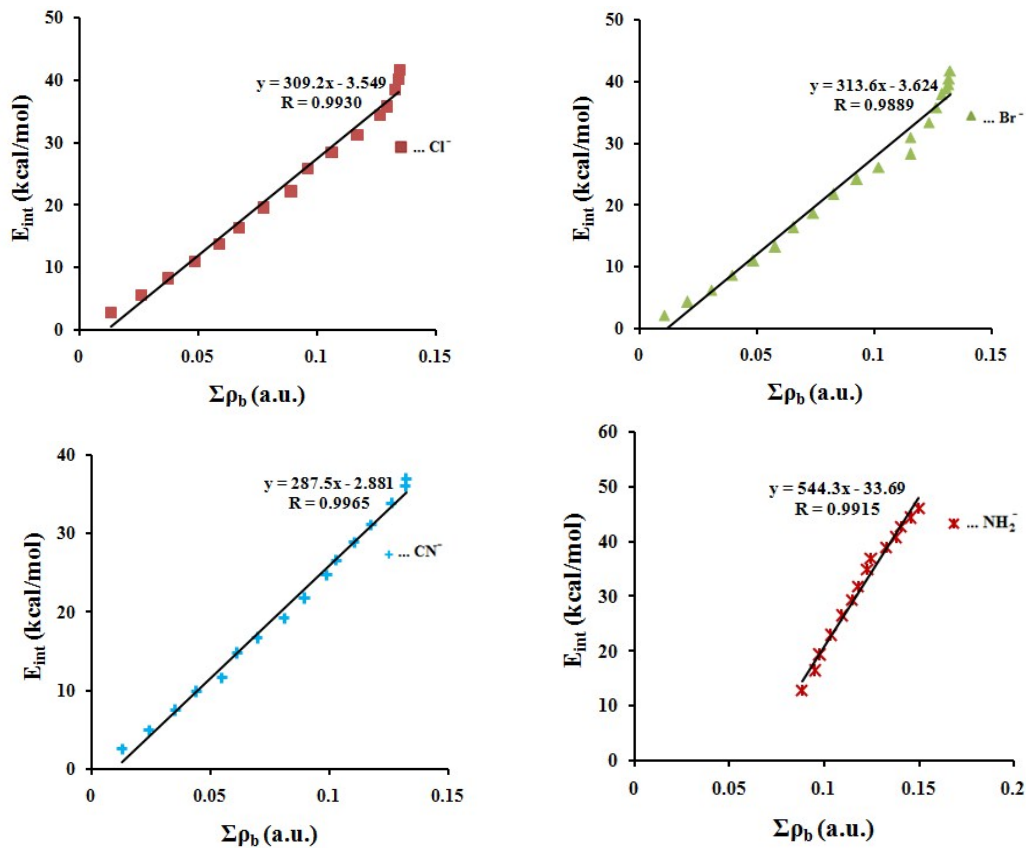
18. **S18** QTAIM features of $\text{X}^-(\text{H}_2)_{n_{\text{max}}+1}$ complexes optimized at M06L/6-311++G(d,p) level

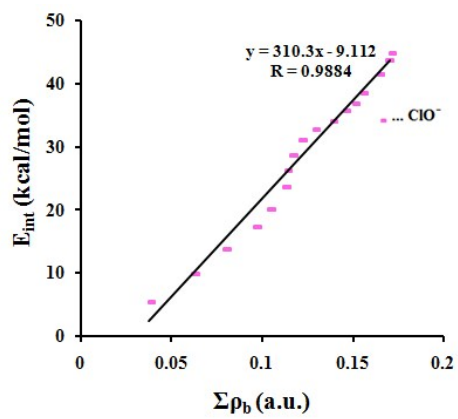
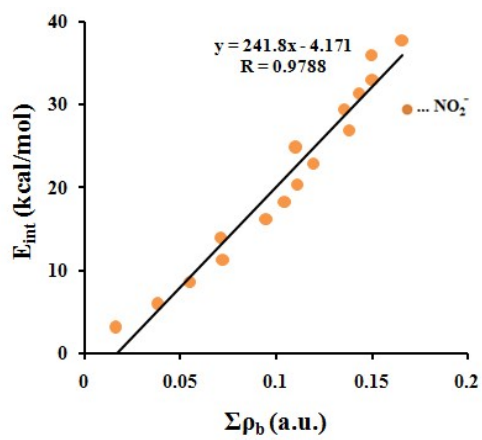
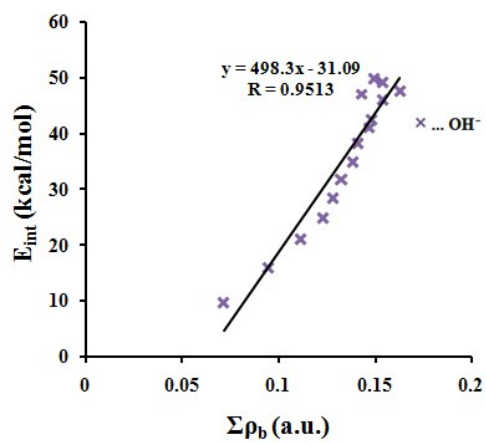
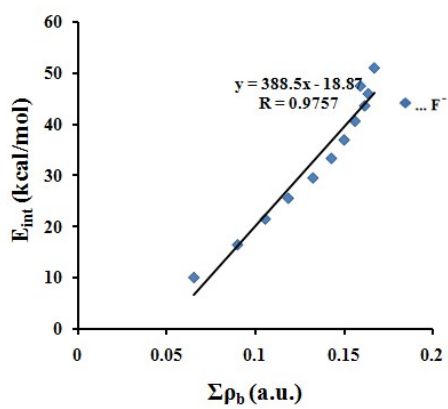


19. Fig. S19 Variation of $\Sigma\rho_b$ values of $X^-(H_2)_n$ complexes with number of H_2 molecules

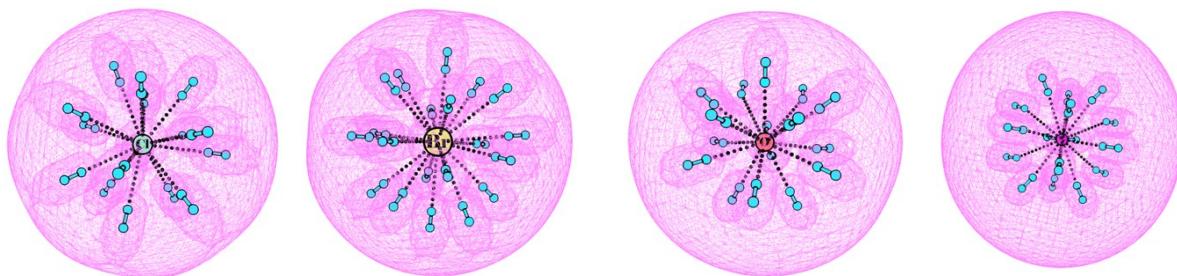


20. Fig. S20 Correlation between E_{int/H_2} and $\Sigma\rho_b$ values of $X^-(H_2)_n$ complexes at M06L/6-311++G(d,p) level





21. Fig. S21 MESP of $X^-(H_2)_{n_{\max}}$ and $X^-(H_2)_{n_{\max} + 1}$ complexes (isosurface value of each complex is given in brackets)

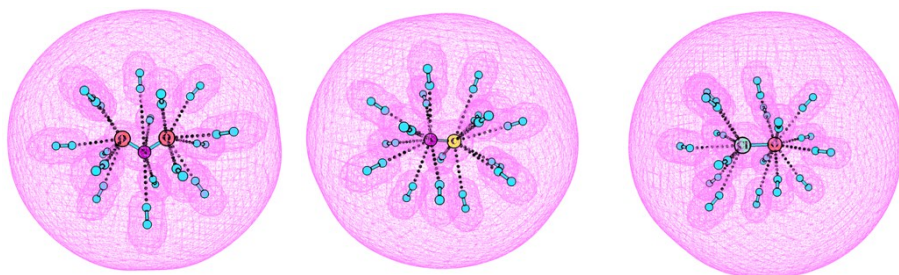


$Cl^-(H_2)_{16}$ (-0.980 a. u.)

$Br^-(H_2)_{20}$ (-0.0922 a. u.)

$OH^-(H_2)_{15}$ (-0.1042 a. u.)

$NH_2^-(H_2)_{15}$ (-0.0880 a. u.)

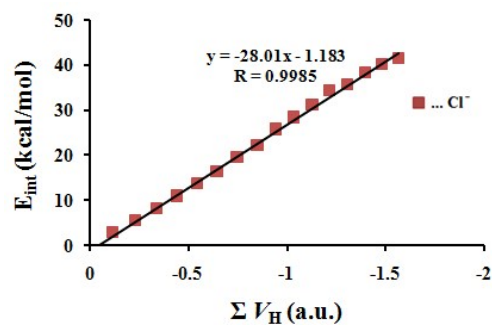
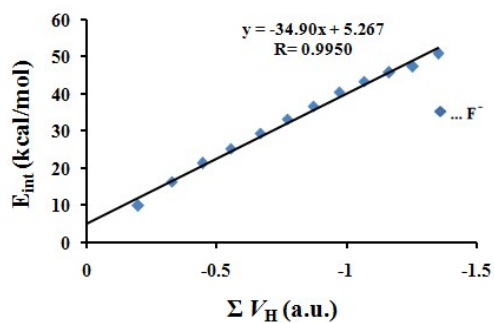


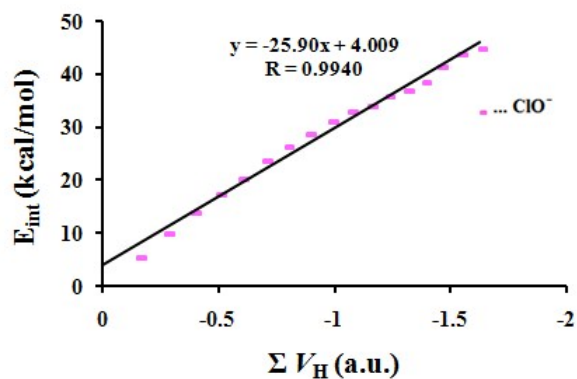
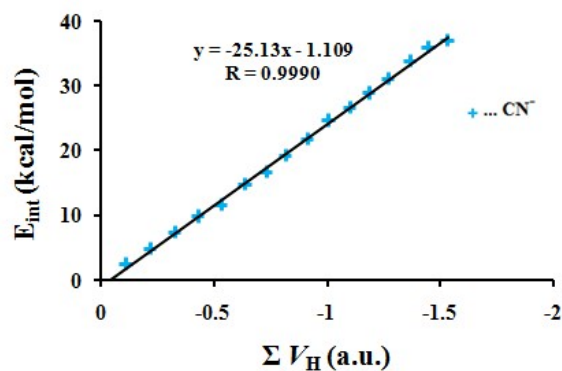
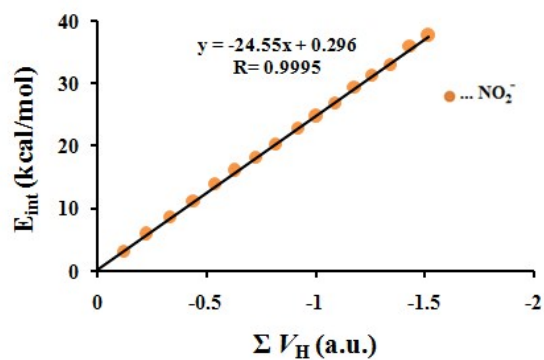
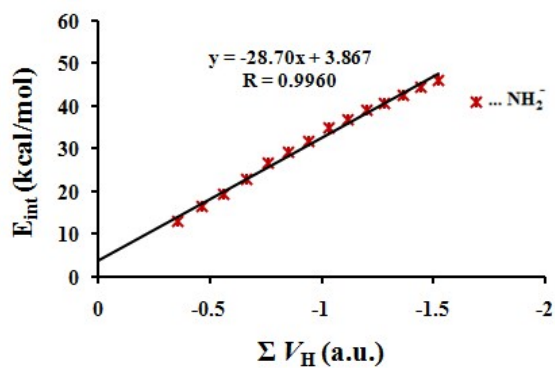
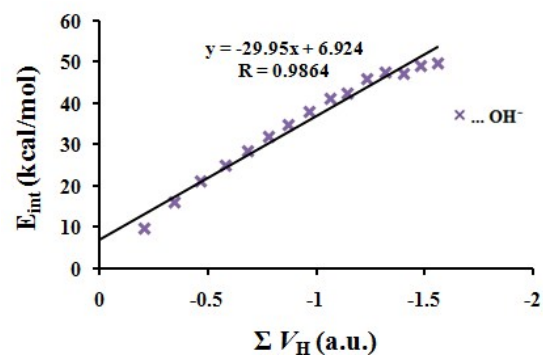
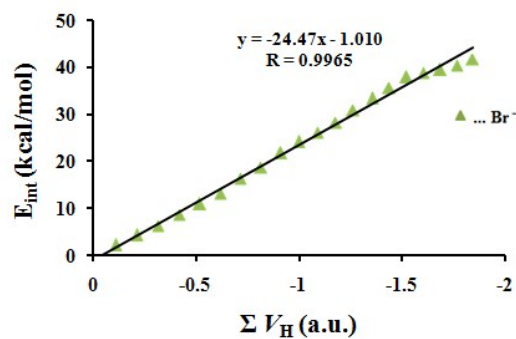
$NO_2^-(H_2)_{16}$ (-0.0900 a. u.)

$CN^-(H_2)_{16}$ (-0.090 a. u.)

$ClO^-(H_2)_{17}$ (-0.0800 a.u.)

22. Fig. S22 Correlation between E_{int} and ΣV_H of $X^-(H_2)_n$ complexes at M06L/6-311++G(d,p) level





23. Table S1 BSSE corrected $E_{\text{int/H}_2}$ (kcal/mol) of anion complexes with $n = 1-3$ at aug-cc-pVnZ basis set ($n = T, Q$) and extrapolation to CBS.

Anion	n	HF			MP2			CCSD(T)		
		T	Q	CBS	T	Q	CBS	T	Q	CBS
F ⁻	1	4.47	4.51	4.53	5.76	5.94	6.12	6.21	6.41	6.59
	2	4.29	4.31	4.33	5.36	5.51	5.67	5.76	5.93	6.08
	3	4.05	4.07	4.08	4.99	5.12	5.26	5.35	5.49	5.63
Cl ⁻	1	1.17	1.17	1.17	2.26	2.34	2.44	2.32	2.41	2.51
	2	1.16	1.15	1.15	2.23	2.31	2.40	2.29	2.38	2.47
	3	1.14	1.14	1.14	2.19	2.27	2.36	2.25	2.34	2.42
Br ⁻	1	0.57	0.57	0.57	1.75	1.85	1.96	1.78	1.89	1.99
	2	0.60	0.60	0.59	1.74	1.84	1.95	1.78	1.87	1.97
	3	0.59	0.58	0.58	1.72	1.81	1.92	1.75	1.85	1.94
OH ⁻	1	3.85	3.86	3.87	4.84	4.96	5.09	5.22	5.54	5.85
	2	3.64	3.65	3.65	4.47	4.60	4.73	4.85	4.99	5.13
	3	3.39	3.40	3.41	4.15	4.27	4.40	4.52	4.65	4.78
NH ₂ ⁻	2	2.48	2.47	2.46	3.79	3.86	3.95	4.02	4.10	4.18
	3	2.20	2.20	2.20	3.30	3.38	3.48	3.56	3.65	3.74
NO ₂ ⁻	1	1.49	1.49	1.49	2.13	2.18	2.24	2.24	2.30	2.36
	2	1.45	1.46	1.46	2.32	2.38	2.46	2.43	2.50	2.57
	3	1.42	1.43	1.43	2.21	2.27	2.33	2.32	2.38	2.44
CN ⁻	1	1.17	1.17	1.16	1.45	1.96	2.54	1.98	2.02	2.06
	2	0.96	0.96	0.96	1.62	1.90	2.21	1.91	1.95	1.99
	3	0.84	0.83	0.83	1.68	1.87	2.10	1.88	1.92	1.97
ClO ⁻	1	1.65	1.67	1.68	3.80	3.92	4.05	3.82	3.94	4.05
	2	1.67	1.69	1.70	1.20	3.77	3.66	3.69	3.80	3.90
	3	1.64	1.66	1.67	3.52	3.62	3.72	3.54	3.65	3.74

24. Table S2 BSSE correction of E_{int} (kcal/mol) of anion complexes with $n = 1-3$.

Anion	n	HF		MP2		CCSD(T)	
		T	Q	T	Q	T	Q
F ⁻	1	0.05	0.01	0.50	0.33	0.53	0.29
	2	0.09	0.03	0.85	0.51	0.90	0.44
	3	0.14	0.04	1.17	0.68	1.24	0.59
Cl ⁻	1	0.01	0.00	0.31	0.16	0.31	0.12
	2	0.03	0.01	0.59	0.31	0.59	0.23
	3	0.04	0.01	0.86	0.44	0.85	0.32
Br ⁻	1	0.01	0.00	0.77	0.51	0.76	0.44
	2	0.02	0.01	1.50	1.07	1.47	0.92
	3	0.03	0.01	2.20	1.58	2.15	1.36
OH ⁻	1	0.04	0.01	0.40	0.23	0.40	0.19
	2	0.08	0.03	0.80	0.45	0.80	0.38
	3	0.13	0.05	1.16	0.63	1.17	0.54
NH ₂ ⁻	2	0.09	0.04	0.67	0.38	0.59	0.28
	3	0.19	0.09	1.14	0.63	1.00	0.48
NO ₂ ⁻	1	0.06	0.02	0.28	0.14	0.28	0.13
	2	0.13	0.04	0.61	0.32	0.63	0.28
	3	0.19	0.06	0.87	0.45	0.89	0.38
CN ⁻	1	0.04	0.01	0.23	0.11	0.21	0.08
	2	0.04	0.01	0.39	0.18	0.35	0.13
	3	0.07	0.02	0.58	0.28	0.53	0.19
ClO ⁻	1	0.06	0.02	0.47	0.27	0.50	0.23
	2	0.11	0.04	0.87	0.50	0.91	0.42
	3	0.16	0.05	1.30	0.73	1.35	0.61

25. Table S3 Average $\nabla^2(\rho_b)$ values (a. u.) of X...H bond in complexes optimized at M06L/6-311++G(d,p) level

n	F ⁻	Cl ⁻	Br ⁻	OH ⁻	NH ₂ ⁻	NO ₂ ⁻	CN ⁻	ClO ⁻
1	0.1678	0.0378	0.0253	0.1228	-	0.0452	0.0300	0.1063
2	0.1421	0.0367	0.0252	0.1185	0.0821	0.0560	0.0287	0.0929
3	0.1168	0.0354	0.0249	0.1031	0.0709	0.0521	0.0281	0.0793
4	0.0994	0.0343	0.0242	0.0890	0.0607	0.0517	0.0268	0.0721
5	0.0888	0.0330	0.0238	0.0776	0.0527	0.0417	0.0301	0.0659
6	0.0790	0.0315	0.0237	0.0652	0.0471	0.0475	0.0279	0.0582
7	0.0704	0.0311	0.0228	0.0576	0.0422	0.0451	0.0273	0.0484
8	0.0632	0.0314	0.0228	0.0506	0.0375	0.0417	0.0276	0.0427
9	0.0576	0.0300	0.0224	0.0462	0.0356	0.0398	0.0267	0.0392
10	0.0519	0.0299	0.0228	0.0423	0.0336	0.0338	0.0266	0.0375
11	0.0448	0.0300	0.0229	0.0393	0.0312	0.0387	0.0249	0.0367
12	0.0430	0.0298	0.0241	0.0383	0.0295	0.0337	0.0245	0.0354
13	-	0.0279	0.0219	0.0290	0.0274	0.0342	0.0241	0.0337
14	-	0.0263	0.0217	0.0292	0.0262	0.0319	0.0239	0.0321
15	-	0.0244	0.0206	0.0265	0.0250	0.0301	0.0233	0.0321
16	-	0.0227	0.0195	-	-	0.0309	0.0216	0.0308
17	-	-	0.0185	-	-	-	-	0.0294
18	-	-	0.0174	-	-	-	-	-
19	-	-	0.0164	-	-	-	-	-
20	-	-	0.0155	-	-	-	-	-

26. Table S4 ΣV_H values (a. u.) of $X^-(H_2)_n$ complexes at M06L/6-311++G(d,p) level.

n	F ⁻	Cl ⁻	Br ⁻	OH ⁻	NH ₂ ⁻	NO ₂ ⁻	CN ⁻	ClO ⁻
1	-0.201	-0.1202	-0.1112	-0.2114	-	-0.1232	-0.1157	-0.1539
2	-0.3307	-0.2335	-0.2178	-0.3514	-0.3572	-0.2262	-0.2225	-0.2745
3	-0.4482	-0.3407	-0.3197	-0.4717	-0.469	-0.3366	-0.33	-0.3918
4	-0.5575	-0.4473	-0.4218	-0.5845	-0.5659	-0.4424	-0.4317	-0.5004
5	-0.6682	-0.5485	-0.5214	-0.6906	-0.6668	-0.5432	-0.5358	-0.5966
6	-0.7737	-0.6471	-0.6194	-0.7861	-0.7658	-0.6345	-0.6424	-0.6982
7	-0.8728	-0.7504	-0.7173	-0.873	-0.8545	-0.7299	-0.7361	-0.7914
8	-0.973	-0.8525	-0.816	-0.971	-0.9424	-0.8219	-0.8215	-0.8856
9	-1.0686	-0.947	-0.9136	-1.0663	-1.0342	-0.9223	-0.9155	-0.9835
10	-1.1651	-1.039	-1.0007	-1.1461	-1.1229	-1.0045	-1.011	-1.0685
11	-1.2561	-1.1303	-1.0928	-1.2372	-1.2034	-1.0904	-1.1029	-1.1522
12	-1.3531	-1.2199	-1.1797	-1.3203	-1.286	-1.1796	-1.1879	-1.2264
13	-	-1.3088	-1.2638	-1.4046	-1.3667	-1.2623	-1.2722	-1.3099
14	-	-1.4013	-1.3556	-1.4864	-1.4439	-1.3475	-1.3695	-1.3844
15	-	-1.4826	-1.4401	-1.5629	-1.5267	-1.4323	-1.4521	-1.4518
16	-	-1.5677	-1.5246	-	-	-1.5184	-1.5363	-1.5384
17	-	-	-1.6033	-	-	-	-	-1.626
18	-	-	-1.6876	-	-	-	-	-
19	-	-	-1.7676	-	-	-	-	-
20	-	-	-1.8435	-	-	-	-	-

27. Cartesian coordinates of optimized geometry of complexes at M06L/6-311++G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

H₂F⁻				H₄F⁻			
9	0.000000000	0.355589000	0.000000000	9	-0.000032000	0.083507000	-0.000008000
1	-0.000188000	-1.182920000	0.000000000	1	1.674708000	-0.135349000	0.000169000
1	0.000188000	-2.017380000	0.000000000	1	2.467453000	-0.240415000	-0.000115000
				1	-2.467329000	-0.240433000	-0.000040000
				1	-1.674545000	-0.135368000	0.000059000
H₆F⁻				H₈F⁻			
9	0.038904000	-0.018554000	-0.082281000	9	0.000090000	-0.004343000	-0.001588000
1	1.816306000	-0.188481000	0.090328000	1	-1.590978000	-2.116105000	-0.127810000
1	2.590585000	-0.277112000	0.177666000	1	-1.124580000	-1.497814000	-0.097893000
1	-1.709005000	-1.904019000	0.153108000	1	1.115553000	1.501830000	-0.099287000
1	-1.172442000	-1.335881000	0.091667000	1	1.576724000	2.123567000	-0.129185000
1	-1.112635000	2.284938000	0.150436000	1	-1.497332000	1.124165000	0.100916000
1	-0.762943000	1.587541000	0.077327000	1	-2.114702000	1.590965000	0.133322000
				1	2.129003000	-1.573371000	0.132902000

				1	1.505505000	-1.114147000	0.101325000
H₁₀F⁻				H₁₂F⁻			
9	-0.057344000	0.014563000	-0.013445000	9	-0.003059000	-0.001655000	-0.185387000
1	-1.967832000	0.002532000	-0.022747000	1	-0.937820000	-1.183042000	1.133066000
1	-2.738709000	-0.003429000	-0.024864000	1	-1.781764000	0.243449000	-0.955672000
1	0.034388000	-0.787440000	1.737004000	1	0.678246000	-1.671779000	-0.939619000
1	0.073416000	-1.108442000	2.435629000	1	1.116671000	1.405942000	-0.952761000
1	0.146708000	2.680226000	-0.295223000	1	-0.564953000	1.416970000	1.110863000
1	0.085560000	1.916340000	-0.214514000	1	0.946886000	-2.329884000	-1.228648000
1	0.117639000	-1.178896000	-1.508287000	1	-1.293270000	-1.633470000	1.638391000
1	0.192334000	-1.657960000	-2.106928000	1	-2.483614000	0.340714000	-1.250452000
1	2.669821000	0.000692000	0.072842000	1	-0.779417000	1.957749000	1.606990000
1	1.902774000	0.005312000	0.048094000	1	1.558217000	1.960203000	-1.247095000
				1	2.070070000	-0.284964000	1.627380000
				1	1.498279000	-0.206995000	1.126040000
H₁₄F⁻				H₁₆F⁻			
1	-0.327312000	-1.958886000	-0.011183000	1	1.769259000	-0.207359000	1.065075000
1	1.250987000	-0.632582000	-1.409910000	1	1.398842000	1.100275000	-1.066142000
1	-0.952933000	1.884439000	0.004630000	1	-1.398342000	-1.104062000	-1.064273000
1	-1.406834000	-0.201254000	1.384816000	1	-0.209697000	-1.768026000	1.065425000
1	1.715574000	-0.924098000	-1.941052000	1	1.914516000	1.506801000	-1.449370000
1	-0.451960000	-2.707978000	-0.015577000	1	2.422600000	-0.283853000	1.446453000
1	-1.954187000	-0.329964000	1.901067000	1	-0.287769000	-2.420845000	1.447438000
1	-1.326129000	2.550071000	0.006224000	1	-1.913996000	-1.511080000	-1.446916000
1	1.744006000	-0.972391000	1.894251000	1	0.284506000	2.425828000	1.442378000
1	1.272376000	-0.667296000	1.377426000	1	0.208553000	1.771811000	1.062147000
9	0.024678000	0.117853000	0.000539000	9	0.000402000	-0.000102000	0.001940000
1	1.536892000	1.454125000	0.009120000	1	-1.101652000	1.396692000	-1.066607000
1	2.110607000	1.957317000	0.012163000	1	-1.508754000	1.911549000	-1.450323000
1	-1.996088000	-0.318229000	-1.860706000	1	1.510343000	-1.915782000	-1.445161000
1	-1.437098000	-0.193953000	-1.356121000	1	1.103447000	-1.399760000	-1.062833000
				1	-1.770847000	0.210328000	1.062482000
				1	-2.424624000	0.288403000	1.442765000
H₁₈F⁻				H₂₀F⁻			
1	-1.504924000	1.190627000	0.800748000	1	-0.955746000	1.628361000	0.997241000
1	-1.728283000	-0.166200000	-1.260521000	1	0.949084000	0.442943000	1.856404000
1	1.701556000	0.220456000	-1.287514000	1	0.954255000	-1.854378000	0.439944000
1	1.217226000	1.491803000	0.782543000	1	-0.951091000	-1.627075000	-0.999855000
1	-2.351196000	-0.227566000	-1.688894000	1	1.291453000	0.600073000	2.514066000
1	-2.049692000	1.623177000	1.105287000	1	-1.295740000	2.205592000	1.351541000
1	1.660308000	2.031742000	1.080478000	1	-1.287109000	-2.205555000	-1.355966000
1	2.315810000	0.298638000	-1.725517000	1	1.297743000	-2.511104000	0.598572000
1	-1.633894000	-2.083912000	1.021869000	1	1.293674000	2.514284000	-0.599631000
1	-1.199015000	-1.529427000	0.739012000	1	0.950822000	1.856945000	-0.442367000
9	-0.001131000	0.001587000	-0.046051000	1	2.318829000	0.002997000	0.002288000
1	0.181656000	-1.689080000	-1.309583000	1	3.072382000	0.003753000	0.002464000
1	0.247801000	-2.298874000	-1.755722000	1	-1.288971000	-1.360305000	2.202532000
1	-0.278516000	2.373227000	-1.650578000	1	-0.951565000	-1.003054000	1.625557000
1	-0.205089000	1.744655000	-1.232515000	1	0.953925000	-0.442034000	-1.854170000
1	1.520611000	-1.219720000	0.721030000	1	1.296913000	-0.600504000	-2.511175000

