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

Massive dihydrogen uptake by anionic carbon chains

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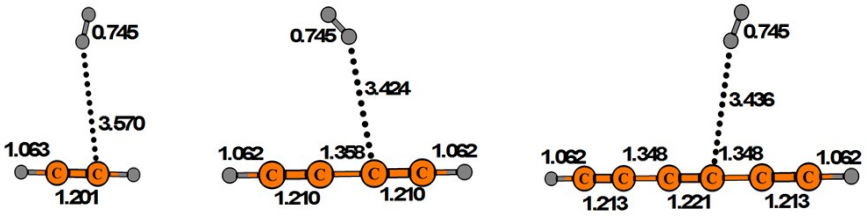
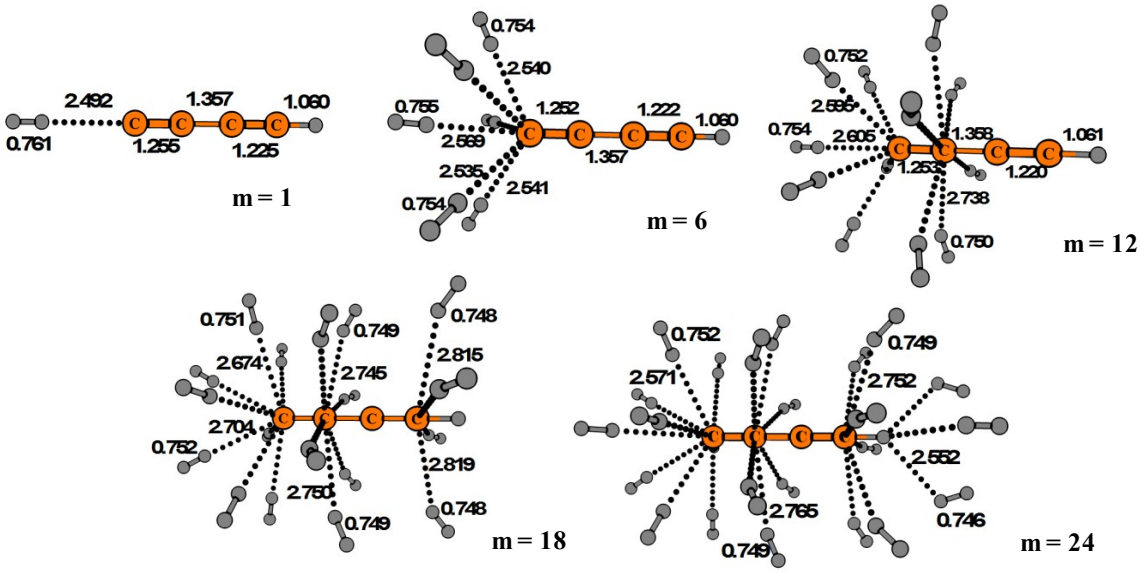
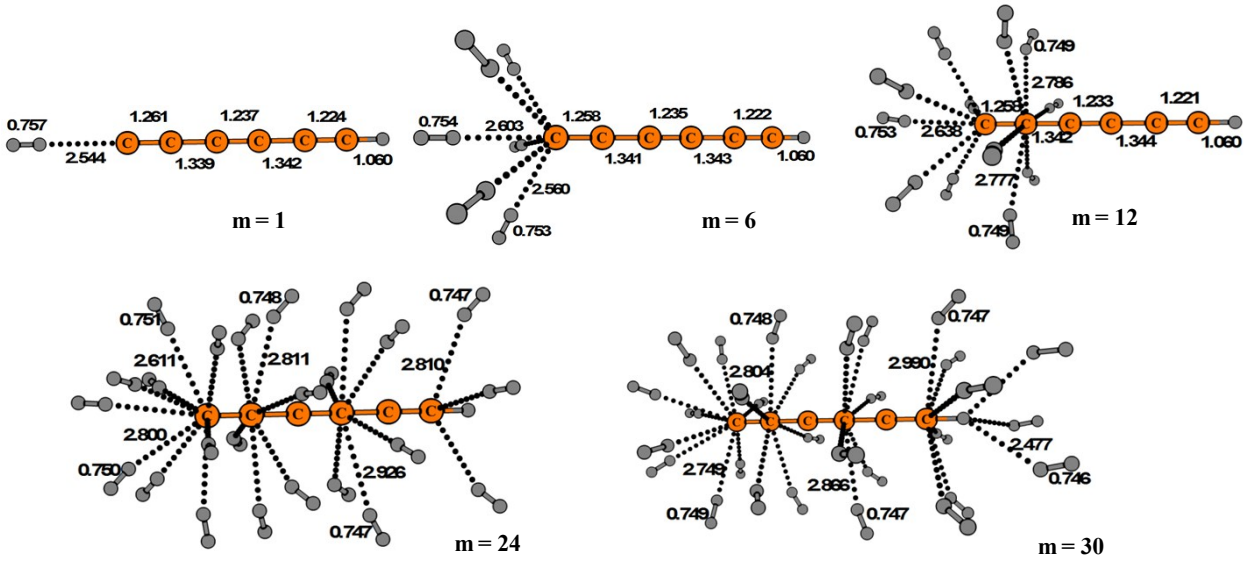
1. **Fig. S1** Optimized geometries of H_2 complexes of $(C_2)_nH_2$, n = 1 – 3 at M06L/6-311++G(d,p) level.



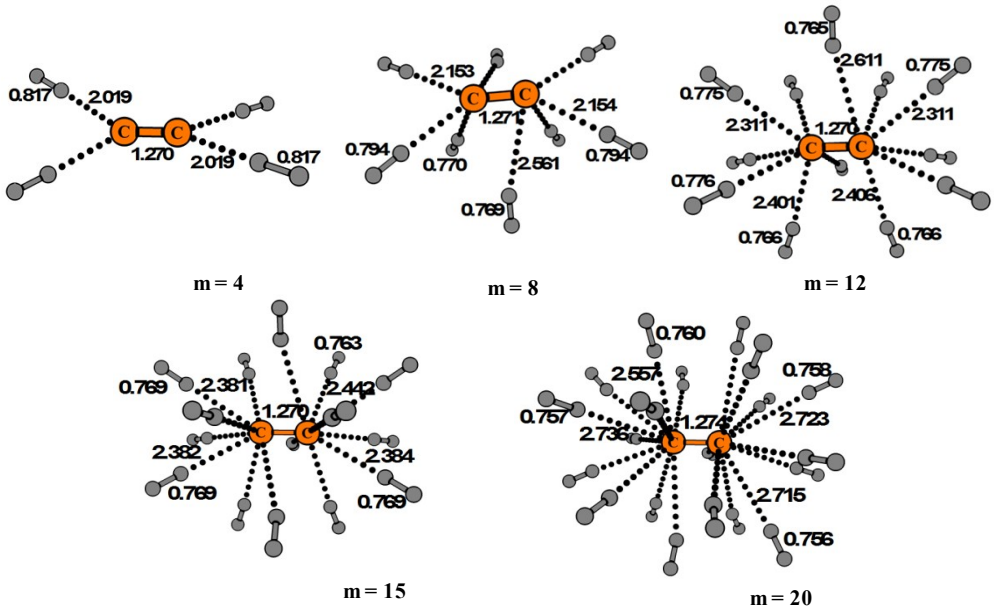
2. **Fig. S2** Optimized geometries of $(HC_4)^-(H_2)_m$ complexes at M06L/6-311++G(d,p) level.



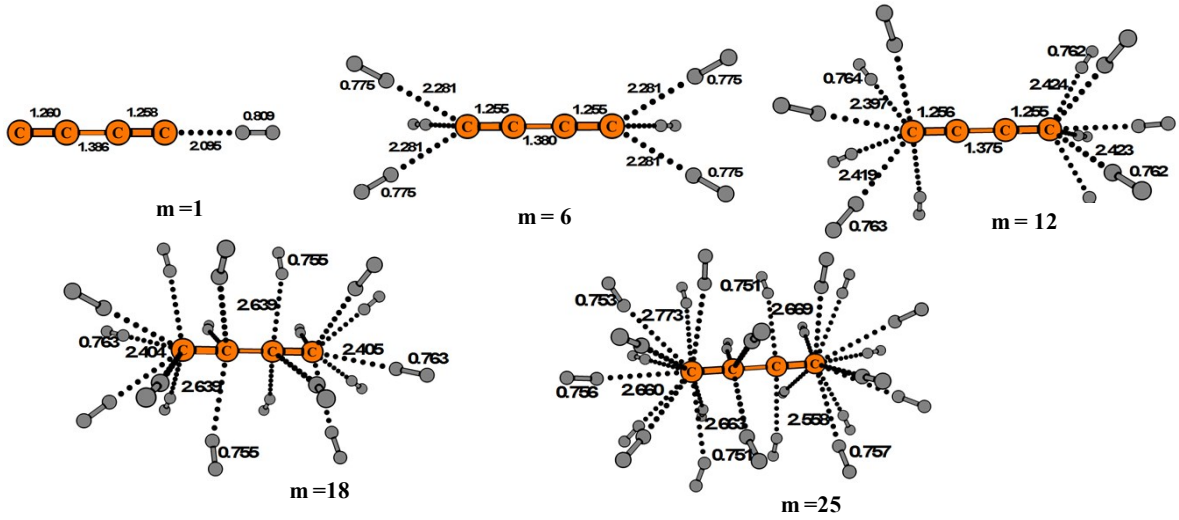
3. **Fig. S3** Optimized geometries of $(HC_6)^-(H_2)_m$ complexes at M06L/6-311++G(d,p) level.



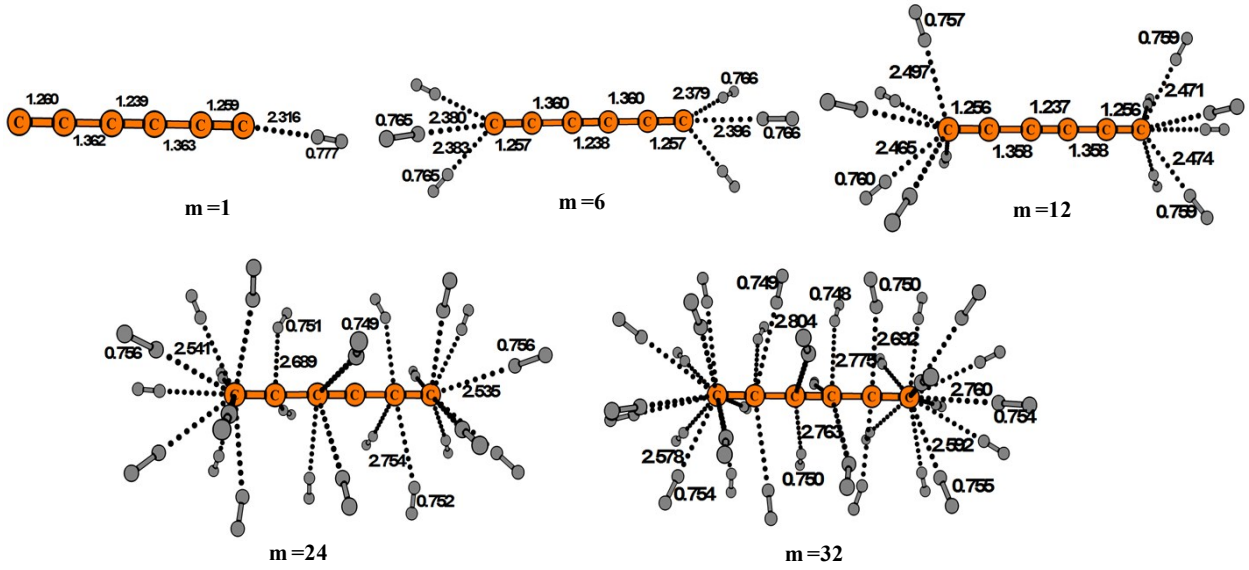
4. **Fig. S4** Optimized geometries of $(C_2)^{2-}(H_2)_m$ complexes at M06L/6-311++G(d,p) level.



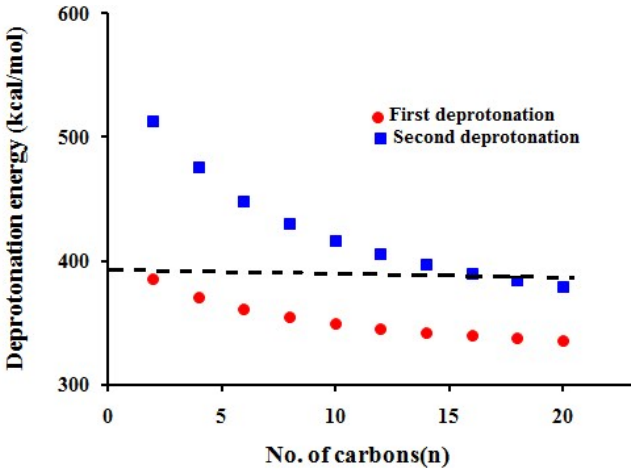
5. **Fig. S5** Optimized geometries of $(C_4)^{2-}(H_2)_m$ complexes at M06L/6-311++G(d,p) level.



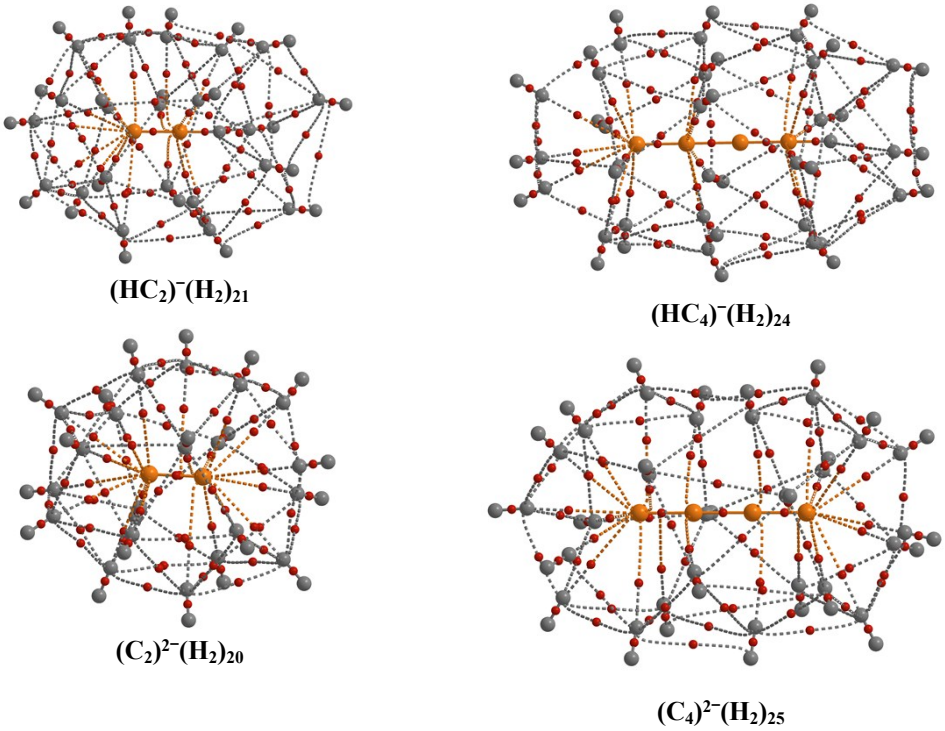
6. **Fig. S6** Optimized geometries of $(C_6)^{2-}(H_2)_m$ complexes at M06L/6-311++G(d,p) level.



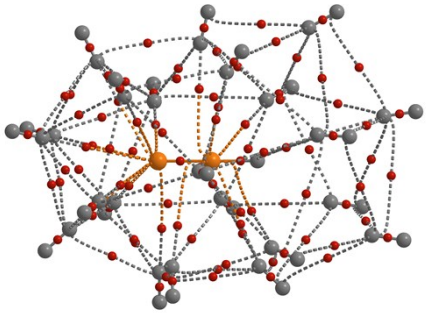
7. **Fig. S7** Deprotonation energy versus number of carbons.



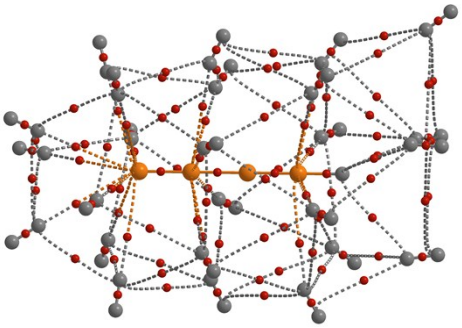
8. Fig. S8 QTAIM features of $(HC_n)^-(H_2)_{mmax}$ and $(C_n)^{2-}(H_2)_{mmax}$ complexes at M06L/6311++G(d,p) level.



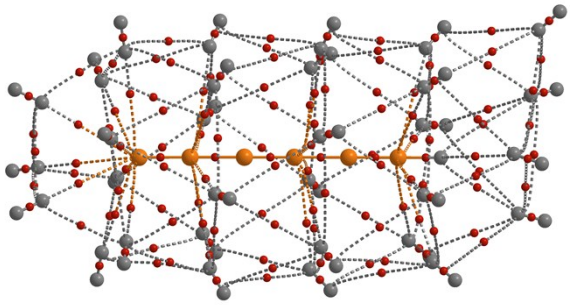
9. Fig. S9 QTAIM features of $(HC_n)^-(H_2)_{mmax+1}$ and $(C_n)^{2-}(H_2)_{mmax+1}$ complexes at M06L/6311++G(d,p) level.



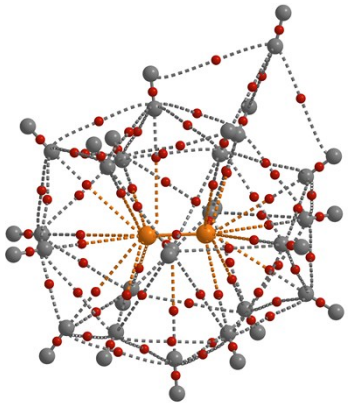
$(HC_2)^-(H_2)_{22}$



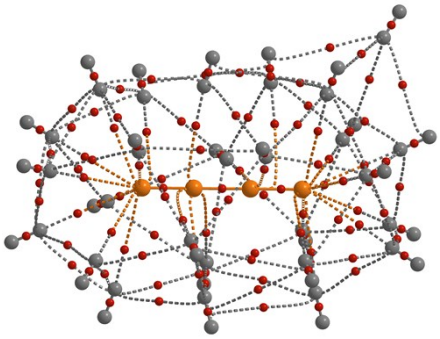
$(HC_4)^-(H_2)_{25}$



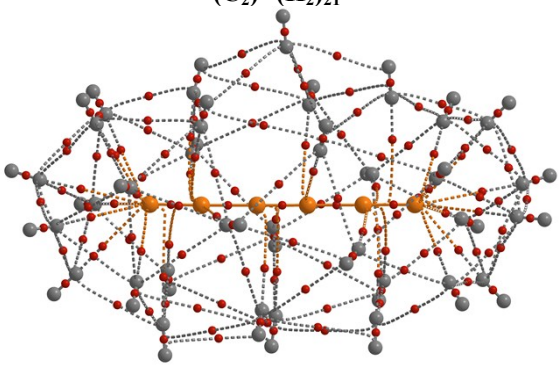
$(HC_6)^-(H_2)_{31}$



$(C_2)^{2-}(H_2)_{21}$

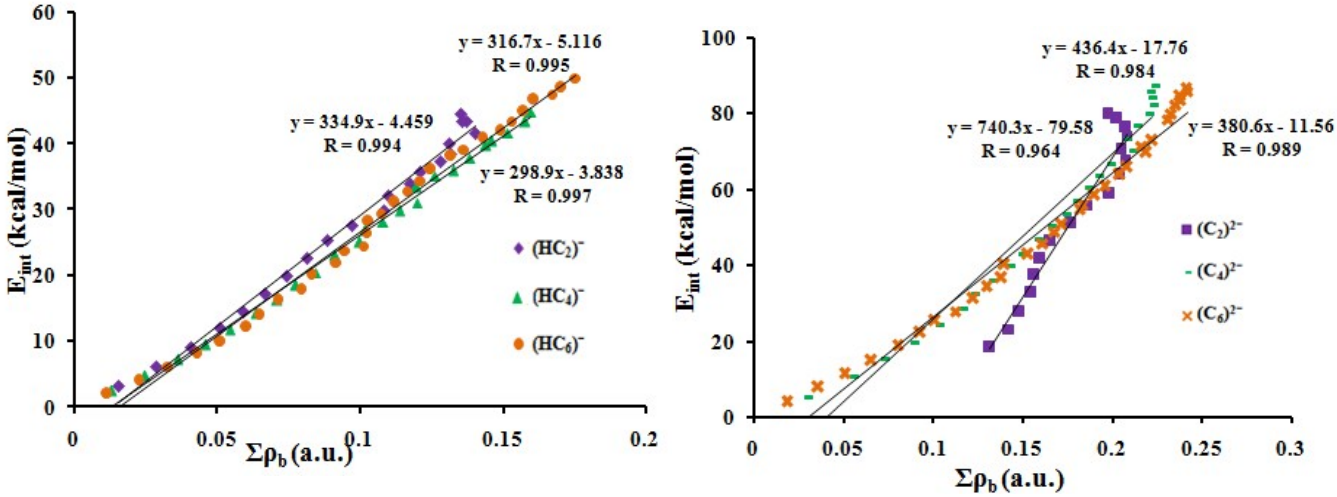


$(C_4)^{2-}(H_2)_{26}$

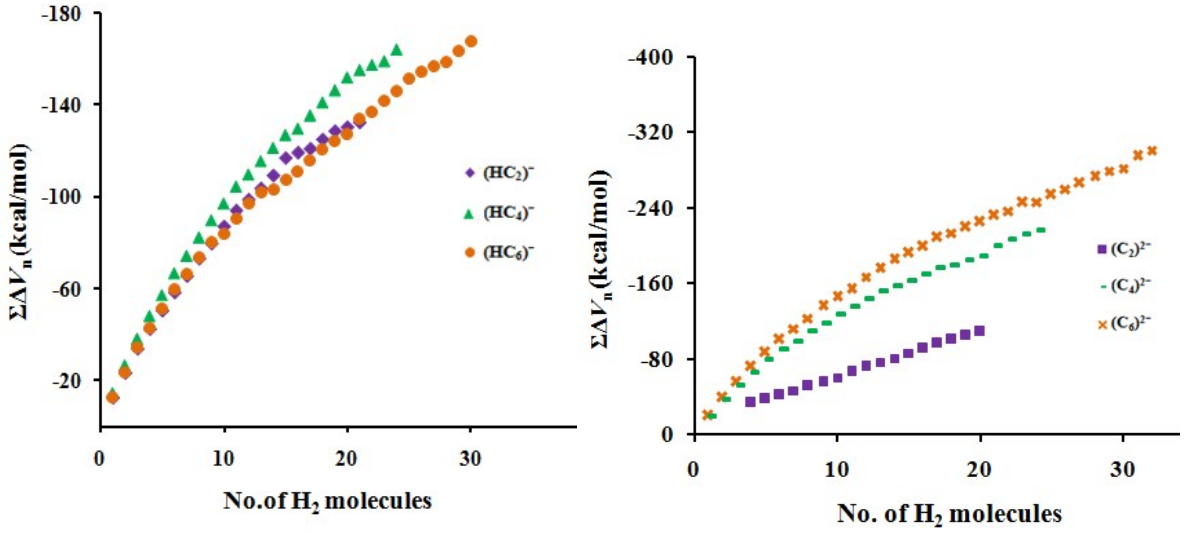


$(C_6)^{2-}(H_2)_{33}$

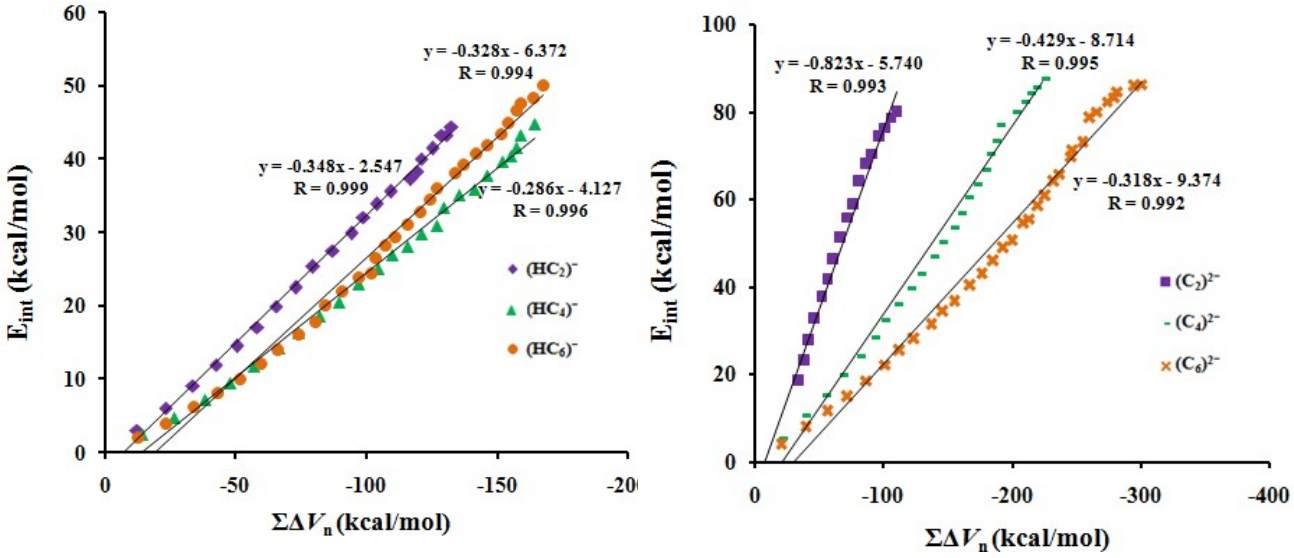
10. Fig. S10 Correlation between E_{int} and $\Sigma\rho_{bcp}$ of anionic polyyne complexes at the M06L/6-311++G(d,p) level.



11. Fig. S11 Correlation between $\Sigma\Delta V_n$ and No. of H_2 molecules of anionic polyyne complexes at the M06L/6-311++G(d,p) level.



12. Fig. S12 Correlation between E_{int} and $\Sigma\Delta V_n$ of anionic polyyne complexes at the M06L/6-311++G(d,p) level.



13. Table S1 Average H-H bond distance (Å) of $(HC_n)^-(H_2)_m$ and $(C_n)^{2-}(H_2)_m$ complexes at M06L/6-311++G(d,p) level.

	$(HC_n)^-(H_2)_m$			$(C_n)^{2-}(H_2)_m$		
m	$(HC_2)^-$	$(HC_4)^-$	$(HC_6)^-$	$(C_2)^{2-}$	$(C_4)^{2-}$	$(C_6)^{2-}$
1	0.767	0.761	0.757	-	0.809	0.777
2	0.763	0.758	0.756	-	0.804	0.776
3	0.761	0.757	0.755	-	0.791	0.771
4	0.759	0.756	0.754	0.817	0.784	0.769
5	0.758	0.755	0.753	0.804	0.779	0.767
6	0.756	0.754	0.753	0.794	0.775	0.765
7	0.756	0.753	0.752	0.788	0.771	0.763
8	0.755	0.753	0.752	0.782	0.769	0.763
9	0.755	0.752	0.751	0.777	0.767	0.761
10	0.754	0.752	0.751	0.774	0.765	0.760
11	0.754	0.752	0.751	0.772	0.764	0.759
12	0.753	0.751	0.751	0.770	0.763	0.759
13	0.753	0.751	0.750	0.769	0.762	0.758
14	0.752	0.751	0.750	0.767	0.761	0.757
15	0.752	0.751	0.750	0.765	0.760	0.757

16	0.752	0.750	0.750	0.764	0.759	0.756
17	0.751	0.750	0.749	0.763	0.759	0.756
18	0.751	0.750	0.749	0.761	0.759	0.755
19	0.751	0.750	0.749	0.760	0.757	0.755
20	0.751	0.750	0.749	0.759	0.757	0.754
21	0.750	0.750	0.749	-	0.756	0.754
22	-	0.750	0.749	-	0.756	0.754
23	-	0.750	0.749	-	0.757	0.754
24	-	0.749	0.749	-	0.755	0.753
25	-	-	0.749	-	0.754	0.753
26	-	-	0.749	-	-	0.753
27	-	-	0.748	-	-	0.752
28	-	-	0.748	-	-	0.752
29	-	-	0.748	-	-	0.752
30	-	-	0.748	-	-	0.752
31	-	-	-	-	-	0.752
32	-	-	-	-	-	0.752

14. Table S2 Average C…H bond distance (Å) of $(HC_n)^-(H_2)_m$ and $(C_n)^{2-}(H_2)_m$ complexes at M06L/6-311++G(d,p) level.

	$(HC_n)^-(H_2)_m$			$(C_n)^{2-}(H_2)_m$		
m	$(HC_2)^-$	$(HC_4)^-$	$(HC_6)^-$	$(C_2)^{2-}$	$(C_4)^{2-}$	$(C_6)^{2-}$
1	2.445	2.492	2.544	-	2.095	2.316
2	2.428	2.499	2.547	-	2.125	2.332
3	2.449	2.510	2.550	-	2.181	2.350
4	2.469	2.524	2.554	2.019	2.219	2.358
5	2.506	2.534	2.562	2.089	2.252	2.369
6	2.534	2.544	2.568	2.153	2.281	2.386
7	2.557	2.589	2.602	2.227	2.323	2.415
8	2.570	2.597	2.626	2.301	2.347	2.420
9	2.599	2.612	2.653	2.318	2.368	2.436
10	2.601	2.628	2.657	2.356	2.395	2.458
11	2.606	2.624	2.697	2.382	2.412	2.465
12	2.655	2.665	2.667	2.399	2.431	2.480
13	2.627	2.691	2.711	2.404	2.446	2.507
14	2.649	2.717	2.725	2.436	2.472	2.521
15	2.651	2.696	2.736	2.455	2.484	2.534
16	2.644	2.711	2.752	2.504	2.509	2.554

17	2.659	2.712	2.768	2.533	2.524	2.564
18	2.622	2.719	2.769	2.539	2.551	2.589
19	2.666	2.726	2.772	2.605	2.557	2.603
20	2.775	2.731	2.774	2.650	2.579	2.614
21	2.755	2.742	2.777	-	2.598	2.607
22	-	2.722	2.778	-	2.620	2.628
23	-	2.701	2.775	-	2.614	2.618
24	-	2.714	2.773	-	2.656	2.648
25	-	-	2.783	-	2.673	2.654
26	-	-	2.784	-	-	2.655
27	-	-	2.829	-	-	2.681
28	-	-	2.807	-	-	2.679
29	-	-	2.799	-	-	2.689
30	-	-	2.784	-	-	2.713
31	-	-	-	-	-	2.730
32	-	-	-	-	-	2.753

15. Table S3 BSSE-corrected E_{int} (kcal/mol) of $(HC_n)^-(H_2)_m$ and $(C_n)^{2-}(H_2)_m$ complexes at M06L/6-311++G(d,p) level.

	$(HC_n)^-(H_2)_m$			$(C_n)^{2-}(H_2)_m$		
m	$(HC_2)^-$	$(HC_4)^-$	$(HC_6)^-$	$(C_2)^{2-}$	$(C_4)^{2-}$	$(C_6)^{2-}$
1	3.1	2.4	2.0	-	5.3	4.0
2	6.0	4.7	4.0	-	10.6	8.0
3	9.1	7.2	6.2	-	15.3	11.5
4	11.9	9.5	8.1	18.5	19.8	15.0
5	14.5	11.7	9.9	23.2	24.1	18.7
6	17.1	14.2	12.2	27.8	28.5	22.2
7	19.9	16.3	14.0	32.7	32.4	25.5
8	22.5	18.5	16.2	37.6	36.2	28.0
9	25.3	20.4	17.9	41.7	39.8	31.3
10	27.5	23.0	20.1	46.3	43.0	34.3
11	29.9	25.1	22.0	51.1	46.9	36.7
12	32.1	26.9	23.8	56.0	50.2	40.3
13	33.9	28.1	24.5	58.8	53.6	43.0
14	35.6	29.7	26.5	63.9	56.8	45.8
15	37.3	31.0	28.2	68.0	60.4	48.9
16	38.4	33.4	29.4	70.4	63.5	50.6
17	40.1	35.1	31.1	74.2	66.7	54.5
18	41.5	35.8	32.8	76.3	70.3	55.6
19	43.3	37.8	34.4	78.7	73.4	58.5
20	43.3	39.7	36.1	79.8	76.8	60.8

21	44.5	40.5	38.2	-	79.8	63.9
22	-	41.6	39.2	-	82.1	65.9
23	-	43.3	40.8	-	84.1	69.7
24	-	44.8	42.0	-	85.6	71.4
25	-	-	43.4	-	87.4	72.9
26	-	-	44.9	-	-	78.5
27	-	-	46.7	-	-	80.0
28	-	-	47.5	-	-	82.3
29	-	-	48.5	-	-	83.3
30	-	-	50.0	-	-	84.6
31	-	-	-	-	-	85.8
32	-	-	-	-	-	86.3

16. Table S4 BSSE-corrected $E_{int/H2}$ (kcal/mol) of $(HC_n)^-(H_2)_m$ and $(C_n)^{2-}(H_2)_m$ complexes at M06L/6-311++G(d,p) level.

	$(HC_n)^-(H_2)_m$			$(C_n)^{2-}(H_2)_m$		
m	$(HC_2)^-$	$(HC_4)^-$	$(HC_6)^-$	$(C_2)^{2-}$	$(C_4)^{2-}$	$(C_6)^{2-}$
1	3.1	2.4	2.0	-	5.3	4.0
2	3.0	2.4	2.0	-	5.3	4.0
3	3.0	2.4	2.1	-	5.1	3.8
4	3.0	2.4	2.0	4.6	5.0	3.7
5	2.9	2.3	2.0	4.6	4.8	3.7
6	2.9	2.4	2.0	4.6	4.7	3.7
7	2.8	2.3	2.0	4.7	4.6	3.6
8	2.8	2.3	2.0	4.7	4.5	3.5
9	2.8	2.3	2.0	4.6	4.4	3.5
10	2.8	2.3	2.0	4.6	4.3	3.4
11	2.7	2.3	2.0	4.6	4.3	3.3
12	2.7	2.2	2.0	4.7	4.2	3.4
13	2.6	2.2	1.9	4.5	4.1	3.3
14	2.5	2.1	1.9	4.6	4.1	3.3
15	2.5	2.1	1.9	4.5	4.0	3.3
16	2.4	2.1	1.8	4.4	4.0	3.2
17	2.4	2.1	1.8	4.4	3.9	3.2
18	2.3	2.0	1.8	4.2	3.9	3.1
19	2.3	2.0	1.8	4.1	3.9	3.1
20	2.2	2.0	1.8	4.0	3.8	3.0

21	2.1	1.9	1.8	-	3.8	3.0
22	-	1.9	1.8	-	3.7	3.0
23	-	1.9	1.8	-	3.7	3.0
24	-	1.9	1.8	-	3.6	3.0
25	-	-	1.7	-	3.5	2.9
26	-	-	1.7	-	-	3.0
27	-	-	1.7	-	-	3.0
28	-	-	1.7	-	-	2.9
29	-	-	1.7	-	-	2.9
30	-	-	1.7	-	-	2.8
31	-	-	-	-	-	2.8
32	-	-	-	-	-	2.7

17. Table S5 Free energy change per H_2 (kacl/mol) of $(HC_n)^-(H_2)_m$ and $(C_n)^{2-}(H_2)_m$ complexes at M06L/6-311++G(d,p) level.

	$(HC_n)^-(H_2)_m$			$(C_n)^{2-}(H_2)_m$		
m	$(HC_2)^-$	$(HC_4)^-$	$(HC_6)^-$	$(C_2)^{2-}$	$(C_4)^{2-}$	$(C_6)^{2-}$
1	6.3	5.1	4.9	-	4.9	3.5
2	3.8	2.5	4.6	-	1.4	4.1
3	4.2	3.6	4.9	-	2.1	3.8
4	4.2	3.8	4.3	0.6	2.5	3.8
5	4.8	4.1	4.4	0.4	1.7	3.8
6	5.0	4.3	4.4	1.2	1.9	4.1
7	5.1	5.4	5.6	1.2	3.0	4.5
8	4.1	4.4	5.5	1.4	3.4	4.1
9	5.1	4.5	4.7	1.5	3.5	3.6
10	4.2	4.5	5.9	1.6	3.6	4.7
11	4.5	4.6	6.1	1.8	3.8	4.6
12	5.5	4.6	6.2	1.8	4.0	3.7
13	5.6	4.6	4.8	1.9	4.0	4.9
14	5.8	4.6	6.3	2.6	4.1	3.8
15	4.4	4.7	6.3	2.1	4.2	5.0
16	4.7	4.7	6.5	2.2	4.3	4.9
17	5.9	4.9	6.3	2.5	3.4	5.0
18	4.9	4.8	6.4	2.6	3.5	5.1
19	6.3	4.9	6.5	3.8	3.4	5.2
20	6.5	4.9	6.6	3.9	4.7	5.3
21	6.6	5.0	6.6	-	3.7	5.4
22	-	5.0	6.5	-	3.7	5.3

23	-	5.1	6.7	-	3.8	4.3
24	-	5.0	6.7	-	4.9	5.6
25	-	-	6.7	-	5.2	4.4
26	-	-	6.7	-	-	5.7
27	-	-	6.7	-	-	5.7
28	-	-	6.7	-	-	5.9
29	-	-	6.7	-	-	5.8
30	-	-	6.8	-	-	5.9
31	-	-	-	-	-	4.5
32	-	-	-	-	-	4.7

18. Table S6 Deprotonation energies (kcal/mol) of polyynes at M06L/6-311++G(d,p) level.

n	first deprotonation energy	second deprotonation energy
2	385.9	513.1
4	370.6	475.2
6	360.9	448.1
8	354.2	429.4
10	349.2	415.7
12	345.4	405.1
14	342.4	396.7
16	339.9	389.8
18	337.8	384.0
20	336.0	379.1

19. Table S7 Average ρ_{bcp} values (a. u.) of $(HC_n)^-(H_2)_m$ and $(C_n)^{2-}(H_2)_m$ complexes at M06L/6-311++G(d,p) level.

m	$(HC_2)^-$	$(HC_4)^-$	$(HC_6)^-$	$(C_2)^{2-}$	$(C_4)^{2-}$	$(C_6)^{2-}$
1	0.0155	0.0130	0.0116	-	0.0290	0.0185
2	0.0144	0.0125	0.0113	-	0.0272	0.0180
3	0.0137	0.0121	0.0110	-	0.0239	0.0169
4	0.0128	0.0115	0.0107	0.0329	0.0219	0.0164
5	0.0118	0.0109	0.0102	0.0284	0.0203	0.0160
6	0.0111	0.0106	0.0101	0.0247	0.0191	0.0155
7	0.0106	0.0101	0.0092	0.0221	0.0174	0.0144
8	0.0102	0.0097	0.0089	0.0195	0.0165	0.0140
9	0.0099	0.0094	0.0088	0.0177	0.0157	0.0136
10	0.0097	0.0091	0.0083	0.0166	0.0148	0.0130
11	0.0098	0.0091	0.0083	0.0161	0.0143	0.0126

12	0.0092	0.0085	0.0079	0.0155	0.0137	0.0116
13	0.0090	0.0083	0.0078	0.0153	0.0133	0.0118
14	0.0086	0.0081	0.0073	0.0146	0.0127	0.0115
15	0.0085	0.0080	0.0069	0.0138	0.0123	0.0112
16	0.0082	0.0075	0.0067	0.0128	0.0119	0.0108
17	0.0077	0.0074	0.0066	0.0122	0.0116	0.0107
18	0.0078	0.0074	0.0065	0.0115	0.0116	0.0102
19	0.0071	0.0073	0.0064	0.0107	0.0109	0.0100
20	0.0069	0.0072	0.0062	0.0099	0.0106	0.0098
21	0.0064	0.0070	0.0063	-	0.0104	0.0097
22	-	0.0069	0.0062	-	0.0101	0.0095
23	-	0.0069	0.0062	-	0.0096	0.0095
24	-	0.0067	0.0062	-	0.0092	0.0090
25	-	-	0.0061	-	-	0.0089
26	-	-	0.0061	-	-	0.0089
27	-	-	0.0060	-	-	0.0086
28	-	-	0.0060	-	-	0.0084
29	-	-	0.0059	-	-	0.0082
30	-	-	0.0059	-	-	0.0079
31	-	-	-	-	-	0.0078
32	-	-	-	-	-	0.0075

20. Table S8 V_{min} values (kcal/mol) of $(HC_n)^-(H_2)_m$ and $(C_n)^{2-}(H_2)_m$ complexes at M06L/6-311++G(d,p) level.

m	$(HC_2)^-$	$(HC_4)^-$	$(HC_6)^-$	$(C_2)^{2-}$	$(C_4)^{2-}$	$(C_6)^{2-}$
1	-75.0	-50.7	-39.6	-	-140.9	-113.5
2	-73.9	-50.0	-39.2	-	-133.8	-110.1
3	-72.2	-48.6	-38.2	-	-129.9	-109.5
4	-70.8	-48.1	-37.9	-146.7	-127.9	-105.7
5	-67.9	-47.4	-37.6	-146.2	-125.8	-106.1
6	-66.9	-46.6	-36.7	-145.3	-122.6	-100.4
7	-65.5	-46.2	-36.3	-134.6	-113.2	-99.7
8	-64.3	-45.6	-36.2	-133.9	-113.7	-100.2
9	-64.0	-45.2	-36.0	-131.8	-111.5	-100.1
10	-60.5	-44.9	-35.8	-130.5	-111.1	-98.5
11	-59.8	-44.5	-35.1	-129.0	-110.7	-99.2
12	-55.4	-44.4	-35.1	-127.6	-109.4	-98.2
13	-54.7	-44.3	-35.1	-125.0	-109.2	-97.3