1	2.071599000	-1.663225000	0.997209000	1	-0.953554000	0.998000000	-1.626885000
1	0.018636000	-0.047042000	2.160740000	1	-1.292011000	1.352759000	-2.204790000
1	0.025587000	-0.063566000	2.916389000	9	-0.002039000	0.000462000	0.000376000
				1	-2.315642000	-0.002440000	0.000429000
				1	-3.069302000	-0.003411000	0.000423000
H₂₂F⁻				H₂₄F⁻			
1	0.780697000	-1.778669000	-1.211706000	1	1.075249000	-0.759875000	-1.822778000
1	1.948933000	0.193591000	-1.199895000	1	-0.255132000	-2.182301000	-0.483576000
1	-0.810121000	1.850059000	0.828326000	1	-1.077440000	0.766199000	1.818835000
1	-2.006170000	-0.201040000	0.834446000	1	0.258558000	2.181837000	0.482287000
1	2.611322000	0.258004000	-1.556852000	1	-0.343099000	-2.914003000	-0.646421000
1	1.048077000	-2.387303000	-1.570449000	1	1.436573000	-1.014639000	-2.434507000
1	-2.685407000	-0.263833000	1.159038000	1	0.346052000	2.913926000	0.643508000
1	-1.084488000	2.474786000	1.152472000	1	-1.439019000	1.023863000	2.429174000
1	2.331725000	-1.362404000	1.154609000	1	-1.700922000	-0.657182000	-2.387191000
1	1.739457000	-1.018554000	0.835763000	1	-1.273580000	-0.493642000	-1.786967000
1	1.504902000	1.344961000	0.831127000	1	-2.022219000	-0.890960000	0.421954000
1	2.014892000	1.798203000	1.155355000	1	-2.701069000	-1.189026000	0.563150000
1	-2.262593000	1.319227000	-1.560038000	1	1.700259000	0.653377000	2.388595000
1	-1.686024000	0.986008000	-1.203770000	1	1.273200000	0.490072000	1.788070000
1	0.000565000	0.000317000	2.094298000	1	-1.779523000	1.325764000	-0.367473000
1	0.001389000	0.000508000	2.850153000	1	-2.377859000	1.769297000	-0.489377000
1	-0.430077000	-1.972841000	0.831116000	1	0.134907000	1.409222000	-1.747554000
1	-0.578456000	-2.639535000	1.153851000	1	0.181586000	1.883175000	-2.333094000
9	0.000226000	-0.000845000	-0.112694000	9	0.000961000	-0.001137000	0.000439000
1	-1.458184000	-1.293243000	-1.207875000	1	2.023127000	0.890323000	-0.419080000
1	-1.956152000	-1.734418000	-1.565475000	1	2.701638000	1.189257000	-0.560166000
1	0.558755000	2.540939000	-1.575349000	1	-0.186667000	-1.878082000	2.337672000
1	0.414926000	1.892841000	-1.214901000	1	-0.137995000	-1.405423000	1.751266000
				1	2.376295000	-1.772688000	0.485510000
				1	1.778428000	-1.328261000	0.364208000
H₂₆F⁻							
1	0.841778000	1.095724000	-2.739885000				
9	0.263729000	-0.000122000	0.000309000				
1	0.694719000	0.821372000	-2.052466000				
1	0.834653000	-2.922619000	0.419360000				
1	0.691472000	-2.189063000	0.315019000				
1	-2.104597000	-1.802987000	0.258059000				
1	-1.508684000	-1.343779000	0.191374000				
1	2.053337000	-0.507480000	1.269892000				
1	2.652919000	-0.679455000	1.694567000				
1	0.690741000	1.366649000	1.738465000				
1	0.834003000	1.824929000	2.320647000				
1	-1.508779000	0.840713000	1.064862000				
1	-2.106456000	1.128050000	1.426445000				
1	-0.155418000	-0.822251000	2.055532000				
1	-0.295339000	-1.097571000	2.744076000				
1	-1.506738000	0.504652000	-1.261829000				
1	-2.102857000	0.677760000	-1.692029000				
1	-0.151330000	-1.368452000	-1.741131000				
1	-0.287916000	-1.827833000	-2.323977000				
1	2.656487000	-1.128541000	-1.427740000				

1	2.055030000	-0.844980000	-1.070946000
1	-4.088680000	-0.001046000	0.005506000
1	-4.835554000	0.000833000	-0.007454000
1	2.655408000	1.804972000	-0.258845000
1	2.056935000	1.350120000	-0.192568000
1	-0.288169000	2.927918000	-0.421418000
1	-0.150526000	2.193468000	-0.316297000

H₂Cl⁻	H₄Cl⁻		
17	0.000000000	0.308872000	0.000000000
1	0.024715000	-2.245811000	0.000000000
1	-0.024715000	-3.005012000	0.000000000
17	0.000115000	-0.049348000	-0.000069000
1	2.560395000	0.160466000	-0.025983000
1	3.312097000	0.258994000	0.020219000
1	-3.312908000	0.258339000	-0.023084000
1	-2.561539000	0.161122000	0.030027000
H₆Cl⁻	H₈Cl⁻		
17	0.032622000	-0.016099000	-0.072355000
1	2.596976000	-0.260654000	0.171176000
1	3.342465000	-0.359495000	0.271266000
1	-2.230141000	-2.460752000	0.225109000
1	-1.702900000	-1.916887000	0.182269000
1	-1.450304000	2.973144000	0.224946000
1	-1.110675000	2.298320000	0.155273000
17	-0.000143000	-0.004583000	-0.000067000
1	-2.867316000	-1.760666000	-0.000372000
1	-2.213876000	-1.377410000	-0.000231000
1	2.199734000	1.392500000	-0.000054000
1	2.848800000	1.783109000	-0.000138000
1	-2.199179000	1.393126000	0.000433000
1	-2.848132000	1.783926000	0.000727000
1	2.867992000	-1.759835000	0.000493000
1	2.214405000	-1.376840000	0.000288000
H₁₀Cl⁻	H₁₂Cl⁻		
17	-0.000048000	-0.149743000	-0.017082000
1	2.356176000	1.014332000	-0.035591000
1	2.068602000	-1.751538000	0.039714000
1	0.000127000	2.482437000	0.101146000
1	-2.356806000	1.014303000	-0.056172000
1	-2.067863000	-1.752364000	0.061465000
1	0.000217000	3.237839000	0.135138000
1	3.032214000	1.353721000	-0.038477000
1	2.675680000	-2.203057000	0.058448000
1	-2.674729000	-2.203721000	0.088382000
1	-3.032796000	1.353680000	-0.063652000
17	-0.001842000	-0.002229000	-0.000866000
1	0.097249000	2.632155000	0.270747000
1	2.326654000	1.239688000	-0.268776000
1	-2.235900000	1.398608000	-0.262747000
1	-0.086376000	-2.636741000	-0.251509000
1	2.245256000	-1.384662000	0.261437000
1	-2.873235000	1.800438000	-0.320498000
1	0.121228000	3.384799000	0.333147000
1	2.991609000	1.593600000	-0.327510000
1	2.885422000	-1.782125000	0.317310000
1	-0.112606000	-3.390138000	-0.303381000
1	-2.997115000	-1.584893000	0.312057000
1	-2.330864000	-1.232843000	0.254449000
H₁₄Cl⁻	H₁₆Cl⁻		
1	-1.936996000	-0.048445000	1.619530000
1	-0.254099000	2.055918000	0.999634000
1	2.277548000	1.072525000	0.562525000
1	-2.542103000	0.071768000	2.055076000
1	2.882066000	1.500177000	0.710340000
1	-0.371860000	2.752391000	1.265520000
1	-2.753241000	-1.995361000	-0.812836000
1	2.383029000	1.328887000	0.128353000
1	1.486050000	-0.987753000	1.625065000
1	-1.441611000	-1.054230000	1.618928000
1	-2.441552000	1.210721000	0.135998000
1	1.907310000	-1.369784000	2.121395000
1	3.067894000	1.631412000	0.226689000
1	-3.141407000	1.476714000	0.233458000

1	-2.099115000	-1.656191000	-0.646002000	1	-1.846820000	-1.454204000	2.114454000
1	-1.924731000	1.062045000	-0.908096000	1	2.693761000	-1.478029000	-1.412893000
1	-2.504644000	1.480644000	-1.148930000	1	2.089559000	-1.098503000	-1.166322000
1	0.645303000	1.712848000	-1.568336000	1	0.055461000	-2.450975000	-0.070879000
1	0.774359000	2.333223000	-1.978896000	1	0.071748000	-3.203483000	-0.033991000
17	0.134779000	-0.389715000	-0.011032000	1	-2.035201000	-1.180217000	-1.174407000
1	2.424296000	-1.681067000	0.014811000	1	-2.618397000	-1.586232000	-1.429147000
1	3.091979000	-2.035315000	0.023206000	17	-0.002562000	0.224101000	-0.202112000
H₁₈Cl⁺				1	-0.082217000	2.830309000	0.199669000
1	-1.267984000	-2.259514000	0.146050000	1	-0.104052000	3.575647000	0.319528000
1	1.356319000	-2.273249000	-0.795917000	H₂₀Cl⁺			
1	1.299414000	2.306332000	-0.800236000	1	1.405364000	-2.271093000	-0.208807000
1	-1.326853000	2.223691000	0.161012000	1	2.362617000	0.000584000	-1.593133000
1	1.740777000	-2.920404000	-0.847055000	1	-1.402113000	2.270107000	-0.211992000
1	-1.620045000	-2.895286000	0.347896000	1	-2.225779000	0.005935000	1.148893000
1	-1.693257000	2.849287000	0.369018000	1	3.044962000	0.000890000	-1.914527000
1	1.670094000	2.961634000	-0.849911000	1	1.803271000	-2.908461000	-0.145990000
1	1.021525000	-1.714077000	2.308617000	1	-2.853051000	0.009006000	1.566455000
1	0.796905000	-1.345061000	1.690938000	1	-1.799479000	2.907776000	-0.149220000
1	2.591132000	0.030980000	0.151502000	1	2.853768000	0.000075000	1.566550000
1	3.316260000	0.042625000	0.358656000	1	2.225807000	-0.000013000	1.149949000
1	0.767521000	1.361974000	1.691907000	1	1.404778000	2.269082000	-0.200264000
1	0.983161000	1.733225000	2.311457000	1	1.796633000	2.910097000	-0.136870000
1	-1.567517000	-0.025339000	1.690314000	1	-3.035855000	-0.005090000	-1.926126000
1	-2.007950000	-0.037909000	2.301872000	1	-2.356048000	0.001825000	-1.599422000
17	-0.000633000	0.001151000	-0.505095000	1	-0.004328000	1.359767000	1.964542000
1	-2.648007000	-0.025653000	-0.799205000	1	-0.006153000	1.736283000	2.617249000
1	-3.400734000	-0.032815000	-0.850291000	1	0.000299000	-1.359325000	1.966107000
H₂₂Cl⁺				1	0.000522000	-1.734784000	2.619446000
1	0.020492000	-2.357472000	-1.402350000	17	0.001191000	-0.001845000	-0.363628000
1	2.324327000	-0.800965000	-1.244841000	1	-1.416058000	-2.263881000	-0.198869000
1	0.071178000	2.386713000	1.063342000	1	-1.819398000	-2.897418000	-0.132286000
1	-2.269570000	0.721055000	1.054691000	H₂₄Cl⁺			
1	2.981047000	-1.037084000	-1.529092000	1	-2.017843000	1.769648000	-0.098380000
1	0.029015000	-3.032902000	-1.736822000	1	-1.000141000	0.793032000	2.364785000
1	-2.908888000	0.914741000	1.403357000	1	2.023050000	-1.753108000	0.090654000
1	0.095907000	3.061578000	1.398206000	1	1.028677000	-0.769161000	-2.346924000
1	1.684310000	-2.529214000	1.403858000	1	-1.275059000	1.016081000	3.029913000
1	1.315182000	-1.969856000	1.059508000	1	-2.580601000	2.269540000	-0.130402000
1	2.270674000	0.675474000	1.094814000	1	1.324900000	-0.983950000	-3.005398000
1	2.908498000	0.857777000	1.452302000	1	2.593942000	-2.244182000	0.111638000
1	-1.830139000	2.551113000	-1.571787000	1	0.737596000	3.209233000	0.960303000
1	-1.412617000	1.998078000	-1.274839000	1	0.571863000	2.504140000	0.753282000
1	-0.072815000	-0.091860000	2.494956000	1	1.750789000	0.287209000	2.008734000
1	-0.095077000	-0.131442000	3.247207000	1	2.249777000	0.371604000	2.566788000
1	-1.470767000	-1.928688000	0.930059000	1	-0.691551000	-3.210918000	-1.020971000
1	-1.887337000	-2.474731000	1.239757000	1	-0.540269000	-2.508851000	-0.793406000
17	0.006979000	0.022337000	-0.182621000	1	2.425669000	0.921943000	-0.632425000
				1	3.107762000	1.182838000	-0.817200000
				1	0.116308000	1.854462000	-1.918590000
				1	0.153174000	2.379900000	-2.456100000
				17	-0.012211000	-0.007095000	0.008209000

1	-2.298019000	-0.684589000	-1.345796000	1	-1.726085000	-0.263065000	-2.038633000
1	-2.957078000	-0.884571000	-1.651907000	1	-2.215521000	-0.332109000	-2.607110000
1	1.904026000	2.458920000	-1.643659000	1	-0.139718000	-2.380766000	2.483185000
1	1.479002000	1.918201000	-1.336408000	1	-0.110032000	-1.858464000	1.940961000
				1	-3.131812000	-1.198717000	0.794442000
				1	-2.447284000	-0.935722000	0.621294000
H₂₆Cl⁺				H₂₈Cl⁺			
1	-1.360230000	-0.468396000	-2.240852000	1	1.354013000	-2.092248000	1.180201000
1	-1.648793000	2.101708000	-0.576135000	1	2.094236000	1.345434000	-1.173766000
1	1.458316000	0.490734000	2.214084000	1	-2.219745000	1.141661000	-1.168700000
1	2.278247000	-1.378658000	0.427784000	1	-2.484283000	-0.111683000	1.193568000
1	-2.091398000	2.691112000	-0.727809000	1	2.671440000	1.716247000	-1.481810000
1	-1.738357000	-0.600774000	-2.879601000	1	1.725681000	-2.668565000	1.488772000
1	2.918253000	-1.758001000	0.541070000	1	-3.165381000	-0.140443000	1.510931000
1	1.878708000	0.625862000	2.823719000	1	-2.831419000	1.454053000	-1.474713000
1	0.616012000	2.277068000	-2.503565000	1	3.180694000	0.155016000	1.476340000
1	0.471716000	1.775859000	-1.960866000	1	2.495217000	0.122784000	1.168809000
1	0.483881000	2.531649000	0.800734000	1	-0.124089000	2.483946000	-1.183968000
1	0.625809000	3.237948000	1.018607000	1	-0.155544000	3.166540000	-1.497857000
1	0.127876000	-2.327487000	2.555003000	1	-2.683689000	-1.715257000	-1.472912000
1	0.085689000	-1.815931000	2.003802000	1	-2.104729000	-1.346443000	-1.165904000
1	2.423649000	1.125115000	-0.264747000	1	-1.339061000	2.101657000	1.164301000
1	3.101140000	1.445724000	-0.331085000	1	-1.707595000	2.682310000	1.468577000
1	1.525914000	-0.576558000	-2.134052000	1	1.149560000	2.214547000	1.174257000
1	1.970738000	-0.733595000	-2.720537000	1	1.462400000	2.825584000	1.481220000
17	-0.035537000	-0.012859000	0.013971000	17	0.000368000	-0.002695000	0.000727000
1	0.373905000	-2.533401000	-0.933152000	1	-1.137546000	-2.214077000	1.188449000
1	0.491183000	-3.233169000	-1.184027000	1	-1.446757000	-2.824437000	1.500397000
1	-1.630172000	1.106147000	2.830878000	1	-0.017130000	0.003763000	-3.417879000
1	-1.281120000	0.848742000	2.214625000	1	-0.013041000	0.000489000	-2.664276000
1	-3.577975000	0.112235000	0.170501000	1	2.817542000	-1.456994000	-1.504556000
1	-2.827496000	0.086786000	0.141626000	1	2.210207000	-1.142693000	-1.191676000
1	-1.800178000	-2.113954000	0.213284000	1	0.111611000	-2.491644000	-1.188036000
1	-2.271188000	-2.698159000	0.263202000	1	0.141929000	-3.173434000	-1.503628000
				1	0.004420000	0.005007000	3.417585000
				1	0.004804000	0.004705000	2.663912000
H₃₀Cl⁺				H₃₂Cl⁺			
1	-1.206383000	-0.015094000	2.531296000	1	2.655836000	1.046169000	0.029570000
1	2.378808000	-1.282373000	0.728615000	1	-1.080327000	2.171965000	-1.498081000
1	0.002953000	0.018657000	-2.692634000	1	-1.743418000	-1.966937000	-0.653725000
1	-1.200317000	2.203178000	-1.254215000	1	-0.569762000	-2.133812000	1.798072000
1	3.017904000	-1.625625000	0.924432000	1	-1.370796000	2.740766000	-1.892703000
1	-1.541356000	-0.019824000	3.203756000	1	3.352531000	1.325601000	0.041995000
1	-1.532361000	2.788852000	-1.587847000	1	-0.724598000	-2.692959000	2.274656000
1	0.005349000	0.023905000	-3.445655000	1	-2.230489000	-2.510454000	-0.838055000
1	1.532541000	-0.023445000	3.205461000	1	1.084869000	3.426372000	-0.242852000
1	1.200806000	-0.017917000	2.531329000	1	0.852230000	2.713964000	-0.195984000
1	2.380859000	0.006915000	-1.468281000	1	-2.376047000	-0.484279000	1.506599000
1	3.020346000	0.009830000	-1.862759000	1	-3.000972000	-0.610554000	1.903077000
1	-3.015395000	0.014568000	-1.869628000	1	1.009321000	-3.470576000	-0.092717000
1	-2.376504000	0.010609000	-1.474071000	1	0.800459000	-2.749870000	-0.070400000
1	1.209948000	2.201287000	-1.248526000	1	-0.383183000	0.103415000	2.817048000

1	1.542379000	2.788908000	-1.578307000	1	-0.485497000	0.125639000	3.560547000
1	2.382614000	1.266167000	0.746324000	1	-1.340322000	2.015963000	1.199751000
1	3.022156000	1.605260000	0.947792000	1	-1.712353000	2.575995000	1.538336000
17	-0.000261000	-0.000518000	-0.000132000	17	0.001058000	-0.001904000	-0.002993000
1	-2.380571000	1.272782000	0.741330000	1	1.864096000	-0.968958000	1.703796000
1	-3.018862000	1.615711000	0.940572000	1	2.378349000	-1.243908000	2.179810000
1	1.535827000	-2.766613000	-1.619614000	1	-1.660019000	-0.063590000	-3.196603000
1	1.200835000	-2.186101000	-1.280056000	1	-1.311799000	-0.056670000	-2.531503000
1	-0.004827000	-2.993229000	1.702286000	1	1.546247000	1.192221000	-2.861880000
1	-0.002010000	-2.338556000	1.330256000	1	1.212614000	0.932499000	-2.239258000
1	-2.385172000	-1.275038000	0.725397000	1	2.446828000	-1.133632000	-0.943002000
1	-3.026050000	-1.615734000	0.919818000	1	3.089857000	-1.430317000	-1.192311000
1	0.002641000	2.971823000	1.741993000	1	1.600933000	2.056153000	2.494230000
1	0.002493000	2.321882000	1.361546000	1	1.263725000	1.623722000	1.981501000
1	-1.538280000	-2.767012000	-1.618980000	1	0.555383000	-2.117096000	-2.862584000
1	-1.205934000	-2.184971000	-1.279389000	1	0.437615000	-1.674924000	-2.267308000
				1	-2.731454000	0.569597000	-0.616654000
				1	-3.447844000	0.720859000	-0.782488000
H₃₄Cl⁻							
1	-2.971756000	-0.116197000	-0.626507000				
1	-0.193775000	2.847824000	0.139924000				
1	1.910384000	-0.302266000	1.835692000				
1	2.088641000	-1.813895000	-0.031818000				
1	-0.190264000	3.597650000	0.174588000				
1	-3.706350000	-0.145318000	-0.777940000				
1	2.671929000	-2.285805000	-0.047850000				
1	2.488234000	-0.375573000	2.310704000				
1	-2.308601000	2.387388000	-1.660407000				
1	-1.867694000	1.889701000	-1.312081000				
1	4.331076000	-0.057075000	-0.087636000				
1	5.077122000	-0.066320000	-0.060718000				
1	0.019727000	-3.124448000	1.524047000				
1	-0.015997000	-2.452826000	1.186639000				
1	0.433451000	-2.180447000	-1.758782000				
1	0.600563000	-2.738651000	-2.232110000				
1	0.509266000	1.829683000	-2.030241000				
1	0.680199000	2.325366000	-2.567998000				
17	-0.173672000	-0.013052000	-0.003444000				
1	-1.754842000	-2.246213000	-0.758353000				
1	-2.187827000	-2.824894000	-0.962019000				
1	0.700150000	2.187984000	2.713717000				
1	0.515635000	1.733460000	2.145401000				
1	-2.517258000	1.782942000	1.792391000				
1	-2.007791000	1.387777000	1.403917000				
1	-2.285806000	-1.240553000	1.457348000				
1	-2.838658000	-1.558226000	1.853760000				
1	-1.284682000	-0.308376000	-3.266322000				
1	-1.035595000	-0.239640000	-2.559425000				
1	-0.480588000	-0.558149000	3.520025000				
1	-0.420733000	-0.437215000	2.781275000				
1	2.006835000	1.583369000	0.065062000				
1	2.599481000	2.047114000	0.082687000				
1	2.478604000	-0.171357000	-2.339050000				

1	1.909347000	-0.134925000	-1.849363000	
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H₂Br				H₄Br			
35	0.000000000	0.000000000	0.172165000	35	0.000000000	0.006519000	0.000000000
1	0.000000000	0.000000000	-2.634084000	1	2.809906000	-0.049112000	-0.000005000
1	0.000000000	0.000000000	-3.391680000	1	3.566826000	-0.064966000	0.000004000
				1	-3.566833000	-0.064975000	0.000001000
				1	-2.809913000	-0.049100000	-0.000001000
H₆Br⁻				H₈Br⁻			
35	-0.012199000	-0.006644000	0.000280000	35	0.000000000	0.017367000	-0.000004000
1	-2.805941000	-0.387629000	-0.001521000	1	3.188195000	1.661449000	0.000012000
1	-3.555295000	-0.490622000	-0.001933000	1	2.511357000	1.325576000	0.000009000
1	2.393480000	-2.650424000	-0.001834000	1	-2.420847000	-1.456516000	0.000007000
1	1.884496000	-2.090828000	-0.001408000	1	-3.075089000	-1.834436000	0.000009000
1	1.405056000	3.273274000	-0.001774000	1	2.420847000	-1.456513000	0.000021000
1	1.105154000	2.578781000	-0.001345000	1	3.075089000	-1.834433000	0.000027000
				1	-3.188194000	1.661451000	0.000030000
				1	-2.511356000	1.325579000	0.000022000
H₁₀Br⁻				H₁₂Br⁻			
35	-0.000007000	-0.167892000	0.000199000	35	0.000236000	0.000014000	-0.080761000
1	2.414021000	1.341905000	-0.057078000	1	2.184799000	1.805042000	0.186914000
1	2.540525000	-1.433683000	0.018906000	1	2.655609000	-0.988646000	0.192681000
1	0.000312000	2.679307000	0.075756000	1	-0.473003000	2.791394000	0.216646000
1	-2.413509000	1.342040000	-0.055101000	1	-2.185358000	-1.803607000	0.188551000
1	-2.541349000	-1.432970000	0.016983000	1	0.470355000	-2.791876000	0.214782000
1	-0.000014000	3.433946000	0.094971000	1	-0.599719000	3.530932000	0.296594000
1	3.059197000	1.733370000	-0.073435000	1	2.765226000	2.282067000	0.257308000
1	3.221017000	-1.761037000	0.022666000	1	3.359556000	-1.250449000	0.265759000
1	-3.221613000	-1.760785000	0.020295000	1	0.596285000	-3.531607000	0.294309000
1	-3.058334000	1.734120000	-0.070932000	1	-2.766012000	-2.280263000	0.259500000
				1	-3.360065000	1.248975000	0.263086000
				1	-2.655949000	0.987548000	0.190500000
H₁₄Br⁻				H₁₆Br⁻			
1	-2.160346000	0.174706000	1.643981000	1	2.359072000	1.354964000	0.791784000
1	-0.420223000	2.292449000	1.067040000	1	1.478440000	-1.143678000	1.806610000
1	2.234872000	1.548113000	0.510313000	1	-1.279736000	-1.282032000	1.859979000
1	-2.815658000	0.294782000	1.996707000	1	-2.593572000	0.957072000	0.657255000
1	2.760909000	2.061272000	0.678302000	1	1.903850000	-1.555471000	2.271996000
1	-0.538900000	2.965637000	1.384823000	1	2.981291000	1.658544000	1.090442000
1	-3.066889000	-1.939190000	-0.551677000	1	-3.318727000	1.092930000	0.812122000
1	-2.395720000	-1.609326000	-0.455455000	1	-1.686399000	-1.706726000	2.330431000
1	-2.189371000	1.206130000	-0.872182000	1	3.183167000	-1.441927000	-0.803637000
1	-2.811982000	1.553892000	-1.115888000	1	2.514854000	-1.106224000	-0.709463000
1	0.380702000	2.128428000	-1.534068000	1	0.207355000	-2.674661000	-0.083451000
1	0.454057000	2.796972000	-1.874870000	1	0.305373000	-3.414757000	0.018693000
35	0.122377000	-0.304568000	-0.034921000	1	-2.276731000	-1.553226000	-0.649330000
1	2.801414000	-1.250465000	0.136460000	1	-2.822159000	-2.071721000	-0.683072000