14	-54.2	-44.2	-35.0	-123.1	-108.3	-96.5
15	-55.0	-44.6	-35.0	-122.7	-107.4	-96.3
16	-45.8	-44.6	-35.1	-122.2	-107.0	-96.3
17	-44.9	-44.7	-34.6	-121.5	-106.8	-96.0
18	-44.7	-45.0	-34.8	-117.9	-108.3	-96.3
19	-43.7	-44.4	-34.8	-117.2	-107.1	-96.3
20	-40.3	-44.9	-34.8	-116.9	-105.4	-97.2
21	-40.2	-37.1	-34.6	-	-104.8	-95.4
22	-	-36.7	-35.5	-	-104.2	-93.3
23	-	-36.6	-35.7	-	-103.2	-94.6
24	-	-36.4	-36.1	-	-101.0	-93.8
25	-	-	-35.7	-	-	-93.6
26	-	-	-35.7	-	-	-93.6
27	-	-	-36.1	-	-	-93.9
28	-	-	-30.6	-	-	-92.3
29	-	-	-29.2	-	-	-90.6
30	-	-	-30.3	-	-	-90.6
31	-	-	-	-	-	-91.5
32	-	-	-	-	-	-113.5

21. Table S9 $\Sigma\Delta V_n$ values (kcal/mol) of $(HC_n)^-(H_2)_m$ and $(C_n)^{2-}(H_2)_m$ complexes at M06L/6-311++G(d,p) level.

m	$(HC_2)^-$	$(HC_4)^-$	$(HC_6)^-$	$(C_2)^{2-}$	$(C_4)^{2-}$	$(C_6)^{2-}$
1	-12.3	-14.4	-12.7	-	-19.3	-20.1
2	-23.1	-26.5	-23.4	-	-37.4	-39.0
3	-33.7	-38.1	-34.2	-	-52.6	-55.8
4	-42.3	-48.0	-43.2	-34.4	-66.9	-72.2
5	-50.4	-57.1	-51.4	-38.2	-79.5	-87.0
6	-58.3	-66.6	-59.9	-41.8	-91.2	-101.4
7	-65.5	-74.2	-66.2	-46.7	-99.5	-112.8
8	-73.1	-82.2	-73.9	-51.6	-109.5	-123.7
9	-79.7	-89.8	-80.5	-55.8	-118.6	-136.7
10	-87.2	-97.1	-84.2	-60.7	-127.3	-145.9
11	-94.2	-104.4	-90.7	-66.8	-136.7	-154.7
12	-98.9	-109.7	-97.1	-72.4	-144.1	-167.6
13	-103.8	-115.6	-101.8	-76.9	-152.5	-175.9
14	-109.4	-121.3	-103.5	-81.1	-158.2	-185.5
15	-117.1	-127.0	-107.5	-86.8	-163.7	-193.0
16	-119.4	-129.7	-111.0	-91.2	-170.5	-199.5

17	-121.1	-135.5	-115.8	-96.5	-177.6	-209.0
18	-125.2	-141.2	-120.6	-101.1	-180.5	-213.8
19	-128.8	-146.5	-124.4	-105.4	-185.3	-220.3
20	-130.6	-152.1	-127.2	-109.7	-188.9	-225.6
21	-132.6	-155.3	-133.8	-	-200.6	-232.5
22	-	-157.6	-137.1	-	-207.7	-237.4
23	-	-159.2	-141.7	-	-212.7	-246.0
24	-	-164.2	-146.4	-	-216.6	-246.8
25	-	-	-151.5	-	-	-254.3
26	-	-	-154.3	-	-	-260.6
27	-	-	-157.3	-	-	-266.2
28	-	-	-158.8	-	-	-273.3
29	-	-	-163.8	-	-	-279.4
30	-	-	-167.9	-	-	-282.1
31	-	-	-	-	-	-295.1
32	-	-	-	-	-	-301.3

21. Table S10 H_2 affinity of anionic carbon chains.

Anion	Molecular weight	m_{max}	Weight percent of H_2 (wt%)
HC_2^-	25.029	21	62.8
HC_4^-	49.051	24	49.7
HC_6^-	73.072	30	45.3
C_2^{2-}	24.021	20	62.7
C_4^{2-}	49.051	25	50.7
C_6^{2-}	73.072	32	46.9

22. Cartesian coordinates in Å unit of optimized geometry of $(H_2C_n)(H_2)$ complexes at M06L/6-311++G(d,p) level.

C_2H_4			**C_4H_4**		
SCF Energy = -78.50984 a. u.			SCF Energy = -154.67613 a. u.		
6	0.442939000	0.612578000	-0.000227000		
6	0.530953000	-0.585003000	-0.001219000		
			6	-0.698064000	-0.241906000	0.000024000

1	0.606461000	-1.645338000	-0.001974000	6	0.659333000	-0.282124000	-0.000027000
1	-3.773094000	-0.042385000	-0.049672000	6	1.868588000	-0.314998000	-0.000097000
1	-3.044276000	-0.150661000	0.059927000	6	-1.907198000	-0.201261000	0.000143000
1	0.367559000	1.672929000	0.000399000	1	-2.969067000	-0.169315000	0.000200000
				1	-0.010026000	3.112181000	-0.000195000
				1	0.512606000	3.642589000	-0.000175000
				1	2.930535000	-0.343725000	-0.000088000
C_6H_4							
SCF Energy = -230.84608 a. u.							
6	3.087987000	-0.346612000	-0.000320000				
6	1.876542000	-0.288595000	-0.000212000				
6	0.530516000	-0.219238000	-0.000125000				
1	4.149163000	-0.398126000	-0.000513000				
6	-0.688994000	-0.151118000	-0.000081000				
6	-2.034829000	-0.077031000	-0.000180000				
6	-3.245803000	-0.009697000	-0.000336000				
1	-4.306599000	0.049292000	-0.000479000				
1	1.338727000	3.119961000	0.050490000				
1	1.666194000	3.782614000	-0.041972000				

23. Cartesian coordinates in Å unit of optimized geometry of $(H_2C_n)(H_2)$ complexes at CCSD/aug-cc-pVTZ level.

C_2H_4				**C_4H_4**			
CCSDT Energy = -78.36477 a. u.				CCSDT Energy = -154.37732 a. u.			
6	0.406169000	0.622449000	-0.000042000	6	0.666459000	-0.258907000	0.022215000
6	0.475218000	-0.599258000	-0.000040000	6	-0.729534000	-0.230653000	-0.022257000
1	0.536396000	-1.674529000	-0.000083000	6	-1.953445000	-0.157490000	0.009687000
1	-3.465678000	-0.086808000	-0.003010000	6	1.890941000	-0.322877000	-0.009672000
1	-2.703608000	-0.075505000	0.003641000	1	2.966192000	-0.352410000	0.008413000
1	0.344571000	1.697697000	-0.000059000	1	0.466897000	2.770112000	0.000875000
				1	0.348844000	3.522750000	-0.001682000
				1	-3.028460000	-0.120893000	-0.007449000
C_6H_4							
CCSDT Energy = -230.39198 a. u.							
6	3.234054000	-0.160002000	0.004083000				
6	2.007118000	-0.170385000	-0.011181000				

6	0.616681000	-0.174834000	0.026872000
1	4.309617000	-0.152904000	-0.012848000
6	-0.612227000	-0.177811000	-0.025585000
6	-2.002675000	-0.175269000	0.011666000
6	-3.229583000	-0.168749000	-0.005235000
1	-4.305330000	-0.164513000	0.010197000
1	-0.040702000	2.858905000	-0.005132000
1	-0.043796000	3.620805000	0.004069000

24. Cartesian coordinates in Å unit of optimized geometry of $(HC_n)^-(H_2)_m$ and $(C_n)^{2-}(H_2)_m$ complexes at M06L/6-311++G(d,p) level.

$C_2H_3^-$

SCF Energy = -77.89940 a. u.

6	-0.278924000	-0.054156000	-0.000089000
6	0.964054000	0.020001000	-0.000027000
1	2.034346000	0.088423000	0.000269000
1	-3.454599000	0.095213000	-0.000792000
1	-2.690526000	0.021293000	0.001217000

$C_2H_5^-$

SCF Energy = -79.0758 a. u.

6	-0.015249000	-0.107158000	-0.007342000
6	1.223582000	0.006869000	0.002532000
1	2.291212000	0.104044000	0.011541000
1	-2.199066000	-1.183365000	0.001258000
1	-2.880823000	-1.528701000	0.009878000
1	-2.510234000	1.864105000	0.004331000
1	-1.951090000	1.345654000	0.001850000

$C_2H_7^-$

SCF Energy = -80.25260 a. u.

6	0.207124000	-0.044801000	0.027510000
6	1.449084000	-0.001409000	0.001202000
1	2.519780000	0.037873000	-0.022966000
1	-1.785221000	-0.988078000	-1.040084000
1	-2.405129000	-1.287594000	-1.364612000
1	-2.245647000	1.953824000	-0.463605000
1	-1.692974000	1.444800000	-0.345167000
1	-2.494647000	-0.492099000	1.713746000
1	-1.833411000	-0.391466000	1.350418000

$C_2H_9^-$

SCF Energy = -81.42890 a. u.

6	0.292128000	-0.005290000	0.014177000
6	1.534431000	0.001521000	-0.001579000
1	2.605748000	0.007779000	-0.016481000
1	-1.852488000	0.001523000	1.248375000
1	-2.524752000	0.011473000	1.602796000
1	-1.381318000	-2.751362000	-0.044105000
1	-1.022255000	-2.083827000	-0.017388000
1	-2.531034000	0.009130000	-1.569497000
1	-1.858572000	0.000812000	-1.215999000
1	-1.018196000	2.079686000	-0.017859000

	1 -1.376490000 2.747403000 -0.045433000
$C_2H_{11}^-$ SCF Energy = -82.60480 a. u. 6 0.278700000 -0.278589000 0.099744000 6 1.520193000 -0.303059000 0.125779000 1 2.591181000 -0.322378000 0.145849000 1 -1.852672000 -0.804179000 1.234259000 1 -2.517206000 -0.942862000 1.575718000 1 -1.683085000 -2.368231000 -1.398683000 1 -1.236722000 -1.898337000 -1.005883000 1 -2.512946000 0.790046000 -1.166098000 1 -1.875234000 0.513998000 -0.861135000 1 -0.917093000 1.607445000 1.201662000 1 -1.249406000 2.208959000 1.519011000 1 0.185086000 2.687836000 -1.466599000 1 0.274745000 2.017592000 -1.131236000	**$C_2H_{13}^-$** SCF Energy = -83.78069 a. u. 6 0.299171000 -0.013399000 0.256655000 6 1.540541000 -0.008416000 0.295330000 1 2.611399000 -0.003768000 0.326911000 1 -1.893225000 1.212472000 0.225853000 1 -2.562385000 1.565790000 0.183666000 1 -1.704368000 -0.099660000 2.808305000 1 -1.191352000 -0.087541000 2.251889000 1 -2.566252000 -1.578027000 0.060723000 1 -1.897486000 -1.227734000 0.127319000 1 -1.025779000 0.077062000 -1.857526000 1 -1.375774000 0.129803000 -2.526260000 1 0.090404000 2.932568000 -1.315723000 1 0.193809000 2.266799000 -0.975414000 1 0.089747000 -2.857929000 -1.487456000 1 0.192988000 -2.198942000 -1.134198000
$C_2H_{15}^-$ SCF Energy = -84.95693 a. u. 6 0.160169000 -0.253236000 -0.246409000 6 0.787162000 -1.324930000 -0.270517000 1 1.332022000 -2.247009000 -0.290747000 1 -1.629434000 1.361082000 0.488672000 1 -2.161983000 1.852007000 0.711732000 1 -1.872445000 0.985417000 -2.458000000 1 -1.375630000 0.747283000 -1.939328000 1 0.436164000 2.944656000 -0.859994000 1 0.336448000 2.204348000 -0.737505000 1 0.600793000 1.290404000 1.690730000 1 0.726343000 1.660236000 2.337390000 1 -1.404123000 -0.783144000 2.677392000 1 -1.054929000 -0.706634000 2.013023000 1 -3.019538000 -1.167929000 -0.166895000 1 -2.281980000 -1.033037000 -0.251209000 1 3.118747000 1.436466000 -0.047573000 1 2.565556000 0.924854000 -0.066134000	**$C_2H_{17}^-$** SCF Energy = -86.13307 a. u. 6 0.000355000 -0.301136000 -0.050851000 6 -0.000887000 -1.540900000 -0.119106000 1 -0.002252000 -2.610480000 -0.179055000 1 1.252355000 1.894287000 0.179799000 1 1.652542000 2.532685000 0.249323000 1 -1.650807000 2.533108000 0.253118000 1 -1.251005000 1.894607000 0.182898000 1 -2.864237000 0.173126000 -1.722208000 1 -2.222987000 0.010736000 -1.360122000 1 -2.241249000 -0.256887000 1.311638000 1 -2.881294000 -0.160683000 1.698221000 1 -0.002593000 1.813599000 -2.548440000 1 -0.001766000 1.332733000 -1.965193000 1 2.221352000 0.009022000 -1.362307000 1 2.862681000 0.170231000 -1.724811000 1 2.882989000 -0.162307000 1.694877000 1 2.242526000 -0.257790000 1.308747000 1 0.003592000 1.243981000 2.835995000 1 0.003343000 0.892248000 2.167263000
$C_2H_{19}^-$ SCF Energy = -87.30944 a. u. 6 -0.020371000 -0.014234000 -0.248668000 6 0.082486000 0.164768000 -1.473162000 1 0.172783000 0.320409000 -2.529264000 1 -0.011550000 1.240473000 1.964508000 1 0.029665000 1.600829000 2.627748000 1 1.418274000 -1.281719000 2.432673000 1 1.087387000 -0.986810000 1.819983000 1 -0.054788000 -3.256693000 0.272012000 1 -0.134857000 -2.516388000 0.149746000	**$C_2H_{21}^-$** SCF Energy = -88.48485 a. u. 6 -0.003362000 -0.006465000 -0.133098000 6 0.018575000 -0.093300000 -1.371761000 1 0.037242000 -0.168626000 -2.440259000 1 -2.052351000 0.103426000 1.359332000 1 -2.689299000 0.137951000 1.763247000 1 -0.019937000 1.870983000 2.590139000 1 -0.016834000 1.420154000 1.983430000 1 2.650063000 0.118810000 1.803675000 1 2.017293000 0.087988000 1.392932000

1	2.250309000	-1.438552000	-0.500755000
1	2.911483000	-1.794479000	-0.442095000
1	-1.905365000	-1.043258000	2.241125000
1	-1.410018000	-0.823701000	1.713775000
1	-2.101826000	1.332619000	0.421175000
1	-2.717089000	1.671095000	0.695492000
1	0.335692000	3.456650000	-0.168039000
1	0.227290000	2.718202000	-0.267625000
1	2.810874000	1.354425000	0.847528000
1	2.191936000	1.050229000	0.543030000
1	-3.074432000	-1.414475000	-0.788143000
1	-2.398460000	-1.092055000	-0.701894000

1	1.394563000	2.207910000	-0.103613000
1	1.800479000	2.837943000	-0.025504000
1	-0.032320000	-1.483615000	2.829179000
1	-0.026567000	-1.126831000	2.162870000
1	-1.392305000	-2.204160000	0.170007000
1	-1.794798000	-2.824647000	0.314189000
1	-3.396359000	-0.099994000	-1.386965000
1	-2.664306000	-0.081371000	-1.211633000
1	-1.775342000	2.851000000	-0.067627000
1	-1.374090000	2.216905000	-0.137331000
1	2.692113000	-0.097258000	-1.164986000
1	3.426092000	-0.120880000	-1.331229000
1	1.758043000	-2.836185000	0.342574000
1	1.367338000	-2.210910000	0.186726000

$C_2H_{23}^-$

SCF Energy = -89.66010 a. u.

6	-0.000228000	-0.003693000	-0.010803000
6	0.003066000	0.026081000	-1.252457000
1	0.005171000	0.051635000	-2.323628000
1	1.713964000	1.328012000	1.289734000
1	2.240978000	1.736008000	1.643627000
1	-0.002628000	-0.046900000	3.322784000
1	-0.002486000	-0.037338000	2.567038000
1	-2.849991000	-0.133721000	1.616889000
1	-2.179900000	-0.104379000	1.271041000
1	-0.596689000	-2.117966000	1.248917000
1	-0.779212000	-2.767922000	1.586153000
1	-0.986598000	2.651122000	1.650572000
1	-0.754876000	2.026727000	1.295728000
1	0.729306000	2.588309000	-0.931135000
1	0.932672000	3.299254000	-1.074055000
1	3.408625000	0.133419000	-1.116962000
1	2.671042000	0.106850000	-0.966872000
1	2.367155000	-1.609934000	1.602998000
1	1.810433000	-1.233176000	1.260072000
1	1.172006000	-3.181375000	-1.162221000
1	0.917419000	-2.490319000	-1.004342000
1	-2.094731000	-1.637757000	-0.994306000
1	-2.675162000	-2.091037000	-1.152086000
1	-2.839615000	1.902057000	-1.098856000
1	-2.223912000	1.494103000	-0.951526000

$C_2H_{25}^-$

SCF Energy = --90.83568 a. u.

6	-0.109777000	0.057728000	-0.001293000
6	0.508922000	-0.063345000	-1.072251000
1	1.029520000	-0.167101000	-2.003260000
1	-0.519984000	2.161518000	1.415503000
1	-0.620846000	2.825276000	1.759340000
1	-1.524342000	-0.004749000	3.038259000
1	-1.192419000	0.036598000	2.361171000
1	-2.630439000	-1.956376000	0.729128000
1	-2.098543000	-1.446387000	0.570339000
1	0.078712000	-1.917212000	1.624467000
1	0.113737000	-2.462789000	2.142858000
1	-3.201598000	1.129273000	0.548537000
1	-2.471621000	0.972115000	0.442517000
1	-1.036279000	2.272557000	-1.350128000
1	-1.346485000	2.893665000	-1.640709000
1	1.855408000	3.028777000	-0.065930000
1	1.510919000	2.363843000	-0.136513000
1	2.061244000	0.330716000	2.423316000
1	1.531381000	0.300414000	1.886794000
1	2.627312000	-2.440357000	0.245732000
1	2.105850000	-1.922134000	0.088863000
1	3.097406000	0.398808000	-0.424551000
1	3.833578000	0.504208000	-0.526059000
1	-0.370578000	-2.611994000	-1.081772000
1	-0.486234000	-3.343754000	-1.213686000
1	-2.637550000	-0.533259000	-2.449500000
1	-2.103018000	-0.377954000	-1.943449000

$C_2H_{27}^-$

SCF Energy = -92.01063 a. u.

6	0.132153000	-0.182351000	0.042379000
6	-0.443481000	0.536095000	-0.792941000
1	-0.931294000	1.154839000	-1.519263000
1	0.009673000	-2.139488000	1.780932000
1	-0.019390000	-2.681631000	2.304104000
1	2.407927000	-0.667205000	2.448324000
1	1.876924000	-0.620667000	1.914273000

$C_2H_{29}^-$

SCF Energy = -93.18534 a. u.

6	-0.221708863	-0.045819870	0.121105918
6	0.598352887	0.239672843	-0.769039008
1	1.293195953	0.483626201	-1.547731268
1	-2.340372110	0.292314866	1.619706253
1	-2.886476152	0.468210738	2.109198912
1	-0.457024989	-0.917167362	3.401873096

1	3.386238000	0.163532000	-0.493029000
1	2.650601000	0.055036000	-0.371674000
1	1.581590000	1.697415000	1.176157000
1	1.920393000	2.293301000	1.486627000
1	2.256362000	-2.750071000	-0.033721000
1	1.735460000	-2.205947000	0.000883000
1	-0.668489000	-2.473812000	-0.826288000
1	-0.978498000	-3.145691000	-0.968407000
1	-2.734798000	-1.486406000	1.282528000
1	-2.113612000	-1.182663000	0.985199000
1	-0.830176000	0.852555000	2.994142000
1	-0.545349000	0.560980000	2.359301000
1	-0.707695000	3.628172000	0.607725000
1	-0.579766000	2.896929000	0.494199000
1	-2.677680000	1.271785000	0.498747000
1	-3.344405000	1.596825000	0.616034000
1	-3.307254000	-0.885461000	-1.872591000
1	-2.643263000	-0.771628000	-1.541146000
1	1.532335000	2.127481000	-1.513257000
1	1.862058000	2.729067000	-1.820434000
1	1.528151000	-1.213038000	-3.050459000
1	1.201924000	-0.926673000	-2.435535000
1	-0.391844111	-0.621066232	2.712578983
1	1.353891525	-2.760965892	1.228097097
1	1.027079064	-2.145400986	0.941338062
1	1.724103928	0.324348082	1.975544086
1	2.254702018	0.362087945	2.506774013
1	-1.936481809	-2.631881569	1.404531142
1	-1.597145839	-2.018330183	1.127245967
1	-2.638248101	-0.687148300	-0.600157910
1	-3.310910173	-0.812722061	-0.914408232
1	-2.650617619	2.223266773	-0.555312255
1	-2.130105118	1.711955077	-0.373200138
1	-0.315658462	2.560780256	2.120003124
1	-0.312006081	2.010939164	1.604286028
1	2.743443775	2.688801462	0.249216025
1	2.212364134	2.159361211	0.228148950
1	0.033484749	2.810277274	-1.210440039
1	-0.054148062	3.542277050	-1.353414207
1	-1.575649072	0.425003945	-3.323115117
1	-1.243618924	0.340890692	-2.653342352
1	3.092862158	-0.550314705	-0.009544241
1	3.828163471	-0.662579658	-0.105604199
1	-0.962234742	-2.911926403	-1.601606274
1	-0.825041836	-2.251109434	-1.268796119
1	2.119289264	-2.518829200	-2.123820080
1	1.685139020	-2.077817114	-1.700451293

$C_2H_{31}^-$

SCF Energy = -94.35982 a. u.

6	0.001446000	-0.003896000	0.290822000
6	-0.004693000	0.009998000	-0.953306000
1	-0.009915000	0.022312000	-2.025170000
1	1.140832000	-0.812115000	2.559451000
1	1.489650000	-1.058537000	3.179850000
1	-1.611307000	-0.792328000	3.195709000
1	-1.232186000	-0.606475000	2.571947000
1	-2.594308000	1.822620000	1.174981000
1	-1.997722000	1.404350000	0.981286000
1	-2.401307000	-1.115307000	0.534835000
1	-3.080541000	-1.429886000	0.607099000
1	0.174830000	1.763568000	3.206455000
1	0.131683000	1.347046000	2.580377000
1	2.234859000	1.015611000	0.952942000
1	2.900411000	1.319940000	1.133859000
1	2.774585000	-1.970699000	0.574648000
1	2.162895000	-1.537995000	0.510541000
1	-0.288569000	-3.182398000	1.108297000
1	-0.219309000	-2.452395000	0.933132000
1	-1.859937000	-2.663373000	-1.970085000
1	-1.500601000	-2.141409000	-1.567630000
1	1.064429000	-2.380623000	-1.578611000
1	1.314752000	-2.961919000	-1.982312000
1	3.244274000	-0.234678000	-1.963784000
1	2.610849000	-0.201997000	-1.562347000
1	-2.624267000	0.279071000	-1.532951000
1	-3.257578000	0.368842000	-1.925822000

$C_2H_{33}^-$

SCF Energy = -95.53349 a. u.

6	-0.428137000	-0.156095000	0.020369000
6	0.684069000	0.394607000	-0.068682000
1	1.637686000	0.877126000	-0.147718000
1	-2.554290000	-0.636915000	1.550926000
1	-3.137498000	-0.750278000	2.013680000
1	-2.712907000	-2.680217000	-0.398562000
1	-2.235375000	-2.108179000	-0.289232000
1	-1.296594000	-0.906431000	-3.075249000
1	-1.103899000	-0.734694000	-2.367067000
1	-0.005836000	-2.564017000	-0.974796000
1	0.145932000	-3.243357000	-1.259453000
1	-3.701061000	0.224987000	-0.892556000
1	-2.988162000	0.112931000	-0.677909000
1	-1.773614000	1.831693000	0.952423000
1	-2.171826000	2.409578000	1.226521000
1	-0.650177000	0.338426000	3.394704000
1	-0.594652000	0.228017000	2.652951000
1	-0.367465000	-2.707933000	2.070780000
1	-0.411652000	-2.127779000	1.590702000
1	2.520302000	-2.481284000	0.488531000
1	1.961315000	-1.991859000	0.376849000
1	1.840779000	-0.295985000	2.266092000
1	2.362596000	-0.346739000	2.803584000
1	1.055511000	2.740388000	2.379164000
1	0.793149000	2.191966000	1.939334000
1	1.739919000	-1.071219000	-2.043973000
1	2.230031000	-1.306962000	-2.562173000

1	0.318703000	3.377351000	0.634129000
1	0.247595000	2.633042000	0.553860000
1	1.914717000	2.655748000	-1.939582000
1	1.533881000	2.145312000	-1.542344000
1	-1.421999000	2.962495000	-1.910213000
1	-1.139916000	2.388216000	-1.517643000

1	-1.767030000	2.227042000	-2.086742000
1	-1.453555000	1.716589000	-1.632480000
1	0.491347000	3.772127000	-0.594044000
1	0.329500000	3.046110000	-0.497595000
1	4.511319000	0.065939000	-0.082233000
1	3.818074000	-0.205869000	-0.024169000
1	1.111609000	1.638081000	-3.213708000
1	0.840928000	1.307643000	-2.596701000

$C_2H_{35}^-$

SCF Energy = -96.70795 a. u.

6	-0.606487000	0.010053000	-0.082020000
6	0.587572000	-0.009998000	0.267663000
1	1.613326000	-0.019790000	0.578850000
1	-3.058547000	-0.710391000	0.730457000
1	-3.726573000	-0.855969000	1.045213000
1	-3.189500000	-0.933165000	-2.146831000
1	-2.665031000	-0.725500000	-1.648361000
1	-1.160170000	1.560660000	-2.919287000
1	-1.070136000	1.217061000	-2.253983000
1	-0.425878000	-1.197580000	-2.433613000
1	-0.349332000	-1.529642000	-3.103903000
1	-3.575680000	1.718595000	-0.586311000
1	-2.914596000	1.371030000	-0.494342000
1	-1.612491000	1.184959000	1.975599000
1	-1.913333000	1.499270000	2.590613000
1	-1.412338000	-1.909483000	2.698356000
1	-1.213857000	-1.415330000	2.168375000
1	-1.437808000	-3.158551000	-0.347771000
1	-1.305654000	-2.423190000	-0.246848000
1	1.651630000	-2.923352000	-1.231600000
1	1.166898000	-2.395822000	-1.007479000
1	1.043285000	-2.362210000	1.550534000
1	1.365200000	-2.964093000	1.861861000
1	0.992742000	0.146279000	3.651568000
1	0.667530000	0.073405000	2.979668000
1	1.848168000	-0.060051000	-2.092216000
1	2.385454000	-0.059587000	-2.617083000
1	-1.084015000	3.404735000	0.092180000
1	-0.965623000	2.669038000	-0.004995000
1	1.396159000	2.925324000	1.820550000
1	1.068817000	2.329669000	1.502395000
1	4.223633000	-1.463302000	-0.163421000
1	3.490364000	-1.568769000	-0.071656000
1	4.126362000	2.005809000	-0.119928000
1	3.586543000	1.491466000	-0.137902000
1	1.446006000	2.841960000	-1.517713000
1	1.121931000	2.236184000	-1.214834000

$C_2H_{37}^-$

SCF Energy = -97.88197 a. u.

6	-0.735153000	-0.000322000	-0.001063000
6	0.509287000	0.000062000	-0.000631000
1	1.581125000	0.000106000	-0.000558000
1	-3.052230000	-0.642472000	1.210437000
1	-3.682059000	-0.839219000	1.572601000
1	-3.678738000	-0.947692000	-1.517026000
1	-3.049718000	-0.730591000	-1.165218000
1	-1.748086000	1.465013000	-2.771139000
1	-1.534748000	1.129436000	-2.130732000
1	-1.019984000	-1.356386000	-2.271130000
1	-1.101923000	-1.741958000	-2.911367000
1	-3.679662000	1.783237000	-0.063849000
1	-3.049391000	1.371888000	-0.052578000
1	-1.541926000	1.278195000	2.040503000
1	-1.757885000	1.664661000	2.650614000
1	-1.106577000	-1.650743000	2.962751000
1	-1.024190000	-1.287570000	2.309624000
1	-1.750096000	-3.131532000	0.117253000
1	-1.537947000	-2.408788000	0.087557000
1	1.140484000	-3.098916000	-1.314060000
1	0.811238000	-2.474731000	-1.056683000
1	1.231601000	-2.101603000	1.477724000
1	1.690990000	-2.591285000	1.814089000
1	1.132329000	0.412592000	3.341238000
1	0.805681000	0.324372000	2.670581000
1	1.236355000	-0.227532000	-2.560019000
1	1.696619000	-0.272431000	-3.151695000
1	-1.106125000	3.391440000	-0.053190000
1	-1.022657000	2.644356000	-0.040618000
1	1.691550000	2.867543000	1.340193000
1	1.232335000	2.332211000	1.082348000
1	3.974395000	-1.654635000	-0.757494000
1	3.227709000	-1.663384000	-0.763442000
1	3.974095000	1.485855000	-1.045594000
1	3.227452000	1.497772000	-1.052196000
1	1.141370000	2.691948000	-2.019605000
1	0.812804000	2.154280000	-1.610721000
1	3.968818000	0.159883000	1.814889000
1	3.222192000	0.168242000	1.826674000

$C_2H_{39}^-$

SCF Energy = -99.05655 a. u.

6	-0.731808000	-0.000871000	0.022185000

$C_2H_{41}^-$

SCF Energy = -100.22856 a. u.

6	0.803276000	-0.010064000	-0.025685000

6	0.513002000	0.011742000	0.030998000
1	1.585019000	0.014240000	0.023727000
1	-3.133592000	1.335511000	-0.128448000
1	-3.798103000	1.680225000	-0.199843000
1	-3.746980000	-1.048259000	-1.561983000
1	-3.128448000	-0.772625000	-1.236544000
1	-0.961140000	-1.653316000	-2.898221000
1	-0.886351000	-1.309235000	-2.232753000
1	-1.793255000	-2.476299000	-0.196894000
1	-2.111440000	-3.152845000	-0.271456000
1	-2.140105000	1.315496000	-2.789036000
1	-1.844773000	1.012459000	-2.167486000
1	-0.971758000	2.551569000	-0.426301000
1	-1.076935000	3.287360000	-0.547160000
1	-2.144873000	1.913933000	2.400291000
1	-1.901193000	1.420219000	1.887488000
1	-3.526324000	-0.980663000	1.566963000
1	-2.907430000	-0.720035000	1.222883000
1	-0.833804000	-2.453861000	2.455955000
1	-0.817266000	-1.922984000	1.924158000
1	0.077433000	0.185251000	2.819588000
1	0.198818000	0.288203000	3.553739000
1	0.680805000	2.869392000	2.110159000
1	0.460485000	2.340892000	1.625268000
1	0.699041000	-2.663654000	-0.174115000
1	1.027082000	-3.335927000	-0.248597000
1	0.927231000	1.425208000	-3.068965000
1	0.623864000	1.130766000	-2.447964000
1	2.220700000	-1.869384000	2.381393000
1	1.619871000	-1.568983000	2.049240000
1	4.076519000	-1.674194000	-0.058614000
1	3.345966000	-1.779780000	0.052352000
1	2.164538000	-1.497303000	-2.669305000
1	1.649924000	-1.284231000	-2.168661000
1	2.142975000	3.040902000	-0.573275000
1	1.611668000	2.514235000	-0.538839000
1	4.185883000	0.895474000	-1.715609000
1	3.456634000	0.787705000	-1.599746000
1	2.774744000	0.991093000	1.712118000
1	3.507409000	1.098224000	1.815392000

6	-0.440171000	0.037562000	0.022653000
1	-1.511754000	0.066830000	0.070485000
1	3.301162000	0.889041000	0.924992000
1	3.924533000	1.182606000	1.224104000
1	3.960546000	-1.662536000	0.276892000
1	3.295201000	-1.323944000	0.192572000
1	1.276059000	-3.195022000	0.833437000
1	1.162752000	-2.462526000	0.699771000
1	1.912246000	-1.962823000	-1.605629000
1	2.310727000	-2.420176000	-2.048002000
1	2.440747000	-0.931408000	2.873975000
1	2.110530000	-0.786813000	2.214602000
1	1.121459000	1.486073000	2.140560000
1	1.289771000	1.989673000	2.673415000
1	2.389296000	3.074175000	-0.457702000
1	2.062188000	2.403595000	-0.372946000
1	3.390784000	0.553738000	-2.037120000
1	2.860798000	0.380566000	-1.528638000
1	0.654381000	-0.357421000	-3.516257000
1	0.749404000	-0.248202000	-2.779358000
1	0.204999000	1.961376000	-1.932801000
1	0.168375000	2.492594000	-2.463567000
1	-0.424836000	3.537256000	0.577027000
1	-0.117426000	2.860985000	0.472247000
1	-0.547422000	-2.143522000	-1.598092000
1	-0.830776000	-2.754894000	-1.931756000
1	-0.524961000	-1.168995000	3.240393000
1	-0.378677000	-0.851885000	2.574668000
1	-1.950427000	1.806306000	2.647550000
1	-1.597393000	1.513540000	2.055152000
1	-2.274311000	0.195981000	-2.913032000
1	-1.735329000	0.182195000	-2.392306000
1	-3.927577000	-1.921462000	-1.080236000
1	-3.195348000	-2.018789000	-0.972710000
1	-1.761952000	-3.031660000	1.020530000
1	-1.256690000	-2.514450000	0.822586000
1	-3.715384000	-0.898594000	2.176241000
1	-2.985338000	-1.003235000	2.061196000
1	-4.261613000	0.844820000	-0.217821000
1	-4.927670000	0.937042000	0.105301000
1	-2.750856000	2.731797000	-1.062908000
1	-2.088854000	2.403179000	-0.948621000

$C_2H_{43}^-$

SCF Energy = -101.40226 a. u.

6	-0.877746303	-0.010186133	-0.042369106
6	0.365233904	0.011136006	0.031706184
1	1.436014013	0.036675688	0.101342735
1	-3.239921045	-1.594566100	-0.006167032
1	-3.780903180	-2.115060080	-0.000902247
1	-4.288419088	0.733891055	0.821405860
1	-3.610441430	0.625137193	0.517380830
1	-1.900970311	2.156454970	2.222290970
1	-1.694900223	1.651385978	1.702313997
1	-2.409369944	2.275400257	-0.631235961

$C_2H_{45}^-$

SCF Energy = -102.57327 a. u.

6	-1.015554000	-0.025719000	-0.007014000
6	0.226672000	0.010122000	0.078649000
1	1.298539000	0.040601000	0.140401000
1	-3.622417000	0.843026000	0.780700000
1	-4.299459000	1.082243000	1.000428000
1	-4.166264000	0.093710000	-1.815129000
1	-3.525552000	0.068084000	-1.424747000
1	-1.320173000	0.654648000	-3.268584000
1	-1.255767000	0.501704000	-2.533982000
1	-2.202708000	-1.762573000	-1.923440000

1	-2.922956044	2.820335346	-0.677987183
1	-2.691381201	-0.996906436	2.707018388
1	-2.364229008	-0.723242951	2.087878361
1	-1.181843301	-2.510305213	0.909238170
1	-1.107227192	-3.246145228	1.043312106
1	-1.708209031	-2.704693184	-2.046962376
1	-1.521770890	-2.177868127	-1.545339387
1	-3.282201249	0.028214673	-2.337552125
1	-2.752324428	0.018436006	-1.800417108
1	-0.921311349	2.123556020	-2.834629482
1	-0.909270979	1.601394074	-2.295511109
1	-0.037854165	-0.615445312	-2.695688174
1	0.084294232	-0.731689149	-3.428251524
1	1.143654166	-3.200102045	-0.900534263
1	0.802840205	-2.543470339	-0.770086250
1	-0.031916267	2.734784319	-0.262224261
1	0.085246221	3.472687067	-0.176164165
1	0.186017974	-0.242030328	3.497953164
1	-0.113429143	-0.155404012	2.814720246
1	1.564358017	-2.508785416	2.146329163
1	1.127169237	-2.073613330	1.720584370
1	2.030893909	1.832137051	-2.398359353
1	1.572824324	1.418007169	-1.973307253
1	3.279977117	2.862200146	0.266417990
1	2.550088229	2.739837961	0.365987981
1	1.152859205	2.439364240	2.459933360
1	0.734311222	2.004421288	2.015373140
1	4.077697532	-2.276523171	0.283225189
1	3.347969514	-2.161886974	0.389578174
1	3.313218444	0.055034963	2.367013010
1	2.580543967	0.156389869	2.259991145
1	4.163035301	0.575896192	-0.695500304
1	4.893480354	0.473741170	-0.583887297
1	3.042679222	-1.183807078	-2.448562399
1	2.376750400	-1.079535876	-2.126043153

1	-2.464204000	-2.223788000	-2.454145000
1	-2.783111000	2.706188000	-1.158846000
1	-2.436027000	2.090843000	-0.902253000
1	-1.651222000	2.088000000	1.411256000
1	-1.820402000	2.680948000	1.842489000
1	-2.519827000	-0.140369000	3.089156000
1	-2.221816000	-0.119998000	2.399682000
1	-3.630698000	-1.994802000	0.660749000
1	-3.066377000	-1.521994000	0.495495000
1	-1.072057000	-3.577309000	-0.192647000
1	-1.055891000	-2.827853000	-0.156243000
1	-0.603990000	-1.878329000	2.028282000
1	-0.560229000	-2.392548000	2.575311000
1	0.358116000	0.925015000	3.366334000
1	0.127016000	0.727604000	2.678728000
1	0.275360000	-1.692818000	-2.010267000
1	0.516098000	-2.139479000	-2.565631000
1	0.104769000	3.043516000	-1.651068000
1	-0.061606000	2.403495000	-1.294020000
1	1.086960000	3.177526000	1.316710000
1	0.702754000	2.580773000	1.074300000
1	1.826469000	-3.026042000	0.342094000
1	1.287829000	-2.506362000	0.292450000
1	3.538438000	-1.903657000	-2.025739000
1	2.820079000	-1.742757000	-1.899758000
1	1.914867000	0.744621000	-2.834373000
1	1.362580000	0.609733000	-2.345004000
1	3.563017000	1.236607000	1.733166000
1	2.818423000	1.286953000	1.764920000
1	4.894595000	0.760311000	-1.190396000
1	4.159362000	0.682637000	-1.091370000
1	3.961728000	-1.524683000	0.864426000
1	4.699512000	-1.635616000	0.884337000
1	2.372135000	-1.357466000	2.902817000
1	1.751891000	-1.218157000	2.509024000
1	2.490910000	2.953429000	-0.860327000
1	3.141644000	3.297969000	-0.985096000

$C_4H_3^-$

SCF Energy = -154.088774 a. u.

6	-0.000025000	0.000006000	-0.931320000
6	0.000017000	-0.000677000	0.425319000
6	0.000010000	-0.001549000	1.680396000
6	0.000061000	0.000935000	-2.155997000
1	-0.000261000	0.000807000	-3.216162000
1	-0.000328000	0.002625000	4.172509000
1	0.000209000	0.004279000	4.933263000

$C_4H_5^-$

SCF Energy = -155.26408 a. u.

6	-1.189959000	-0.000862000	0.000026000
6	0.166623000	-0.008683000	-0.000442000
6	1.420769000	-0.016875000	-0.000896000
6	-2.413966000	0.006281000	0.000408000
1	-3.474137000	0.012059000	0.000990000
1	3.550121000	1.292905000	0.000823000
1	4.185950000	1.705971000	0.001313000
1	3.593018000	-1.250639000	0.000817000
1	4.244245000	-1.639460000	0.001478000

$C_4H_7^-$

SCF Energy = -156.439914 a. u.

6	-1.414836000	0.000343000	0.000263000
6	-0.057887000	-0.003429000	0.003673000

$C_4H_9^-$

SCF Energy = -157.615364 a. u.

6	1.562432341	-0.000156107	-0.000039159
6	0.205292726	-0.000278347	-0.000528119

6	1.195185000	-0.006080000	0.008728000
6	-2.638336000	0.001627000	-0.002795000
1	-3.698477000	0.003719000	-0.004365000
1	3.226575000	-0.989391000	-1.090686000
1	3.832444000	-1.289631000	-1.430664000
1	3.215711000	1.444377000	-0.321410000
1	3.817631000	1.892099000	-0.422771000
1	3.856560000	-0.575268000	1.818022000
1	3.244796000	-0.440665000	1.392655000

6	-1.047314273	-0.000292106	-0.001054121
6	2.785556230	-0.000091018	0.000332852
1	3.845695113	0.000052918	0.000923943
1	-2.456779992	2.084422305	0.000127003
1	-2.857007859	2.724867008	0.000628133
1	-2.459710576	-2.082960188	-0.000364074
1	-2.860510483	-2.722979962	0.002658057
1	-3.886695238	0.001337231	1.655836888
1	-3.234401197	0.000895897	1.273127964
1	-3.889729540	-0.000572041	-1.653298954
1	-3.236663430	-0.000157166	-1.271909269

$C_4H_{11}^-$

SCF Energy = -158.79066 a. u.

6	-1.659002426	-0.000133882	0.009986633
6	-0.303466219	-0.000329677	-0.057318892
6	0.947060056	-0.000264059	-0.124804867
6	-2.880205402	-0.000024871	0.070908693
1	-3.939094369	0.000274114	0.124476777
1	2.030860042	-2.089814091	-1.045947937
1	2.346528029	-2.722231176	-1.309489320
1	2.029053960	2.090277122	-1.045868032
1	2.344183245	2.723060397	-1.309196156
1	4.215491054	0.001727235	-0.719515426
1	3.470380383	0.000269880	-0.592721382
1	2.945053957	-1.682366131	1.858012231
1	2.494202878	-1.292740860	1.394782109
1	2.943802982	1.682974156	1.858051919
1	2.493221255	1.293085355	1.394785813

$C_4H_{13}^-$

SCF Energy = -159.966612 a. u.