1	3.483931000	-1.563506000	0.208736000	35	-0.007508000	0.184777000	-0.292218000
				1	-0.294390000	2.844673000	0.680512000
				1	-0.398893000	3.575051000	0.836761000
H₁₈Br⁻				H₂₀Br⁻			
1	2.341733000	1.311312000	0.535024000	1	1.444638000	-2.430747000	-0.027030000
1	0.036762000	2.861087000	-0.291849000	1	2.706686000	0.129434000	-1.263590000
1	-2.496377000	-1.398503000	-0.295859000	1	-1.428843000	2.409517000	0.211528000
1	-0.032717000	-2.683933000	0.529358000	1	-2.292990000	-0.047814000	1.430376000
1	0.045435000	3.612201000	-0.230394000	1	3.388766000	0.200801000	-1.575448000
1	2.952495000	1.652170000	0.815702000	1	1.788313000	-3.094755000	0.067931000
1	-0.040723000	-3.383619000	0.809301000	1	-2.953115000	-0.097897000	1.788638000
1	-3.151274000	-1.766030000	-0.232936000	1	-1.772052000	3.067229000	0.343750000
1	0.023548000	1.917495000	2.650628000	1	2.951174000	-0.171484000	1.782554000
1	0.019308000	1.523282000	2.009338000	1	2.291539000	-0.109958000	1.425118000
1	-2.309251000	1.370380000	0.533889000	1	1.494183000	2.370230000	0.200686000
1	-2.911379000	1.725271000	0.815563000	1	1.842279000	3.025655000	0.331560000
1	-1.329904000	-0.748992000	2.007355000	1	-3.382508000	0.298571000	-1.569717000
1	-1.675534000	-0.943873000	2.647094000	1	-2.700467000	0.216502000	-1.260326000
1	1.311164000	-0.782185000	2.007788000	1	0.038555000	1.252646000	2.263470000
1	1.652220000	-0.987176000	2.646889000	1	0.096761000	1.586534000	2.935805000
35	-0.000148000	0.000549000	-0.469306000	1	-0.036677000	-1.485264000	2.149988000
1	2.461366000	-1.458149000	-0.295989000	1	-0.091516000	-1.831025000	2.816394000
1	3.108302000	-1.839953000	-0.235203000	35	-0.000092000	0.004244000	-0.344668000
				1	-1.516095000	-2.387740000	-0.040967000
				1	-1.865408000	-3.048985000	0.052662000
H₂₂Br⁻				H₂₄Br⁻			
1	-2.714585000	0.343043000	-1.064731000	1	2.124024000	1.542058000	1.094523000
1	-1.185595000	-2.468829000	-1.059953000	1	-0.335125000	0.904221000	2.673564000
1	2.409951000	-0.305727000	1.293264000	1	-2.125792000	-1.543014000	-1.096051000
1	1.043337000	2.200837000	1.279602000	1	0.331419000	-0.904168000	-2.673637000
1	-1.500266000	-3.126105000	-1.251778000	1	-0.423765000	1.145216000	3.381939000
1	-3.436554000	0.433830000	-1.260537000	1	2.689025000	1.947671000	1.383996000
1	1.314900000	2.774379000	1.684631000	1	0.418557000	-1.145915000	-3.381999000
1	3.045276000	-0.382626000	1.689689000	1	-2.690342000	-1.949994000	-1.384086000
1	-2.683149000	-1.461112000	1.706013000	1	2.021104000	-1.599289000	2.507465000
1	-2.126290000	-1.155045000	1.302235000	1	1.599867000	-1.262797000	1.981149000
1	0.449954000	-2.382875000	1.293108000	1	-1.345105000	-1.761635000	1.780308000
1	0.571562000	-3.008754000	1.693485000	1	-1.704300000	-2.228427000	2.250102000
1	3.041398000	1.638610000	-1.274634000	1	-2.026109000	1.602047000	-2.501402000
1	2.400741000	1.294362000	-1.077304000	1	-1.602753000	1.265258000	-1.977016000
1	0.000565000	0.006984000	2.635381000	1	0.494517000	-2.780586000	-0.349228000
1	0.008797000	0.007161000	3.387957000	1	0.625260000	-3.516632000	-0.441735000
1	-1.759122000	1.674523000	1.287571000	1	2.639640000	-0.737107000	-0.773535000
1	-2.219820000	2.117459000	1.685504000	1	3.338567000	-0.931757000	-0.976057000
35	-0.000719000	-0.000880000	-0.265419000	35	0.000719000	-0.000272000	-0.000104000
1	-0.510783000	2.681506000	-1.070260000	1	1.341915000	1.766245000	-1.781149000
1	-0.639926000	3.397766000	-1.265759000	1	1.698911000	2.234533000	-2.251107000
1	2.522935000	-2.372955000	-1.259920000	1	-3.332078000	0.933511000	0.979074000
1	1.991846000	-1.875628000	-1.063895000	1	-2.634555000	0.736364000	0.773998000
				1	-0.629521000	3.514949000	0.437749000
				1	-0.498519000	2.778769000	0.346776000

H₂₆Br⁻				H₂₈Br⁻			
1	0.227690000	2.004727000	-1.945093000	1	2.615380000	-0.151779000	-1.265071000
1	2.753348000	0.590405000	-0.749057000	1	-0.160784000	-2.616473000	1.262864000
1	-0.204648000	-2.097582000	1.941374000	1	-2.186379000	1.440163000	1.265690000
1	-2.468034000	-1.474657000	0.215703000	1	-1.166449000	2.344900000	-1.265121000
1	3.434490000	0.882317000	-0.877020000	1	-0.199937000	-3.300060000	1.573788000
1	0.257561000	2.536521000	-2.478128000	1	3.299021000	-0.189988000	-1.575999000
1	-3.021158000	-1.983741000	0.228924000	1	-1.475062000	2.956400000	-1.575516000
1	-0.236902000	-2.637787000	2.465013000	1	-2.755736000	1.817669000	1.580085000
1	1.514836000	-0.895573000	-3.112843000	1	1.481822000	-2.947672000	-1.582133000
1	1.185055000	-0.751609000	-2.452063000	1	1.171649000	-2.337363000	-1.270898000
1	2.007514000	-2.052148000	-0.004751000	1	-2.344081000	-1.172461000	1.258455000
1	2.538495000	-2.584806000	-0.012704000	1	-2.955141000	-1.482339000	1.568497000
1	-2.517651000	0.423292000	2.651157000	1	0.192496000	3.289248000	1.591221000
1	-1.984989000	0.383572000	2.121101000	1	0.154483000	2.607378000	1.276336000
1	-0.384344000	-2.670309000	-0.920713000	1	-2.609326000	0.160902000	-1.270307000
1	-0.498164000	-3.399045000	-1.067596000	1	-3.293622000	0.200953000	-1.579639000
1	-1.468363000	-0.467014000	-2.365323000	1	-1.441653000	-2.179036000	-1.275769000
1	-1.809352000	-0.574192000	-3.027349000	1	-1.818751000	-2.746994000	-1.593205000
35	0.010656000	0.037542000	0.076553000	35	0.000034000	-0.000035000	-0.000320000
1	-2.568116000	1.216931000	-0.630266000	1	1.446784000	2.188593000	-1.252701000
1	-3.293695000	1.367876000	-0.757631000	1	1.823778000	2.758721000	-1.566316000
1	2.669484000	-0.275728000	2.543940000	1	-0.008106000	-0.012913000	3.593224000
1	2.131884000	-0.243162000	2.018737000	1	-0.006171000	-0.009779000	2.839823000
1	1.975417000	2.957907000	1.119090000	1	2.749330000	-1.826867000	1.579087000
1	1.630936000	2.343827000	0.855130000	1	2.181813000	-1.447999000	1.262990000
1	-0.963543000	2.707018000	0.722712000	1	2.339617000	1.164403000	1.275618000
1	-1.280704000	3.378990000	0.838296000	1	2.949525000	1.472295000	1.589871000
				1	0.008249000	0.012184000	-3.593541000
				1	0.006073000	0.009143000	-2.840135000
H₃₀Br⁻				H₃₂Br⁻			
1	-1.266658000	2.289676000	-1.330355000	1	-2.460958000	1.350384000	0.976499000
1	2.487588000	1.366710000	0.775162000	1	0.805543000	-1.047963000	2.661959000
1	0.003464000	-2.480015000	1.445707000	1	1.289675000	-1.932517000	-1.726513000
1	-1.271366000	-2.298815000	-1.308981000	1	0.942382000	0.729332000	-2.723506000
1	3.127542000	1.709632000	0.968518000	1	1.009310000	-1.310454000	3.335478000
1	-1.595492000	2.874430000	-1.669265000	1	-3.081715000	1.693934000	1.222650000
1	-1.599696000	-2.886404000	-1.643393000	1	1.182261000	0.914432000	-3.410682000
1	0.004789000	-3.130738000	1.824190000	1	1.627914000	-2.432891000	-2.174886000
1	1.591438000	2.870873000	-1.676420000	1	-0.786830000	1.271380000	3.412018000
1	1.263164000	2.286678000	-1.335962000	1	-0.625586000	1.014641000	2.724840000
1	2.485495000	-1.361795000	0.788104000	1	2.781534000	0.400070000	-0.974036000
1	3.125811000	-1.701616000	0.986110000	1	3.485083000	0.500232000	-1.217100000
1	-3.124165000	-1.699417000	1.001538000	1	-1.406146000	-0.875841000	-3.333020000
1	-2.484645000	-1.359941000	0.800246000	1	-1.120534000	-0.700699000	-2.660875000
1	1.260323000	-2.300689000	-1.315384000	1	1.319047000	2.497641000	-0.918395000
1	1.586230000	-2.888245000	-1.652350000	1	1.654507000	3.128151000	-1.150828000
1	2.481052000	-0.009551000	-1.579474000	1	1.997136000	1.340477000	1.610756000
1	3.119614000	-0.011685000	-1.975477000	1	2.517717000	1.693371000	2.023202000
35	0.000127000	0.000044000	-0.000142000	35	-0.000061000	-0.001003000	-0.000350000
1	-2.489899000	-0.005717000	-1.569280000	1	-1.401169000	1.952676000	-1.614909000
1	-3.131357000	-0.007605000	-1.960673000	1	-1.764475000	2.460489000	-2.034383000

1	1.601781000	0.013239000	3.318697000	1	0.535853000	-3.524398000	1.072472000
1	1.271825000	0.010780000	2.643311000	1	0.423709000	-2.813260000	0.858544000
1	0.006941000	3.149575000	1.794110000	1	-2.388005000	-1.705714000	2.171862000
1	0.005863000	2.494984000	1.422473000	1	-1.894522000	-1.354771000	1.725912000
1	-2.481622000	1.371128000	0.786566000	1	-2.839047000	-0.387539000	-0.797251000
1	-3.120165000	1.715175000	0.982952000	1	-3.556573000	-0.483652000	-0.997163000
1	-0.010169000	-0.019124000	-3.622906000	1	-0.452707000	3.513170000	1.149081000
1	-0.008639000	-0.016075000	-2.870243000	1	-0.363051000	2.804113000	0.918506000
1	-1.584862000	0.012367000	3.327325000	1	-1.733280000	-3.117599000	-1.065919000
1	-1.258628000	0.010648000	2.650127000	1	-1.381615000	-2.488956000	-0.853053000
				1	2.524830000	-1.355892000	0.798316000
				1	3.161845000	-1.697246000	1.002663000
H₃₄Br⁻				H₃₆Br⁻			
1	-2.055601000	-1.789608000	1.267391000	1	-1.240403000	-2.721018000	-0.576155000
1	1.952580000	-1.892254000	1.282911000	1	2.271349000	-1.934926000	0.714970000
1	1.623622000	0.708655000	-2.303804000	1	2.271287000	1.935088000	-0.714842000
1	0.075362000	2.630279000	-1.425151000	1	-1.240657000	2.720941000	0.576114000
1	2.444600000	-2.356210000	1.608755000	1	2.830089000	-2.404302000	0.888894000
1	-2.573080000	-2.228107000	1.589058000	1	-1.540097000	-3.393108000	-0.722422000
1	0.095674000	3.289392000	-1.784099000	1	-1.540543000	3.392938000	0.722417000
1	2.073969000	0.889027000	-2.878354000	1	2.830058000	2.404450000	-0.888703000
1	-0.055565000	-1.645884000	3.357729000	1	0.123260000	-3.366220000	1.863472000
1	-0.044222000	-1.324526000	2.679309000	1	0.118230000	-2.714174000	1.493300000
1	2.094491000	2.210210000	0.012323000	1	1.044152000	2.257824000	1.582720000
1	2.604693000	2.760336000	0.015217000	1	1.312667000	2.824487000	1.996738000
1	-2.010813000	0.998286000	-2.888540000	1	-2.469190000	1.608034000	-2.206221000
1	-1.570904000	0.796010000	-2.313217000	1	-1.958424000	1.277081000	-1.765144000
1	-1.973749000	2.317697000	0.006882000	1	-2.860860000	0.920895000	0.784793000
1	-2.454181000	2.894015000	0.008682000	1	-3.548689000	1.137890000	0.989838000
1	1.613142000	0.689839000	2.314107000	1	0.890418000	-0.560880000	2.728861000
1	2.060322000	0.863827000	2.893104000	1	1.126720000	-0.711994000	3.426245000
35	-0.000513000	0.001482000	-0.000508000	35	0.004872000	0.000003000	-0.000006000
1	-3.039223000	0.136322000	-0.008393000	1	-2.860682000	-0.921165000	-0.785043000
1	-3.789247000	0.158022000	-0.011372000	1	-3.548498000	-1.138164000	-0.990129000
1	2.450565000	-2.348855000	-1.607563000	1	3.439141000	-0.554967000	-1.518146000
1	1.955534000	-1.886751000	-1.283613000	1	2.758450000	-0.423292000	-1.231201000
1	-0.096422000	-3.664945000	-0.004671000	1	1.313021000	-2.824399000	-1.996659000
1	-0.076323000	-2.913397000	-0.005730000	1	1.044418000	-2.257756000	-1.582672000
1	-2.044756000	-1.785702000	-1.287046000	1	-1.053906000	-1.086628000	-2.559233000
1	-2.560369000	-2.222876000	-1.613523000	1	-1.327784000	-1.374095000	-3.196618000
1	-2.024388000	0.975420000	2.886220000	1	-2.469248000	-1.608193000	2.206021000
1	-1.582579000	0.779461000	2.310172000	1	-1.958461000	-1.277205000	1.764996000
1	-0.038079000	-1.619918000	-3.374513000	1	1.126893000	0.712169000	-3.426161000
1	-0.030437000	-1.303677000	-2.693666000	1	0.890566000	0.561010000	-2.728795000
1	3.044275000	-0.019516000	0.004299000	1	2.758344000	0.423478000	1.231351000
1	3.794347000	-0.038671000	0.005273000	1	3.438988000	0.555182000	1.518394000
1	0.086762000	3.274350000	1.811714000	1	-1.328238000	1.373875000	3.196514000
1	0.067964000	2.617880000	1.447883000	1	-1.054188000	1.086540000	2.559143000
				1	0.123147000	3.366294000	-1.863249000
				1	0.118158000	2.714195000	-1.493169000
H₃₈Br⁻				H₄₀Br⁻			

1	2.252725000	2.097243000	-0.497710000	1	-2.467563000	1.585614000	-1.213072000
1	-0.555356000	1.840148000	2.332313000	1	-1.661695000	-2.411512000	-1.217212000
1	-3.319182000	-0.001382000	-0.235051000	1	2.466820000	-1.581303000	-1.216384000
1	-0.293769000	-2.762038000	-1.230145000	1	1.983304000	0.397097000	2.425874000
1	-0.697350000	2.300184000	2.908035000	1	-2.058419000	-2.977231000	-1.507359000
1	2.798965000	2.593351000	-0.630841000	1	-3.053402000	1.953116000	-1.501752000
1	-0.345445000	-3.446768000	-1.532637000	1	2.444796000	0.487152000	3.009525000
1	-4.066342000	-0.001312000	-0.284203000	1	3.052536000	-1.948842000	-1.505264000
1	2.299900000	1.624911000	2.401499000	1	-3.627533000	-0.729261000	0.012374000
1	1.831917000	1.296476000	1.913902000	1	-2.890815000	-0.581099000	0.005599000
1	-2.027924000	-2.047788000	0.603907000	1	2.408662000	-1.667112000	1.211591000
1	-2.542350000	-2.575464000	0.751083000	1	2.974882000	-2.064816000	1.499434000
1	0.115553000	-0.854070000	-3.603785000	1	2.063925000	2.984456000	-1.494588000
1	0.101259000	-0.696396000	-2.869399000	1	1.665138000	2.418456000	-1.207878000
1	2.027923000	-2.047794000	-0.603791000	1	-0.297905000	1.463884000	2.571817000
1	2.542347000	-2.575480000	-0.750948000	1	-0.371600000	1.832586000	3.222003000
1	-0.101216000	-0.696127000	2.869484000	1	-1.575882000	-2.467263000	1.211249000
1	-0.115473000	-0.853757000	3.603879000	1	-1.942973000	-3.054610000	1.497447000
35	-0.000003000	0.002577000	0.000003000	35	-0.000410000	0.000015000	-0.000342000
1	2.310985000	0.053001000	-2.037788000	1	-0.581969000	2.892254000	-0.007066000
1	2.874642000	0.064543000	-2.532566000	1	-0.731512000	3.628673000	-0.012936000
1	-2.799019000	2.593395000	0.630670000	1	0.490697000	-2.425345000	-3.014822000
1	-2.252772000	2.097288000	0.497575000	1	0.400527000	-1.967950000	-2.427906000
1	-0.000048000	3.706717000	-0.000154000	1	-1.858601000	-0.368802000	-3.210509000
1	-0.000015000	2.955455000	-0.000122000	1	-1.484355000	-0.294824000	-2.563547000
1	0.555342000	1.839987000	-2.332467000	1	-0.396196000	1.976160000	-2.421873000
1	0.697330000	2.299991000	-2.908217000	1	-0.486915000	2.437159000	-3.005872000
1	4.066391000	-0.001255000	0.284201000	1	-2.974970000	2.060803000	1.505430000
1	3.319229000	-0.001326000	0.235043000	1	-2.410961000	1.662305000	1.214380000
1	-2.299907000	1.624732000	-2.401605000	1	1.864632000	0.381523000	-3.206139000
1	-1.831929000	1.296313000	-1.913990000	1	1.488334000	0.304145000	-2.560773000
1	-2.310958000	0.053108000	2.037773000	1	0.580237000	-2.892619000	-0.016913000
1	-2.874630000	0.064670000	2.532534000	1	0.728195000	-3.629314000	-0.027185000
1	0.345445000	-3.446631000	1.532955000	1	0.371302000	-1.847385000	3.214111000
1	0.293760000	-2.761968000	1.230316000	1	0.295790000	-1.473322000	2.567197000
1	-2.615090000	-1.588372000	-2.358549000	1	3.627003000	0.729653000	0.018544000
1	-2.109948000	-1.272856000	-1.903148000	1	2.890858000	0.578951000	0.007404000
1	2.109983000	-1.272716000	1.903218000	1	-1.983059000	-0.403797000	2.421351000
1	2.615129000	-1.588213000	2.358627000	1	-2.444161000	-0.497204000	3.004798000
				1	1.575787000	2.460713000	1.221690000
				1	1.941411000	3.048377000	1.509202000
H₄₂Br⁻							
1	-3.005689000	0.139307000	-1.361709000				
1	-1.067707000	2.891410000	0.907903000				
1	0.884225000	-0.196428000	2.987140000				
1	2.599587000	-1.415144000	-0.603819000				
1	-1.295785000	3.574084000	1.116611000				
1	-3.682421000	0.174677000	-1.681689000				
1	3.245553000	-1.757122000	-0.770788000				
1	1.127798000	-0.253274000	3.693626000				
1	-1.847072000	2.717187000	-1.849786000				

1	-1.510894000	2.169644000	-1.460104000
1	2.689784000	-0.033735000	1.369449000
1	3.355919000	-0.034515000	1.713425000
1	-1.256966000	-3.647184000	0.901515000
1	-1.040835000	-2.952760000	0.720635000
1	1.052880000	-0.952681000	-2.544739000
1	1.363222000	-1.190566000	-3.185973000
1	0.806227000	2.960901000	-0.632307000
1	1.044086000	3.656801000	-0.776192000
35	-0.150433000	-0.001620000	0.005247000
1	-1.568133000	-2.006461000	-1.636397000
1	-1.934974000	-2.511698000	-2.054486000
1	-1.208787000	1.630555000	3.411049000
1	-0.992907000	1.322053000	2.763107000
1	-3.425143000	1.284723000	1.218600000
1	-2.757345000	1.028021000	0.989963000
1	-2.940088000	-1.438879000	0.490513000
1	-3.595264000	-1.777233000	0.624018000
1	-1.441649000	0.113970000	-3.688180000
1	-1.188240000	0.091606000	-2.983251000
1	-1.693692000	-1.445899000	3.072283000
1	-1.379887000	-1.149128000	2.457825000
1	1.242118000	2.000633000	1.661858000
1	1.593546000	2.509830000	2.088434000
1	6.083150000	-0.009637000	-0.263047000
1	5.338985000	-0.023268000	-0.212157000
1	1.595679000	-2.714105000	1.831542000
1	1.234185000	-2.172258000	1.456929000
1	0.715080000	1.551457000	-2.614407000
1	0.944837000	1.908271000	-3.232111000
1	0.696192000	-2.881801000	-0.972504000
1	0.889307000	-3.566318000	-1.208847000
1	2.470970000	1.081554000	-0.855084000
1	3.125308000	1.380093000	-1.072506000

H₃O⁻				H₅O⁻			
8	-0.339645000	-0.113065000	0.000004000	8	0.000006000	-0.175512000	-0.107857000
1	-0.582167000	0.818381000	0.000000000	1	-0.000464000	-0.967731000	0.438972000
1	2.078020000	0.074725000	0.000052000	1	2.371609000	0.739956000	0.143398000
1	1.221309000	0.011413000	-0.000081000	1	1.614967000	0.445782000	0.068598000
				1	-2.371431000	0.740101000	0.143406000
				1	-1.614730000	0.445989000	0.068483000
H₇O⁻				H₉O⁻			
8	-0.027424000	-0.082621000	0.113979000	8	-0.001746000	-0.001789000	0.198861000
1	-0.039809000	-0.162868000	1.073466000	1	-0.004998000	-0.001223000	1.161643000
1	2.270276000	-1.260695000	-0.447291000	1	-0.109531000	2.639047000	-0.443905000
1	1.575068000	-0.905016000	-0.285204000	1	-0.078925000	1.877380000	-0.258846000
1	-2.509132000	-0.730053000	-0.467460000	1	2.646512000	0.121844000	-0.423454000
1	-1.749540000	-0.542703000	-0.302778000	1	1.883923000	0.086029000	-0.244741000
1	0.273631000	1.744550000	-0.177898000	1	-1.885539000	-0.079443000	-0.247954000
1	0.398900000	2.517754000	-0.304668000	1	-2.648418000	-0.110605000	-0.427266000

	1	0.123151000	-2.639812000	-0.447112000
	1	0.087796000	-1.878904000	-0.259251000
H₁₁O⁻				
8	-0.006451000	0.000824000	-0.430682000	
1	-0.011799000	0.001076000	-1.392685000	
1	0.415697000	-2.660959000	0.163814000	
1	0.296079000	-1.909585000	-0.008061000	
1	2.662702000	0.398425000	0.153382000	
1	1.909655000	0.286170000	-0.015474000	
1	-1.913208000	-0.289310000	0.000551000	
1	-2.664960000	-0.404157000	0.175676000	
1	0.014723000	-0.004493000	2.476546000	
1	0.009112000	-0.003167000	1.721259000	
1	-0.279515000	1.913337000	-0.001961000	
1	-0.386879000	2.666070000	0.172409000	
H₁₃O⁻				
8	-0.144474000	0.000002000	0.351496000	
1	-0.179421000	0.000000000	1.313158000	
1	2.211942000	-1.667271000	0.407432000	
1	1.581963000	-1.227068000	0.371496000	
1	-2.936923000	0.000068000	0.013096000	
1	-2.165774000	0.000046000	0.087132000	
1	0.750864000	0.000017000	-1.591113000	
1	1.021877000	0.000021000	-2.297979000	
1	-0.820212000	-2.577422000	-0.612906000	
1	-0.641315000	-1.881090000	-0.334208000	
1	-0.641221000	1.881123000	-0.334186000	
1	-0.820080000	2.577462000	-0.612892000	
1	1.582039000	1.226973000	0.371529000	
1	2.212051000	1.667127000	0.407477000	
H₁₅O⁻				
8	0.015791000	-0.182073000	-0.243495000	
1	0.014570000	-0.289981000	-1.199428000	
1	2.610828000	0.967811000	-1.143694000	
1	1.973564000	0.669599000	-0.847487000	
1	-0.061853000	1.934180000	-0.051793000	
1	-0.136409000	2.691891000	0.045765000	
1	1.358573000	-1.697860000	0.082386000	
1	1.890900000	-2.252429000	0.166722000	
1	-2.635039000	0.861032000	-1.150043000	
1	-1.991445000	0.583220000	-0.849346000	
1	-1.831144000	-2.288783000	0.160274000	
1	-1.302900000	-1.730657000	0.080046000	
1	-1.322908000	0.367109000	1.389441000	
1	-1.802246000	0.566084000	1.942029000	
1	1.319294000	0.431406000	1.383875000	
1	1.789891000	0.643960000	1.939210000	
H₁₇O⁻				
8	-0.004509000	-0.038714000	0.325830000	
1	-0.005550000	-0.103490000	1.285678000	
1	0.133285000	-2.681358000	-0.875716000	
1	0.084483000	-1.997600000	-0.535069000	
1	2.604659000	-1.416373000	0.854016000	
1	1.942340000	-1.075178000	0.691944000	
1	-1.677562000	1.307281000	0.713956000	
1	-2.231228000	1.796764000	0.912114000	
1	2.131875000	1.901270000	0.905942000	
1	1.592292000	1.394824000	0.711453000	
1	-0.059620000	1.859100000	-0.867115000	
1	-0.069273000	2.418063000	-1.379540000	
1	-1.426046000	-0.122216000	-1.354709000	
1	-1.938033000	-0.134638000	-1.912950000	
1	1.422863000	-0.039263000	-1.354407000	
1	1.935739000	-0.036028000	-1.911804000	
1	-1.875861000	-1.200892000	0.672943000	
1	-2.528288000	-1.560556000	0.836620000	
H₁₉O⁻				
8	-0.000158000	-0.000521000	-0.284596000	
1	-0.006707000	0.004566000	-1.246823000	
1	1.065035000	-2.717889000	-1.191950000	
1	0.807978000	-2.061211000	-0.909551000	
1	-2.897326000	0.461119000	-1.166181000	
1	-2.197173000	0.350872000	-0.893605000	
1	0.923732000	1.157151000	1.355264000	
1	1.213758000	1.520528000	1.953299000	
1	-1.938446000	0.309419000	1.935050000	
1	-1.473452000	0.233614000	1.341598000	
1	0.522860000	-1.390827000	1.346858000	
1	0.684508000	-1.835753000	1.938315000	
1	2.184386000	-0.347531000	-0.032829000	
1	2.933655000	-0.464185000	0.046181000	
H₂₁O⁻				
8	0.002810000	0.049043000	-0.197900000	
1	-0.029580000	-0.404854000	-1.045731000	
1	2.533784000	0.007222000	-1.955497000	
1	1.946464000	0.085107000	-1.482446000	
1	-2.511785000	0.376199000	-1.965378000	
1	-1.924382000	0.362871000	-1.486716000	
1	0.077523000	1.095866000	1.757578000	
1	0.121773000	1.470523000	2.409641000	
1	-2.638193000	0.155060000	1.256318000	
1	-1.977419000	0.123930000	0.882261000	
1	-0.126288000	-1.328819000	1.492556000	
1	-0.172161000	-1.805710000	2.086175000	
1	1.957987000	-0.205218000	0.878660000	
1	2.614052000	-0.278221000	1.256102000	

1	-1.390230000	-1.721119000	-0.061385000	1	-1.496099000	-1.882661000	-0.328740000
1	-1.868427000	-2.310942000	0.009187000	1	-1.885426000	-2.510064000	-0.487023000
1	1.413040000	1.714012000	-0.898722000	1	1.357654000	1.921024000	-0.254618000
1	1.858074000	2.262155000	-1.178470000	1	1.822647000	2.519121000	-0.218982000
1	-0.781808000	2.064884000	-0.066445000	1	-0.993988000	2.053228000	-0.239802000
1	-1.052195000	2.775308000	-0.003024000	1	-1.346146000	2.727468000	-0.222071000
				1	1.467359000	-2.778015000	-0.450418000
				1	1.179742000	-2.096398000	-0.298669000
H₂₃O⁻				H₂₅O⁻			
8	0.000556000	0.000026000	-0.127695000	8	0.130549000	-0.018679000	-0.024076000
1	0.001184000	0.001849000	-1.089777000	1	-0.803859000	0.111889000	0.159691000
1	2.428481000	1.458310000	-1.511567000	1	-1.381704000	-2.723908000	-0.252153000
1	1.886180000	1.132198000	-1.097799000	1	-0.942953000	-2.107604000	-0.211114000
1	-2.819123000	0.248542000	-1.513902000	1	-1.356375000	2.160048000	1.913370000
1	-2.188487000	0.191417000	-1.100746000	1	-0.883764000	1.727273000	1.518036000
1	-0.001746000	-0.000501000	2.123425000	1	1.020000000	0.829373000	-1.911498000
1	-0.002041000	-0.002624000	2.876063000	1	1.344059000	1.105703000	-2.539482000
1	-2.340309000	-1.407584000	1.182699000	1	1.386815000	2.713560000	0.249859000
1	-1.758326000	-1.057409000	0.844248000	1	1.070437000	2.025721000	0.180866000
1	0.461194000	-2.000627000	0.847247000	1	2.373311000	0.015230000	0.008595000
1	0.614505000	-2.661763000	1.186628000	1	3.125814000	-0.001379000	-0.019778000
1	2.042110000	-0.177891000	0.847622000	1	1.007306000	-1.567407000	-1.398383000
1	2.718639000	-0.236022000	1.186538000	1	1.340054000	-2.077288000	-1.849718000
1	-0.856638000	-2.021183000	-1.100796000	1	1.082152000	0.424210000	1.971468000
1	-1.105590000	-2.603435000	-1.513997000	1	1.394095000	0.577073000	2.648141000
1	0.800320000	1.887516000	0.847377000	1	-2.862204000	-0.180997000	-0.237954000
1	1.065220000	2.512893000	1.186011000	1	-3.471584000	0.068995000	0.115751000
1	-1.549843000	1.343799000	0.847595000	1	-0.932866000	1.884038000	-1.116568000
1	-2.063629000	1.788330000	1.185615000	1	-1.379432000	2.426638000	-1.393193000
1	2.137741000	-1.855838000	-1.509376000	1	1.373163000	-2.384394000	1.377578000
1	1.657639000	-1.439965000	-1.099122000	1	1.051856000	-1.790395000	1.030557000
1	-0.637564000	2.759160000	-1.506543000	1	-1.355629000	-1.134219000	2.608281000
1	-0.494367000	2.140621000	-1.095880000	1	-0.903610000	-0.925317000	2.041884000
				1	-1.386360000	-0.574940000	-2.655994000
				1	-0.953112000	-0.452470000	-2.045637000
H₂₇O⁻				H₂₉O⁻			
8	-0.000386000	-0.000045000	-0.107301000	8	-0.075322000	0.004534000	-0.090004000
1	-0.001152000	-0.000921000	-1.070798000	1	0.345403000	-0.067483000	0.772743000
1	-2.218874000	-1.997601000	-1.487771000	1	2.997789000	0.734594000	-1.035600000
1	-1.742339000	-1.569803000	-1.090209000	1	2.265376000	0.608404000	-0.907449000
1	0.903974000	2.801213000	1.203614000	1	-0.822461000	0.070918000	3.229417000
1	0.694072000	2.144955000	0.895805000	1	-0.743789000	-0.021876000	2.488475000
1	2.230959000	-0.721135000	-1.092865000	1	-2.080816000	-0.576134000	-1.250704000
1	2.839831000	-0.918118000	-1.491128000	1	-2.622187000	-0.765662000	-1.738302000
1	2.871078000	0.613587000	1.210665000	1	-3.020502000	0.724558000	1.031186000
1	2.199874000	0.469979000	0.896937000	1	-2.346358000	0.596897000	0.715819000
1	1.512473000	-1.674752000	0.894872000	1	-1.478358000	1.625959000	-1.139264000
1	1.972566000	-2.185897000	1.205504000	1	-1.916161000	2.081123000	-1.550476000
1	0.488110000	-2.288024000	-1.095264000	1	0.341598000	0.054041000	-2.204812000
1	0.621581000	-2.910607000	-1.498742000	1	0.445916000	0.136599000	-2.951110000

1	0.001734000	-0.000426000	2.032324000	1	-0.702428000	2.123529000	0.955990000
1	0.002347000	-0.000005000	2.787398000	1	-0.827587000	2.782800000	1.303519000
1	1.739886000	1.568581000	-1.092363000	1	1.667931000	-1.577717000	-0.946340000
1	2.216677000	1.997263000	-1.488704000	1	2.191607000	-2.079246000	-1.155575000
1	-0.901305000	-2.793959000	1.205769000	1	-1.713526000	-1.588697000	0.794410000
1	-0.691199000	-2.139398000	0.894228000	1	-2.215394000	-2.097578000	1.040089000
1	-2.840377000	0.916964000	-1.489136000	1	0.953388000	2.822360000	-1.254893000
1	-2.231655000	0.720504000	-1.090357000	1	0.665514000	2.187603000	-0.964458000
1	-2.875664000	-0.614320000	1.212984000	1	2.971224000	-0.860462000	1.646470000
1	-2.204405000	-0.469893000	0.899911000	1	2.464412000	-0.685560000	1.123291000
1	-0.622831000	2.911148000	-1.498582000	1	2.076276000	2.103896000	1.601116000
1	-0.489131000	2.288203000	-1.095749000	1	1.632378000	1.699517000	1.150448000
1	-1.506522000	1.671198000	0.894000000	1	0.679606000	-2.796408000	1.514715000
1	-1.966618000	2.181621000	1.206069000	1	0.466348000	-2.273892000	1.017045000
				1	-0.585788000	-2.835583000	-1.447009000
				1	-0.486833000	-2.162772000	-1.118705000
H₃₁O⁻				H₃₃O⁻			
8	-0.079129000	-0.214522000	0.003038000	8	0.609576000	-0.178163000	-0.038306000
1	0.219151000	0.701484000	-0.017773000	1	0.422699000	0.725036000	0.237553000
1	2.865885000	0.267105000	1.517738000	1	1.575954000	-2.931493000	-0.869838000
1	2.210901000	0.063269000	1.206766000	1	1.352511000	-2.243928000	-0.662408000
1	-1.768261000	-1.089480000	-2.621556000	1	-0.804387000	2.735820000	2.324864000
1	-1.379054000	-0.882083000	-2.009779000	1	-0.593461000	2.041991000	2.144633000
1	-1.923725000	1.203016000	1.129947000	1	-0.864174000	0.772786000	-1.543639000
1	-2.390362000	1.708083000	1.438142000	1	-1.338784000	1.166967000	-1.985993000
1	-3.214142000	-0.861446000	-0.044178000	1	-0.120408000	3.788433000	-0.310961000
1	-2.476440000	-0.703740000	-0.032027000	1	0.101977000	3.113213000	-0.540712000
1	-1.432638000	-0.837403000	1.982729000	1	1.577770000	1.435955000	-1.589459000
1	-1.853765000	-1.031294000	2.577609000	1	1.831323000	2.023185000	-1.991447000
1	0.192673000	0.904103000	2.157486000	1	0.859538000	-0.611824000	-2.303224000
1	0.320762000	1.373530000	2.735384000	1	0.948706000	-0.768556000	-3.038231000
1	-0.637264000	-2.285991000	0.024239000	1	2.318791000	1.219399000	0.990933000
1	-0.849497000	-3.010221000	0.038525000	1	2.713714000	1.778178000	1.310242000
1	2.223078000	2.273970000	-0.012435000	1	-2.990213000	-2.529103000	0.704127000
1	2.439001000	2.988644000	-0.042548000	1	-3.604395000	-2.932446000	0.840074000
1	-1.874213000	1.183408000	-1.211517000	1	-2.756917000	2.252083000	0.021068000
1	-2.330891000	1.682798000	-1.543007000	1	-3.265506000	2.796620000	0.072351000
1	0.954974000	-1.788985000	2.642678000	1	3.487580000	-0.411974000	-1.063708000
1	0.707568000	-1.423133000	2.031277000	1	2.776915000	-0.350303000	-0.807208000
1	2.913270000	0.207372000	-1.450762000	1	-0.366925000	-2.595084000	1.559585000
1	2.250103000	0.015216000	-1.150187000	1	-0.130869000	-1.984961000	1.178493000
1	2.285513000	-2.402517000	0.071755000	1	2.710287000	-1.527981000	1.735772000
1	1.733792000	-1.888054000	0.056759000	1	2.191925000	-1.187964000	1.299747000
1	0.409155000	1.289101000	-2.776555000	1	-2.187040000	-0.045392000	1.122633000
1	0.265103000	0.832527000	-2.192573000	1	-1.501075000	-0.145975000	0.809340000
1	-0.383555000	3.653879000	-0.029881000	1	-4.203607000	-0.274065000	-1.333469000
1	-0.625861000	2.947528000	0.004474000	1	-3.479320000	-0.334975000	-1.159495000
1	0.759810000	-1.493986000	-1.956342000	1	0.469065000	-0.136700000	2.370949000
1	1.021963000	-1.880525000	-2.548692000	1	0.404524000	-0.013573000	3.114171000
				1	-0.954836000	-1.468926000	-0.998386000
				1	-1.457970000	-1.929139000	-1.331910000

H₂CN⁻				H₄CN⁻			
1	2.657877000	-0.033747000	0.020727000	1	-2.126569000	-1.249354000	-0.001454000
6	0.162540000	0.096771000	-0.001600000	6	0.094133000	-0.079408000	-0.006542000
7	-1.006528000	-0.060180000	0.000503000	7	1.268597000	0.022861000	0.003759000
1	3.412575000	-0.125621000	-0.014648000	1	-2.800128000	-1.598819000	0.009040000
				1	-2.539804000	1.836398000	0.003981000
				1	-1.978476000	1.328198000	0.001373000
H₆CN⁻				H₈CN⁻			
1	-1.744269000	1.372106000	-0.494748000	1	1.771297000	0.127235000	1.293953000
6	0.321647000	0.020371000	0.002456000	6	-0.400581000	-0.107133000	0.004950000
7	1.499768000	-0.011616000	0.000309000	7	-1.578227000	-0.070373000	-0.001626000
1	-2.396403000	1.733947000	-0.623905000	1	2.436254000	0.212398000	1.643480000
1	-2.410640000	-0.335098000	1.769542000	1	2.462632000	0.219252000	-1.583735000
1	-1.752561000	-0.249157000	1.406686000	1	1.795355000	0.136439000	-1.238088000
1	-2.373626000	-1.445012000	-1.176867000	1	1.832833000	-2.537761000	-0.037683000
1	-1.750754000	-1.117699000	-0.897612000	1	1.308835000	-1.994520000	-0.036279000
				1	0.750794000	2.150418000	-0.009024000
				1	1.093074000	2.821951000	-0.050940000
H₁₀CN⁻				H₁₂CN⁻			
6	-0.604715000	0.013054000	-0.786226000	1	0.055250000	0.148046000	2.515423000
7	0.551447000	-0.090236000	-0.576467000	6	-0.643232000	-0.058729000	-0.977587000
1	-2.787904000	-1.704620000	0.922847000	7	0.520042000	-0.088118000	-0.782471000
1	-2.336724000	-1.280630000	0.490697000	1	0.148015000	0.051071000	1.775801000
1	-2.483793000	1.897578000	1.127529000	1	-2.446221000	-1.880625000	1.087465000
1	-2.062132000	1.463744000	0.676529000	1	-2.034796000	-1.450436000	0.624949000
1	0.730125000	-1.943577000	1.005056000	1	-2.548811000	1.741232000	1.024479000
1	0.880091000	-2.473396000	1.519412000	1	-2.128855000	1.315921000	0.565017000
1	2.690121000	-0.057351000	0.393410000	1	1.050173000	-2.097760000	0.498335000
1	3.364951000	-0.014260000	0.731938000	1	1.255988000	-2.634847000	0.984670000
1	0.819980000	2.007834000	0.764804000	1	2.500710000	0.257871000	0.462735000
1	0.953443000	2.658006000	1.120401000	1	3.049369000	0.402794000	0.960900000
				1	0.609421000	2.224060000	0.255355000
				1	0.708856000	2.891869000	0.587689000
H₁₄CN⁻				H₁₆CN⁻			
1	3.244615000	-0.250388000	1.051505000	1	-3.556961000	-1.644445000	-0.225462000
6	0.640789000	-0.098685000	-0.977576000	6	-0.688479000	-0.009933000	-0.643110000
7	-0.497511000	0.043039000	-0.701460000	7	0.490468000	0.006717000	-0.624730000
1	2.706025000	-0.234269000	0.523905000	1	-2.898420000	-1.291559000	-0.333422000
1	1.864749000	2.608015000	0.585334000	1	-0.887021000	-1.826572000	2.187994000
1	1.565261000	2.000405000	0.258818000	1	-0.850927000	-1.318587000	1.635789000
1	1.312910000	-2.766373000	0.897998000	1	-0.757090000	2.095771000	2.011307000
1	1.120229000	-2.230435000	0.407004000	1	-0.723199000	1.576900000	1.469111000
1	-1.095363000	2.200056000	0.315265000	1	1.389272000	-2.194853000	-0.015444000
1	-1.238984000	2.860498000	0.646482000	1	1.716554000	-2.856950000	0.129553000
1	-2.666420000	0.258664000	0.368767000	1	2.903813000	-0.162454000	-0.776999000
1	-3.335603000	0.335043000	0.707596000	1	3.647436000	-0.260678000	-0.703371000
1	-1.553218000	-1.966226000	0.197919000	1	1.573850000	2.133512000	-0.204991000
1	-1.873795000	-2.579991000	0.493629000	1	1.912094000	2.795846000	-0.086237000
1	-0.163596000	-0.016485000	1.789523000	1	1.685666000	0.043835000	1.515306000

1	-0.248966000	0.072319000	2.531930000	1	2.027856000	0.098596000	2.183204000
				1	-2.912021000	1.237250000	-0.328091000
				1	-3.573305000	1.586965000	-0.226476000
H₁₈CN⁻				H₂₀CN⁻			
1	-3.513597000	-1.572765000	-1.250331000	1	3.751574000	0.431643000	-1.378690000
6	-0.588407000	-0.123282000	-0.580285000	6	0.536387000	-0.071893000	-0.612456000
7	0.588344000	-0.057200000	-0.547751000	7	-0.636274000	-0.053792000	-0.491756000
1	-2.848644000	-1.238746000	-1.124300000	1	3.017597000	0.315453000	-1.247904000
1	-0.113019000	-1.536034000	2.563615000	1	0.020532000	1.457932000	2.529831000
1	-0.055828000	-1.206486000	1.891416000	1	-0.049758000	1.124492000	1.860934000
1	-0.606192000	1.932663000	2.124288000	1	0.141051000	-1.970582000	2.277781000
1	-0.515042000	1.575618000	1.469528000	1	0.069866000	-1.622276000	1.616337000
1	1.825444000	-2.117767000	0.009142000	1	-1.466536000	2.225079000	-0.128694000
1	2.173592000	-2.769074000	0.152379000	1	-1.787765000	2.896835000	-0.021447000
1	2.936389000	-0.045550000	-1.137289000	1	-2.925442000	0.220492000	-1.254814000
1	3.674647000	-0.126016000	-1.265088000	1	-3.656341000	0.326962000	-1.402286000
1	1.550731000	2.189030000	-0.461836000	1	-1.847106000	-2.174887000	-0.415382000
1	1.884012000	2.860446000	-0.395016000	1	-2.192974000	-2.839934000	-0.350176000
1	2.093408000	0.336465000	1.339671000	1	-2.346411000	-0.094310000	1.244820000
1	2.455531000	0.442868000	1.990570000	1	-2.876913000	-0.103475000	1.778313000
1	-2.698780000	1.330002000	-0.723755000	1	2.164438000	-2.032148000	-0.387153000
1	-3.357961000	1.692255000	-0.779410000	1	2.681087000	-2.578589000	-0.346492000
1	-2.470033000	-0.293888000	1.190297000	1	2.375788000	0.016842000	1.186650000
1	-3.002618000	-0.312929000	1.722093000	1	2.904444000	0.027752000	1.722166000
				1	1.788985000	2.925483000	-0.023191000
				1	1.469482000	2.255136000	-0.143580000
H₂₂CN⁻				H₂₄CN⁻			
1	-3.769836000	-0.367242000	-1.436506000	1	-3.605976000	-0.822839000	-1.306783000
6	-0.548745000	0.037260000	-0.585582000	6	-0.524564000	0.011597000	-0.335615000
7	0.620238000	0.043115000	-0.430220000	7	0.653016000	0.043108000	-0.290629000
1	-3.036499000	-0.256159000	-1.299840000	1	-2.880690000	-0.679610000	-1.158181000
1	-0.144690000	-1.898990000	2.348867000	1	-0.155963000	-0.681158000	3.074213000
1	-0.069725000	-1.551485000	1.688220000	1	-0.056284000	-0.559993000	2.340659000
1	-0.049906000	1.606431000	2.486376000	1	0.033952000	2.643570000	1.875692000
1	0.023350000	1.270413000	1.818194000	1	0.046606000	2.103675000	1.354070000
1	1.325619000	-2.347739000	-0.414949000	1	1.275062000	-2.208968000	0.659439000
1	1.646131000	-3.024056000	-0.345096000	1	1.557876000	-2.833604000	0.966471000
1	2.824978000	-0.359330000	-1.380799000	1	2.688930000	-0.912687000	-1.165799000
1	3.497840000	-0.468998000	-1.700243000	1	3.310185000	-1.224413000	-1.455550000
1	2.352455000	1.706692000	0.153808000	1	2.413671000	1.743942000	-0.426374000
1	2.867564000	2.219002000	0.346989000	1	2.946439000	2.274175000	-0.446952000
1	2.291111000	-0.510068000	1.299693000	1	2.374388000	0.082447000	1.452382000
1	2.805392000	-0.698450000	1.814764000	1	2.903938000	0.095377000	1.986134000
1	-2.310436000	1.824574000	0.059552000	1	-2.337102000	1.845217000	-0.518392000
1	-2.814273000	2.347985000	0.255122000	1	-2.863520000	2.382466000	-0.538145000
1	-2.371841000	-0.363274000	1.203292000	1	-2.462765000	0.242573000	1.362398000
1	-2.889275000	-0.533047000	1.722161000	1	-2.996135000	0.275122000	1.892234000
1	-1.747872000	-3.046448000	-0.375108000	1	-1.900109000	-2.765323000	0.878082000
1	-1.597113000	-2.317175000	-0.478385000	1	-1.599981000	-2.143138000	0.581637000
1	0.106379000	2.751522000	-0.664020000	1	0.100989000	2.483947000	-1.478503000
1	0.011446000	3.490472000	-0.577057000	1	0.005540000	3.212715000	-1.628149000

	1	-0.111762000	-2.736178000	-2.382855000
	1	-0.111017000	-2.188657000	-1.869638000
H₂₆CN⁻				
1	3.656362000	-0.782140000	0.627169000	
6	0.454649000	0.000568000	0.026234000	
7	-0.710542000	0.063693000	0.192347000	
1	2.925695000	-0.648931000	0.500066000	
1	-0.631006000	-1.445068000	-2.977124000	
1	-0.535789000	-1.115785000	-2.309717000	
1	-0.490705000	2.250398000	-2.452883000	
1	-0.464618000	1.726775000	-1.915299000	
1	-1.467044000	-2.341845000	0.065367000	
1	-1.791412000	-3.015481000	-0.006398000	
1	-2.383103000	-0.556504000	1.799327000	
1	-2.898322000	-0.754814000	2.311339000	
1	-2.413993000	1.847285000	0.398998000	
1	-2.785477000	2.496150000	0.475508000	
1	-2.809010000	-0.161931000	-1.036280000	
1	-3.363221000	-0.189269000	-1.544028000	
1	2.309217000	1.746532000	-0.417973000	
1	2.837696000	2.279358000	-0.471600000	
1	2.030760000	-0.166106000	-2.023434000	
1	2.544249000	-0.187815000	-2.572898000	
1	1.650006000	-3.044141000	-0.730901000	
1	1.335469000	-2.373421000	-0.606106000	
1	0.090561000	2.671832000	0.732276000	
1	0.195595000	3.404245000	0.855206000	
1	0.610913000	-2.274179000	2.575401000	
1	0.566888000	-1.747107000	2.042870000	
1	1.840225000	1.035793000	2.949165000	
1	1.685965000	0.896913000	2.228118000	
H₂₈CN⁻				
1	3.577378000	0.085843000	-1.398223000	
6	0.527442000	-0.008011000	-0.016457000	
7	-0.649213000	0.006993000	0.053931000	
1	2.904311000	0.037265000	-1.063392000	
1	0.188724000	3.025285000	1.647888000	
1	0.083144000	2.301713000	1.481777000	
1	-0.083633000	-0.448834000	3.375973000	
1	-0.177209000	-0.341130000	2.638524000	
1	-1.194792000	2.288323000	-0.968885000	
1	-1.475820000	2.913151000	-1.275606000	
1	-2.741366000	0.257985000	-1.245627000	
1	-3.404909000	0.337511000	-1.589886000	
1	-2.497446000	-1.360609000	0.946232000	
1	-3.019812000	-1.850792000	1.173911000	
1	-2.383646000	1.160376000	1.342460000	
1	-2.972889000	1.481758000	1.681534000	
1	2.339739000	-1.473082000	1.115461000	
1	2.789924000	-1.912031000	1.528011000	
1	2.440834000	1.005156000	1.405817000	
1	3.035261000	1.308102000	1.753492000	
1	1.908117000	2.815984000	-1.174368000	
1	1.602647000	2.191541000	-0.889620000	
1	-0.126825000	-2.592771000	0.851904000	
1	-0.059502000	-3.268910000	1.169179000	
1	0.113483000	0.469752000	-3.379067000	
1	0.205647000	0.355736000	-2.642772000	
1	1.731250000	-2.596900000	-1.751534000	
1	1.446004000	-1.986479000	-1.419333000	
1	-1.315925000	-1.843474000	-1.547166000	
1	-1.532848000	-2.361356000	-2.045451000	
H₃₀CN⁻				
1	-3.283148000	1.961953000	-0.057568000	
6	-0.525017000	-0.004972000	-0.000223000	
7	0.654190000	0.004310000	0.003300000	
1	-2.692593000	1.496630000	-0.041895000	
1	-0.083276000	-1.808958000	-2.896106000	
1	-0.068581000	-1.413371000	-2.258286000	
1	1.492347000	-3.194734000	0.110711000	
1	1.248914000	-2.485321000	0.086601000	
1	1.271237000	1.154762000	-2.195161000	
1	1.516137000	1.485103000	-2.822972000	
1	2.643900000	1.496772000	-0.066032000	
1	3.233345000	1.962271000	-0.087556000	
1	2.630266000	-0.722924000	1.325140000	
1	3.219981000	-0.952901000	1.730043000	
1	2.614133000	-0.817835000	-1.289675000	
1	3.197552000	-1.076059000	-1.686456000	
1	-2.701889000	-0.675198000	1.313670000	
H₃₂CN⁻				
1	3.585793000	1.420119000	0.729157000	
6	0.516481000	-0.000187000	0.000583000	
7	-0.663224000	0.002221000	-0.001241000	
1	2.932360000	1.093093000	0.553804000	
1	-0.670642000	-1.889565000	2.783218000	
1	-0.571313000	-1.462519000	2.173826000	
1	-1.345025000	-3.264444000	-0.608896000	
1	-1.134349000	-2.560810000	-0.458865000	
1	-2.026865000	0.731988000	1.992472000	
1	-2.442188000	0.963041000	2.573455000	
1	-1.176024000	2.547541000	0.461154000	
1	-1.390620000	3.248715000	0.617453000	
1	-2.032230000	-0.759248000	-1.977135000	
1	-2.443334000	-0.997156000	-2.558438000	
1	-2.877253000	-1.122024000	0.559892000	
1	-3.524189000	-1.460670000	0.734372000	
1	2.942342000	-1.062245000	-0.566320000	

1	-3.301971000	-0.886994000	1.714658000	1	3.598938000	-1.379577000	-0.747645000
1	-2.714456000	-0.772571000	-1.249634000	1	2.166602000	-0.809764000	1.925502000
1	-3.322682000	-1.009090000	-1.623507000	1	2.592425000	-1.059772000	2.491351000
1	-1.629136000	1.511532000	-2.818413000	1	0.813228000	1.774400000	2.858575000
1	-1.374357000	1.177596000	-2.196454000	1	0.703049000	1.380488000	2.229093000
1	-1.392872000	-2.489079000	0.093799000	1	1.251102000	-2.575995000	0.364697000
1	-1.648071000	-3.194600000	0.113763000	1	1.471186000	-3.279796000	0.500269000
1	-0.033684000	3.411616000	-0.121134000	1	1.424900000	3.294205000	-0.497675000
1	-0.022666000	2.661425000	-0.095603000	1	1.209603000	2.588362000	-0.365165000
1	-1.602203000	1.706169000	2.712542000	1	2.562841000	1.091659000	-2.497482000
1	-1.352967000	1.326706000	2.114917000	1	2.142156000	0.836025000	-1.930320000
1	1.291804000	1.310500000	2.098047000	1	-0.608460000	1.451326000	-2.178602000
1	1.538996000	1.685579000	2.699265000	1	-0.710348000	1.879905000	-2.786501000
1	-0.045082000	-1.249136000	2.354056000	1	0.718975000	-1.374564000	-2.230608000
1	-0.058207000	-1.600185000	3.017478000	1	0.830765000	-1.767492000	-2.860424000
				1	-2.898648000	1.090896000	-0.552869000
				1	-3.551091000	1.419458000	-0.726158000
H₃₄CN⁻							
1	-1.530819000	-3.581764000	0.007569000				
6	-0.270986000	-0.374323000	0.048326000				
7	0.716994000	0.266880000	-0.017567000				
1	-1.276574000	-2.874937000	0.019740000				
1	0.150696000	0.760038000	3.336713000				
1	0.186754000	0.586406000	2.607499000				
1	-1.329097000	3.020083000	0.456626000				
1	-0.962435000	2.368645000	0.392763000				
1	2.613442000	0.267483000	1.642641000				
1	3.178280000	0.256848000	2.136994000				
1	2.851083000	-1.129387000	-0.421266000				
1	3.490138000	-1.506528000	-0.530677000				
1	0.784258000	2.326055000	-1.479200000				
1	0.826511000	2.943426000	-1.903764000				
1	1.507296000	2.432311000	1.008438000				
1	1.726864000	3.071723000	1.334655000				
1	-2.845984000	-0.910829000	-0.276360000				
1	-3.578994000	-1.041853000	-0.384354000				
1	-1.435585000	-1.624408000	2.116692000				
1	-1.719301000	-1.957936000	2.726581000				
1	1.404934000	-2.676443000	1.933295000				
1	1.105487000	-2.116021000	1.534001000				
1	-2.284344000	0.587632000	1.611259000				
1	-2.825807000	0.873842000	2.044137000				
1	1.126415000	-3.111712000	-1.579156000				
1	0.882439000	-2.495930000	-1.228311000				
1	-1.527057000	-1.853789000	-2.778152000				
1	-1.276909000	-1.534361000	-2.146819000				
1	1.203312000	-0.058668000	-2.500143000				
1	1.418937000	-0.123322000	-3.216473000				
1	-1.531305000	0.978754000	-1.830394000				
1	-1.941575000	1.335823000	-2.347562000				
1	2.934327000	1.304939000	-0.728287000				
1	3.585652000	1.612431000	-0.940440000				
1	-3.827528000	1.944224000	-0.354855000				