6	-1.772599319	-0.017424748	-0.007205807
6	-0.415290897	-0.031377036	-0.013564930
6	0.836682148	-0.038801922	-0.015548815
6	-2.994994001	-0.004399580	-0.001570069
1	-4.055248246	0.008729308	0.004197963
1	1.939360533	2.209064185	0.411324184
1	2.259173566	2.876131266	0.556206035
1	2.164128040	-1.972901374	0.959969335
1	2.540370418	-2.554558189	1.258121026
1	4.155621528	0.138510028	0.043964046
1	3.401678359	0.093672840	0.032327967
1	2.447188126	1.406975940	-2.498273310
1	2.062737150	1.077268880	-1.940117256
1	2.576077182	-1.937698916	-2.062377309
1	2.183573187	-1.495963974	-1.593719946
1	2.026885391	0.303876860	2.196962959
1	2.375667175	0.398913919	2.858754144

$C_4H_{15}^-$

SCF Energy = -161.141927 a. u.

6	-1.763285270	-0.154303323	0.008412331
6	-0.406116021	-0.136694950	0.014429076
6	0.845542163	-0.109308969	0.016310301
6	-2.985279365	-0.165654175	0.003419014
1	-4.045356335	-0.175821258	-0.001927793
1	2.184319856	1.701396932	1.185681953
1	2.518294731	2.297392334	1.503843953
1	1.971453016	-2.373374250	0.164323294
1	2.302290399	-3.046527928	0.236018874
1	4.163744399	-0.371997847	-0.074629867
1	3.418336330	-0.271620861	-0.008021798
1	2.647691798	1.951966064	-1.827936971
1	2.227207027	1.498846932	-1.397037992
1	2.274956277	-1.303133901	-2.702487044
1	1.960683201	-1.015991213	-2.080742935
1	2.412207393	-0.764176928	2.831525328
1	2.074728306	-0.640292829	2.168789033
1	-0.068761292	2.586989876	-0.080101031
1	-0.186963085	3.322114972	-0.172718691

$C_4H_{17}^-$

SCF Energy = -162.317161 a. u.

6	-1.747888858	-0.284849234	-0.001161015
6	-0.390668808	-0.264075323	-0.001697071
6	0.860272341	-0.210175974	-0.001739935
6	-2.969319380	-0.289785399	-0.000532352
1	-4.029577328	-0.295358165	0.000100015
1	2.218063373	1.958719953	0.003177709
1	2.579809999	2.619723193	0.000784770
1	2.057920050	-2.030996040	1.310049719
1	2.392883427	-2.575165410	1.709365813
1	4.194119173	-0.313526936	0.008281624
1	3.440050589	-0.279198150	0.009209801
1	2.447253214	0.686790047	-2.747509444
1	2.099297477	0.469779749	-2.115209308
1	2.403069560	-2.560719400	-1.724903515
1	2.065727531	-2.019966399	-1.322960056
1	-0.311067850	2.686802230	1.791794165
1	-0.142944004	2.055705972	1.421735752
1	2.441303145	0.668914968	2.752360941
1	2.093887169	0.456400031	2.118239906
1	-0.146769956	2.066284225	-1.408912200

			1 -0.317395222 2.699122005 -1.774823451
$C_4H_{19}^-$			**$C_4H_{21}^-$**
SCF Energy = -163.492047 a. u.			SCF Energy = -164.668125 a. u.
6 1.739102000 0.106000000 0.000063000			6 1.730609000 -0.000026000 -0.182649000
6 0.381613000 0.105126000 0.000067000			6 0.373214000 -0.000076000 -0.182565000
6 -0.870545000 0.086937000 0.000141000			6 -0.878591000 -0.000033000 -0.148082000
6 2.960088000 0.100849000 -0.000104000			6 2.951179000 -0.000137000 -0.171478000
1 4.020364000 0.096614000 0.000209000			1 4.011530000 -0.000113000 -0.162101000
1 -2.222381000 -2.091065000 0.001398000			1 -2.241050000 -2.073673000 0.513908000
1 -2.574504000 -2.756926000 0.001653000			1 -2.590012000 -2.710083000 0.714239000
1 -2.110268000 1.879048000 1.322777000			1 -2.240324000 2.074118000 0.513887000
1 -2.441080000 2.429548000 1.716540000			1 -2.589709000 2.710318000 0.714241000
1 -4.212938000 0.148660000 0.001175000			1 -4.206777000 0.000010000 -0.451445000
1 -3.458546000 0.131764000 0.000846000			1 -3.456360000 0.000344000 -0.373987000
1 -2.462298000 -0.820312000 -2.746554000			1 -2.231133000 -1.779533000 -2.572749000
1 -2.115129000 -0.601109000 -2.114875000			1 -1.935891000 -1.357459000 -2.023330000
1 -2.440939000 2.427902000 -1.718308000			1 -2.230832000 1.779599000 -2.572813000
1 -2.110268000 1.877726000 -1.323970000			1 -1.935646000 1.357498000 -2.023379000
1 0.309253000 -2.829876000 1.804609000			1 0.183121000 -1.869195000 2.713501000
1 0.136876000 -2.198895000 1.436668000			1 0.038325000 -1.463799000 2.098480000
1 -2.459330000 -0.818283000 2.749226000			1 -2.707492000 0.000341000 2.628896000
1 -2.112888000 -0.599604000 2.116952000			1 -2.323567000 0.000209000 1.981093000
1 0.134572000 -2.196742000 -1.439381000			1 0.193676000 -2.685419000 -0.550711000
1 0.305700000 -2.827388000 -1.808413000			1 0.393466000 -3.401741000 -0.649612000
1 0.358619000 3.543705000 -0.001434000			1 0.394176000 3.401505000 -0.649985000
1 0.193628000 2.811769000 -0.000118000			1 0.194229000 2.685234000 -0.551006000
			1 0.183296000 1.869490000 2.713236000
			1 0.038500000 1.463978000 2.098288000
$C_4H_{23}^-$			**$C_4H_{25}^-$**
SCF Energy = -165.843649 a. u.			SCF Energy = -167.018216 a. u.
6 -1.711658000 -0.007684000 -0.006432000			6 -1.673016000 -0.196657000 -0.019785000
6 -0.354184000 -0.005031000 -0.004947000			6 -0.322396000 -0.058300000 -0.006727000
6 0.898250000 -0.000326000 -0.000387000			6 0.926262000 0.045494000 0.002902000
6 -2.932006000 -0.009191000 -0.007135000			6 -2.886677000 -0.320190000 -0.031749000
1 -3.992424000 -0.013177000 -0.000770000			1 -3.941722000 -0.427943000 -0.037440000
1 2.202247000 -2.135463000 -0.541148000			1 2.196300000 0.519286000 2.193906000
1 2.542825000 -2.786457000 -0.706206000			1 2.531713000 0.654421000 2.853863000
1 2.166463000 2.072442000 -0.804604000			1 2.223816000 0.950504000 -2.029199000
1 2.501229000 2.700298000 -1.051004000			1 2.562584000 1.217350000 -2.645940000
1 4.246398000 0.019756000 0.038613000			1 4.261327000 0.440048000 0.067198000
1 3.492292000 0.013614000 0.026321000			1 3.513063000 0.348213000 0.054623000
1 2.487239000 -1.539862000 2.458908000			1 -0.524443000 1.706171000 2.958612000
1 2.163039000 -1.178449000 1.883330000			1 -0.290950000 1.357915000 2.336675000
1 2.469206000 1.847671000 2.249136000			1 1.979226000 3.130202000 0.303302000
1 2.145665000 1.417665000 1.722465000			1 1.765164000 2.411353000 0.229351000
1 -0.268990000 -2.192275000 -2.636391000			1 2.835671000 -2.304330000 1.429906000
1 -0.116206000 -1.720157000 -2.073111000			1 2.435095000 -1.758154000 1.101964000
1 2.524081000 -0.142735000 -2.882572000			1 2.863171000 -1.981085000 -1.823009000
1 2.186895000 -0.115539000 -2.209876000			1 2.467796000 -1.503272000 -1.397096000
1 -0.147273000 -2.505181000 0.979189000			1 0.014310000 -1.416167000 2.334612000
1 -0.335275000 -3.185809000 1.233754000			1 -0.128286000 -1.788737000 2.969672000
1 -0.374713000 1.837285000 -2.875132000			1 -0.064644000 -1.207570000 -3.256895000

1	-0.165897000	1.446610000	-2.269266000
1	-0.187499000	0.168808000	2.672991000
1	-0.396735000	0.225346000	3.391597000
1	-0.374180000	3.299093000	0.844601000
1	-0.170801000	2.599904000	0.662581000
1	0.070932000	-0.956105000	-2.563217000
1	-1.040016000	2.685794000	0.229021000
1	-1.399063000	3.338902000	0.294490000
1	-0.540115000	2.197532000	-2.622492000
1	-0.299289000	1.748350000	-2.072525000
1	0.064663000	-3.461500000	-0.323494000
1	0.178659000	-2.723263000	-0.253738000

$C_4H_{27}^-$

SCF Energy = -168.191962 a. u.

6	-1.531408000	-0.298229000	-0.129199000
6	-0.187804000	-0.128209000	-0.041133000
6	1.050526000	0.048851000	0.029100000
6	-2.739879000	-0.448547000	-0.206260000
1	-3.789903000	-0.579522000	-0.274794000
1	2.699615000	-1.231905000	-1.476088000
1	3.145971000	-1.618341000	-1.942947000
1	2.161235000	0.728094000	2.250234000
1	2.443759000	0.927764000	2.918647000
1	4.374039000	0.478312000	0.281691000
1	3.628596000	0.379743000	0.227517000
1	0.348724000	-3.205215000	-1.544857000
1	0.425739000	-2.540110000	-1.207149000
1	2.633515000	-2.389393000	1.534103000
1	2.306128000	-1.808178000	1.183670000
1	2.702146000	1.606607000	-2.428504000
1	2.375572000	1.257943000	-1.847314000
1	2.283339000	3.127484000	0.446336000
1	2.043580000	2.420623000	0.351991000
1	0.259006000	-0.230225000	-2.736305000
1	0.134401000	-0.307265000	-3.472050000
1	-0.652100000	2.582493000	2.014100000
1	-0.371614000	2.039485000	1.579066000
1	-0.391687000	-2.662843000	1.256012000
1	-0.610450000	-3.309206000	1.562886000
1	-0.356752000	-0.634170000	3.376556000
1	-0.124417000	-0.502926000	2.675761000
1	-0.437479000	2.874630000	-1.692241000
1	-0.190326000	2.268203000	-1.325920000
1	-3.482485000	2.965081000	0.213389000
1	-3.106757000	2.319640000	0.161156000

$C_4H_{29}^-$

SCF Energy = -169.366341 a. u.

6	-1.392394000	-0.485797000	-0.002197000
6	-0.067402000	-0.193446000	-0.001451000
6	1.151995000	0.095066000	-0.000082000
6	-2.584333000	-0.748106000	-0.003063000
1	-3.621764000	-0.968156000	-0.003525000
1	2.584830000	-0.168771000	-2.124141000
1	2.967938000	-0.253308000	-2.766384000
1	2.576006000	-0.184542000	2.130386000
1	2.956423000	-0.272843000	2.773692000
1	4.455364000	0.715755000	0.008967000
1	3.713212000	0.583639000	0.008084000
1	0.357435000	-2.184548000	-2.798669000
1	0.463349000	-1.721261000	-2.218663000
1	3.069388000	-2.559147000	-0.004739000
1	2.659730000	-1.926847000	-0.004965000
1	2.326227000	2.775920000	-1.621992000
1	2.097048000	2.164046000	-1.249054000
1	2.318967000	2.761146000	1.650115000
1	2.088329000	2.154431000	1.269696000
1	-0.100766000	0.995151000	-2.448233000
1	-0.328542000	1.241887000	-3.119042000
1	-0.349506000	1.213494000	3.123063000
1	-0.109598000	0.980147000	2.451718000
1	0.066321000	-3.063399000	-0.014553000
1	-0.062968000	-3.800202000	-0.009918000
1	0.345700000	-2.202594000	2.786400000
1	0.454045000	-1.737145000	2.208647000
1	-0.686606000	3.196771000	0.006549000
1	-0.381379000	2.511355000	0.005900000
1	-3.330355000	2.197887000	1.797280000
1	-2.932222000	1.668485000	1.448659000
1	-2.923181000	1.672469000	-1.449073000
1	-3.320623000	2.203878000	-1.795451000

$C_4H_{31}^-$

SCF Energy = -170.540116 a. u.

6	1.318473000	0.074681000	-0.243361000
6	-0.030061000	0.057834000	-0.097328000
6	-1.274874000	0.022907000	0.043023000
6	2.531893000	0.090020000	-0.375190000
1	3.586484000	0.095422000	-0.487905000
1	-2.848386000	-0.113440000	-1.990991000
1	-3.270356000	-0.157596000	-2.612469000
1	-2.422650000	1.188108000	2.037964000

$C_4H_{33}^-$

SCF Energy = -171.7157594 a. u.

6	-1.399773000	-0.117070000	-0.300301000
6	-0.059652000	-0.030855000	-0.099878000
6	1.178553000	0.047155000	0.082781000
6	-2.603799000	-0.197010000	-0.480757000
1	-3.649741000	-0.264264000	-0.641998000
1	3.401033000	1.028251000	1.252241000
1	4.015213000	1.322689000	1.570981000
1	2.217851000	-0.661285000	-2.320959000

1	-2.717354000	1.537734000	2.635477000
1	-4.617791000	0.031800000	0.395154000
1	-3.867982000	0.027997000	0.319322000
1	-0.396819000	1.150206000	-3.365301000
1	-0.523091000	0.916380000	-2.664205000
1	-2.729123000	2.859789000	-0.721481000
1	-2.425172000	2.195419000	-0.537794000
1	-2.996289000	-2.769465000	-0.610024000
1	-2.645293000	-2.123809000	-0.450119000
1	-2.670182000	-1.769836000	2.497422000
1	-2.390164000	-1.358146000	1.933608000
1	-0.464216000	-1.800561000	-2.049450000
1	-0.327338000	-2.276859000	-2.612609000
1	0.307192000	-0.362107000	3.302310000
1	0.051996000	-0.291445000	2.600468000
1	0.322088000	2.728387000	-0.999845000
1	0.606308000	3.380498000	-1.232103000
1	0.159730000	2.849423000	1.927692000
1	-0.083685000	2.262630000	1.529118000
1	0.096310000	-3.214111000	0.947983000
1	-0.106914000	-2.522643000	0.739878000
1	2.984657000	-2.176734000	2.291568000
1	2.648864000	-1.720316000	1.802367000
1	2.476175000	-2.677838000	-0.916994000
1	2.747001000	-3.351971000	-1.097435000
1	3.318201000	3.295657000	0.818651000
1	2.925216000	2.694784000	0.606883000

1	2.359345000	-0.789100000	-3.046777000
1	4.482867000	-0.756419000	-0.565538000
1	3.754163000	-0.621705000	-0.438181000
1	1.627637000	3.257127000	1.211402000
1	1.539237000	2.581273000	0.896872000
1	2.725527000	2.225305000	-1.832946000
1	2.473147000	1.714453000	-1.340703000
1	2.457464000	-1.994291000	2.329079000
1	2.233854000	-1.490998000	1.815654000
1	2.377489000	-3.044060000	-0.820262000
1	2.076930000	-2.414495000	-0.543193000
1	1.392025000	0.818425000	2.660173000
1	1.489217000	0.945279000	3.393526000
1	-0.282823000	-2.507203000	-2.559308000
1	-0.083307000	-1.996834000	-2.049370000
1	-0.321994000	2.589311000	-0.915308000
1	-0.647052000	3.251509000	-1.044845000
1	-0.081036000	1.075815000	-3.420483000
1	0.040955000	0.759971000	-2.752547000
1	-0.374114000	-3.401616000	0.757346000
1	-0.239478000	-2.674478000	0.638323000
1	-0.593403000	-0.846566000	2.468669000
1	-0.912712000	-1.130535000	3.083812000
1	-1.310105000	2.276949000	2.190792000
1	-0.883182000	1.841384000	1.756757000
1	-3.176577000	-2.157808000	1.386018000
1	-3.611445000	-2.598346000	1.806519000
1	-3.855384000	2.992566000	-0.061638000
1	-3.333580000	2.456372000	-0.075177000

$C_4H_{35}^-$

SCF Energy = -172.8904684 a. u.

6	-1.287536931	0.172632436	-0.214696206
6	0.055607004	0.039222089	-0.071698755
6	1.296465210	-0.084384192	0.059997058
6	-2.495018870	0.291982543	-0.345136810
1	-3.544511236	0.396930563	-0.457295928
1	3.743920570	0.690555672	0.935213894
1	4.370963330	0.983340977	1.228899859
1	2.041984406	-1.443851128	-2.142603226
1	2.167553404	-1.782920392	-2.800336150
1	4.328277247	-1.640581237	-0.436545830
1	3.663926433	-1.304667457	-0.329521848
1	2.280237466	3.194148271	0.408150179
1	2.150458333	2.462327887	0.304330894
1	3.107708755	1.299376743	-2.308923107
1	2.771603413	0.988867175	-1.710958107
1	2.489893259	-1.681473409	2.691481215
1	2.218958212	-1.344873286	2.074803979
1	1.770503248	-3.469824218	-0.129419821
1	1.665056214	-2.733047030	-0.031186003
1	1.810808562	1.150797001	2.398712315
1	1.901292580	1.483697116	3.065283028
1	-0.833207041	-2.686564100	-1.992340171
1	-0.409701197	-2.239366991	-1.566973211

$C_4H_{37}^-$

SCF Energy = -174.063552 a. u.

6	-1.211752000	0.001587000	-0.000813000
6	0.145617000	-0.003051000	0.004253000
6	1.399742000	-0.006216000	0.008011000
6	-2.432096000	0.006290000	-0.006558000
1	-3.492841000	0.012503000	-0.013403000
1	3.831056000	-0.789967000	-0.879684000
1	4.490033000	-1.017910000	-1.160971000
1	2.052115000	0.529340000	2.548075000
1	2.188460000	0.681060000	3.270582000
1	4.499784000	1.005972000	1.147192000
1	3.837004000	0.777793000	0.875168000
1	2.133775000	-3.137093000	-1.169291000
1	1.995934000	-2.447301000	-0.906912000
1	2.958370000	-2.228854000	1.898700000
1	2.643176000	-1.707010000	1.456959000
1	2.944921000	2.213330000	-1.898117000
1	2.630945000	1.692835000	-1.453944000
1	2.139207000	3.129565000	1.168571000
1	2.001881000	2.438436000	0.909481000
1	2.032026000	-0.533571000	-2.543740000
1	2.166250000	-0.682849000	-3.267128000
1	-0.620853000	2.151379000	2.605570000
1	-0.277505000	1.728125000	2.091987000

1	0.207590414	2.428731482	-1.453671070
1	0.093406664	3.088506501	-1.788814368
1	0.037977464	0.325215404	-3.562398486
1	0.164359278	0.217202919	-2.832238130
1	-0.975050886	-2.914917842	1.458034137
1	-0.659418883	-2.305570239	1.157772086
1	-3.796178411	-2.923778915	-0.520248970
1	-3.270667302	-2.391602818	-0.498631021
1	-0.404505735	-0.143770050	2.638060243
1	-0.737386800	-0.217700874	3.304923062
1	-0.613097881	2.991645368	1.660858251
1	-0.314607516	2.379428566	1.349965030
1	-3.315310282	-0.954649516	1.993408051
1	-3.822190118	-1.163495667	2.502825292
1	-3.020109812	3.705244592	-0.632828255
1	-2.687633567	3.039922737	-0.548577945

1	-0.153871000	-2.667070000	0.536543000
1	-0.454527000	-3.335736000	0.691280000
1	-0.317712000	-1.252068000	3.192561000
1	-0.018024000	-0.998634000	2.554397000
1	-0.452791000	3.320409000	-0.696405000
1	-0.145185000	2.656264000	-0.535984000
1	-3.348555000	3.184765000	1.131782000
1	-2.901754000	2.617561000	0.934877000
1	-0.045374000	0.991006000	-2.532885000
1	-0.349905000	1.237698000	-3.171340000
1	-0.627198000	-2.158776000	-2.602771000
1	-0.285658000	-1.735395000	-2.088090000
1	-3.356950000	-2.485188000	2.285899000
1	-2.920634000	-2.029992000	1.882883000
1	-2.753633000	2.085707000	-1.905373000
1	-3.175556000	2.551835000	-2.311398000
1	-3.351878000	-3.177969000	-1.135542000
1	-2.903599000	-2.611860000	-0.938889000

$C_4H_{39}^-$

SCF Energy = -175.238577 a. u.