1	-4.476548000	2.305010000	-0.430378000	
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H₂ClO⁻				H₄ClO⁻			
8	0.895831000	-0.559750000	0.000000000	8	0.908435000	0.000027000	-0.000004000
17	-0.698917000	0.128965000	0.000000000	17	-0.820590000	-0.000029000	0.000001000
1	2.624406000	1.434348000	0.000000000	1	1.807913000	-2.554368000	0.000009000
1	2.090525000	0.851238000	0.000000000	1	1.533595000	-1.826079000	0.000001000
				1	1.807634000	2.554523000	0.000011000
				1	1.533405000	1.826201000	-0.000002000
H₆ClO⁻				H₈ClO⁻			
8	0.764813000	-0.000016000	-0.318890000	8	-0.728202000	-0.000049000	0.000601000
17	-0.912596000	0.000010000	0.085540000	17	0.993749000	0.000393000	-0.000638000
1	1.528981000	-2.636265000	-0.693979000	1	-1.486471000	0.839795000	2.583625000
1	1.307280000	-1.904791000	-0.589512000	1	-1.278079000	0.611366000	1.881630000
1	1.529051000	2.636203000	-0.694049000	1	-1.490286000	2.583172000	-0.839261000
1	1.307325000	1.904739000	-0.589561000	1	-1.280294000	1.881549000	-0.611742000
1	1.683874000	0.000032000	1.490448000	1	-1.276710000	-1.882537000	0.613146000
1	2.039108000	0.000046000	2.173599000	1	-1.484821000	-2.584620000	0.840852000
				1	-1.490638000	-0.841798000	-2.581805000
				1	-1.280817000	-0.613216000	-1.880414000
H₁₀ClO⁻				H₁₂ClO⁻			
8	-0.562313000	0.002422000	0.002982000	8	0.518395000	-0.000108000	0.000470000
17	1.158202000	-0.000811000	-0.001092000	17	-1.201312000	-0.000197000	-0.000721000
1	-1.221860000	1.864225000	-2.060730000	1	1.098320000	1.775127000	2.252793000
1	-1.049432000	1.365473000	-1.507339000	1	0.959294000	1.312657000	1.665154000
1	-1.227156000	-2.051198000	-1.869604000	1	1.104783000	-2.758955000	-0.779754000
1	-1.053292000	-1.500344000	-1.368639000	1	0.960631000	-2.040682000	-0.575360000
1	-1.043990000	1.507003000	1.372409000	1	2.604403000	0.001661000	0.003732000
1	-1.214556000	2.059334000	1.873077000	1	3.356991000	0.000515000	0.004478000
1	-3.432927000	0.003619000	0.004795000	1	1.099586000	-1.596121000	2.381899000
1	-2.680917000	0.002575000	0.003317000	1	0.958585000	-1.179402000	1.761416000
1	-1.047604000	-1.375473000	1.499872000	1	0.963345000	-0.082762000	-2.118006000
1	-1.219195000	-1.880802000	2.047554000	1	1.106987000	-0.112172000	-2.864297000
				1	0.960704000	1.991631000	-0.732350000
				1	1.101510000	2.692711000	-0.991198000
H₁₄ClO⁻				H₁₆ClO⁻			
8	-0.492694000	-0.008242000	0.086941000	8	-0.449034000	0.005521000	-0.003089000
17	1.222902000	0.006309000	-0.089113000	17	1.273225000	0.011602000	-0.125687000
1	-0.353784000	2.824909000	-1.069191000	1	-0.733933000	-0.213449000	2.929994000
1	-0.432232000	2.145568000	-0.749151000	1	-0.642065000	-0.123792000	2.181995000
1	-1.283033000	0.016807000	-1.925814000	1	0.087062000	-2.850662000	1.273356000
1	-1.608662000	0.049292000	-2.612555000	1	-0.025352000	-2.178477000	0.953884000
1	-0.476975000	1.351340000	1.802456000	1	-0.545673000	1.886573000	-1.286471000
1	-0.449342000	1.874349000	2.351890000	1	-0.546236000	2.450213000	-1.790045000
1	-0.314389000	-2.817798000	-1.107136000	1	-0.524952000	-2.302624000	-1.952213000
1	-0.398683000	-2.140124000	-0.784694000	1	-0.527483000	-1.751165000	-1.435010000
1	-0.427704000	-1.890124000	2.346645000	1	-2.027994000	0.064224000	-1.659128000
1	-0.459460000	-1.367029000	1.797273000	1	-2.577030000	0.073903000	-2.176797000
1	-2.314179000	-1.298598000	0.146321000	1	-2.171436000	1.289257000	0.608184000
1	-2.986393000	-1.632598000	0.214238000	1	-2.834610000	1.622346000	0.742574000
1	-2.334831000	1.255820000	0.168882000	1	-2.165561000	-1.332909000	0.507327000

1	-3.008124000	1.586867000	0.240222000	1	-2.829501000	-1.670164000	0.626708000
				1	-0.051743000	2.066167000	1.149502000
				1	0.063949000	2.729156000	1.487529000
H₁₈ClO⁻				H₂₀ClO⁻			
8	-0.436215000	-0.000588000	-0.000023000	8	-0.511897000	0.209013000	0.000199000
17	1.291379000	0.000698000	-0.000492000	17	0.871754000	-0.825188000	-0.000319000
1	0.110745000	2.260712000	2.254200000	1	3.763014000	1.219795000	-0.002514000
1	-0.011500000	1.735428000	1.730490000	1	3.095027000	0.877275000	-0.002019000
1	0.113328000	-3.083841000	0.827762000	1	-1.971936000	-2.695455000	0.003937000
1	-0.009876000	-2.367648000	0.635353000	1	-1.617422000	-2.032793000	0.002435000
1	-2.155732000	0.382980000	-1.439082000	1	-1.474158000	1.798546000	-1.318554000
1	-2.799830000	0.484452000	-1.817261000	1	-1.886019000	2.325680000	-1.665561000
1	-2.797335000	-1.819219000	0.490966000	1	-3.526840000	0.071803000	0.003165000
1	-2.152891000	-1.441535000	0.389820000	1	-2.775926000	0.005416000	0.001537000
1	-2.154019000	1.054695000	1.056009000	1	-1.470067000	1.801621000	1.318697000
1	-2.798510000	1.330696000	1.332808000	1	-1.880939000	2.331323000	1.662960000
1	-0.634166000	2.159283000	-0.580921000	1	0.539312000	2.205625000	-0.001663000
1	-0.672251000	2.889373000	-0.777750000	1	0.901705000	2.869956000	-0.002121000
1	-0.629013000	-0.577054000	2.161245000	1	-1.287098000	-0.572944000	1.956216000
1	-0.665485000	-0.772113000	2.891900000	1	-1.517169000	-0.859877000	2.617865000
1	-0.014341000	0.632512000	-2.367863000	1	0.620802000	0.992720000	-2.069116000
1	0.108732000	0.824498000	-3.084201000	1	0.973181000	1.229088000	-2.689799000
1	-0.632422000	-1.582678000	-1.580222000	1	-1.291326000	-0.575339000	-1.953295000
1	-0.669168000	-2.117703000	-2.114695000	1	-1.522308000	-0.863208000	-2.614212000
				1	0.978090000	1.232148000	2.687985000
				1	0.625445000	0.994713000	2.067880000
H₂₂ClO⁻				H₂₄ClO⁻			
8	0.608238000	-0.000355000	0.180338000	8	-0.717284000	0.001033000	0.000622000
17	-0.906237000	0.001011000	-0.648497000	17	1.008300000	-0.001374000	-0.001514000
1	-0.859848000	1.651303000	2.314808000	1	-0.467761000	-2.575350000	-1.655852000
1	-0.462249000	1.249129000	1.815206000	1	-0.575306000	-1.946612000	-1.252853000
1	1.579256000	-2.015426000	0.717850000	1	2.431113000	3.254668000	-0.001815000
1	1.958925000	-2.631944000	0.933207000	1	2.029143000	2.621141000	-0.001519000
1	1.640955000	-1.670317000	-2.187419000	1	-1.819854000	0.005500000	2.019174000
1	1.416558000	-1.261034000	-1.594537000	1	-2.255091000	0.008054000	2.636448000
1	2.844871000	0.000382000	-0.146720000	1	-0.455490000	2.575989000	1.658795000
1	3.597527000	0.000277000	-0.116993000	1	-0.564563000	1.947414000	1.255988000
1	1.519466000	-0.002215000	2.253626000	1	-2.514461000	1.374903000	0.000078000
1	1.925012000	-0.003528000	2.888353000	1	-3.183696000	1.720345000	0.000111000
1	1.416525000	1.264173000	-1.591821000	1	-2.521967000	-1.364356000	0.003267000
1	1.640834000	1.675371000	-2.183408000	1	-3.192637000	-1.706924000	0.004134000
1	-3.054965000	-0.002899000	1.156972000	1	-0.567006000	1.946169000	-1.258050000
1	-3.715606000	-0.003465000	1.513202000	1	-0.457210000	2.574137000	-1.661588000
1	-0.763654000	-2.733704000	-0.488728000	1	2.016676000	-2.630335000	0.004103000
1	-0.798227000	-3.482640000	-0.504280000	1	2.416477000	-3.265219000	0.005790000
1	1.957877000	2.629072000	0.938465000	1	0.827214000	0.000637000	2.742167000
1	1.578585000	2.012777000	0.721711000	1	0.877545000	0.000757000	3.490207000
1	-0.797639000	3.484339000	-0.497916000	1	-2.258424000	0.001393000	-2.634056000
1	-0.763168000	2.735370000	-0.483751000	1	-1.822314000	0.001180000	-2.017410000
1	-0.859116000	-1.656250000	2.311490000	1	0.871903000	-0.008840000	-3.494594000
1	-0.461796000	-1.253107000	1.812434000	1	0.822229000	-0.006847000	-2.746521000
				1	-0.465631000	-2.570120000	1.664741000

				1	-0.573710000	-1.942581000	1.260016000
H₂₆ClO⁻				H₂₈ClO⁻			
8	-0.721769000	-0.001278000	0.315956000	8	0.820089000	0.192114000	-0.345794000
17	0.698951000	0.000291000	-0.666360000	17	-0.669898000	-0.182385000	0.437031000
1	3.494524000	1.901024000	0.379303000	1	-2.342064000	1.362624000	-2.433468000
1	2.838811000	1.547846000	0.287227000	1	-1.820769000	1.105663000	-1.961520000
1	-2.373743000	-2.662487000	0.846122000	1	-0.410278000	-2.409162000	3.187834000
1	-1.949220000	-2.058443000	0.697718000	1	-0.322188000	-1.953638000	2.598272000
1	-1.695280000	1.187081000	-1.495889000	1	3.071174000	0.019720000	-0.124999000
1	-1.962610000	1.558437000	-2.094245000	1	3.822801000	0.020963000	-0.169284000
1	-3.759833000	-0.005481000	0.133154000	1	1.904477000	-2.383741000	0.965618000
1	-3.008379000	-0.004427000	0.084155000	1	1.680764000	-1.750188000	0.623648000
1	-1.959675000	2.055763000	0.693611000	1	1.918640000	-1.427973000	-1.701367000
1	-2.386492000	2.658410000	0.840867000	1	2.308608000	-1.897174000	-2.143781000
1	0.492377000	2.764506000	-1.137224000	1	1.353594000	1.167243000	-2.205171000
1	0.536458000	3.492375000	-1.311674000	1	1.656751000	1.485031000	-2.821216000
1	-1.260265000	-0.000459000	2.390613000	1	-0.561088000	-2.838555000	-0.408614000
1	-1.577268000	-0.000373000	3.077393000	1	-0.630182000	-3.561117000	-0.596652000
1	-1.693111000	-1.195036000	-1.494120000	1	-0.123891000	2.340251000	-0.612456000
1	-1.958155000	-1.568658000	-2.092074000	1	-0.488507000	2.997399000	-0.664726000
1	0.557502000	2.494476000	1.654431000	1	1.700081000	0.301591000	1.838734000
1	0.208136000	1.896088000	1.358380000	1	1.928965000	0.327190000	2.556344000
1	3.505003000	-1.884026000	0.381058000	1	-0.613233000	-1.107572000	-2.790373000
1	2.848145000	-1.533087000	0.288629000	1	-0.217922000	-0.793623000	-2.231299000
1	1.855105000	0.004000000	2.624458000	1	-3.453590000	1.958772000	0.674839000
1	1.303951000	0.004955000	2.115939000	1	-2.803120000	1.609251000	0.542507000
1	0.546914000	-3.493194000	-1.310034000	1	-3.560988000	-1.461385000	-1.116987000
1	0.500769000	-2.765970000	-1.133460000	1	-2.887793000	-1.186359000	-0.932841000
1	0.217481000	-1.895862000	1.360403000	1	-0.353935000	2.670974000	2.504767000
1	0.570840000	-2.492193000	1.655731000	1	-0.335684000	2.086908000	2.035419000
				1	2.414407000	2.743988000	0.435418000
				1	1.992521000	2.136555000	0.288178000
H₃₀ClO⁻				H₃₂ClO⁻			
8	-1.107667000	-0.098557000	0.001889000	8	-1.160403000	0.001802000	-0.001072000
17	0.604537000	0.084428000	-0.001104000	17	0.561492000	-0.000778000	0.000167000
1	2.532299000	-2.348379000	-1.737655000	1	2.104728000	-1.155028000	-3.041744000
1	2.009436000	-1.919264000	-1.413584000	1	1.654051000	-0.945966000	-2.480392000
1	-1.930668000	2.853668000	-0.028761000	1	-1.091150000	2.363980000	1.899196000
1	-1.738633000	2.123405000	-0.021120000	1	-1.172049000	1.778835000	1.428082000
1	-0.925548000	-1.126685000	2.032247000	1	-1.176019000	-2.125093000	0.821767000
1	-0.773703000	-1.452332000	2.696900000	1	-1.098581000	-2.826570000	1.091556000
1	-3.523639000	0.453583000	1.716085000	1	-3.516025000	-0.288578000	1.864608000
1	-2.871463000	0.352169000	1.352748000	1	-2.875011000	-0.225086000	1.474230000
1	-2.578247000	-1.830653000	0.019978000	1	-2.871615000	-1.160211000	-0.944076000
1	-3.149157000	-2.322680000	0.025013000	1	-3.510693000	-1.473204000	-1.191050000
1	2.016622000	-1.876912000	1.461613000	1	1.645455000	-2.632247000	-0.388256000
1	2.536935000	-2.299393000	1.798248000	1	2.097022000	-3.224985000	-0.469856000
1	-2.870801000	0.324117000	-1.359007000	1	-2.867249000	1.399749000	-0.545426000
1	-3.523184000	0.417659000	-1.724104000	1	-3.504849000	1.773926000	-0.689797000
1	3.328235000	0.337020000	-0.009962000	1	3.236412000	-0.008288000	0.010469000
1	4.065230000	0.459638000	-0.010869000	1	3.983651000	-0.004844000	-0.010031000
1	-0.828079000	1.348404000	2.014486000	1	-0.767783000	-0.374311000	2.421848000

1	-0.702301000	1.789926000	2.609245000	1	-0.601299000	-0.487593000	3.145697000
1	-0.090347000	-3.197373000	0.036770000	1	-0.595139000	-2.479294000	-1.999864000
1	-0.361342000	-2.496918000	0.029394000	1	-0.761677000	-1.909602000	-1.539235000
1	2.299711000	0.852116000	-3.013805000	1	2.109221000	2.021995000	-2.547270000
1	1.815516000	0.709721000	-2.458811000	1	1.657991000	1.653823000	-2.075286000
1	-0.772496000	-1.510080000	-2.664983000	1	-1.082940000	0.469014000	-2.996193000
1	-0.925134000	-1.170336000	-2.007670000	1	-1.167346000	0.351979000	-2.254556000
1	1.632963000	3.404409000	-0.041174000	1	2.098455000	1.195943000	3.032551000
1	1.311547000	2.725661000	-0.033410000	1	1.649055000	0.973808000	2.475226000
1	2.311194000	0.932568000	2.984014000	1	2.090728000	-2.066501000	2.525130000
1	1.825566000	0.773790000	2.434760000	1	1.641060000	-1.686131000	2.061402000
1	-0.828378000	1.309703000	-2.038268000	1	-0.755296000	2.287698000	-0.884624000
1	-0.707927000	1.736628000	-2.644654000	1	-0.585874000	2.970485000	-1.148372000
				1	2.112337000	3.209667000	0.529343000
				1	1.658286000	2.621440000	0.430662000
H₃₄ClO⁻				H₃₆ClO⁻			
8	1.125924000	-0.002823000	0.003481000	8	-0.898651000	-0.517472000	0.000667000
17	-0.597855000	-0.001237000	0.019172000	17	0.681849000	0.172238000	0.001819000
1	-1.846253000	-0.019137000	-3.382627000	1	2.458362000	-0.630809000	-3.048992000
1	-1.453146000	-0.016732000	-2.744405000	1	1.973871000	-0.559384000	-2.481465000
1	0.852832000	-1.648138000	2.586779000	1	-1.506250000	1.997297000	1.755090000
1	0.979093000	-1.248290000	1.959773000	1	-1.412070000	1.379805000	1.334153000
1	2.520861000	1.943163000	0.000443000	1	-1.488231000	-2.584207000	0.988519000
1	3.029610000	2.497997000	-0.001892000	1	-1.764840000	-3.219452000	1.283933000
1	3.571649000	0.030988000	1.828059000	1	-3.479103000	-0.551321000	1.552403000
1	2.916855000	0.024322000	1.457634000	1	-2.801714000	-0.492294000	1.228037000
1	2.911878000	0.024487000	-1.461269000	1	-2.125884000	-2.102149000	-1.299966000
1	3.565941000	0.030197000	-1.832752000	1	-2.588013000	-2.582305000	-1.647668000
1	-1.892599000	2.174235000	-1.393970000	1	2.927414000	-1.606992000	-0.290368000
1	-2.398028000	2.630096000	-1.707681000	1	3.613550000	-1.904055000	-0.342633000
1	2.577391000	-1.914268000	0.003301000	1	-2.934160000	0.129912000	-1.183078000
1	3.103598000	-2.452297000	0.000952000	1	-3.602889000	0.260442000	-1.500728000
1	-3.303963000	-0.039442000	-0.371499000	1	3.106995000	1.330403000	-0.477317000
1	-3.844575000	-0.036854000	0.144553000	1	3.638217000	1.570075000	-0.009275000
1	0.963179000	1.271976000	1.946198000	1	-0.610055000	-0.674482000	2.324543000
1	0.832013000	1.679931000	2.566817000	1	-0.448170000	-0.700209000	3.060340000
1	0.822664000	1.668699000	-2.550774000	1	0.588116000	-2.809609000	-1.491151000
1	0.953964000	1.265396000	-1.926821000	1	0.174329000	-2.291965000	-1.132724000
1	-2.337497000	-2.682011000	-1.701410000	1	1.340808000	2.367107000	-2.802642000
1	-1.844404000	-2.215017000	-1.384409000	1	1.048046000	1.907288000	-2.288059000
1	0.851833000	-1.652061000	-2.561884000	1	-0.737089000	-0.204787000	-3.038532000
1	0.975690000	-1.252820000	-1.933649000	1	-0.828595000	-0.309972000	-2.296937000
1	-1.971088000	-0.009983000	3.364962000	1	1.472246000	2.165034000	2.913426000
1	-1.582114000	-0.010745000	2.724221000	1	1.177234000	1.740134000	2.370898000
1	-2.473640000	2.626810000	1.632570000	1	3.089831000	-0.545644000	2.606038000
1	-1.959187000	2.165289000	1.342659000	1	2.499502000	-0.488367000	2.147937000
1	0.353926000	-2.599783000	0.015404000	1	-3.824549000	2.194287000	0.449231000
1	0.194438000	-3.332162000	0.016487000	1	-4.418548000	2.641802000	0.518092000
1	-2.405209000	-2.672569000	1.648816000	1	0.960944000	3.774448000	0.180674000
1	-1.914495000	-2.196881000	1.341083000	1	0.762021000	3.052924000	0.139848000
1	0.282105000	2.638518000	0.010868000	1	0.852217000	-2.340174000	1.222910000
1	0.122828000	3.370696000	0.009699000	1	1.272758000	-2.866574000	1.550491000
				1	-1.459858000	2.422731000	-1.311262000

	1	-1.328662000	1.742797000	-1.020026000
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H₄N⁻				H₆N⁻			
7	0.322316000	-0.000002000	-0.127348000	7	0.000015000	-0.158267000	0.000205000
1	0.517868000	-0.801214000	0.471176000	1	-0.001564000	-0.803620000	-0.800811000
1	0.517388000	0.801475000	0.470980000	1	-0.000625000	-0.808423000	0.797348000
1	-2.571817000	-0.000039000	0.127884000	1	2.484463000	0.836126000	0.000417000
1	-0.719651000	-0.000211000	-0.178605000	1	1.720829000	0.523099000	0.000342000
				1	-2.483484000	0.836944000	0.000261000
				1	-1.719727000	0.523743000	0.001007000
H₈N⁻				H₁₀N⁻			
7	-0.037133000	-0.401722000	0.041531000	7	-0.001379000	-0.380053000	0.001896000
1	-0.069266000	-1.229865000	-0.565252000	1	-0.096872000	-1.029635000	-0.787984000
1	-0.058097000	-0.817310000	0.981373000	1	0.081357000	-1.021442000	0.799874000
1	2.651684000	0.096509000	-0.267597000	1	2.816882000	-0.590494000	-0.489745000
1	1.859295000	-0.044197000	-0.164711000	1	2.039631000	-0.495153000	-0.352614000
1	-2.643003000	0.375275000	-0.265699000	1	-2.826072000	-0.572298000	0.475332000
1	-1.867149000	0.150483000	-0.165021000	1	-2.047834000	-0.480113000	0.342993000
1	0.147274000	1.762593000	0.035191000	1	1.068795000	1.396808000	0.644563000
1	0.239191000	2.518565000	0.121002000	1	1.401587000	2.019251000	0.948303000
				1	-1.378381000	2.029043000	-0.949223000
				1	-1.049441000	1.404407000	-0.644775000
H₁₂N⁻				H₁₄N⁻			
7	-0.211371000	-0.447831000	-0.081930000	7	-0.001849000	-0.549879000	0.003236000
1	-0.208783000	-1.200548000	0.616440000	1	0.072895000	-1.190230000	0.802631000
1	-0.225820000	-0.972055000	-0.965253000	1	-0.081280000	-1.201365000	-0.786661000
1	-3.069882000	-0.541307000	0.186305000	1	-2.919046000	-0.915902000	0.645030000
1	-2.285049000	-0.478105000	0.095115000	1	-2.166685000	-0.800681000	0.484548000
1	2.739131000	-1.084171000	0.098963000	1	2.910278000	-0.933446000	-0.637373000
1	1.983188000	-0.918019000	0.022631000	1	2.158278000	-0.814157000	-0.476461000
1	-1.112467000	1.579572000	-0.062213000	1	-0.916248000	1.293831000	0.919233000
1	-1.430027000	2.276054000	-0.094394000	1	-1.201659000	1.915481000	1.257725000
1	1.298455000	1.190833000	1.892917000	1	2.005802000	1.040749000	1.661809000
1	0.964820000	0.825745000	1.310272000	1	1.557664000	0.634378000	1.199357000
1	1.196278000	0.995750000	-1.050647000	1	0.925415000	1.274688000	-0.926849000
1	1.629753000	1.461069000	-1.476630000	1	1.213739000	1.893827000	-1.267821000
				1	-1.549889000	0.624016000	-1.215675000
				1	-1.996324000	1.027964000	-1.682145000
H₁₆N⁻				H₁₈N⁻			
7	-0.000088000	-0.406953000	-0.093906000	7	0.000082000	-0.314808000	0.001923000
1	0.002500000	-0.985105000	-0.942785000	1	-0.061283000	-0.951558000	0.804924000
1	0.002971000	-1.117098000	0.647727000	1	0.065174000	-0.969324000	-0.786317000
1	2.341214000	0.959113000	-1.497605000	1	-2.620738000	-2.021690000	-0.928422000
1	1.785891000	0.619396000	-1.094828000	1	-2.054664000	-1.574094000	-0.688101000
1	-0.001954000	1.923051000	-0.148597000	1	2.623465000	-2.023685000	0.921408000
1	-0.002750000	2.681423000	-0.175335000	1	2.056645000	-1.575094000	0.684788000
1	2.192565000	-1.336587000	0.065132000	1	-0.607834000	1.667328000	1.001003000
1	2.868786000	-1.691210000	0.130289000	1	-0.781768000	2.297063000	1.386618000

1	-2.342538000	0.954443000	-1.498835000	1	2.315494000	1.172230000	1.319667000
1	-1.787075000	0.615526000	-1.095677000	1	1.759061000	0.794413000	0.951523000
1	-2.863640000	-1.694168000	0.131148000	1	0.606800000	1.667829000	-1.002596000
1	-2.187529000	-1.338920000	0.065712000	1	0.780574000	2.298572000	-1.386777000
1	-1.488722000	0.649101000	1.251900000	1	-1.754062000	0.792342000	-0.955045000
1	-1.929795000	0.977626000	1.781658000	1	-2.309515000	1.169967000	-1.324901000
1	1.485267000	0.651660000	1.253499000	1	2.156568000	-0.143030000	-1.138656000
1	1.925423000	0.980423000	1.783940000	1	2.780828000	-0.126786000	-1.572581000
				1	-2.164554000	-0.144825000	1.134544000
				1	-2.790766000	-0.126005000	1.565460000
H₂₀N⁻				H₂₂N⁻			
7	0.069881000	0.002121000	0.412139000	7	-0.000710000	0.000169000	-0.412300000
1	0.113404000	-0.794088000	1.059018000	1	0.000373000	-0.792479000	-1.064505000
1	0.114497000	0.798625000	1.058571000	1	0.000034000	0.792591000	-1.064826000
1	2.831733000	-0.003196000	2.117250000	1	-2.891276000	-0.002507000	-1.754799000
1	2.225926000	-0.001807000	1.657358000	1	-2.223510000	-0.001998000	-1.383585000
1	-2.659766000	-1.590453000	1.203921000	1	2.890321000	-0.002810000	-1.755001000
1	-2.071163000	-1.160018000	0.989437000	1	2.222745000	-0.002656000	-1.383470000
1	0.511202000	0.000595000	-1.896734000	1	-0.000643000	-1.148746000	1.621086000
1	0.626726000	0.000300000	-2.646614000	1	-0.000300000	-1.586055000	2.238742000
1	-2.424391000	-0.003473000	-1.521961000	1	2.611301000	0.002100000	1.402068000
1	-1.836752000	-0.002033000	-1.036478000	1	1.994790000	0.001284000	0.953897000
1	-0.497697000	1.902472000	-0.861122000	1	0.001855000	1.151683000	1.619999000
1	-0.609123000	2.594958000	-1.138184000	1	0.002010000	1.590025000	2.236905000
1	1.968730000	1.156798000	-0.396064000	1	-1.995314000	0.001056000	0.954403000
1	2.539910000	1.601882000	-0.635449000	1	-2.611410000	0.000656000	1.403115000
1	-2.073078000	1.155847000	0.990836000	1	1.557662000	1.984714000	-0.139869000
1	-2.663626000	1.583630000	1.205621000	1	1.889641000	2.661893000	-0.147563000
1	1.968353000	-1.154976000	-0.399483000	1	-1.555828000	-1.986083000	-0.136325000
1	2.539113000	-1.600159000	-0.639415000	1	-1.886863000	-2.663705000	-0.143197000
1	-0.491936000	-1.903186000	-0.860001000	1	1.558919000	-1.984144000	-0.137347000
1	-0.601230000	-2.596563000	-1.135478000	1	1.889175000	-2.662107000	-0.145667000
				1	-1.889414000	2.662067000	-0.149308000
				1	-1.559299000	1.984034000	-0.138655000
H₂₄N⁻				H₂₆N⁻			
7	0.049503000	0.083211000	-0.211793000	7	0.005317000	-0.001397000	-0.140790000
1	-0.019285000	1.078340000	0.029225000	1	0.128337000	-0.775081000	-0.803771000
1	0.116258000	0.119481000	-1.236086000	1	-0.126678000	0.793609000	-0.776190000
1	3.185882000	-0.238251000	-0.962346000	1	-3.241087000	-0.249764000	0.383356000
1	2.461751000	-0.160613000	-0.740181000	1	-2.490519000	-0.203159000	0.270041000
1	-2.545949000	1.327164000	-1.800545000	1	2.246638000	1.070425000	-2.426537000
1	-1.995699000	1.001029000	-1.391535000	1	1.817532000	0.814151000	-1.859029000
1	-0.381174000	0.009307000	2.072361000	1	1.182626000	-1.572226000	1.158566000
1	-0.493530000	0.142291000	2.806657000	1	1.493268000	-2.179721000	1.483167000
1	-2.988139000	-0.392311000	0.806884000	1	3.235964000	0.245798000	0.436130000
1	-2.277760000	-0.298930000	0.549441000	1	2.487498000	0.197638000	0.309468000
1	-0.674573000	-1.947170000	0.822094000	1	0.958813000	0.590195000	1.990486000
1	-0.885103000	-2.600377000	1.142687000	1	1.237195000	0.790794000	2.665706000
1	1.567429000	-1.144588000	1.176401000	1	-0.979518000	-0.763178000	1.915952000
1	2.027575000	-1.540726000	1.633579000	1	-1.269650000	-1.025324000	2.564952000
1	-1.579000000	-1.381758000	-1.333736000	1	1.259306000	2.157986000	0.222086000

1	-1.981292000	-1.842560000	-1.779745000	1	1.495998000	2.874009000	0.244052000
1	1.917887000	1.165905000	1.105935000	1	-1.309565000	-2.179581000	0.030505000
1	2.392188000	1.583579000	1.522768000	1	-1.556482000	-2.891018000	-0.012871000
1	-1.778230000	1.987031000	0.880271000	1	2.105788000	-1.549980000	-1.217952000
1	-2.076108000	2.609385000	1.176709000	1	2.515434000	-2.061684000	-1.586360000
1	1.182486000	-2.646079000	-1.260179000	1	-1.489162000	2.029501000	1.657896000
1	0.961449000	-2.020282000	-0.902777000	1	-1.174356000	1.455579000	1.279771000
1	1.919701000	2.603520000	-1.579922000	1	-2.233677000	-0.839050000	-2.526929000
1	1.596718000	2.004130000	-1.255409000	1	-1.802717000	-0.642893000	-1.937508000
				1	-2.463390000	2.231334000	-1.408989000
				1	-2.064816000	1.691421000	-1.070467000
H₂₈N⁻				H₃₀N⁻			
7	-0.000836000	-0.025340000	0.002519000	7	-0.048986000	-0.173483000	0.057290000
1	0.010194000	0.624755000	-0.791717000	1	0.091766000	0.776673000	-0.305782000
1	-0.010375000	0.613292000	0.806033000	1	-0.098786000	-0.012696000	1.069827000
1	-3.247669000	-0.654203000	-0.265529000	1	-3.218785000	0.519766000	-0.694185000
1	-2.503534000	-0.517759000	-0.196969000	1	-2.504939000	0.332204000	-0.515665000
1	2.209618000	1.597635000	2.190759000	1	1.830441000	-0.509612000	3.009705000
1	1.862340000	1.190521000	1.661092000	1	1.571391000	-0.475648000	2.304362000
1	1.572950000	-0.471743000	-1.948777000	1	1.797252000	-0.223241000	-1.634546000
1	1.915006000	-0.502691000	-2.619763000	1	2.285471000	-0.130253000	-2.203828000
1	3.239408000	-0.688285000	0.254269000	1	2.689283000	-1.955126000	0.293629000
1	2.496476000	-0.543176000	0.190522000	1	2.064356000	-1.530706000	0.217641000
1	1.041420000	-2.189236000	-0.474216000	1	0.483931000	-2.084665000	-1.392989000
1	1.344194000	-2.860471000	-0.646934000	1	0.633968000	-2.663371000	-1.854710000
1	-0.929338000	-1.337917000	-1.705999000	1	-0.810432000	-0.043880000	-2.172705000
1	-1.144260000	-1.673949000	-2.348049000	1	-0.917527000	0.135547000	-2.898141000
1	0.927198000	-1.334074000	1.719229000	1	-0.039360000	-2.370913000	0.885165000
1	1.136816000	-1.666110000	2.364925000	1	-0.080846000	-3.010030000	1.283297000
1	-1.842049000	1.195282000	-1.685717000	1	-1.328862000	2.395126000	-0.741339000
1	-2.177091000	1.603145000	-2.222425000	1	-1.443839000	3.101184000	-0.967625000
1	2.106836000	1.543783000	-0.728693000	1	2.427239000	0.720121000	0.411920000
1	2.597785000	2.063970000	-0.968910000	1	3.095008000	1.057831000	0.525791000
1	-1.373155000	-2.833811000	0.669591000	1	-2.221993000	-2.291847000	-1.015707000
1	-1.064526000	-2.166531000	0.491185000	1	-1.723957000	-1.775679000	-0.772454000
1	-2.579302000	2.099666000	0.933393000	1	-2.190673000	1.882676000	1.919360000
1	-2.090503000	1.573726000	0.701244000	1	-1.818929000	1.412989000	1.462283000
1	-1.950532000	-0.460098000	2.624325000	1	-2.629895000	-1.201760000	1.878729000
1	-1.606371000	-0.435824000	1.954255000	1	-2.122509000	-0.976424000	1.367612000
1	0.033825000	3.578917000	0.013817000	1	0.827979000	2.848101000	1.743021000
1	0.030491000	2.828566000	0.011422000	1	0.700855000	2.193351000	1.398072000
				1	1.556596000	2.890858000	-1.637214000
				1	1.438698000	2.203806000	-1.364551000
H₃₂N⁻				H₃₄N⁻			
7	-0.029883000	-0.004600000	0.198966000	7	-0.168018000	-0.057254000	0.179512000
1	-0.067181000	0.793732000	-0.446278000	1	0.180116000	0.594653000	-0.533399000
1	0.194289000	-0.781951000	-0.433770000	1	-0.989913000	-0.462417000	-0.284524000
1	2.682576000	1.761362000	0.930767000	1	2.666841000	-1.617192000	0.337171000
1	2.084365000	1.316826000	0.791277000	1	1.991368000	-1.272241000	0.300577000
1	-1.165091000	-2.980044000	-1.662771000	1	-3.788014000	-0.357032000	-1.009126000
1	-1.114766000	-2.360331000	-1.243337000	1	-3.151026000	-0.141944000	-0.679022000
1	-2.308772000	0.957774000	0.620503000	1	-0.341483000	2.476826000	0.749347000

1	-2.957081000	1.335723000	0.722149000	1	-0.309861000	3.229174000	0.816058000
1	-2.747683000	-1.754138000	0.765088000	1	-2.874919000	1.553878000	1.359675000
1	-2.144292000	-1.311382000	0.642988000	1	-2.235588000	1.220917000	1.125859000
1	-1.239198000	-0.085016000	2.354040000	1	-0.407223000	0.954496000	2.445835000
1	-1.589115000	-0.100945000	3.023339000	1	-0.455503000	1.250182000	3.141351000
1	-0.152841000	1.971247000	1.474531000	1	1.677721000	0.992825000	1.120264000
1	-0.243321000	2.681136000	1.710761000	1	2.279712000	1.424961000	1.260844000
1	0.060704000	-1.961133000	1.490838000	1	-1.641958000	-1.007647000	1.783810000
1	0.137776000	-2.669553000	1.735832000	1	-2.164046000	-1.424644000	2.133069000
1	1.239682000	2.434565000	-1.179464000	1	4.486639000	0.244728000	0.036687000
1	1.312126000	3.033959000	-1.622993000	1	5.215345000	0.403446000	0.003044000
1	-2.165712000	-0.203795000	-1.380916000	1	-1.732245000	1.844673000	-1.079751000
1	-2.721120000	-0.235866000	-1.893754000	1	-2.100967000	2.311047000	-1.542387000
1	1.375846000	0.122804000	3.106315000	1	1.102717000	-1.270384000	2.887619000
1	1.063685000	0.100954000	2.417451000	1	0.812076000	-0.986191000	2.251700000
1	2.818171000	0.228443000	-1.733757000	1	0.932273000	-2.392750000	-2.038207000
1	2.244490000	0.195707000	-1.244059000	1	0.731743000	-1.885575000	-1.512674000
1	2.909610000	-1.330873000	0.922402000	1	0.082961000	-3.230882000	0.778989000
1	2.261565000	-0.960500000	0.795367000	1	0.107576000	-2.487710000	0.641556000
1	0.099928000	-0.015334000	-3.356115000	1	-0.830910000	-0.045603000	-3.278099000
1	0.023272000	-0.019690000	-2.609002000	1	-0.628253000	-0.125581000	-2.558680000
1	-1.666160000	2.766214000	-1.801131000	1	1.031176000	2.965612000	-2.105600000
1	-1.571529000	2.168035000	-1.360589000	1	0.723719000	2.548549000	-1.566370000
1	1.709929000	-2.241496000	-1.239414000	1	-1.595043000	-2.443860000	-1.118360000
1	1.845027000	-2.824235000	-1.689061000	1	-2.155355000	-2.841645000	-1.416273000
				1	2.532410000	0.301269000	-2.106755000
				1	2.024041000	0.076841000	-1.600808000

H₂NO₂⁻				H₄NO₂⁻			
7	-0.474489000	-0.504486000	-0.002585000	7	0.029599000	0.258249000	0.000728000
8	0.784179000	-0.609416000	0.001657000	8	-1.059200000	-0.375249000	0.002691000
8	-0.934629000	0.665368000	0.001153000	8	1.074816000	-0.446067000	-0.002865000
1	1.992041000	1.273141000	-0.001415000	1	3.219663000	1.533972000	0.003674000
1	2.532987000	1.810648000	-0.002975000	1	2.668470000	1.008888000	0.001950000
				1	-3.441359000	1.297922000	-0.006576000
				1	-2.778889000	0.922003000	-0.002744000
H₆NO₂⁻				H₈NO₂⁻			
7	-0.018852000	-0.446167000	-0.000691000	7	-0.000012000	0.575103000	0.000000000
8	1.065442000	0.195290000	0.002727000	8	-1.065218000	-0.096670000	0.017239000
8	-1.067250000	0.251028000	0.004506000	8	1.065215000	-0.096638000	-0.017238000
1	0.185841000	3.284136000	-0.013900000	1	-3.166193000	1.977030000	0.052715000
1	0.164459000	2.526361000	-0.007889000	1	-2.619211000	1.450733000	0.043956000
1	3.109775000	-1.913007000	-0.007545000	1	0.149346000	-2.037167000	1.205420000
1	2.572035000	-1.375697000	-0.005158000	1	0.148769000	-2.630317000	1.674241000
1	-2.659373000	-1.231354000	-0.007196000	1	2.619162000	1.450811000	-0.043957000
1	-3.226315000	-1.737821000	-0.011348000	1	3.166129000	1.977123000	-0.052717000
				1	-0.149239000	-2.037164000	-1.205425000
				1	-0.148650000	-2.630311000	-1.674248000
H₁₀NO₂⁻				H₁₂NO₂⁻			
7	0.363162000	-0.624582000	-0.003440000	7	0.138798000	-0.842968000	-0.006210000

8	1.076082000	0.412883000	-0.001854000	8	1.134285000	-0.073272000	-0.004860000
8	-0.881621000	-0.433085000	-0.001046000	8	-0.988123000	-0.281020000	-0.005599000
1	3.838095000	-0.670993000	0.007061000	1	3.378342000	-2.046566000	0.008505000
1	3.129832000	-0.400705000	0.004661000	1	2.808650000	-1.548017000	0.004812000
1	-2.533960000	1.098159000	-0.011298000	1	-2.535835000	1.378588000	-0.013446000
1	-3.175220000	1.496833000	-0.015509000	1	-3.128236000	1.842806000	-0.016137000
1	-0.326976000	1.899522000	1.247477000	1	-0.230996000	1.758918000	-1.211734000
1	-0.583850000	2.437640000	1.711471000	1	-0.290554000	2.357071000	-1.668550000
1	-1.656097000	-2.509974000	0.001236000	1	-2.731270000	-1.646535000	0.023365000
1	-1.927009000	-3.217696000	0.001564000	1	-3.352597000	-2.079504000	0.037571000
1	-0.300800000	1.928553000	-1.222092000	1	-0.248975000	1.743871000	1.222345000
1	-0.561834000	2.472358000	-1.677294000	1	-0.306620000	2.337037000	1.685794000
H₁₄NO₂⁻				1	2.042143000	2.003483000	0.021184000
				1	2.455065000	2.633960000	0.033436000
7	-0.070893000	-0.869861000	-0.105689000	H₁₆NO₂⁻			
8	-1.149003000	-0.236411000	0.020000000	7	-0.005839000	-0.850267000	-0.080543000
8	0.964510000	-0.164013000	-0.248634000	8	-1.070003000	-0.182897000	-0.164135000
1	-3.607200000	-1.877937000	0.412707000	8	1.060557000	-0.184935000	-0.159955000
1	-2.967040000	-1.487563000	0.309746000	1	0.025686000	1.215619000	-2.897208000
1	-0.023910000	1.781895000	1.057630000	1	0.029499000	0.954043000	-2.192363000
1	0.023293000	2.387125000	1.505990000	1	-3.073703000	-2.452260000	0.082594000
1	2.355361000	0.267661000	1.558661000	1	-2.573428000	-1.890044000	0.020666000
1	2.826839000	0.407999000	2.126774000	1	0.010173000	1.407188000	1.531117000
1	1.996397000	1.847340000	-0.582273000	1	0.000155000	1.814784000	2.162801000
1	2.456917000	2.433468000	-0.690064000	1	2.683008000	0.456807000	1.352135000
1	2.564077000	-1.757078000	-0.346535000	1	3.233359000	0.674983000	1.814511000
1	3.104985000	-2.284828000	-0.368047000	1	1.422529000	2.100648000	-0.434455000
1	-0.498443000	1.721487000	-1.328167000	1	1.653242000	2.815236000	-0.511347000
1	-0.573487000	2.310422000	-1.794162000	1	2.547843000	-1.911380000	0.013505000
1	-2.560990000	1.527151000	0.303040000	1	3.044437000	-2.476874000	0.074155000
1	-3.124594000	2.015270000	0.403601000	1	-1.374743000	2.110494000	-0.451082000
				1	-1.587956000	2.830161000	-0.532328000
				1	-2.686457000	0.507754000	1.333787000
				1	-3.237201000	0.737375000	1.790040000
H₁₈NO₂⁻				H₂₀NO₂⁻			
7	-0.043186000	-0.518382000	-0.572631000	7	0.021740000	-0.670978000	-0.624284000
8	-1.077877000	0.170458000	-0.385284000	8	0.678143000	0.239278000	-0.035657000
8	1.052722000	0.070985000	-0.374352000	8	-1.222473000	-0.562352000	-0.582945000
1	0.121574000	2.657208000	-2.062637000	1	-1.911510000	1.565428000	1.745951000
1	0.109760000	2.114415000	-1.541894000	1	-1.580878000	1.145391000	1.213858000
1	-3.047870000	-2.147192000	-0.766974000	1	2.692908000	0.011230000	1.140631000
1	-2.528435000	-1.602961000	-0.719457000	1	3.324648000	-0.013764000	1.548084000
1	0.178493000	0.610067000	1.894137000	1	0.088096000	-0.774334000	2.891542000
1	0.078945000	0.704104000	2.632309000	1	0.164822000	-0.498245000	2.197837000
1	-0.138899000	-2.581641000	1.830339000	1	1.410285000	-2.447360000	0.363409000
1	-0.074466000	-2.236125000	1.166992000	1	1.793686000	-2.963699000	0.751153000
1	2.581244000	-0.462606000	1.287646000	1	2.512976000	-0.765518000	-1.332223000
1	3.095256000	-0.638717000	1.806471000	1	3.130025000	-0.995023000	-1.694395000
1	1.628664000	2.126933000	0.526839000	1	-2.736533000	-1.178901000	1.060653000
1	1.930640000	2.748320000	0.829918000	1	-3.264362000	-1.412287000	1.541405000
1	2.181893000	-1.917048000	-0.805328000	1	0.844278000	2.022770000	1.443730000

1	2.522872000	-2.580330000	-0.913190000	1	1.038989000	2.577276000	1.913018000
1	-1.249918000	2.276772000	0.568807000	1	-3.720568000	1.150090000	-0.937360000
1	-1.382956000	2.943944000	0.896218000	1	-3.063951000	0.807463000	-0.807587000
1	-2.490181000	-0.141792000	1.458745000	1	-0.822316000	2.803185000	-1.045183000
1	-3.013077000	-0.176223000	1.996568000	1	-0.611112000	2.138553000	-0.760840000
				1	2.699227000	2.317903000	-1.070684000
				1	2.213742000	1.791280000	-0.844191000
H₂₂NO₂⁻				H₂₄NO₂⁻			
7	-0.035556000	-0.529552000	-0.553853000	7	-0.466256000	0.086753000	-0.057029000
8	1.052922000	0.018590000	-0.238267000	8	0.789207000	0.217406000	0.013179000
8	-1.072785000	0.126214000	-0.280436000	8	-0.895799000	-1.087573000	-0.068710000
1	-1.565097000	2.718305000	1.307189000	1	1.066996000	-1.149617000	2.840505000
1	-1.347542000	2.103677000	0.928018000	1	0.984148000	-0.937765000	2.124847000
1	2.552886000	-0.669647000	1.398483000	1	1.251515000	-1.651219000	-2.521727000
1	3.071354000	-0.853320000	1.910008000	1	1.045063000	-1.387497000	-1.849139000
1	-0.013505000	0.184454000	2.812895000	1	0.528240000	2.579963000	-0.284840000
1	0.004698000	0.277089000	2.068113000	1	0.459517000	3.320669000	-0.394487000
1	-0.078542000	-2.435059000	0.981816000	1	-0.811291000	1.360597000	-3.015539000
1	-0.087188000	-2.933696000	1.542516000	1	-0.758042000	1.136880000	-2.301942000
1	2.307110000	-1.850507000	-0.912255000	1	-2.200242000	1.910390000	-0.005951000
1	2.710527000	-2.447455000	-1.131070000	1	-2.745353000	2.429015000	0.019275000
1	-2.569862000	-0.468695000	1.419502000	1	-0.308465000	1.641588000	2.020393000
1	-3.090706000	-0.629421000	1.936005000	1	-0.413058000	2.020474000	2.658090000
1	1.558661000	1.951523000	1.034606000	1	-2.979098000	-0.657689000	-1.027553000
1	1.842123000	2.525574000	1.431710000	1	-3.636971000	-0.516198000	-1.365363000
1	-2.878709000	-2.297211000	-1.057919000	1	2.345830000	1.437835000	1.246870000
1	-2.430266000	-1.718687000	-0.883249000	1	2.885152000	1.780122000	1.641781000
1	-3.827507000	1.166937000	-1.080752000	1	2.282499000	1.132919000	-1.537771000
1	-3.149971000	0.889694000	-0.913745000	1	2.802406000	1.407787000	-2.004731000
1	0.321644000	2.857528000	-1.511442000	1	-3.028343000	-0.320478000	2.177166000
1	0.275878000	2.211883000	-1.128288000	1	-2.548749000	-0.477655000	1.621775000
1	3.735059000	1.122141000	-1.162124000	1	3.450338000	-1.342825000	0.139033000
1	3.066750000	0.843325000	-0.963425000	1	2.755565000	-1.054419000	0.111426000
				1	1.043635000	-3.471151000	0.325189000
				1	0.645233000	-2.837653000	0.226146000
H₂₆NO₂⁻				H₂₈NO₂⁻			
7	0.214430000	-0.391448000	-0.150416000	7	-0.098724000	0.426285000	-0.003158000
8	-0.923008000	0.085838000	0.111581000	8	0.926348000	-0.278147000	0.190543000
8	1.107591000	0.442638000	-0.428554000	8	-1.109337000	-0.181648000	-0.433265000
1	2.692141000	-1.221021000	1.993343000	1	-0.901799000	-2.628561000	1.650239000
1	2.275733000	-0.944819000	1.435399000	1	-0.722072000	-2.120471000	1.126495000
1	-0.902247000	1.794175000	-2.611334000	1	-1.082798000	1.497898000	-3.159753000
1	-0.681255000	1.519517000	-1.947842000	1	-1.091554000	1.130719000	-2.506082000
1	-2.596363000	0.075739000	1.727986000	1	2.215890000	1.605641000	0.948127000
1	-3.158869000	0.115219000	2.223394000	1	2.633906000	2.185472000	1.180585000
1	-3.578221000	0.032244000	-1.460610000	1	0.015012000	3.648566000	-0.636991000
1	-2.918652000	0.032539000	-1.102145000	1	-0.015467000	2.917151000	-0.465634000
1	-1.987152000	-2.044975000	0.145245000	1	-0.216104000	2.074628000	1.915741000
1	-2.328055000	-2.715394000	0.143053000	1	-0.273196000	2.494900000	2.535164000
1	-0.482901000	-1.465298000	2.180669000	1	1.456321000	-0.589225000	2.421367000
1	-0.458280000	-1.822290000	2.838621000	1	1.637020000	-0.697581000	3.142684000

1	-0.439097000	-1.585107000	-2.238420000	1	-2.560279000	1.626562000	-0.083636000
1	-0.634273000	-1.860988000	-2.907526000	1	-3.023929000	2.202147000	0.059226000
1	0.181610000	1.385611000	1.902556000	1	1.544231000	-2.573690000	0.166930000
1	0.371385000	1.642171000	2.582180000	1	1.858579000	-3.256779000	0.189125000
1	-1.875544000	2.234997000	0.261048000	1	1.942479000	1.340291000	-1.618300000
1	-2.290783000	2.857490000	0.344507000	1	2.292670000	1.741581000	-2.144241000
1	0.931190000	-3.574214000	0.047462000	1	-2.234273000	0.021420000	2.761035000
1	0.756639000	-2.844075000	-0.007840000	1	-1.934844000	-0.009855000	2.076155000
1	3.641407000	1.722726000	0.750277000	1	-1.094021000	-3.108549000	-1.547520000
1	3.017941000	1.399318000	0.486180000	1	-1.014142000	-2.417297000	-1.258497000
1	3.235614000	-1.497494000	-1.493142000	1	-3.844015000	-1.483275000	0.129522000
1	2.712948000	-1.027314000	-1.221985000	1	-3.171414000	-1.176462000	0.003344000
1	0.774224000	3.528323000	-0.223399000	1	1.367372000	-1.371631000	-2.716092000
1	0.763190000	2.775254000	-0.258979000	1	1.152679000	-1.197277000	-2.017813000
				1	3.976426000	-0.645918000	-0.135805000
				1	3.242304000	-0.516042000	-0.051491000
H₃₀NO₂⁻				H₃₂NO₂⁻			
7	0.050898000	-0.475521000	0.013956000	7	-0.048066000	0.464663000	-0.010466000
8	-1.057535000	0.115258000	-0.001085000	8	1.064542000	-0.120855000	0.020069000
8	1.070510000	0.261279000	0.007057000	8	-1.061876000	-0.279350000	-0.013269000
1	-0.524334000	3.313478000	0.026664000	1	-0.891849000	-1.343152000	2.928238000
1	-0.472334000	2.561970000	0.018979000	1	-0.889147000	-1.178301000	2.196114000
1	3.592472000	0.234759000	-1.819398000	1	-2.519696000	-3.050363000	-0.199319000
1	2.987065000	0.191470000	-1.377766000	1	-2.065451000	-2.455633000	-0.141189000
1	-1.811494000	-0.991807000	2.084378000	1	1.902750000	2.146073000	-0.592495000
1	-2.030984000	-1.281789000	2.739736000	1	2.234500000	2.785914000	-0.800442000
1	2.599670000	-2.597477000	-0.067463000	1	-0.420394000	1.665262000	-2.972998000
1	2.197410000	-1.964332000	-0.043561000	1	-0.336422000	1.473743000	-2.253183000
1	0.890734000	-1.717688000	2.110132000	1	-0.363617000	3.051179000	0.221680000
1	1.103222000	-1.995229000	2.772574000	1	-0.463335000	3.788596000	0.324281000
1	-2.436549000	1.511836000	1.340071000	1	1.328924000	1.478278000	2.002180000
1	-2.951969000	1.870201000	1.750780000	1	1.486291000	1.844602000	2.636584000
1	2.980672000	0.153027000	1.387282000	1	-2.504425000	1.625238000	-0.532960000
1	3.585212000	0.189706000	1.831024000	1	-2.970852000	2.187966000	-0.704524000
1	-2.419708000	1.540237000	-1.328272000	1	2.024083000	-1.275797000	1.915911000
1	-2.936711000	1.902397000	-1.733755000	1	2.396140000	-1.555010000	2.504142000
1	0.887331000	-1.586379000	-2.178432000	1	0.027457000	-1.646630000	-1.784251000
1	1.089560000	-1.854103000	-2.847686000	1	0.074005000	-1.981218000	-2.455579000
1	0.303570000	1.549285000	2.786395000	1	-1.915470000	1.814278000	2.487263000
1	0.407144000	1.338727000	2.073272000	1	-1.645826000	1.451778000	1.890198000
1	0.300472000	1.578909000	-2.747100000	1	0.400165000	-3.278578000	0.619008000
1	0.395947000	1.355894000	-2.036318000	1	0.338339000	-2.546894000	0.452494000
1	2.572508000	2.963980000	0.027603000	1	-3.992045000	-0.423395000	1.126369000
1	2.107926000	2.373719000	0.019870000	1	-3.295450000	-0.337872000	0.861797000
1	-2.050313000	-1.240237000	-2.755338000	1	3.043667000	-2.431363000	-0.801106000
1	-1.828618000	-0.959863000	-2.096583000	1	2.488373000	-1.964213000	-0.611014000
1	-3.957219000	-1.082060000	-0.001607000	1	4.127145000	0.503528000	0.520442000
1	-3.244540000	-0.843495000	-0.000375000	1	3.393216000	0.413732000	0.393127000
1	-1.059755000	-3.439316000	-0.048231000	1	2.639946000	0.189553000	-2.749395000
1	-0.736474000	-2.759470000	-0.032343000	1	2.257296000	0.128671000	-2.107754000
				1	-2.546127000	-0.516226000	-1.893978000
				1	-3.027060000	-0.614742000	-2.460777000

H₃₄NO₂⁻				
7	-0.123595000	0.483612000	0.036937000	
8	-1.186314000	-0.187191000	-0.007333000	
8	0.945552000	-0.171518000	-0.061859000	
1	-0.283480000	-3.283085000	-0.672810000	
1	-0.275410000	-2.546275000	-0.517487000	
1	2.779691000	-0.363872000	2.548395000	
1	2.328556000	-0.315537000	1.951811000	
1	-1.896514000	1.357938000	-1.834025000	
1	-2.140952000	1.778211000	-2.404530000	
1	0.118936000	3.827804000	-0.166589000	
1	0.053546000	3.081690000	-0.109870000	
1	1.020137000	1.685813000	-2.041679000	
1	1.183902000	2.058569000	-2.669525000	
1	-2.295122000	-1.456546000	-1.748242000	
1	-2.742107000	-1.771025000	-2.261728000	
1	2.765868000	-0.176912000	-1.631494000	
1	3.350736000	-0.232349000	-2.097085000	
1	-2.392804000	-2.150208000	0.746472000	
1	-2.885656000	-2.666099000	0.977744000	
1	0.230880000	1.626828000	2.195605000	
1	0.349619000	1.861828000	2.897870000	
1	0.223440000	-1.086763000	-3.001359000	
1	0.329066000	-0.999860000	-2.263593000	
1	0.039449000	-2.054374000	2.363948000	
1	0.044653000	-1.701159000	1.701128000	
1	2.702661000	-2.695273000	0.050659000	
1	2.183188000	-2.154108000	0.009508000	
1	-2.508022000	-0.002642000	2.923569000	
1	-2.185496000	-0.027934000	2.247595000	
1	-4.340465000	0.182989000	-0.089664000	
1	-3.591335000	0.158261000	-0.060208000	
1	-2.507341000	2.620182000	0.978776000	
1	-2.134099000	2.020797000	0.725938000	
1	4.586372000	-0.452655000	0.406669000	
1	5.326555000	-0.489965000	0.496394000	
1	2.918121000	2.208544000	0.373183000	
1	2.434687000	1.641569000	0.269599000	

28. Cartesian coordinates of optimized geometry of complexes at CCSD/6-311++G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