6	1.102135000	0.070847000	-0.206457000
6	-0.245721000	0.016418000	-0.057644000
6	-1.491291000	-0.033215000	0.080284000
6	2.314258000	0.121034000	-0.341352000
1	3.367884000	0.163875000	-0.458576000
1	-4.038206000	0.768438000	-0.361650000
1	-4.730375000	1.018933000	-0.514705000
1	-1.763108000	-0.948200000	2.581116000
1	-1.814085000	-1.211447000	3.282279000
1	-4.391725000	-1.310867000	1.466909000
1	-3.778585000	-1.016058000	1.147001000
1	-2.455427000	3.204878000	-0.493121000
1	-2.266536000	2.489459000	-0.366521000
1	-2.779513000	1.838290000	2.483118000
1	-2.528439000	1.397526000	1.926938000
1	-3.232856000	-2.002226000	-1.929503000
1	-2.877350000	-1.543454000	-1.450035000
1	-2.030264000	-3.327457000	0.845302000
1	-1.940224000	-2.600790000	0.679642000
1	-2.459800000	0.844488000	-2.255223000
1	-2.689661000	1.091309000	-2.925923000
1	0.864770000	-2.509206000	2.020983000
1	0.464220000	-2.011964000	1.629398000
1	0.028204000	2.574493000	0.829833000
1	0.345328000	3.222875000	1.031090000
1	0.666512000	0.783585000	3.172016000
1	0.299320000	0.616516000	2.540607000
1	0.295028000	-3.128348000	-1.356357000
1	-0.009964000	-2.511440000	-1.059924000
1	3.381566000	-3.187573000	0.082105000
1	2.914970000	-2.603640000	0.043027000
1	-0.343542000	-0.561319000	-2.728669000
1	-0.119540000	-0.691500000	-3.431563000
1	0.122696000	2.573902000	-2.378212000

$C_4H_{41}^-$

SCF Energy = -176.413576 a. u.

6	-1.035700949	-0.001787032	0.000948815
6	0.320981986	-0.001212874	0.000239188
6	1.575036285	-0.000083081	-0.000060855
6	-2.256851007	-0.002739551	-0.000079906
1	-3.318100104	-0.003404726	-0.001291722
1	4.022485295	1.176888614	-0.002556984
1	4.682996399	1.535665497	-0.003144900
1	2.207113108	-2.281632377	-1.247613154
1	2.354055047	-2.929871332	-1.596435154
1	4.683083184	-1.533953609	0.011463038
1	4.022386339	-1.175474653	0.008666865
1	2.350976293	2.914087033	-1.625721940
1	2.205864250	2.270146056	-1.268282817
1	3.094800535	-0.013135238	-2.938956247
1	2.793364240	-0.009657485	-2.249241967
1	3.092019179	0.016288605	2.941359241
1	2.791559216	0.011105843	2.251241199
1	2.348759041	-2.912181466	1.629997163
1	2.205030796	-2.269296197	1.270105303
1	2.204138603	2.280996836	1.248066129
1	2.349799403	2.929152181	1.597595111
1	-0.409950440	-3.368604252	0.015087902
1	-0.068557029	-2.701910240	0.015101131
1	0.087775159	1.287715264	-2.386852923
1	-0.218928566	1.606595887	-2.991541120
1	-0.216855249	-1.638095162	-2.976985041
1	0.089427780	-1.312242100	-2.375812169
1	-0.221817873	-1.593438953	2.995072320
1	0.090696747	-1.282930972	2.389027313
1	-3.099133438	-2.932779161	1.754058006
1	-2.673472255	-2.407210901	1.433633244
1	0.077305917	1.319512996	2.370343122
1	-0.226686833	1.644247377	2.973236350
1	-0.411662857	3.367540076	-0.017427924

1	-0.128708000	2.053462000	-1.902120000
1	3.281215000	2.430223000	2.134930000
1	2.811770000	2.007712000	1.733445000
1	2.432637000	-1.617368000	-2.601109000
1	2.820223000	-1.985363000	-3.124866000
1	2.969322000	3.480283000	-1.142855000
1	2.579234000	2.861395000	-0.985461000
1	3.077864000	-0.766845000	2.229155000
1	3.578858000	-0.937081000	2.758513000

1	-0.070783807	2.700591001	-0.016213991
1	-2.973323135	-0.020514614	-3.456202137
1	-2.574134043	-0.013491903	-2.823223066
1	-2.582655914	0.014633338	2.826525132
1	-2.983484925	0.024922132	3.458440557
1	-3.098044920	2.933650716	-1.758538021
1	-2.673619895	2.407241593	-1.437923284
1	-2.673540519	-2.425314055	-1.411278151
1	-3.097217287	-2.956434972	-1.725023109
1	-2.677742715	2.422904182	1.401633367
1	-3.104722079	2.952625425	1.713331996

$C_4H_{43}^-$

SCF Energy = -177.586407 a. u.

6	0.952316000	0.114861000	0.117102000
6	-0.396969000	0.022723000	0.008499000
6	-1.644308000	-0.068418000	-0.085233000
6	2.167174000	0.192686000	0.215185000
1	3.220538000	0.276847000	0.312319000
1	-4.104549000	0.885782000	-0.705895000
1	-4.771156000	1.180642000	-0.889359000
1	-1.704743000	-0.724403000	2.542795000
1	-1.756994000	-0.921220000	3.265346000
1	-4.545604000	-0.588022000	1.676957000
1	-3.929996000	-0.478367000	1.259544000
1	-2.371732000	3.012522000	-1.431822000
1	-2.232711000	2.334352000	-1.142070000
1	-3.017870000	2.326568000	1.763633000
1	-2.730569000	1.771751000	1.344784000
1	-4.280403000	-1.878037000	-1.345702000
1	-3.728906000	-1.460011000	-1.051864000
1	-2.727677000	-3.103772000	1.117653000
1	-2.534730000	-2.430284000	0.848050000
1	-2.381911000	0.131986000	-2.531306000
1	-2.562247000	0.202728000	-3.258269000
1	0.416802000	-3.005147000	1.407925000
1	0.059197000	-2.416822000	1.112701000
1	-0.123036000	2.783632000	0.288498000
1	0.169265000	3.459520000	0.424389000
1	-0.095594000	1.762713000	3.059302000
1	-0.313986000	1.416213000	2.432999000
1	-1.304532000	-3.065515000	-1.759817000
1	-1.361848000	-2.408151000	-1.401813000
1	3.613486000	-2.710600000	1.569243000
1	3.060492000	-2.257925000	1.348160000
1	0.125962000	-0.748999000	-2.618551000
1	0.482985000	-0.921298000	-3.253405000
1	0.444163000	2.177838000	-2.611859000
1	0.100634000	1.745862000	-2.105709000
1	2.868161000	2.745771000	2.444107000
1	2.462286000	2.266558000	2.036686000
1	1.884271000	-2.335149000	-1.177682000
1	2.123990000	-2.976442000	-1.480467000
1	3.063691000	3.309677000	-1.043924000
1	2.614110000	2.747052000	-0.840118000

$C_4H_{45}^-$

SCF Energy = -178.75989 a. u.

6	0.790381000	0.019266000	0.145284000
6	-0.558961000	-0.013136000	0.007772000
6	-1.808076000	-0.027818000	-0.105782000
6	2.005513000	0.053644000	0.268766000
1	3.055839000	0.093650000	0.414694000
1	-4.198441000	-1.204658000	-0.568114000
1	-4.846637000	-1.561142000	-0.702467000
1	-1.670535000	2.139805000	-1.708257000
1	-1.638709000	2.744964000	-2.151431000
1	-4.555614000	1.428071000	-1.547132000
1	-3.969251000	1.090488000	-1.218846000
1	-2.329896000	-3.293841000	-1.007186000
1	-2.240220000	-2.574294000	-0.813249000
1	-2.687561000	-0.769567000	-3.206799000
1	-2.524526000	-0.583836000	-2.496052000
1	-4.721216000	0.534373000	1.613358000
1	-4.100267000	0.410142000	1.207894000
1	-3.079021000	3.061045000	0.712903000
1	-2.843686000	2.372298000	0.529061000
1	-2.739441000	-1.711096000	1.607513000
1	-2.972641000	-2.219233000	2.110606000
1	0.072928000	3.228784000	1.011373000
1	-0.257836000	2.592467000	0.795092000
1	0.028191000	-1.966106000	-1.862810000
1	0.399293000	-2.432332000	-2.316684000
1	0.322848000	0.547071000	-3.341220000
1	-0.044493000	0.427297000	-2.700051000
1	-1.918593000	1.256758000	3.116935000
1	-1.873918000	0.971262000	2.424095000
1	3.294548000	3.208476000	1.152385000
1	2.758853000	2.708999000	1.000898000
1	-0.300015000	-1.059527000	2.621683000
1	-0.052917000	-1.286896000	3.290384000
1	0.207275000	-3.303984000	0.911050000
1	-0.129795000	-2.674936000	0.683798000
1	3.220787000	-0.660321000	-2.868225000
1	2.726826000	-0.515518000	-2.323793000
1	1.390594000	1.116814000	2.853236000
1	1.564608000	1.436183000	3.507495000
1	2.973532000	-3.209530000	-0.625399000
1	2.535023000	-2.617204000	-0.492949000

1	1.542942000	-0.571551000	2.950774000
1	1.723790000	-0.791352000	3.642788000
1	2.814988000	0.359191000	-2.493909000
1	3.306317000	0.414541000	-3.056104000
1	4.634070000	-1.539575000	-1.075165000
1	5.379381000	-1.550213000	-1.107163000

1	1.574549000	2.306273000	-1.506887000
1	1.781090000	2.929560000	-1.866515000
1	2.516363000	-1.790165000	2.244240000
1	2.999830000	-2.173877000	2.668336000
1	4.859187000	-1.377766000	-0.328316000
1	5.525557000	-1.149823000	-0.081733000
1	4.289747000	1.605020000	-1.314050000
1	5.024617000	1.734115000	-1.325103000

$C_4H_{47}^-$

SCF Energy = -179.934358 a. u.

6	-0.651275000	0.023533000	0.010878000
6	0.705075000	0.023760000	-0.000667000
6	1.959554000	0.008554000	-0.009276000
6	-1.872797000	0.017986000	0.020978000
1	-2.933450000	0.012467000	0.036848000
1	4.391720000	1.182758000	-0.011336000
1	5.054127000	1.538908000	-0.011501000
1	1.827649000	-1.647897000	-2.140584000
1	1.815539000	-2.124689000	-2.720725000
1	4.741308000	-1.114073000	-1.656819000
1	4.150445000	-0.854684000	-1.270108000
1	2.586090000	3.382070000	-0.006232000
1	2.467508000	2.640797000	-0.007657000
1	3.022873000	1.487668000	-2.782097000
1	2.807291000	1.144880000	-2.147773000
1	4.736491000	-1.100595000	1.657039000
1	4.147674000	-0.844929000	1.264906000
1	3.118617000	-3.230958000	0.010862000
1	2.893396000	-2.514653000	0.003690000
1	2.799957000	1.152576000	2.134912000
1	3.016316000	1.497042000	2.767919000
1	-0.043376000	-3.311657000	0.017501000
1	0.325222000	-2.659358000	0.014664000
1	0.266451000	2.406387000	-1.351389000
1	-0.051392000	2.981542000	-1.710702000
1	-0.026506000	0.378357000	-3.433340000
1	0.313062000	0.314433000	-2.769414000
1	1.805479000	-2.109062000	2.722899000
1	1.817023000	-1.634397000	2.141055000
1	-3.124184000	-3.293254000	-0.011948000
1	-2.622380000	-2.738599000	-0.000051000
1	0.297929000	0.331101000	2.769841000
1	-0.016863000	0.383715000	3.446755000
1	-0.053415000	2.982668000	1.712717000
1	0.264408000	2.415888000	1.340322000
1	-2.999228000	1.472687000	-2.823193000
1	-2.499189000	1.233754000	-2.319112000
1	-1.473680000	-1.720876000	2.256975000
1	-1.710367000	-2.186285000	2.793692000
1	-2.650517000	3.442397000	-0.011592000
1	-2.261313000	2.802760000	-0.009279000
1	-1.455115000	-1.725416000	-2.234321000
1	-1.686547000	-2.195287000	-2.769285000
1	-2.495829000	1.241346000	2.377009000

$C_4H_{49}^-$

SCF Energy = -181.108839 a. u.

6	-0.626149000	-0.000381000	0.000837000
6	0.730641000	0.006471000	0.001742000
6	1.985248000	0.010445000	0.002248000
6	-1.847849000	-0.007257000	-0.000075000
1	-2.909021000	-0.024017000	-0.000462000
1	4.361405000	-0.569550000	1.252776000
1	4.992632000	-0.740320000	1.622193000
1	2.379129000	2.676453000	-0.269928000
1	2.468835000	3.417051000	-0.348350000
1	5.004957000	1.764798000	-0.188545000
1	4.371929000	1.363524000	-0.139959000
1	2.436836000	-1.408593000	3.125067000
1	2.371434000	-1.102398000	2.443477000
1	3.058809000	1.843025000	2.556818000
1	2.847850000	1.414245000	1.976011000
1	4.986498000	-1.056152000	-1.450797000
1	4.361402000	-0.810194000	-1.114918000
1	3.045031000	1.287138000	-2.881312000
1	2.845588000	0.993605000	-2.218211000
1	2.816954000	-2.414507000	0.244362000
1	3.012289000	-3.136934000	0.319222000
1	-0.029282000	2.670032000	-2.111315000
1	0.298675000	2.167623000	-1.663316000
1	0.278769000	0.334520000	2.716296000
1	-0.059561000	0.457384000	3.372837000
1	-0.017108000	3.039033000	1.545390000
1	0.291905000	2.448064000	1.204899000
1	2.441751000	-2.008864000	-2.777614000
1	2.363250000	-1.570341000	-2.174163000
1	-3.096229000	1.318157000	-2.903372000
1	-2.579952000	1.096578000	-2.408091000
1	0.272827000	-2.504255000	-1.048100000
1	-0.064251000	-3.135774000	-1.267773000
1	-0.062600000	-2.826946000	1.873296000
1	0.265447000	-2.242121000	1.540156000
1	-3.103727000	1.872935000	2.582234000
1	-2.589508000	1.550407000	2.143528000
1	0.280300000	-0.211246000	-2.717898000
1	-0.054504000	-0.224305000	-3.387541000
1	-2.531423000	-1.426084000	3.161524000
1	-2.154626000	-1.162494000	2.570552000
1	-2.086722000	2.811623000	-0.278768000
1	-2.457745000	3.458637000	-0.344844000
1	-2.434036000	-2.697884000	0.273138000

1	-3.022752000	1.498186000	2.843350000
1	-4.621356000	1.762622000	-0.092720000
1	-5.314892000	1.495304000	-0.027499000
1	-4.229372000	-1.185670000	-1.739446000
1	-4.972601000	-1.118861000	-1.738129000
1	-4.266667000	-1.146432000	1.786436000
1	-4.978934000	-1.167672000	1.565392000

1	-2.950303000	-3.238851000	0.317140000
1	-4.584495000	-0.747228000	1.793776000
1	-5.288315000	-0.755136000	1.545683000
1	-4.513137000	1.960915000	-0.196866000
1	-5.247897000	1.830456000	-0.183147000
1	-2.128385000	-1.652256000	-2.304522000
1	-2.517068000	-2.026752000	-2.823513000
1	-5.276205000	-1.052525000	-1.383678000
1	-4.569742000	-1.086138000	-1.621882000

$C_4H_{51}^-$

SCF Energy = -182.281408 a. u.

6	-0.476227000	0.144987000	-0.031801000
6	0.872945000	0.004207000	0.001845000
6	2.120442000	-0.126701000	0.032952000
6	-1.691068000	0.271872000	-0.060217000
1	-2.746921000	0.378650000	-0.084279000
1	4.352297000	-1.387735000	1.034062000
1	4.937468000	-1.757756000	1.325073000
1	2.741807000	2.371584000	0.869060000
1	2.887972000	3.068514000	1.104879000
1	5.270895000	1.250824000	0.691327000
1	4.611490000	0.925638000	0.538056000
1	2.244068000	-2.698420000	2.349954000
1	2.237685000	-2.141052000	1.848045000
1	3.130159000	0.414118000	3.158492000
1	2.934757000	0.293915000	2.442297000
1	5.135951000	-0.807335000	-1.613343000
1	4.503708000	-0.661657000	-1.235058000
1	3.471321000	2.097309000	-2.034103000
1	3.209203000	1.573404000	-1.562415000
1	2.746096000	-2.515691000	-0.693287000
1	2.877473000	-3.222121000	-0.915441000
1	0.494249000	3.347203000	-0.904562000
1	0.732329000	2.671370000	-0.687265000
1	0.216461000	-0.737514000	2.587646000
1	-0.163016000	-0.868219000	3.219732000
1	0.270464000	2.231567000	2.596600000
1	0.569631000	1.800809000	2.062155000
1	2.620293000	-0.875569000	-3.306568000
1	2.531063000	-0.717385000	-2.578764000
1	-2.576306000	2.702391000	-2.323351000
1	-2.116476000	2.255608000	-1.936166000
1	0.323229000	-1.811485000	-1.981192000
1	-0.041007000	-2.253665000	-2.463499000
1	-0.280817000	-3.225263000	0.590892000
1	0.119012000	-2.598533000	0.501128000
1	-2.737383000	1.179282000	3.075979000
1	-2.254968000	0.978121000	2.539289000
1	0.574644000	0.909268000	-2.589667000
1	0.257606000	1.196792000	-3.204119000
1	-2.871647000	-2.188998000	2.110032000
1	-2.396270000	-1.755814000	1.725734000
1	-1.657873000	3.002750000	0.752250000
1	-1.964871000	3.661660000	0.931447000

$C_6H_3^-$

SCF Energy = -230.27353 a. u.

6	0.000349786	0.001025016	-3.395276373
6	-0.000155049	0.000815991	-2.171722263
6	0.000183095	-0.000075672	-0.829458350
1	-0.001412903	0.002162218	-4.455452299
6	-0.000035984	-0.000787945	0.407704082
6	-0.000203204	-0.001817724	1.746891888
6	0.000103719	-0.002480783	3.007686318
1	-0.000438159	0.007353447	5.551558302
1	0.000396354	0.010413150	6.308940594

1	-2.406086000	-2.241185000	-0.964986000
1	-2.893030000	-2.757641000	-1.204150000
1	-5.132247000	-2.915694000	0.229864000
1	-5.771509000	-3.299508000	0.242311000
1	-4.150842000	2.517374000	0.299195000
1	-4.883778000	2.497638000	0.159808000
1	-2.006212000	-0.334164000	-2.840806000
1	-2.398066000	-0.430347000	-3.471488000
1	-5.055892000	-0.213995000	-1.435561000
1	-4.406696000	-0.165897000	-1.801284000
1	-5.391384000	-0.198820000	1.577109000
1	-4.654587000	-0.310516000	1.612262000

$C_6H_5^-$

SCF Energy = -231.44840 a. u.

6	3.639231000	0.038376000	0.019138000
6	2.416207000	0.012982000	0.007894000
6	1.073830000	-0.013712000	-0.004265000
6	-0.162650000	-0.038303000	-0.014502000
6	-1.502170000	-0.063469000	-0.025039000
6	-2.761557000	-0.088450000	-0.031778000
1	-5.301975000	1.991082000	0.058695000
1	-4.758688000	1.466736000	0.043739000
1	-5.765988000	-1.467516000	0.109286000
1	-5.089715000	-1.135250000	0.050645000
1	4.699020000	0.060401000	0.028948000

$C_6H_7^-$

SCF Energy = -232.62365 a. u.

6	-3.868949000	0.053774000	-0.006811000
6	-2.646451000	0.019406000	-0.002064000
6	-1.304063000	-0.017547000	0.002572000
6	-0.068235000	-0.050460000	0.006746000
6	1.271438000	-0.084645000	0.010510000
6	2.529733000	-0.118243000	0.013257000
1	4.693203000	-0.371804000	1.352980000
1	5.355394000	-0.445586000	1.707485000
1	4.932007000	2.116089000	-0.309366000
1	4.399157000	1.584244000	-0.265964000
1	5.361285000	-0.969712000	-1.480357000
1	4.706712000	-0.811560000	-1.139462000
1	-4.928594000	0.084614000	-0.010568000

$C_6H_9^-$

SCF Energy = -233.79853 a. u.

6	-4.036320000	0.007729000	0.005467000
6	-2.813772000	0.001075000	0.001944000
6	-1.470886000	-0.005820000	-0.001867000
1	-5.096540000	0.013846000	0.008629000
6	-0.235171000	-0.010704000	-0.005348000
6	1.104984000	-0.014866000	-0.008773000
6	2.363285000	-0.015462000	-0.012127000
1	3.759247000	2.109929000	-0.004498000
1	4.141402000	2.759185000	-0.000369000
1	4.561275000	0.042784000	1.301776000
1	5.205043000	0.054789000	1.694669000
1	5.258326000	0.032118000	-1.637862000
1	4.603869000	0.020769000	-1.262889000
1	4.248860000	-2.720868000	0.016161000
1	3.845792000	-2.084263000	0.008603000

$C_6H_{11}^-$

SCF Energy = -234.97340 a. u.

6	-4.162744000	0.000247000	0.064915000
6	-2.941006000	0.000179000	0.028628000
6	-1.598517000	0.000022000	-0.010605000
1	-5.222573000	0.000197000	0.095228000
6	-0.363734000	-0.000355000	-0.046869000
6	0.976129000	-0.000971000	-0.085648000
6	2.233364000	-0.001707000	-0.128221000
1	3.764864000	1.301376000	1.441690000
1	4.191383000	1.693069000	1.923292000
1	3.768540000	-1.300157000	1.441920000
1	4.196375000	-1.690639000	1.923421000
1	5.546190000	0.010390000	-0.643713000
1	4.800198000	0.000452000	-0.534119000
1	3.683178000	-2.745603000	-1.272526000
1	3.369110000	-2.110512000	-1.017921000
1	3.364655000	2.110525000	-1.018001000
1	3.677128000	2.746411000	-1.272464000

$C_6H_{13}^-$

SCF Energy = -236.14894 a. u.

6	4.302542000	-0.000228000	0.001251000
6	3.080494000	-0.000045000	0.000047000

$C_6H_{15}^-$

SCF Energy = -237.32351 a. u.

6	-4.361034000	-0.032006000	0.017088000
6	-3.139672000	-0.002625000	-0.002939000

6	1.737614000	0.000083000	-0.000817000
1	5.362879000	-0.000764000	0.001979000
6	0.502612000	-0.000018000	-0.001450000
6	-0.838204000	-0.000985000	-0.001158000
6	-2.095756000	-0.002939000	0.000500000
1	-3.367572000	-0.059968000	-2.221811000
1	-3.719394000	-0.078717000	-2.886914000
1	-3.361316000	-2.136482000	-0.628452000
1	-3.706640000	-2.777580000	-0.819012000
1	-5.452311000	0.006575000	0.003613000
1	-4.698564000	0.004686000	0.003379000
1	-3.713333000	-1.639918000	2.384587000
1	-3.367306000	-1.257819000	1.836093000
1	-3.350229000	2.100407000	-0.746306000
1	-3.695223000	2.730560000	-0.970704000
1	-3.704927000	1.773127000	2.290627000
1	-3.361886000	1.360692000	1.762684000

6	-1.796676000	0.028331000	-0.024592000
6	-0.562331000	0.052907000	-0.042420000
6	0.778428000	0.076759000	-0.062104000
6	2.035668000	0.087084000	-0.076634000
1	2.642964000	-1.260149000	2.079530000
1	2.775522000	-1.601615000	2.735427000
1	4.430450000	-0.921840000	0.153372000
1	5.101929000	-1.252597000	0.236793000
1	4.200922000	1.391748000	2.071503000
1	3.703422000	1.140560000	1.565355000
1	4.752387000	1.613577000	-1.296372000
1	4.140371000	1.282732000	-1.008247000
1	3.494505000	-1.147141000	-2.770489000
1	3.184289000	-0.849193000	-2.152971000
1	2.274811000	3.492603000	-0.055266000
1	2.167444000	2.754624000	0.029203000
1	2.356226000	-2.554764000	-0.278706000
1	2.469176000	-3.292019000	-0.195040000
1	-5.420727000	-0.059219000	0.035512000

$C_6H_{17}^-$

SCF Energy = -238.49895 a. u.

6	-4.443822000	0.001221000	0.006963000
6	-3.222282000	0.002776000	-0.005675000
6	-1.878644000	0.004581000	-0.019055000
6	-0.644351000	0.006537000	-0.030556000
6	0.696967000	0.008933000	-0.040968000
6	1.954186000	0.011090000	-0.046756000
1	2.309466000	2.284238000	-1.336374000
1	2.410790000	2.947141000	-1.674262000
1	4.259142000	1.233302000	0.111999000
1	4.924160000	1.578715000	0.184036000
1	4.076874000	0.000416000	-2.608266000
1	3.559038000	0.002323000	-2.062496000
1	4.891492000	-1.622108000	0.160486000
1	4.227744000	-1.273728000	0.091765000
1	3.581949000	-0.091489000	2.837204000
1	3.242397000	-0.036563000	2.168064000
1	2.347424000	-2.924745000	-1.720960000
1	2.251953000	-2.261750000	-1.381879000
1	2.159042000	2.277128000	1.354989000
1	2.242406000	2.940065000	1.696885000
1	2.084026000	-2.299547000	1.318541000
1	2.163737000	-2.964163000	1.657806000
1	-5.503962000	-0.000062000	0.018748000

$C_6H_{19}^-$

SCF Energy = -239.67366 a. u.

6	-4.430370000	-0.000421000	0.061906000
6	-3.209727000	-0.000541000	0.096463000
6	-1.866530000	-0.000730000	0.136399000
6	-0.633478000	-0.000967000	0.178117000
6	0.707275000	-0.001149000	0.215689000
6	1.964697000	-0.001646000	0.215293000
1	3.087394000	2.167780000	1.008445000
1	3.389349000	2.821548000	1.225537000
1	4.547685000	0.008965000	0.584782000
1	5.290632000	0.011631000	0.709306000
1	3.941931000	1.663471000	-1.903123000
1	3.522191000	1.283311000	-1.408024000
1	3.954942000	-1.656788000	-1.898478000
1	3.531608000	-1.279136000	-1.404500000
1	1.059077000	2.449702000	-1.026805000
1	0.903248000	3.100678000	-1.363955000
1	3.408485000	-2.812010000	1.231346000
1	3.102706000	-2.160348000	1.013159000
1	1.191281000	-0.006709000	-3.262898000
1	1.293393000	-0.005513000	-2.520001000
1	2.911126000	0.004341000	2.614261000
1	3.169039000	0.005739000	3.320514000
1	1.073934000	-2.455469000	-1.018572000
1	0.921008000	-3.108186000	-1.353734000
1	-5.490226000	-0.000282000	0.029542000

$C_6H_{21}^-$

SCF Energy = -240.84899 a. u.

6	4.483672000	-0.022051000	0.001347000
6	3.262586000	-0.032067000	-0.001186000
6	1.918646000	-0.041530000	-0.004203000
6	0.684993000	-0.048844000	-0.008204000

$C_6H_{23}^-$

SCF Energy = -242.02422 a. u.

6	-4.458932000	-0.008413000	-0.008569000
6	-3.238221000	-0.011158000	-0.020065000
6	-1.893950000	-0.013439000	-0.030953000
6	-0.660818000	-0.014614000	-0.035561000

6	-0.656591000	-0.046251000	-0.013338000
6	-1.913801000	-0.039659000	-0.019734000
1	-2.058766000	-1.404149000	2.286806000
1	-2.144385000	-1.740897000	2.951943000
1	-4.143922000	0.143759000	1.337499000
1	-4.804822000	0.219172000	1.689450000
1	-4.170801000	-2.516547000	0.049513000
1	-3.653289000	-1.970974000	0.038178000
1	-4.870762000	0.223983000	-1.599973000
1	-4.206224000	0.148968000	-1.254370000
1	-1.045358000	-2.800795000	-0.041596000
1	-0.926972000	-3.534880000	-0.134541000
1	-3.615746000	2.824610000	0.104452000
1	-3.282066000	2.153115000	0.046037000
1	-2.316257000	-1.712631000	-2.942764000
1	-2.216360000	-1.372084000	-2.281126000
1	-1.914856000	1.438406000	2.237758000
1	-1.989925000	1.782963000	2.900045000
1	-2.021517000	1.457528000	-2.249491000
1	-2.045665000	1.973791000	-2.793223000
1	-0.140351000	3.312975000	-0.040684000
1	-0.652862000	2.768040000	-0.035426000
1	5.543868000	-0.011938000	0.003424000

6	0.681009000	-0.011738000	-0.032408000
6	1.938384000	-0.003273000	-0.026677000
1	1.005626000	-2.566315000	-1.017810000
1	0.895239000	-3.235126000	-1.337671000
1	3.428932000	-1.242065000	-1.752052000
1	3.851382000	-1.663105000	-2.209632000
1	3.552181000	-2.732291000	0.997550000
1	3.231969000	-2.110576000	0.721464000
1	5.290361000	0.159672000	0.342862000
1	4.550662000	0.070394000	0.235173000
1	0.714876000	-1.786785000	2.049897000
1	0.513129000	-2.293262000	2.563460000
1	3.761243000	1.820958000	-2.142850000
1	3.348887000	1.388548000	-1.686491000
1	3.108693000	-0.153824000	3.092234000
1	2.969786000	-0.061619000	2.359608000
1	1.061120000	0.077138000	-2.769602000
1	0.944185000	0.176653000	-3.503313000
1	3.105070000	2.142293000	0.844304000
1	3.411630000	2.766731000	1.128949000
1	0.466481000	2.114450000	2.690892000
1	0.673103000	1.614973000	2.172616000
1	0.557199000	3.281632000	-0.989890000
1	0.872516000	2.612981000	-0.867673000
1	-5.519098000	-0.005643000	0.003372000

$C_6H_{25}^-$

SCF Energy = -243.19881 a. u.

6	-4.493303000	-0.145374000	-0.001981000
6	-3.273093000	-0.116877000	0.003480000
6	-1.929047000	-0.087389000	0.009175000
1	-5.553321000	-0.168847000	-0.007230000
6	-0.696442000	-0.058925000	0.014874000
6	0.645338000	-0.025169000	0.018074000
6	1.902949000	-0.015067000	0.021568000
1	3.434701000	-1.759602000	-1.229963000
1	3.857491000	-2.216433000	-1.650394000
1	4.527851000	0.234347000	-0.043449000
1	5.267678000	0.339338000	-0.132916000
1	3.898587000	-2.191333000	1.668001000
1	3.472245000	-1.735895000	1.249436000
1	3.620833000	0.798634000	2.754993000
1	3.285840000	0.658699000	2.096504000
1	1.084537000	-2.772759000	0.041291000
1	0.972907000	-3.507728000	-0.052791000
1	3.188992000	3.011489000	-0.146812000
1	2.868931000	2.334525000	-0.073385000
1	0.961613000	-1.525995000	3.166346000
1	1.064021000	-1.201151000	2.498750000
1	3.194711000	0.599772000	-2.142463000
1	3.521484000	0.729022000	-2.806892000
1	0.842877000	1.644539000	2.247322000
1	0.640425000	2.146001000	2.765246000
1	0.751065000	1.589097000	-2.249685000
1	0.542867000	2.084914000	-2.770475000

$C_6H_{27}^-$

SCF Energy = -244.37181 a. u.

6	4.413770000	-0.133266000	-0.081434000
6	3.193701000	-0.129578000	-0.066140000
6	1.849663000	-0.117924000	-0.048682000
1	5.474090000	-0.138626000	-0.094344000
6	0.617102000	-0.096867000	-0.031786000
6	-0.724352000	-0.072711000	-0.011226000
6	-1.981409000	-0.027783000	-0.002685000
1	-3.384796000	1.042541000	-1.943150000
1	-3.730874000	1.350573000	-2.534749000
1	-4.609785000	-0.040684000	0.073306000
1	-5.362173000	-0.052406000	0.096241000
1	-3.660987000	2.870038000	0.374437000
1	-3.317268000	2.207210000	0.289647000
1	-3.629957000	0.646513000	2.834278000
1	-3.298215000	0.486360000	2.179047000
1	-0.952272000	2.350913000	-1.275760000
1	-0.766987000	2.990843000	-1.619072000
1	-3.314127000	-2.674750000	1.422895000
1	-3.047176000	-2.057031000	1.086054000
1	-0.737051000	2.686489000	2.089467000
1	-0.930007000	2.122207000	1.635669000
1	-3.397743000	-1.498573000	-1.612014000
1	-3.757485000	-1.939871000	-2.102804000
1	-0.898318000	-0.472967000	2.741720000
1	-0.675761000	-0.597252000	3.445992000
1	-1.004158000	-2.559684000	-1.241073000
1	-0.812434000	-3.215619000	-1.547613000

1	0.881623000	-1.584051000	-3.110045000	1	1.711951000	2.761231000	0.211081000
1	0.991750000	-1.258122000	-2.444431000	1	2.049047000	3.425904000	0.265172000
1	-0.294367000	3.555106000	-0.046684000	1	-0.897971000	-0.226758000	-3.483943000
1	0.036244000	2.889239000	0.028592000	1	-1.054088000	-0.170102000	-2.753202000
				1	0.059875000	-3.214639000	1.607742000
				1	-0.266182000	-2.613085000	1.306692000
$C_6H_{29}^-$				**$C_6H_{31}^-$**			
SCF Energy = -245.54684 a. u.				SCF Energy = -246.72146 a. u.			
6	4.487871000	-0.174741000	-0.058872000	6	4.556083000	0.019111000	-0.009211000
6	3.268040000	-0.144698000	-0.039315000	6	3.335868000	0.016470000	-0.000959000
6	1.924290000	-0.111301000	-0.018908000	6	1.991351000	0.014868000	0.006771000
6	0.692657000	-0.069980000	-0.004508000	6	0.759425000	0.011004000	0.009825000
6	-0.649265000	-0.026754000	0.013867000	6	-0.584424000	0.009174000	0.011873000
6	-1.907259000	-0.002085000	0.010439000	6	-1.843450000	0.009424000	0.015990000
1	-1.891345000	2.641809000	-0.469912000	1	-2.526987000	-2.515055000	-0.151189000
1	-1.989243000	3.376549000	-0.586728000	1	-2.833005000	-3.194617000	-0.245034000
1	-3.675271000	1.081198000	-1.654076000	1	-4.204966000	-0.814540000	1.112898000
1	-4.171447000	1.327816000	-2.161419000	1	-4.823405000	-1.101923000	1.427599000
1	-4.749632000	1.641098000	1.047734000	1	-4.747796000	-0.864568000	-1.771256000
1	-4.136515000	1.303202000	0.774800000	1	-4.217711000	-0.664266000	-1.279461000
1	-5.111037000	-1.192630000	-0.305827000	1	-4.914307000	1.707232000	0.014186000
1	-4.436648000	-0.869898000	-0.226655000	1	-4.249101000	1.361113000	0.052167000
1	-2.146218000	1.574077000	2.192677000	1	-2.087016000	-1.231967000	-2.394429000
1	-2.219252000	1.921527000	2.853379000	1	-2.157436000	-1.566066000	-3.062006000
1	-3.130456000	-1.538538000	-2.764961000	1	-2.936134000	1.402260000	2.858799000
1	-2.866595000	-1.208835000	-2.144203000	1	-2.661964000	1.093850000	2.230748000
1	-3.294439000	-1.302245000	2.702797000	1	-2.849194000	1.831155000	-2.602074000
1	-2.995121000	-0.994188000	2.085067000	1	-2.646628000	1.335382000	-2.075142000
1	-1.015695000	0.661396000	-2.645539000	1	-2.179173000	-1.481251000	2.282326000
1	-0.901637000	0.975150000	-3.316585000	1	-2.196417000	-2.004097000	2.818827000
1	-2.656596000	-2.560052000	-0.055839000	1	-2.231652000	2.708800000	0.152934000
1	-2.776532000	-3.294626000	-0.151224000	1	-2.341122000	3.442165000	0.263302000
1	-0.268021000	-0.157286000	2.800856000	1	-0.068615000	-0.121833000	2.796909000
1	-0.136853000	-0.464903000	3.469820000	1	0.263624000	-0.052560000	3.463295000
1	0.723621000	2.912180000	1.698883000	1	-0.007568000	0.245234000	-2.754861000
1	0.218929000	2.397365000	1.502773000	1	0.320434000	0.340322000	-3.420146000
1	-0.143862000	-3.101206000	1.586039000	1	0.541525000	-2.917069000	-1.804109000
1	-0.442661000	-2.488187000	1.278042000	1	0.041707000	-2.403797000	-1.591984000
1	-0.071974000	-2.684786000	-2.066647000	1	0.242503000	3.092998000	-1.580922000
1	-0.492052000	-2.235633000	-1.640353000	1	-0.062850000	2.483984000	-1.272776000
1	1.313280000	3.134767000	-1.728371000	1	0.317336000	2.793284000	1.998817000
1	1.017559000	2.524526000	-1.415635000	1	-0.105663000	2.347579000	1.573094000
1	5.547709000	-0.202292000	-0.075110000	1	0.370442000	-3.183771000	1.525151000
				1	0.045686000	-2.570510000	1.247360000
				1	5.616338000	0.022230000	-0.018754000
$C_6H_{33}^-$				**$C_6H_{35}^-$**			
SCF Energy = -247.89513 a. u.				SCF Energy = -249.06976 a. u.			
6	-4.471266000	-0.304420000	0.015127000	6	-4.381549000	-0.526376000	-0.002468000
6	-3.253437000	-0.233695000	0.006106000	6	-3.166648000	-0.419262000	-0.011239000
6	-1.911442000	-0.151292000	-0.003742000	6	-1.828252000	-0.289583000	-0.020035000
6	-0.680849000	-0.087990000	-0.008200000	6	-0.600312000	-0.182489000	-0.023858000
6	0.661592000	-0.029413000	-0.011429000	6	0.739346000	-0.081670000	-0.026163000

6	1.919851000	0.017649000	-0.018209000
1	2.662167000	-2.503201000	0.011756000
1	2.974711000	-3.181632000	0.089840000
1	4.309383000	-0.701651000	-1.137018000
1	4.930977000	-0.974787000	-1.458067000
1	4.837314000	-0.893020000	1.739303000
1	4.306347000	-0.684188000	1.252155000
1	4.968532000	1.765185000	0.094763000
1	4.304823000	1.419795000	0.032853000
1	2.181382000	-1.361920000	2.316567000
1	2.252634000	-1.700778000	2.981554000
1	3.001294000	1.555775000	-2.782536000
1	2.736118000	1.230198000	-2.159165000
1	2.876178000	1.706423000	2.707149000
1	2.678429000	1.218684000	2.171183000
1	2.323520000	-1.347301000	-2.369083000
1	2.348361000	-1.863569000	-2.911491000
1	2.256406000	2.714734000	0.010053000
1	2.360950000	3.450434000	-0.089890000
1	0.176853000	-0.014718000	-2.790049000
1	-0.153504000	0.061416000	-3.456725000
1	0.074368000	0.024431000	2.760341000
1	-0.256572000	0.103357000	3.426293000
1	-0.395581000	-3.081181000	1.635251000
1	0.105900000	-2.565203000	1.434157000
1	-0.192162000	2.929487000	1.722339000
1	0.103093000	2.320577000	1.403629000
1	-0.279800000	2.802254000	-1.828705000
1	0.148742000	2.355901000	-1.408826000
1	-0.191580000	-3.181934000	-1.708480000
1	0.122091000	-2.569621000	-1.416518000
1	-3.075035000	3.300683000	-0.084620000
1	-2.553271000	2.767138000	-0.089925000
1	-5.529766000	-0.366799000	0.023995000

6	1.995618000	0.003259000	-0.026404000
1	2.819726000	-2.150910000	1.211516000
1	3.091772000	-2.768964000	1.540489000
1	4.462059000	-1.059651000	-0.629957000
1	5.123946000	-1.390775000	-0.756402000
1	4.879338000	0.108292000	2.019622000
1	4.340031000	0.099863000	1.498346000
1	4.997115000	1.710364000	-0.692277000
1	4.340363000	1.367760000	-0.570365000
1	2.255273000	-0.091120000	2.717237000
1	2.162062000	0.000567000	3.455031000
1	3.206197000	0.202913000	-3.133258000
1	2.891039000	0.125301000	-2.455407000
1	2.756700000	2.787438000	1.665378000
1	2.636363000	2.127537000	1.326839000
1	2.527106000	-2.289407000	-1.403069000
1	2.621556000	-2.951822000	-1.741093000
1	2.268177000	2.396288000	-1.293284000
1	2.342419000	3.061626000	-1.630860000
1	0.380800000	-1.363457000	-2.514131000
1	0.079284000	-1.667282000	-3.127334000
1	0.034792000	1.262838000	2.344177000
1	-0.199703000	1.751829000	2.859033000
1	-0.205415000	-2.065216000	2.871067000
1	0.217708000	-1.635743000	2.429910000
1	-0.273061000	3.297743000	0.128715000
1	0.057924000	2.631350000	0.050486000
1	-0.246482000	1.522863000	-2.945872000
1	0.251017000	1.306997000	-2.430991000
1	0.018371000	-3.620027000	-0.034096000
1	0.349467000	-2.954454000	-0.113371000
1	-3.072297000	2.717984000	1.673560000
1	-2.569164000	2.213360000	1.451100000
1	-3.076226000	2.711820000	-1.671506000
1	-2.579859000	2.202640000	-1.443830000
1	-5.437615000	-0.621820000	0.005593000

$C_6H_{37}^-$

SCF Energy = -250.24445 a. u.