H₂F⁻				H₄ F⁻			
9	0.000000000	0.000000000	0.402262000	9	-0.000291000	-0.221080000	-0.000052000
1	0.000000000	0.000000000	-1.422348000	1	-1.793971000	0.375677000	0.000719000
1	0.000000000	0.000000000	-2.198014000	1	-2.523460000	0.619614000	-0.000335000
				1	2.524716000	0.619170000	0.000060000
				1	1.795338000	0.375259000	0.000022000
H₆ F⁻				H₈ F⁻			
9	-0.000818000	-0.000257000	-0.000276000	9	-0.000565000	-0.001393000	-0.000171000
1	1.131286000	-1.590603000	0.000295000	1	-1.688861000	-1.625747000	-1.481568000

1	1.574700000	-2.213441000	0.000532000	1	-1.225282000	-1.179680000	-1.074810000
1	-2.705593000	-0.252619000	0.000539000	1	1.200997000	1.170023000	-1.108860000
1	-1.944335000	-0.181596000	0.000287000	1	1.655673000	1.613360000	-1.528410000
1	1.135549000	2.467512000	0.000528000	1	-1.177706000	1.204169000	1.097923000
1	0.815754000	1.773062000	0.000300000	1	-1.623099000	1.660457000	1.513533000
				1	1.659587000	-1.639966000	1.497514000
				1	1.203776000	-1.190079000	1.086220000
H₁₀ F⁻				H₁₂ F⁻			
9	0.001622000	0.000477000	0.062504000	9	-0.001045000	-0.000178000	-0.147641000
1	1.984419000	-0.228425000	-0.516878000	1	1.127153000	1.205153000	1.239078000
1	2.708167000	-0.312120000	-0.725692000	1	1.814722000	-0.403100000	-1.111925000
1	-0.232700000	-1.940248000	-0.644333000	1	-0.571567000	1.781897000	-1.090007000
1	-0.318238000	-2.648524000	-0.900120000	1	-1.274411000	-1.372962000	-1.088392000
1	0.351822000	2.686814000	-0.775902000	1	0.498425000	-1.571530000	1.240029000
1	0.258253000	1.968448000	-0.553137000	1	-0.777877000	2.426441000	-1.429833000
1	-0.054729000	-0.060940000	2.091328000	1	1.524299000	1.629703000	1.721220000
1	-0.076046000	-0.084252000	2.850643000	1	2.471470000	-0.548858000	-1.459662000
1	-2.675543000	0.354800000	-0.809738000	1	0.674473000	-2.125128000	1.722736000
1	-1.960001000	0.260152000	-0.578709000	1	-1.734929000	-1.869306000	-1.427551000
				1	-2.151335000	0.488226000	1.751660000
				1	-1.591017000	0.361065000	1.261411000
H₁₄ F⁻				H₁₆ F⁻			
1	-1.698041000	-1.286305000	0.002352000	1	0.486536000	-1.833680000	-1.167259000
1	0.490249000	-1.340639000	-1.612983000	1	-0.952956000	-1.640471000	1.167498000
1	0.606967000	2.143331000	0.006479000	1	0.951727000	1.640096000	1.168256000
1	-1.166982000	0.857659000	1.591230000	1	1.834330000	0.486626000	-1.166512000
1	0.635183000	-1.827352000	-2.171020000	1	-1.277822000	-2.198898000	1.554229000
1	-2.299684000	-1.739288000	0.002602000	1	0.652809000	-2.458645000	-1.552939000
1	-1.601320000	1.137648000	2.140880000	1	2.459580000	0.653156000	-1.551608000
1	0.791029000	2.875413000	0.009397000	1	1.276616000	2.198389000	1.555170000
1	0.661864000	-1.868958000	2.129124000	1	-2.458062000	-0.652282000	-1.553604000
1	0.510146000	-1.371395000	1.582639000	1	-1.833239000	-0.486250000	-1.167584000
9	0.076363000	0.052027000	-0.000153000	9	-0.000028000	-0.000114000	-0.000996000
1	2.232357000	-0.031511000	-0.010152000	1	-1.641094000	0.952536000	1.167183000
1	2.986627000	-0.061739000	-0.014026000	1	-2.199787000	1.277418000	1.553507000
1	-1.639676000	1.166736000	-2.096357000	1	2.198850000	-1.277301000	1.554510000
1	-1.195984000	0.878154000	-1.558788000	1	1.640170000	-0.952529000	1.168063000
				1	-0.486015000	1.833751000	-1.167262000
				1	-0.651392000	2.459110000	-1.552682000
H₁₈ F⁻				H₂₀ F⁻			
1	0.817546000	1.511328000	1.442407000	1	1.057732000	0.961458000	1.773497000
1	-1.392569000	0.047939000	1.837924000	1	-1.061797000	1.931176000	0.574642000
1	-1.398953000	-0.040980000	-1.833541000	1	-1.059978000	0.574273000	-1.930440000
1	0.813116000	1.438859000	-1.516758000	1	1.061343000	-0.960573000	-1.771652000
1	-1.841867000	0.063588000	2.439915000	1	-1.412382000	2.568315000	0.764558000
1	1.090760000	2.018415000	1.926442000	1	1.407008000	1.278627000	2.358590000
1	1.085022000	1.922088000	-2.025315000	1	1.412356000	-1.277224000	-2.356015000
1	-1.850118000	-0.054552000	-2.434174000	1	-1.410644000	0.764241000	-2.567570000
1	1.080736000	-1.928489000	2.021821000	1	-1.408040000	-0.770106000	2.566789000
1	0.810295000	-1.444062000	1.513623000	1	-1.058224000	-0.579096000	1.929516000
9	-0.010514000	0.000041000	0.000149000	1	-2.780927000	-0.000017000	0.001540000

1	-1.396051000	-1.836594000	0.046466000	1	-3.527580000	0.000716000	0.002332000
1	-1.846050000	-2.438044000	0.061728000	1	1.409497000	2.359068000	-1.275979000
1	-1.833557000	2.447440000	-0.056489000	1	1.059630000	1.773895000	-0.959600000
1	-1.386507000	1.843758000	-0.042710000	1	-1.060000000	-1.930948000	-0.574575000
1	0.805886000	-1.514599000	-1.445179000	1	-1.410587000	-2.568163000	-0.764360000
1	1.075190000	-2.022831000	-1.930205000	1	1.063896000	-1.773210000	0.957459000
1	2.355801000	-0.005756000	-0.003116000	1	1.415044000	-2.357771000	1.273520000
1	3.105950000	-0.007878000	-0.004181000	9	0.000427000	-0.000303000	-0.000634000
				1	2.776568000	0.003080000	0.001390000
				1	3.523241000	0.004989000	0.002061000

H₂ Cl⁻				H₄Cl⁻			
17	0.000000000	0.000000000	-0.308329000	17	-0.000011000	0.241435000	-0.000001000
1	0.000000000	0.000000000	2.245584000	1	-2.618221000	-0.876716000	0.000100000
1	0.000000000	0.000000000	2.996014000	1	-3.305951000	-1.175519000	-0.000079000
				1	3.306039000	-1.175483000	0.000041000
				1	2.618316000	-0.876673000	-0.000052000
H₆ Cl⁻				H₈ Cl⁻			
17	-0.000631000	-0.002371000	-0.000449000	17	-0.001430000	-0.018315000	-0.356063000
1	2.400622000	-1.534457000	0.001053000	1	-2.739753000	-1.985581000	0.911949000
1	3.032616000	-1.937669000	0.001501000	1	-2.171776000	-1.575959000	0.645183000
1	0.180772000	3.590782000	0.001559000	1	2.121285000	1.632155000	0.600316000
1	0.143034000	2.842065000	0.000957000	1	2.676207000	2.066478000	0.855165000
1	-3.207422000	-1.629839000	0.001480000	1	-2.110885000	1.644741000	0.608879000
1	-2.538895000	-1.290572000	0.001085000	1	-2.662153000	2.082264000	0.866190000
				1	2.739847000	-1.980581000	0.916627000
				1	2.171537000	-1.572163000	0.648757000
H₁₀ Cl⁻				H₁₂Cl⁻			
17	-0.001372000	-0.000452000	-0.353264000	17	-0.001387000	-0.000192000	0.169157000
1	-2.371471000	-1.340454000	0.487578000	1	-0.275389000	-0.028376000	3.035136000
1	-2.003102000	1.840486000	0.490195000	1	1.243631000	2.403046000	-0.764060000
1	0.547945000	-2.662377000	0.492864000	1	-1.855038000	1.880873000	-0.935457000
1	2.703565000	-0.306264000	0.483980000	1	0.500465000	-2.632945000	-0.835938000
1	1.132650000	2.471610000	0.489696000	1	2.708272000	-0.385970000	-0.668753000
1	0.693374000	-3.362032000	0.717799000	1	-2.341106000	2.373909000	-1.221035000
1	-2.994934000	-1.691335000	0.709831000	1	-0.348040000	-0.035076000	3.780696000
1	-2.529368000	2.324388000	0.714112000	1	1.569899000	3.032072000	-1.006465000
1	1.430330000	3.121714000	0.713297000	1	3.417801000	-0.487015000	-0.886129000
1	3.414336000	-0.388053000	0.706128000	1	0.631411000	-3.322636000	-1.096854000
				1	-2.916585000	-1.559287000	-1.288487000
				1	-2.311741000	-1.235334000	-0.988327000
H₁₄Cl⁻				H₁₆Cl⁻			
1	2.041654000	-0.500288000	1.747120000	1	2.572950000	1.409034000	0.273551000
1	-0.763734000	-2.136317000	1.303811000	1	1.602529000	-0.985531000	1.896705000
1	-2.796226000	0.279423000	0.689230000	1	-1.605480000	-0.986269000	1.893984000
1	2.580528000	-0.694039000	2.229556000	1	-2.569782000	1.416123000	0.275695000
1	-3.519145000	0.288191000	0.883748000	1	2.032336000	-1.274404000	2.437188000
1	-0.960963000	-2.758779000	1.669982000	1	3.239496000	1.728587000	0.390859000

1	3.251695000	1.556527000	-0.990522000	1	-3.234853000	1.739434000	0.391029000
1	2.578373000	1.285315000	-0.806494000	1	-2.036558000	-1.275464000	2.433282000
1	1.470340000	-2.136223000	-0.844130000	1	2.846452000	-1.491599000	-1.775755000
1	1.851733000	-2.748107000	-1.044866000	1	2.264632000	-1.151517000	-1.450351000
1	-1.646621000	-1.454395000	-1.672431000	1	-0.001771000	-2.754581000	-0.157042000
1	-2.075203000	-1.900765000	-2.094150000	1	-0.002403000	-3.502466000	-0.137676000
17	-0.012685000	0.247290000	-0.083811000	1	-2.265147000	-1.150429000	-1.451283000
1	-0.796539000	2.998602000	0.147102000	1	-2.847671000	-1.489428000	-1.776555000
1	-1.000254000	3.716919000	0.206823000	17	-0.000052000	0.169541000	-0.169510000
H₁₈Cl⁻				1	0.001650000	3.068901000	-0.181866000
1	-2.552945000	1.357176000	0.118475000	1	0.004507000	3.817410000	-0.180087000
1	-2.476421000	-1.542560000	-1.003209000	H₂₀Cl⁻			
1	2.581699000	-1.362683000	-1.002889000	1	1.536953000	-2.479340000	-0.357869000
1	2.448833000	1.533636000	0.125438000	1	2.048476000	-0.010771000	-2.231137000
1	-3.105966000	-1.935514000	-1.095576000	1	-1.535101000	2.478966000	-0.364030000
1	-3.197130000	1.696403000	0.289361000	1	-2.513919000	0.012919000	1.269937000
1	3.066623000	1.917546000	0.299301000	1	2.588074000	-0.012971000	-2.749700000
1	3.237077000	-1.711002000	-1.094696000	1	1.934001000	-3.111456000	-0.405944000
1	-1.837809000	-1.169564000	2.456518000	1	-3.170459000	0.016007000	1.628576000
1	-1.464437000	-0.927933000	1.855429000	1	-1.930981000	3.111695000	-0.413692000
1	0.100210000	-2.888115000	0.081360000	1	3.172601000	-0.002601000	1.624974000
1	0.126878000	-3.617145000	0.245864000	1	2.515607000	-0.002027000	1.267164000
1	1.524429000	-0.824070000	1.856995000	1	1.551344000	2.468636000	-0.363896000
1	1.912238000	-1.038724000	2.459187000	1	1.950879000	3.099054000	-0.413639000
1	-0.064562000	1.703999000	1.895865000	1	-2.591806000	0.001600000	-2.747219000
1	-0.083106000	2.140220000	2.502793000	1	-2.051297000	0.000872000	-2.229607000
17	0.000588000	0.004799000	-0.462112000	1	0.005624000	1.546428000	2.218682000
1	-0.100384000	2.924017000	-1.010146000	1	0.006995000	1.951953000	2.847530000
1	-0.125230000	3.662728000	-1.124170000	1	-0.002334000	-1.543808000	2.219909000
				1	-0.002971000	-1.948974000	2.848999000
				17	-0.000228000	-0.000442000	-0.170181000
				1	-1.553583000	-2.469377000	-0.354400000
				1	-1.954225000	-3.099292000	-0.401563000

H₂Br⁻				H₄Br⁻			
35	0.000000000	0.000000000	0.188452000	35	0.000022000	0.020807000	0.000000000
1	0.000000000	0.000000000	-2.923906000	1	-3.128614000	-0.181452000	0.000006000
1	0.000000000	0.000000000	-3.671931000	1	-3.876713000	-0.182534000	0.000002000
H₆Br⁻				1	3.876363000	-0.181572000	0.000004000
35	0.012182000	-0.006700000	-0.000280000	1	3.128181000	-0.182694000	0.000003000
1	3.082722000	-0.441776000	0.001526000	H₈Br⁻			
1	3.823710000	-0.545768000	0.001942000	35	0.071077000	-0.001259000	-0.000066000
1	-2.572973000	-2.866059000	0.001832000	1	2.537680000	-2.962068000	0.027897000
1	-2.069960000	-2.312169000	0.001407000	1	2.058755000	-2.387263000	0.022457000
1	-1.491362000	3.544394000	0.001765000	1	-2.577535000	-0.040539000	-1.622077000
1	-1.198520000	2.855874000	0.001340000	1	-3.212773000	-0.050063000	-2.017069000
				1	-2.577533000	0.025413000	1.622756000
				1	-3.212713000	0.031834000	2.017882000
				1	2.482375000	3.005119000	-0.027497000
				1	2.014049000	2.421647000	-0.022028000

H₁₀Br⁻				H₁₂Br⁻			
35	-0.010021000	-0.232769000	-0.175753000	35	0.000017000	-0.000773000	0.001647000
1	-1.714966000	1.928627000	1.262699000	1	1.408696000	-2.465443000	1.247405000
1	-2.771665000	-1.336904000	0.699015000	1	3.133664000	0.109090000	-0.017066000
1	0.136295000	2.663599000	-1.306877000	1	-1.228804000	-2.558958000	-1.245481000
1	1.828317000	1.788856000	1.309734000	1	-1.402287000	2.467329000	1.248815000
1	2.672358000	-1.523664000	0.694423000	1	1.221142000	2.561984000	-1.246096000
1	0.173730000	3.353951000	-1.592030000	1	-1.524830000	-3.176792000	-1.545623000
1	-2.127611000	2.449056000	1.606559000	1	1.748226000	-3.060565000	1.547360000
1	-3.436795000	-1.608171000	0.907976000	1	3.880974000	0.135426000	-0.021697000
1	3.317693000	-1.839995000	0.902052000	1	1.515265000	3.180793000	-1.546079000
1	2.273382000	2.271561000	1.667806000	1	-1.740734000	3.062954000	1.549004000
				1	-3.879651000	-0.126510000	-0.015737000
				1	-3.132246000	-0.102241000	-0.012450000
H₁₄Br⁻				H₁₆Br⁻			
1	-2.144121000	-0.345570000	2.055452000	1	2.742582000	1.564315000	0.229860000
1	0.105710000	2.273799000	1.738559000	1	1.649128000	-0.962704000	2.153439000
1	2.955430000	0.945854000	0.242796000	1	-1.647481000	-0.967667000	2.162073000
1	-2.676026000	-0.384928000	2.579501000	1	-2.767515000	1.513039000	0.198512000
1	3.648140000	1.214204000	0.327365000	1	2.051045000	-1.214397000	2.731404000
1	0.115781000	2.870614000	2.188773000	1	3.394950000	1.910165000	0.346778000
1	-3.236732000	-1.876896000	-1.291460000	1	-3.430085000	1.841668000	0.307208000
1	-2.595613000	-1.564172000	-1.067072000	1	-2.049265000	-1.213697000	2.742499000
1	-2.308056000	1.814980000	-0.299163000	1	3.275095000	-1.790469000	-1.148924000
1	-2.879267000	2.295631000	-0.338056000	1	2.646996000	-1.422331000	-0.979635000
1	0.752434000	2.512443000	-1.440704000	1	0.024888000	-2.961443000	0.320501000
1	0.922146000	3.163855000	-1.766147000	1	0.030332000	-3.697737000	0.449610000
35	0.069848000	-0.216804000	-0.122407000	1	-2.610492000	-1.475321000	-0.976749000
1	2.193131000	-2.405986000	0.590781000	1	-3.227892000	-1.863307000	-1.141680000
1	2.702346000	-2.925698000	0.763603000	35	0.000293000	0.109017000	-0.255955000
				1	-0.038429000	3.105251000	0.670928000
				1	-0.054116000	3.819038000	0.892599000
H₁₈Br⁻				H₂₀Br⁻			
1	0.375600000	-3.005048000	0.463070000	1	-1.571299000	2.687608000	-0.027860000
1	2.950436000	-1.242154000	-0.504775000	1	-3.011798000	-0.137357000	-1.383649000
1	-0.400242000	3.177010000	-0.495134000	1	1.550026000	-2.671740000	0.225219000
1	-2.787341000	1.172947000	0.479754000	1	2.555349000	0.052859000	1.498970000
1	3.639627000	-1.532048000	-0.506533000	1	-3.712389000	-0.171591000	-1.641562000
1	0.463270000	-3.706295000	0.705593000	1	-1.926036000	3.336689000	0.079783000
1	-3.446495000	1.449845000	0.698008000	1	3.137290000	0.070973000	1.967802000
1	-0.492257000	3.919076000	-0.492512000	1	1.914473000	-3.308799000	0.367134000
1	1.964868000	-0.835836000	2.777385000	1	-3.136705000	0.181370000	1.960179000
1	1.581580000	-0.672504000	2.157568000	1	-2.552406000	0.147326000	1.495877000
1	2.413103000	1.822993000	0.479670000	1	-1.664052000	-2.610086000	0.209551000
1	2.983402000	2.253393000	0.699587000	1	-2.046162000	-3.237651000	0.350182000
1	-0.212908000	1.695653000	2.163918000	1	3.701363000	-0.330439000	-1.636282000
1	-0.264550000	2.106246000	2.785638000	1	3.003687000	-0.266191000	-1.376406000
1	-1.366407000	-1.041569000	2.158225000	1	-0.074689000	-1.381607000	2.455057000
1	-1.697699000	-1.294452000	2.777988000	1	-0.092515000	-1.709001000	3.126904000
35	-0.000324000	0.001553000	-0.438185000	1	0.070800000	1.613772000	2.338235000

1	-2.548880000	-1.934618000	-0.504654000	1	0.089827000	1.996106000	2.979385000
1	-3.143780000	-2.386986000	-0.506328000	35	0.000307000	-0.004111000	-0.371731000
				1	1.688583000	2.621435000	-0.034645000
				1	2.065896000	3.260193000	0.056706000

H₃O⁻				H₅O⁻			
8	-0.358651000	-0.086943000	-0.000014000	8	0.000086000	0.360877000	-0.000001000
1	-1.100887000	0.526362000	-0.000063000	1	-0.002629000	1.323484000	0.000007000
1	2.369877000	0.077029000	-0.000499000	1	-2.244667000	-1.298028000	0.000002000
1	1.600215000	0.092150000	0.000671000	1	-1.653256000	-0.808567000	0.000000000
				1	2.245629000	-1.296652000	0.000001000
				1	1.654234000	-0.807249000	0.000001000
H₇O⁻				H₉O⁻			
8	0.027536000	-0.327355000	-0.306352000	8	-0.000023000	-0.003755000	0.478241000
1	0.051494000	-0.911621000	-1.071018000	1	0.001569000	-0.009570000	1.440986000
1	-2.398005000	-0.289708000	1.216184000	1	0.555992000	-2.552628000	-0.858046000
1	-1.762395000	-0.316864000	0.792572000	1	0.414705000	-1.904117000	-0.486505000
1	2.432478000	-0.046486000	1.208558000	1	-2.563955000	-0.539966000	-0.833860000
1	1.802497000	-0.138887000	0.785068000	1	-1.910702000	-0.403391000	-0.468785000
1	-0.143890000	1.783400000	-0.278128000	1	1.907325000	0.420048000	-0.467350000
1	-0.202470000	2.539006000	-0.202420000	1	2.559266000	0.564797000	-0.831555000
				1	-0.552222000	2.552592000	-0.844696000
				1	-0.411793000	1.902274000	-0.476118000
H₁₁O⁻				H₁₃O⁻			
8	0.004768000	-0.001912000	-0.547549000	8	-0.112022000	0.000028000	-0.427213000
1	0.009063000	-0.000828000	-1.509961000	1	-0.012400000	-0.000029000	-1.384704000
1	0.769832000	2.734993000	0.319227000	1	2.372503000	1.840212000	-0.264653000
1	0.574334000	2.035928000	0.094914000	1	1.763907000	1.392280000	-0.272366000
1	-2.726975000	0.786859000	0.315053000	1	-3.109705000	-0.005317000	-0.093122000
1	-2.029403000	0.585423000	0.091486000	1	-2.355520000	-0.004108000	-0.169247000
1	2.035121000	-0.590299000	0.097167000	1	0.625652000	0.000606000	1.655308000
1	2.732082000	-0.792232000	0.322535000	1	0.804218000	0.000936000	2.387217000
1	0.004194000	0.002748000	2.490785000	1	-0.942455000	2.674738000	0.668326000
1	0.005412000	0.002015000	1.739600000	1	-0.735499000	2.005355000	0.380898000
1	-0.601877000	-2.027196000	0.096820000	1	-0.728122000	-2.007295000	0.382421000
1	-0.809931000	-2.722116000	0.322764000	1	-0.932758000	-2.677361000	0.669891000
				1	1.768284000	-1.386965000	-0.274542000
				1	2.378071000	-1.833277000	-0.267725000
H₁₅O⁻				H₁₇O⁻			
8	-0.000909000	0.096362000	-0.289270000	8	-0.000505000	-0.001212000	-0.225709000
1	-0.000400000	-0.005604000	-1.246279000	1	-0.000666000	0.001304000	-1.187872000
1	-2.980256000	-0.753648000	-1.176964000	1	0.001043000	-2.742221000	1.153713000
1	-2.305414000	-0.557309000	-0.908079000	1	0.000650000	-2.074944000	0.801557000
1	0.003121000	-2.208461000	0.042407000	1	-2.485964000	-1.853639000	-1.114028000
1	0.004281000	-2.960657000	0.116291000	1	-1.920749000	-1.436744000	-0.844451000
1	-1.315987000	1.910269000	0.067489000	1	1.914072000	1.446561000	-0.843194000
1	-1.760154000	2.512719000	0.182234000	1	2.476910000	1.866706000	-1.112582000
1	2.977808000	-0.766618000	-1.167910000	1	-2.478719000	1.866053000	-1.109313000
1	2.302835000	-0.567649000	-0.901319000	1	-1.915596000	1.445769000	-0.840702000

1	1.772070000	2.508435000	0.164502000	1	0.001528000	2.067122000	0.815823000
1	1.324630000	1.907469000	0.055119000	1	0.001998000	2.732059000	1.172271000
1	1.319708000	-0.377641000	1.466832000	1	1.538148000	-0.004563000	1.422024000
1	1.734397000	-0.505356000	2.083456000	1	2.005836000	-0.005935000	2.013617000
1	-1.326324000	-0.387655000	1.460959000	1	-1.537646000	-0.003842000	1.422123000
1	-1.743044000	-0.519191000	2.075423000	1	-2.004864000	-0.005038000	2.014115000
				1	1.921262000	-1.436158000	-0.844078000
				1	2.486797000	-1.852793000	-1.113350000
H₁₉O⁻				H₂₁O⁻			
8	-0.000388000	0.000513000	-0.154294000	8	0.000549000	-0.000015000	-0.039074000
1	0.005714000	-0.002268000	-1.116321000	1	-0.002293000	0.004499000	-1.000966000
1	-1.423937000	2.699384000	-1.536918000	1	-2.754171000	0.002719000	-2.393230000
1	-1.125221000	2.132079000	-1.147906000	1	-2.293849000	-0.001679000	-1.805033000
1	3.060178000	-0.126578000	-1.527933000	1	2.740849000	-0.018378000	-2.403593000
1	2.418993000	-0.099965000	-1.140113000	1	2.282329000	-0.017418000	-1.813940000
1	-0.851878000	-1.351528000	1.464596000	1	-0.005751000	-1.379399000	1.821561000
1	-1.114019000	-1.766989000	2.036075000	1	-0.007645000	-1.792143000	2.450036000
1	2.088211000	-0.085614000	2.034455000	1	2.775860000	-0.013056000	1.301722000
1	1.596664000	-0.065687000	1.463512000	1	2.102124000	-0.009028000	0.963269000
1	-0.737884000	1.416961000	1.465307000	1	0.007235000	1.385269000	1.815152000
1	-0.964503000	1.851952000	2.037412000	1	0.009441000	1.799713000	2.442605000
1	-2.451916000	0.101883000	-0.014543000	1	-2.100965000	0.013307000	0.965970000
1	-3.203710000	0.132740000	-0.006815000	1	-2.774812000	0.017181000	1.304200000
1	1.311180000	2.076131000	-0.025236000	1	1.330198000	2.138983000	-0.340228000
1	1.713371000	2.712082000	-0.023039000	1	1.724187000	2.759004000	-0.496323000
1	-1.298558000	-2.034446000	-1.146630000	1	-1.323601000	-2.138210000	-0.334146000
1	-1.642578000	-2.575402000	-1.535668000	1	-1.717230000	-2.759148000	-0.487822000
1	1.137177000	-2.176019000	-0.023998000	1	1.304349000	-2.149141000	-0.337511000
1	1.485820000	-2.842819000	-0.021883000	1	1.691945000	-2.773676000	-0.492016000
				1	-1.689481000	2.777532000	-0.502535000
				1	-1.303108000	2.153190000	-0.344581000

H₂CN⁻				H₄CN⁻			
1	0.624273000	2.903925000	0.000000000	1	-2.222733000	1.576952000	-0.001760000
6	-0.112071000	0.134636000	0.000000000	6	0.141055000	-0.000036000	0.007378000
7	-0.112071000	-1.047941000	0.000000000	7	1.323347000	0.000004000	-0.004449000
1	0.832648000	3.623844000	0.000000000	1	-2.832012000	2.012544000	-0.004791000
				1	-2.832174000	-2.012413000	-0.004706000
				1	-2.222842000	-1.576894000	-0.001870000
H₆CN⁻				H₈CN⁻			
1	1.867402000	-0.786461000	1.606949000	1	-2.922922000	1.115633000	1.086762000
6	-0.348072000	0.000858000	0.008903000	6	-0.535068000	0.006039000	-0.007424000
7	-1.530145000	-0.002092000	-0.001552000	7	0.647062000	-0.013550000	-0.006697000
1	2.432720000	-1.004528000	2.046596000	1	-3.533904000	1.423466000	1.390977000
1	2.405640000	2.296759000	-0.171882000	1	3.208834000	-1.859463000	1.057677000
1	1.845564000	1.801589000	-0.132847000	1	2.627443000	-1.449779000	0.821892000
1	2.403783000	-1.287591000	-1.902133000	1	-3.551438000	-1.420369000	-1.357866000
1	1.844337000	-1.010270000	-1.489240000	1	-2.936736000	-1.109685000	-1.064290000
				1	2.606744000	1.468540000	-0.808389000
				1	3.182958000	1.890274000	-1.035339000

H₁₀CN⁻				H₁₂CN⁻			
6	0.668975000	0.007437000	0.011429000	1	-0.645962000	-0.033642000	2.943575000
7	-0.512891000	-0.008396000	0.038927000	6	0.636590000	-0.028323000	-0.715363000
1	3.642707000	-1.999274000	0.304757000	7	-0.533470000	-0.022839000	-0.545244000
1	3.037547000	-1.563362000	0.240295000	1	-0.533121000	-0.047070000	2.204635000
1	3.678109000	1.987647000	0.011674000	1	3.290838000	2.075378000	0.541669000
1	3.066211000	1.556327000	0.012636000	1	2.766378000	1.617901000	0.267661000
1	-1.712613000	-2.100363000	-0.971189000	1	3.597380000	-1.719708000	0.489225000
1	-2.083838000	-2.685322000	-1.254564000	1	3.006617000	-1.347322000	0.220825000
1	-2.763052000	-0.053881000	1.325599000	1	-1.137704000	2.482607000	0.294254000
1	-3.414597000	-0.067651000	1.694959000	1	-1.388822000	3.160470000	0.485733000
1	-1.747542000	2.166698000	-0.742420000	1	-3.120978000	-0.010804000	-0.168917000
1	-2.126545000	2.773332000	-0.962812000	1	-3.862795000	-0.002884000	-0.064663000
				1	-0.934207000	-2.578348000	0.336117000
				1	-1.122873000	-3.266765000	0.558766000
H₁₄CN⁻				H₁₆CN⁻			
1	4.616423000	0.015901000	0.258597000	1	3.873695000	1.932971000	-0.431337000
6	1.010452000	0.004447000	0.501461000	6	0.842050000	-0.006056000	-0.366700000
7	-0.106111000	0.000850000	0.112087000	7	-0.328708000	-0.004436000	-0.202278000
1	3.870914000	0.013534000	0.327832000	1	3.258956000	1.506317000	-0.420978000
1	0.575295000	-3.084515000	-1.590317000	1	0.020441000	1.748179000	2.896937000
1	0.521390000	-2.442255000	-1.211967000	1	0.039506000	1.385246000	2.244096000
1	0.521292000	3.097132000	-1.581640000	1	-0.142117000	-2.174696000	2.611151000
1	0.476531000	2.452745000	-1.205715000	1	-0.096341000	-1.724804000	2.016289000
1	-2.239727000	-1.561092000	0.127084000	1	-1.154824000	2.572564000	-0.406880000
1	-2.847690000	-1.997287000	0.127887000	1	-1.434263000	3.264440000	-0.453940000
1	-1.244816000	-0.013164000	2.637573000	1	-2.294112000	0.210667000	-1.989094000
1	-1.621658000	-0.017079000	3.283160000	1	-2.852359000	0.272673000	-2.483094000
1	-2.256765000	1.538974000	0.141425000	1	-1.419123000	-2.414970000	-0.736325000
1	-2.869922000	1.967831000	0.145226000	1	-1.758977000	-3.066641000	-0.873935000
1	-1.248840000	-0.001180000	-2.289001000	1	-2.619663000	0.032202000	1.064314000
1	-1.572366000	-0.002180000	-2.963514000	1	-3.272041000	0.042630000	1.431389000
				1	3.244405000	-1.543786000	-0.420256000
				1	3.855469000	-1.975600000	-0.432185000
H₁₈CN⁻				H₂₀CN⁻			
1	-3.410181000	-2.080261000	-1.423813000	1	3.569032000	0.052147000	-2.262157000
6	-0.677756000	-0.015303000	-0.298022000	6	0.578081000	-0.014319000	-0.190033000
7	0.497712000	-0.024025000	-0.173968000	7	-0.602276000	-0.004209000	-0.131921000
1	-2.855393000	-1.646747000	-1.171077000	1	2.958905000	0.039799000	-1.829795000
1	0.346582000	-1.192696000	3.180017000	1	-0.729793000	1.802446000	2.909504000
1	0.292481000	-0.949523000	2.475629000	1	-0.625165000	1.416556000	2.278288000
1	0.506316000	2.605060000	2.204603000	1	-0.810220000	-2.120349000	2.692034000
1	0.421753000	2.060686000	1.699744000	1	-0.689450000	-1.671867000	2.106715000
1	1.365259000	-2.585339000	0.062460000	1	-1.532570000	2.512891000	-0.528177000
1	1.644274000	-3.274978000	0.135775000	1	-1.821050000	3.194759000	-0.631072000
1	2.265574000	-0.649747000	-2.074344000	1	-2.118279000	0.157015000	-2.340536000
1	2.769882000	-0.815637000	-2.601149000	1	-2.557322000	0.201514000	-2.944171000
1	1.650933000	2.220874000	-1.150372000	1	-1.630943000	-2.419559000	-0.802939000
1	2.015435000	2.819541000	-1.410602000	1	-1.952042000	-3.069706000	-0.984669000
1	2.869835000	0.135807000	0.925942000	1	-3.071648000	-0.001552000	0.744940000
1	3.546841000	0.182218000	1.241955000	1	-3.775410000	-0.001327000	0.999967000

1	-2.896023000	1.596042000	-1.087588000	1	2.163155000	-2.385759000	-0.231998000
1	-3.461584000	2.029356000	-1.315823000	1	2.536346000	-3.033342000	-0.237107000
1	-2.962803000	-0.089594000	1.411772000	1	2.851532000	-0.013175000	1.502886000
1	-3.526629000	-0.105068000	1.902781000	1	3.431153000	-0.009841000	1.975695000
				1	2.454462000	3.060407000	-0.171370000
				1	2.096753000	2.404324000	-0.182397000

H₂ClO⁻				H₄ClO⁻			
8	-0.882331000	-0.428342000	-0.000014000	8	-0.858924000	0.000002000	0.000002000
17	0.772638000	0.115533000	-0.000002000	17	0.877005000	-0.000015000	-0.000002000
1	-3.391784000	0.868879000	-0.000484000	1	-2.205398000	2.524062000	0.000004000
1	-2.684417000	0.593789000	0.000636000	1	-1.813300000	1.873805000	0.000004000
				1	-2.205683000	-2.523863000	0.000004000
				1	-1.813308000	-1.873771000	0.000004000
H₆ClO⁻				H₈ClO⁻			
8	0.731766000	0.000747000	-0.166035000	8	-0.659592000	-0.000162000	0.000780000
17	-0.977095000	-0.000614000	0.116654000	17	1.070441000	0.000213000	-0.000657000
1	1.495854000	-2.672948000	-1.053386000	1	-1.760495000	-0.796938000	2.628134000
1	1.288203000	-1.982681000	-0.820780000	1	-1.465817000	-0.595629000	1.962172000
1	1.491413000	2.676394000	-1.050703000	1	-1.761982000	2.627528000	0.795498000
1	1.284877000	1.985556000	-0.818780000	1	-1.467081000	1.961683000	0.594162000
1	2.294686000	-0.000775000	1.318853000	1	-1.466819000	-1.961285000	-0.594683000
1	2.901460000	-0.001090000	1.769951000	1	-1.761794000	-2.626959000	-0.796489000
				1	-1.766321000	0.795546000	-2.624564000
				1	-1.470446000	0.593725000	-1.959297000
H₁₀ClO⁻				H₁₂ClO⁻			
8	-0.520180000	-0.009010000	-0.009518000	8	-0.471292000	0.000905000	0.000497000
17	1.208112000	0.001655000	0.001394000	17	1.256854000	-0.000363000	-0.000597000
1	-1.331391000	-1.824863000	2.230949000	1	-1.212024000	-2.952272000	-0.042762000
1	-1.135185000	-1.364980000	1.665893000	1	-1.040862000	-2.219529000	-0.031835000
1	-1.337674000	2.200720000	1.845361000	1	-1.211761000	2.364991000	1.769924000
1	-1.140959000	1.642649000	1.377401000	1	-1.040418000	1.778393000	1.330722000
1	-1.133378000	-1.661200000	-1.388176000	1	-2.787441000	-0.003842000	0.001362000
1	-1.331544000	-2.220019000	-1.855002000	1	-3.535456000	-0.004505000	0.002074000
1	-3.620160000	-0.006267000	-0.001863000	1	-1.211045000	-0.952086000	2.795583000
1	-2.872297000	-0.004683000	-0.000495000	1	-1.040057000	-0.715854000	2.101818000
1	-1.137910000	1.403218000	-1.635414000	1	-1.042991000	1.815260000	-1.278812000
1	-1.335967000	1.879371000	-2.186208000	1	-1.215326000	2.413882000	-1.701050000
				1	-1.043207000	-0.654408000	-2.120544000
				1	-1.215593000	-0.871092000	-2.820303000
H₁₄ClO⁻				H₁₆ClO⁻			
8	-0.486915000	0.001074000	0.061076000	8	-0.458656000	-0.000330000	0.000506000
17	1.238898000	-0.002130000	-0.071992000	17	1.274044000	0.000063000	-0.014658000
1	-0.185487000	3.115726000	-1.069848000	1	-1.580957000	0.001280000	2.858993000
1	-0.209436000	2.413185000	-0.813365000	1	-1.298124000	0.000935000	2.162560000
1	-1.335505000	-0.002926000	-2.034759000	1	-0.085759000	-2.870910000	1.739033000
1	-1.600199000	-0.004228000	-2.740038000	1	-0.138879000	-2.230690000	1.356478000
1	-0.591722000	1.371934000	1.941719000	1	-0.193795000	2.194301000	-1.385076000
1	-0.598659000	1.814005000	2.550009000	1	-0.147682000	2.827713000	-1.780026000

1	-0.192704000	-3.123395000	-1.052894000	1	-0.146353000	-2.828215000	-1.778294000
1	-0.213631000	-2.419235000	-0.800691000	1	-0.193270000	-2.194825000	-1.383390000
1	-0.611220000	-1.790454000	2.563099000	1	-1.439067000	-0.000652000	-2.112293000
1	-0.601085000	-1.353310000	1.951261000	1	-1.771747000	-0.000767000	-2.786035000
1	-2.426274000	-1.386236000	0.052734000	1	-2.364311000	1.445654000	0.057792000
1	-3.090297000	-1.731872000	0.070959000	1	-3.020687000	1.805842000	0.073012000
1	-2.423205000	1.388690000	0.049689000	1	-2.363879000	-1.446650000	0.057534000
1	-3.086524000	1.735727000	0.067375000	1	-3.020152000	-1.807025000	0.072813000
H₁₈ClO⁻				1	-0.138518000	2.232494000	1.355002000
				1	-0.086318000	2.873086000	1.737041000
8	0.504033000	0.001590000	-0.004015000	8	0.619521000	-0.255690000	0.082548000
17	-1.228347000	-0.004797000	0.012572000	17	-0.913253000	0.456531000	-0.298659000
1	-0.456956000	3.332150000	-1.387826000	1	-4.135557000	-1.529368000	-0.035189000
1	-0.425956000	2.644173000	-1.100740000	1	-3.450246000	-1.235172000	-0.036667000
1	-0.438947000	-2.874832000	-2.185170000	1	-0.356508000	3.979983000	0.825423000
1	-0.410957000	-2.281889000	-1.733141000	1	-0.413162000	3.264853000	0.620639000
1	2.267647000	-0.198568000	1.596643000	1	2.607853000	-1.065806000	-0.975058000
1	2.879902000	-0.252126000	2.025056000	1	3.265567000	-1.341485000	-1.203560000
1	2.848871000	-1.636097000	-1.286461000	1	3.142883000	1.119067000	1.358886000
1	2.243438000	-1.289241000	-1.013665000	1	2.512313000	0.834412000	1.070181000
1	2.235547000	1.515032000	-0.653772000	1	1.696864000	-1.727154000	1.654712000
1	2.838611000	1.923164000	-0.829901000	1	2.120740000	-2.167759000	2.086731000
1	0.667646000	1.901450000	1.440336000	1	0.240268000	-2.440918000	-0.595086000
1	0.688920000	2.498291000	1.894665000	1	0.102415000	-3.143006000	-0.825647000
1	0.633369000	0.306694000	-2.374675000	1	0.316475000	0.615358000	2.410078000
1	0.644173000	0.402407000	-3.118833000	1	0.237914000	0.880234000	3.106103000
1	-0.364595000	-0.366732000	2.845152000	1	0.579752000	-0.660662000	-2.622280000
1	-0.383326000	-0.461888000	3.584950000	1	0.619352000	-0.788359000	-3.357130000
1	0.678920000	-2.200433000	0.913633000	1	1.693841000	1.503899000	-1.308018000
1	0.703328000	-2.892722000	1.202135000	1	2.002646000	2.042212000	-1.727639000
				1	-1.294371000	-2.142988000	2.226408000
				1	-0.919902000	-1.712847000	1.743925000

H₄N⁻				H₆N⁻			
7	-0.323850000	0.000000000	-0.123909000	7	-0.564853000	-0.001588000	0.000013000
1	-0.528958000	0.806678000	0.463590000	1	-1.217445000	-0.001070000	0.797296000
1	-0.529057000	-0.806615000	0.463640000	1	-1.217410000	0.007495000	-0.797245000
1	2.617704000	-0.000002000	0.131887000	1	1.915339000	1.800142000	0.001060000
1	0.707263000	-0.000060000	-0.191757000	1	1.277098000	1.383372000	0.001096000
				1	1.917839000	-1.796936000	-0.000539000
				1	1.278548000	-1.381886000	-0.001762000
H₈N⁻				H₁₀N⁻			
7	0.696701000	-0.015409000	0.072022000	7	-0.107748000	-0.721232000	-0.040214000
1	1.337408000	-0.785420000	-0.167887000	1	0.303917000	-1.313926000	-0.774946000
1	1.341574000	0.787035000	0.106397000	1	-0.223936000	-1.394848000	0.730322000
1	-1.449294000	-1.568761000	-1.445473000	1	2.915598000	0.543076000	-0.111468000
1	-0.940053000	-1.110424000	-1.120324000	1	2.219909000	0.251251000	-0.051494000
1	-1.710024000	-0.361318000	2.016699000	1	-2.840876000	0.854799000	-0.043121000
1	-1.101099000	-0.281300000	1.570594000	1	-2.204239000	0.445071000	-0.091460000

1	-0.926132000	1.439561000	-0.660332000	1	0.204619000	1.008227000	1.484419000
1	-1.429286000	1.988490000	-0.803828000	1	0.213811000	1.530082000	2.032985000
				1	0.115316000	1.858968000	-1.678669000
				1	0.050116000	1.265925000	-1.215073000
H₁₂N⁻				H₁₄N⁻			
7	0.002978000	-0.311101000	-0.617634000	7	0.000296000	-0.561322000	-0.007258000
1	-0.016849000	-1.309264000	-0.869994000	1	0.038044000	-1.201873000	-0.812921000
1	0.010974000	0.133240000	-1.546991000	1	-0.036207000	-1.224457000	0.779976000
1	-2.711902000	-1.245120000	0.880875000	1	3.343851000	-0.818553000	-0.745010000
1	-2.116094000	-0.970543000	0.504304000	1	2.620665000	-0.734953000	-0.549940000
1	2.713770000	-1.241257000	0.891867000	1	-3.340798000	-0.839027000	0.730750000
1	2.116484000	-0.973969000	0.512121000	1	-2.618182000	-0.750073000	0.535908000
1	-1.528056000	1.490168000	-0.105002000	1	1.025785000	1.423055000	-0.858987000
1	-1.925110000	2.122705000	0.009629000	1	1.317914000	2.038691000	-1.184467000
1	-0.004025000	0.345278000	2.447374000	1	-1.939117000	0.832913000	-2.083582000
1	-0.003120000	0.211873000	1.704245000	1	-1.537138000	0.521526000	-1.525278000
1	1.524336000	1.489601000	-0.105659000	1	-1.025775000	1.402687000	0.891191000
1	1.918748000	2.124998000	0.000672000	1	-1.318447000	2.010736000	1.230155000
				1	1.533189000	0.485410000	1.538282000
				1	1.934143000	0.783170000	2.104734000
H₁₆N⁻				H₁₈N⁻			
7	0.000686000	-0.410400000	-0.006508000	7	-0.000918000	-0.236737000	-0.001789000
1	-0.000547000	-1.055075000	-0.809761000	1	-0.018893000	-0.879530000	0.802268000
1	-0.001483000	-1.071575000	0.783224000	1	0.017068000	-0.897236000	-0.791330000
1	2.059648000	0.961170000	-2.006410000	1	-2.855941000	-2.286297000	-1.099929000
1	1.636168000	0.658512000	-1.459765000	1	-2.340914000	-1.804409000	-0.847667000
1	-0.001608000	2.059204000	0.007230000	1	2.846480000	-2.299845000	1.095866000
1	-0.002011000	2.812005000	0.011076000	1	2.333488000	-1.815656000	0.843908000
1	2.619057000	-1.396735000	-0.004666000	1	-0.608272000	1.775400000	1.161805000
1	3.292390000	-1.730805000	-0.004520000	1	-0.780618000	2.367998000	1.593916000
1	-2.061451000	0.960806000	-2.006902000	1	2.490282000	1.269804000	1.378473000
1	-1.637297000	0.658656000	-1.460518000	1	1.933808000	0.917532000	1.008126000
1	-3.292383000	-1.731684000	-0.004317000	1	0.617353000	1.778285000	-1.156040000
1	-2.619437000	-1.396915000	-0.004794000	1	0.793343000	2.374599000	-1.581681000
1	-1.620798000	0.639059000	1.475907000	1	-1.923049000	0.926147000	-1.011012000
1	-2.040033000	0.932666000	2.030649000	1	-2.477430000	1.282117000	-1.381274000
1	1.622620000	0.639403000	1.472652000	1	2.332568000	-0.243987000	-1.359102000
1	2.042363000	0.934112000	2.026472000	1	2.923844000	-0.283803000	-1.821193000
				1	-2.342510000	-0.243244000	1.357874000
				1	-2.934183000	-0.280715000	1.819518000
H₂₀N⁻				H₂₂N⁻			
7	-0.024444000	-0.000292000	-0.304127000	7	-0.000489000	-0.002051000	-0.267135000
1	-0.094162000	-0.795947000	-0.953639000	1	0.002616000	-0.782724000	-0.937751000
1	-0.094746000	0.792743000	-0.956785000	1	-0.000121000	0.800887000	-0.910951000
1	-2.871163000	-0.005966000	-2.625396000	1	-3.111110000	0.000866000	-2.118658000
1	-2.374785000	-0.005156000	-2.064944000	1	-2.515766000	-0.001161000	-1.662686000
1	2.874712000	-1.773333000	-1.408174000	1	3.113044000	-0.003475000	-2.120062000
1	2.324103000	-1.338288000	-1.143322000	1	2.518697000	-0.000928000	-1.662877000
1	-0.610861000	0.004086000	2.061797000	1	-0.000482000	-1.308164000	1.775615000
1	-0.776798000	0.005436000	2.797071000	1	-0.000867000	-1.770508000	2.369028000
1	2.571825000	0.002460000	1.643554000	1	2.834365000	-0.003988000	1.450072000

1	1.987513000	0.001502000	1.165475000	1	2.197574000	-0.003083000	1.045734000
1	0.456099000	2.115315000	0.974211000	1	-0.000678000	1.303831000	1.773915000
1	0.559493000	2.820682000	1.205020000	1	0.000127000	1.773605000	2.361343000
1	-2.206546000	1.297851000	0.366248000	1	-2.197379000	-0.005327000	1.044309000
1	-2.787431000	1.747968000	0.528185000	1	-2.833566000	-0.004491000	1.449617000
1	2.322613000	1.335121000	-1.147377000	1	1.739013000	2.254583000	-0.213757000
1	2.872926000	1.769273000	-1.414344000	1	2.067311000	2.922872000	-0.284103000
1	-2.207887000	-1.295291000	0.371132000	1	-1.713616000	-2.249166000	-0.215717000
1	-2.788558000	-1.744477000	0.536365000	1	-2.038831000	-2.918705000	-0.289796000
1	0.455490000	-2.113627000	0.980574000	1	1.713149000	-2.248654000	-0.209121000
1	0.559273000	-2.818309000	1.213239000	1	2.036776000	-2.918973000	-0.282942000
				1	-2.066765000	2.923117000	-0.280249000
				1	-1.740069000	2.253942000	-0.211013000

H₂NO₂⁻				H₄NO₂⁻			
7	0.500387000	-0.484250000	0.006751000	7	0.000628000	0.207762000	-0.000141000
8	-0.753862000	-0.446804000	-0.005482000	8	-1.066140000	-0.448981000	0.001294000
8	1.093651000	0.617246000	-0.001961000	8	1.066509000	-0.450344000	-0.001212000
1	-2.761827000	0.875009000	0.004250000	1	3.393034000	1.682092000	0.002223000
1	-3.459195000	1.151202000	0.008040000	1	2.824754000	1.191653000	0.001294000
				1	-3.397367000	1.677718000	-0.002058000
				1	-2.827764000	1.188804000	-0.001128000
H₆NO₂⁻				H₈NO₂⁻			
7	0.027151000	-0.431867000	0.000711000	7	-0.000008000	0.536601000	0.000026000
8	-1.065928000	0.180763000	-0.007076000	8	1.062159000	-0.122548000	-0.081978000
8	1.062610000	0.273033000	-0.006853000	8	-1.062120000	-0.122656000	0.081902000
1	-0.287551000	3.604099000	0.026613000	1	3.205268000	2.134900000	-0.736797000
1	-0.244677000	2.856120000	0.016309000	1	2.688113000	1.615934000	-0.576501000
1	-3.184127000	-2.179073000	0.018457000	1	-2.207707000	-2.059077000	-0.802007000
1	-2.668161000	-1.634327000	0.012759000	1	-2.668148000	-2.589304000	-1.063210000
1	2.827999000	-1.380197000	0.013146000	1	-2.688384000	1.615989000	0.576500000
1	3.393001000	-1.873919000	0.019174000	1	-3.205474000	2.134981000	0.736902000
				1	2.207795000	-2.058924000	0.802129000
				1	2.668276000	-2.589076000	1.063413000
H₁₀NO₂⁻				H₁₂NO₂⁻			
7	-0.051266000	-0.667249000	-0.024771000	7	0.118916000	-0.733031000	-0.025929000
8	1.039072000	-0.049242000	0.012127000	8	1.150519000	-0.029236000	0.058712000
8	-1.087511000	0.033802000	0.036203000	8	-0.974621000	-0.119717000	0.033236000
1	3.134628000	-2.445746000	-0.125287000	1	3.438138000	-2.267377000	0.013345000
1	2.629017000	-1.893005000	-0.091863000	1	2.890570000	-1.755548000	0.023243000
1	-1.950443000	2.137245000	-0.801328000	1	-3.076526000	1.061414000	0.146633000
1	-2.321915000	2.732339000	-1.064280000	1	-3.747004000	1.391889000	0.172030000
1	0.342195000	1.705659000	1.855540000	1	-0.646702000	1.900185000	-1.526357000
1	0.376723000	2.159788000	2.449597000	1	-0.678796000	2.453102000	-2.029679000
1	-2.827813000	-1.666435000	-0.079511000	1	-2.460733000	-2.051343000	-0.293226000
1	-3.378518000	-2.173939000	-0.117453000	1	-2.933133000	-2.624825000	-0.391727000
1	2.153217000	1.854434000	-0.968878000	1	-0.119091000	1.635283000	1.905116000
1	2.589284000	2.383924000	-1.269783000	1	-0.160649000	2.073728000	2.510275000
				1	2.388697000	1.974139000	-0.468274000
				1	2.865630000	2.532192000	-0.615456000

H₁₄NO₂⁻				H₁₆NO₂⁻			
7	-0.003964000	-0.742735000	-0.050571000	7	0.008391000	-0.699458000	-0.003385000
8	-1.067212000	-0.079738000	-0.071746000	8	1.128030000	-0.138869000	0.003553000
8	1.060023000	-0.080762000	-0.071594000	8	-0.990086000	0.059159000	-0.003534000
1	-3.039478000	-2.631547000	-0.237816000	1	-2.326792000	2.217653000	1.958311000
1	-2.566939000	-2.052097000	-0.193762000	1	-1.945608000	1.761869000	1.503981000
1	0.023683000	1.905379000	1.521916000	1	2.699437000	-2.999659000	0.012243000
1	0.022549000	2.437495000	2.047787000	1	2.316951000	-2.356233000	0.009730000
1	3.034393000	0.615375000	1.178614000	1	1.251898000	1.886331000	-1.545317000
1	3.652756000	0.844311000	1.531282000	1	1.426970000	2.420543000	-2.039216000
1	1.687861000	1.866327000	-1.446533000	1	-2.489142000	-1.417938000	-1.412137000
1	1.983910000	2.405038000	-1.873996000	1	-2.926025000	-1.820881000	-1.866242000
1	2.552289000	-2.061626000	-0.194276000	1	-1.966418000	1.774812000	-1.477022000
1	3.022168000	-2.643146000	-0.238949000	1	-2.354308000	2.234634000	-1.921504000
1	-1.676007000	1.865044000	-1.458189000	1	-2.486295000	-1.420531000	1.406776000
1	-1.966641000	2.403208000	-1.890058000	1	-2.922053000	-1.823842000	1.861596000
1	-3.016158000	0.647264000	1.198259000	1	1.290427000	1.874937000	1.554374000
1	-3.629125000	0.882126000	1.556438000	1	1.472667000	2.406879000	2.048174000
				1	3.533516000	0.315084000	-0.030625000
				1	4.262481000	0.480230000	-0.039576000
H₁₈NO₂⁻				H₂₀NO₂⁻			
7	-0.094944000	0.546866000	-0.102894000	7	0.086744000	0.616477000	-0.148766000
8	1.010930000	-0.035830000	-0.003378000	8	-0.910118000	-0.143148000	-0.084051000
8	-1.107993000	-0.188828000	-0.119057000	8	1.203897000	0.077738000	0.015924000
1	2.209632000	-1.012928000	-2.881910000	1	2.400402000	-2.119573000	2.070600000
1	1.917323000	-0.821428000	-2.221175000	1	2.051737000	-1.655984000	1.598043000
1	2.690998000	2.608972000	-0.987331000	1	-3.256003000	-0.059849000	0.716090000
1	2.293862000	2.022022000	-0.747477000	1	-3.964327000	-0.113900000	0.949369000
1	-0.384903000	-1.561088000	2.046163000	1	-0.908002000	-0.290312000	3.297643000
1	-0.398591000	-1.902260000	2.711036000	1	-0.868857000	-0.303373000	2.552237000
1	-0.919818000	3.602239000	1.206949000	1	-0.857857000	2.938397000	0.820946000
1	-0.733492000	2.959376000	0.873910000	1	-1.123411000	3.539479000	1.176715000
1	-3.278801000	-0.692810000	0.864864000	1	-2.232380000	1.489141000	-1.590427000
1	-3.947264000	-0.888947000	1.136559000	1	-2.637211000	1.916945000	-2.050796000
1	-1.131855000	-2.540057000	-0.996682000	1	2.331689000	2.346406000	-0.213571000
1	-1.265869000	-3.217190000	-1.286968000	1	2.692161000	2.999900000	-0.264676000
1	-2.637648000	1.417020000	-1.277664000	1	-0.994049000	-2.579727000	0.759898000
1	-3.103132000	1.873572000	-1.645170000	1	-1.152628000	-3.268652000	1.004715000
1	2.020086000	-2.298348000	0.326394000	1	4.244790000	-0.352541000	-0.954267000
1	2.435693000	-2.912060000	0.429552000	1	3.534870000	-0.228786000	-0.756173000
1	2.595265000	0.593827000	1.798816000	1	1.263415000	-2.581846000	-1.976561000
1	3.079626000	0.739294000	2.349869000	1	1.135547000	-2.029838000	-1.488664000
				1	-2.515389000	-1.910399000	-2.277787000
				1	-2.101939000	-1.527547000	-1.786960000