6	4.310741000	-0.152023000	-0.539312000
6	3.096610000	-0.119830000	-0.430198000
6	1.759245000	-0.081546000	-0.294915000
6	0.532233000	-0.050249000	-0.177747000
6	-0.806068000	-0.022769000	-0.063459000
6	-2.061061000	-0.001768000	0.038109000
1	-2.939343000	-0.710073000	-2.324797000
1	-3.242903000	-0.979597000	-2.956773000
1	-4.476973000	-1.336569000	-0.212492000
1	-5.137829000	-1.681037000	-0.301489000
1	-5.091849000	1.301634000	-1.199516000
1	-4.474929000	0.992068000	-0.904910000
1	-5.040473000	0.538786000	1.811750000
1	-4.383769000	0.432065000	1.464033000
1	-2.483484000	1.844110000	-1.961536000
1	-2.513304000	2.367494000	-2.496981000

$C_6H_{39}^-$

SCF Energy = -251.41885 a. u.

6	4.258311000	-0.003143000	-0.483297000
6	3.042852000	-0.012213000	-0.388168000
6	1.703294000	-0.020596000	-0.269350000
6	0.474099000	-0.023376000	-0.168815000
6	-0.866061000	-0.022928000	-0.077733000
6	-2.123080000	-0.020964000	-0.002646000
1	-2.941048000	1.185825000	-2.179228000
1	-3.210374000	1.513758000	-2.798920000
1	-4.596156000	-0.623406000	-1.093729000
1	-5.257115000	-0.748870000	-1.426594000
1	-5.019553000	2.032581000	0.053383000
1	-4.480455000	1.511267000	0.049745000
1	-5.164067000	-0.661521000	1.672746000
1	-4.505650000	-0.544597000	1.331986000
1	-2.395239000	2.723420000	-0.106144000
1	-2.300961000	3.461076000	-0.015011000

1	-2.984526000	-2.229503000	2.356512000
1	-2.798014000	-1.717960000	1.838895000
1	-2.948711000	3.154207000	0.723380000
1	-2.819807000	2.423370000	0.605936000
1	-2.469377000	-2.627101000	-0.614238000
1	-2.580168000	-3.358006000	-0.737580000
1	-2.289072000	0.784375000	2.636091000
1	-2.365902000	1.102329000	3.310630000
1	-0.263095000	-2.647704000	0.765905000
1	0.060969000	-3.312600000	0.876300000
1	-0.304097000	2.640628000	-0.873987000
1	0.022762000	3.305362000	-0.977192000
1	-0.080478000	0.546065000	-3.575795000
1	-0.415816000	0.614372000	-2.911396000
1	0.136753000	2.625886000	2.083169000
1	-0.160937000	2.024107000	1.753372000
1	0.276805000	-0.898196000	3.098666000
1	-0.223430000	-0.695583000	2.580902000
1	-0.133182000	-2.602663000	-2.577249000
1	-0.358537000	-2.106951000	-2.065527000
1	2.881197000	3.275123000	0.423921000
1	2.354640000	2.746316000	0.407681000
1	2.897401000	-2.552694000	2.215480000
1	2.470076000	-2.122672000	1.779931000
1	3.012099000	0.904530000	2.960905000
1	2.511152000	0.707724000	2.443291000
1	5.365958000	-0.182525000	-0.640156000

1	-3.376004000	-3.111788000	0.216640000
1	-3.060698000	-2.434247000	0.137473000
1	-2.939057000	1.673238000	2.770264000
1	-2.816591000	1.334338000	2.111068000
1	-2.653609000	-1.426781000	-2.279523000
1	-2.744912000	-1.765750000	-2.941828000
1	-2.462423000	-1.248087000	2.406171000
1	-2.540093000	-1.584051000	3.071848000
1	-0.532812000	-2.512291000	-1.288565000
1	-0.235131000	-3.126348000	-1.595020000
1	-0.210141000	2.326182000	1.286330000
1	0.028136000	2.837117000	1.777794000
1	0.053430000	2.826446000	-2.055816000
1	-0.371415000	2.388666000	-1.624338000
1	0.105047000	0.104945000	3.307551000
1	-0.226584000	0.028114000	2.641298000
1	0.043379000	-2.902709000	1.597728000
1	-0.447250000	-2.386457000	1.368562000
1	-0.132702000	-0.072410000	-3.594887000
1	-0.464359000	-0.150714000	-2.929423000
1	2.935975000	1.645456000	2.740673000
1	2.435271000	1.428524000	2.231071000
1	2.703230000	-3.491595000	-0.233766000
1	2.180465000	-2.958858000	-0.240685000
1	2.915981000	-1.692149000	2.720218000
1	2.420888000	-1.460596000	2.211286000
1	2.340430000	2.915079000	-0.234698000
1	2.670488000	3.580264000	-0.156379000
1	5.315191000	0.006252000	-0.569222000

$C_6H_{41}^-$

SCF Energy = -252.59347 a. u.

6	-4.209922000	0.030698000	-0.259038000
6	-2.991680000	0.024021000	-0.213674000
6	-1.647955000	0.016245000	-0.157036000
6	-0.415472000	0.010246000	-0.106107000
6	0.926770000	0.003766000	-0.054975000
6	2.185266000	-0.000349000	-0.010225000
1	3.075899000	0.104995000	-2.460650000
1	3.202419000	0.201338000	-3.194843000
1	4.620400000	1.174813000	-0.592763000
1	5.281962000	1.505265000	-0.721802000
1	5.140525000	-1.712881000	-0.877797000
1	4.604739000	-1.230170000	-0.671197000
1	5.124647000	-0.128323000	1.972764000
1	4.580024000	-0.111531000	1.457435000
1	2.510330000	-2.269964000	-1.469432000
1	2.582289000	-2.931790000	-1.814154000
1	3.269009000	2.674470000	1.686399000
1	3.011043000	2.055510000	1.347347000
1	3.059250000	-2.887467000	1.477464000
1	2.934744000	-2.225329000	1.145473000
1	2.634788000	2.392308000	-1.251041000
1	2.722508000	3.057956000	-1.584146000
1	2.456197000	-0.105464000	2.704269000

$C_6H_{43}^-$

SCF Energy = -253.76873 a. u.

6	-4.168120000	0.005430000	0.009918000
6	-2.949178000	0.000051000	0.008938000
6	-1.604234000	-0.000571000	0.008101000
6	-0.370084000	0.005391000	0.006193000
6	0.972998000	0.012856000	0.005143000
6	2.232410000	0.020644000	0.003825000
1	3.036696000	0.547540000	-2.406325000
1	3.165148000	0.664350000	-3.137395000
1	4.649628000	1.354151000	-0.399705000
1	5.309465000	1.697763000	-0.497246000
1	5.251915000	-1.298888000	-1.303448000
1	4.635832000	-0.999185000	-0.997821000
1	5.321077000	-0.460304000	1.689253000
1	4.661466000	-0.362149000	1.345610000
1	2.598029000	-1.940806000	-1.888452000
1	2.680882000	-2.596494000	-2.241437000
1	3.258917000	2.327741000	2.220892000
1	3.063040000	1.812302000	1.711040000
1	3.210225000	-3.042556000	0.985227000
1	3.079486000	-2.370700000	0.676301000
1	2.620801000	2.593391000	-0.796435000
1	2.717207000	3.265866000	-1.113051000
1	2.637145000	-0.637440000	2.641134000

1	2.554792000	-0.205945000	3.440517000
1	0.485501000	2.760913000	0.110684000
1	0.154574000	3.427060000	0.190807000
1	0.383714000	-2.751354000	-0.104792000
1	0.051620000	-3.417668000	-0.031837000
1	-0.049965000	-1.528943000	-3.146244000
1	0.454976000	-1.328800000	-2.633149000
1	-0.059430000	-1.845569000	2.724247000
1	0.366905000	-1.422950000	2.277940000
1	-0.003635000	1.687758000	2.836556000
1	0.421449000	1.266852000	2.387382000
1	0.180224000	1.805168000	-3.088242000
1	0.492954000	1.512217000	-2.475706000
1	-2.722221000	-3.067991000	1.542338000
1	-2.217502000	-2.560705000	1.329601000
1	-2.636612000	3.018812000	1.673266000
1	-2.131487000	2.515738000	1.451459000
1	-2.712764000	-0.059817000	3.278382000
1	-2.188994000	-0.053242000	2.746416000
1	-2.279786000	-2.564735000	-1.544286000
1	-2.575900000	-3.175267000	-1.855935000
1	-2.446250000	3.246576000	-1.729978000
1	-2.145535000	2.634470000	-1.425643000
1	-5.269440000	0.035922000	-0.300783000

1	2.744045000	-0.754152000	3.373562000
1	0.523726000	2.668978000	0.725707000
1	0.192241000	3.329679000	0.839061000
1	0.489718000	-2.678294000	-0.599328000
1	0.165869000	-3.346574000	-0.690206000
1	0.082869000	-0.925345000	-3.206478000
1	0.588949000	-0.730870000	-2.691120000
1	0.273799000	-2.439344000	2.440776000
1	0.504149000	-1.935425000	1.938346000
1	0.101020000	1.058437000	3.195360000
1	0.580367000	0.838070000	2.665146000
1	0.199100000	2.186919000	-2.622927000
1	0.495698000	1.858584000	-2.019631000
1	-2.636545000	-3.333304000	1.032953000
1	-2.131865000	-2.820436000	0.833476000
1	-2.518880000	2.714992000	2.321108000
1	-2.221360000	2.114001000	1.992267000
1	-2.503725000	-0.789739000	3.456429000
1	-2.178646000	-0.688483000	2.791726000
1	-2.180104000	-2.122695000	-1.984233000
1	-2.600013000	-2.564961000	-2.414690000
1	-2.071007000	0.674403000	-2.824521000
1	-2.594524000	0.695649000	-3.356603000
1	-2.486510000	3.389917000	-1.116373000
1	-2.169641000	2.775193000	-0.834105000
1	-5.228448000	0.007402000	0.013454000

$C_6H_{45}^-$

SCF Energy = -254.94210 a. u.

6	-4.014797000	-0.354814000	0.020971000
6	-2.798629000	-0.269102000	0.015108000
6	-1.457195000	-0.174209000	0.009238000
6	-0.225849000	-0.090193000	0.006169000
6	1.113444000	0.004291000	0.007120000
6	2.369742000	0.093478000	0.013330000
1	3.035798000	2.315334000	1.189116000
1	3.142811000	2.981546000	1.519484000
1	4.766923000	0.317004000	1.407606000
1	5.429715000	0.388738000	1.752117000
1	5.210011000	1.996110000	-0.917127000
1	4.683681000	1.503115000	-0.711106000
1	5.496327000	-1.199585000	-0.975872000
1	4.873154000	-0.892692000	-0.692003000
1	2.547988000	2.465164000	-1.379272000
1	2.546536000	3.009077000	-1.894316000
1	3.663028000	-2.574493000	1.595125000
1	3.378715000	-1.958978000	1.271736000
1	3.292992000	0.030731000	-3.209372000
1	3.165898000	0.124811000	-2.475177000
1	2.731923000	0.128993000	2.727040000
1	2.841217000	0.226609000	3.461928000
1	2.936303000	-2.209531000	-1.327333000
1	3.025947000	-2.875918000	-1.658822000
1	0.721926000	-1.470403000	2.347393000
1	0.428411000	-1.785873000	2.958731000

$C_6H_{47}^-$

SCF Energy = -256.11651 a. u.

6	-3.878812000	0.544173000	-0.084480000
6	-2.666707000	0.412038000	-0.068909000
6	-1.329967000	0.266954000	-0.050997000
6	-0.103151000	0.133955000	-0.029694000
6	1.231215000	-0.011023000	-0.005866000
6	2.483120000	-0.147250000	0.016446000
1	3.000434000	-2.638892000	0.487390000
1	3.114792000	-3.371797000	0.606977000
1	4.802093000	-1.333498000	-0.957744000
1	5.415898000	-1.651442000	-1.249639000
1	5.310317000	-1.100597000	1.907255000
1	4.784239000	-0.893316000	1.414349000
1	5.723038000	1.265387000	-0.199611000
1	5.054103000	0.933371000	-0.127189000
1	2.691120000	-1.143057000	2.575771000
1	2.593564000	-1.277661000	3.306394000
1	3.801291000	0.692322000	-2.957056000
1	3.484888000	0.555070000	-2.289777000
1	3.647634000	1.807834000	2.488906000
1	3.432910000	1.311376000	1.968104000
1	2.731928000	-1.915868000	-2.055992000
1	2.747833000	-2.440343000	-2.590702000
1	3.190731000	2.445912000	-0.425426000
1	3.310157000	3.176504000	-0.542834000
1	0.774325000	-0.356236000	-2.736631000
1	0.441901000	-0.437763000	-3.401872000

1	0.501800000	1.274906000	-2.430762000
1	0.172444000	1.406682000	-3.089316000
1	-0.030524000	3.279206000	0.028574000
1	0.491497000	2.743799000	0.032996000
1	0.426197000	-1.722803000	-3.026546000
1	0.729170000	-1.418511000	-2.414280000
1	0.420731000	-3.406839000	0.231938000
1	0.922861000	-2.884088000	0.048663000
1	0.268241000	1.900795000	2.856151000
1	0.507438000	1.412436000	2.342588000
1	-2.476843000	-0.452411000	-3.443913000
1	-1.969025000	-0.272368000	-2.926851000
1	-2.268811000	-3.176219000	1.922173000
1	-1.840540000	-2.729920000	1.504011000
1	-2.155570000	-3.352176000	-1.681434000
1	-1.861233000	-2.740426000	-1.369901000
1	-2.244359000	2.227569000	-1.500183000
1	-2.665590000	2.673838000	-1.925823000
1	-2.153636000	2.284477000	1.398299000
1	-2.657538000	2.792964000	1.611146000
1	-2.332757000	-0.097500000	3.581125000
1	-2.003062000	-0.172396000	2.915065000
1	-5.009467000	2.283808000	-0.052263000
1	-5.539310000	2.810596000	-0.058649000
1	-5.071716000	-0.441890000	0.025701000

1	0.713721000	0.585327000	2.684268000
1	0.395330000	0.867128000	3.299642000
1	-0.016058000	-2.630048000	1.993865000
1	0.483585000	-2.125233000	1.760365000
1	0.749885000	3.236542000	1.267006000
1	1.054946000	2.618948000	0.975502000
1	0.700276000	2.563816000	-2.266772000
1	1.115496000	2.120053000	-1.831035000
1	0.133809000	-3.206518000	-1.078403000
1	0.469890000	-2.549328000	-0.958156000
1	-2.138899000	2.623493000	2.606373000
1	-1.715340000	2.187782000	2.172560000
1	-2.141697000	1.568447000	-3.305840000
1	-1.639563000	1.362228000	-2.793128000
1	-1.848744000	3.841556000	-0.640647000
1	-1.525499000	3.174801000	-0.546613000
1	-2.074837000	-0.629810000	2.651438000
1	-2.398353000	-0.739766000	3.315687000
1	-2.177379000	-2.450360000	0.401647000
1	-2.704647000	-2.979334000	0.424668000
1	-2.448693000	-1.873559000	-2.762161000
1	-2.023980000	-1.450192000	-2.317168000
1	-4.824240000	-1.567303000	1.704001000
1	-5.431641000	-1.877005000	2.009355000
1	-4.864578000	-1.828909000	-1.175378000
1	-5.378166000	-2.332884000	-1.378033000
1	-4.932006000	0.669748000	-0.092721000

$C_6H_{49}^-$

SCF Energy = -257.29039 a. u.

6	-3.770215000	-0.017045000	0.519316000
6	-2.556398000	-0.008678000	0.396969000
6	-1.218823000	0.001410000	0.262308000
6	0.009073000	0.010301000	0.137442000
6	1.343223000	0.018703000	-0.007640000
6	2.594296000	0.027212000	-0.153574000
1	3.165193000	-1.072920000	-2.441933000
1	3.264935000	-1.403365000	-3.109178000
1	4.863658000	0.771457000	-1.620683000
1	5.516311000	0.909318000	-1.964006000
1	5.510091000	-1.917454000	-0.592074000
1	4.970635000	-1.397526000	-0.557844000
1	5.821037000	0.712831000	1.116931000
1	5.154682000	0.596422000	0.792236000
1	2.969362000	-2.712954000	-0.401454000
1	2.873861000	-3.450286000	-0.311072000
1	3.797556000	3.160856000	-0.119351000
1	3.477950000	2.483138000	-0.067004000
1	3.940503000	-1.717712000	2.378918000
1	3.653003000	-1.385379000	1.769861000
1	2.712749000	1.545673000	-2.424410000
1	2.781436000	1.891097000	-3.085952000
1	3.299217000	1.190549000	2.219574000
1	3.402294000	1.519640000	2.885038000
1	0.783316000	2.535745000	-1.128079000

$C_6H_{51}^-$

SCF Energy = -258.46460 a. u.

6	-3.682048000	0.047532000	-0.420169000
6	-2.465996000	0.034226000	-0.320149000
6	-1.126176000	0.021588000	-0.211996000
6	0.104153000	0.009086000	-0.113702000
6	1.441226000	-0.004021000	-0.000779000
6	2.695998000	-0.016381000	0.109212000
1	3.313338000	-0.291873000	2.634659000
1	3.429175000	-0.392462000	3.369814000
1	5.049262000	-1.320127000	0.890564000
1	5.664551000	-1.647788000	1.167658000
1	5.620580000	1.422066000	1.495260000
1	5.012115000	1.105187000	1.191721000
1	5.911676000	0.214589000	-1.358450000
1	5.244234000	0.139845000	-1.024063000
1	2.946090000	2.163605000	1.771782000
1	2.899286000	2.825782000	2.119236000
1	3.940550000	-2.632266000	-1.576780000
1	3.660407000	-2.021511000	-1.241095000
1	3.775327000	2.906777000	-1.122848000
1	3.636556000	2.242203000	-0.801768000
1	2.964506000	-2.497922000	1.231850000
1	3.038151000	-3.167322000	1.560494000
1	3.359401000	0.247283000	-2.520260000
1	3.474063000	0.348586000	-3.253962000
1	0.981926000	-2.728952000	-0.413450000

1	0.283531000	3.053129000	-1.332343000
1	1.000559000	-2.453049000	1.316417000
1	0.781619000	-2.971036000	1.809312000
1	0.252601000	-2.735263000	-1.795085000
1	0.746762000	-2.224388000	-1.562516000
1	0.886408000	-0.306266000	3.450582000
1	1.212637000	-0.224504000	2.782384000
1	0.660382000	2.861906000	1.830194000
1	1.151564000	2.349782000	1.594167000
1	0.199306000	0.087729000	-3.352123000
1	0.536369000	0.160203000	-2.688312000
1	-1.966428000	-1.856604000	3.252794000
1	-1.468706000	-1.633978000	2.742843000
1	-2.195512000	3.431555000	0.588257000
1	-1.671622000	2.899772000	0.563558000
1	-1.820840000	1.551401000	3.532788000
1	-1.526831000	1.245359000	2.918135000
1	-1.757036000	-2.872728000	0.150624000
1	-2.086118000	-3.538535000	0.230571000
1	-2.097076000	-1.287787000	-2.234356000
1	-2.530759000	-1.705464000	-2.676603000
1	-2.399960000	1.907938000	-2.567538000
1	-2.095807000	1.590063000	-1.963481000
1	-4.610406000	-2.413056000	-0.679112000
1	-5.121468000	-2.920930000	-0.877951000
1	-4.778551000	0.078121000	-2.125320000
1	-5.309610000	0.085507000	-2.650879000
1	-4.823965000	-0.026233000	0.641679000
1	-4.651925000	2.453017000	-0.489091000
1	-5.163843000	2.963782000	-0.678032000

1	0.651607000	-3.394718000	-0.497948000
1	0.942670000	2.754310000	0.220146000
1	0.610052000	3.420334000	0.147358000
1	0.288409000	1.286274000	3.043269000
1	0.791934000	1.083530000	2.529146000
1	1.005464000	2.186358000	-2.745869000
1	1.224888000	1.689951000	-2.231429000
1	0.819389000	-1.556546000	-3.051193000
1	1.241157000	-1.138082000	-2.597185000
1	0.442129000	-1.889889000	2.792671000
1	0.763671000	-1.591429000	2.186813000
1	-1.902852000	3.140436000	-1.858651000
1	-1.469914000	2.697317000	-1.441781000
1	-1.974978000	-2.804570000	-2.238526000
1	-1.477955000	-2.301608000	-1.997886000
1	-1.704180000	0.424934000	-3.798304000
1	-1.377558000	0.340034000	-3.131965000
1	-1.850327000	2.323166000	1.368902000
1	-2.144101000	2.933147000	1.685307000
1	-1.845401000	-0.310447000	2.580660000
1	-2.373142000	-0.329822000	3.108902000
1	-2.149930000	-3.225137000	1.152031000
1	-1.841578000	-2.610865000	0.858913000
1	-4.370284000	2.790163000	-0.388598000
1	-4.895030000	3.321959000	-0.402440000
1	-4.590501000	1.207610000	2.017832000
1	-4.930149000	1.498267000	2.616750000
1	-4.559940000	-1.643923000	1.775633000
1	-5.072042000	-1.870047000	2.270488000
1	-4.738722000	0.055779000	-0.516530000
1	-4.355060000	-2.712719000	-0.900617000
1	-4.881872000	-3.241645000	-0.930769000

$C_6H_{53}^-$

SCF Energy = -259.63883 a. u.

6	-3.589937000	0.006538000	-0.208830000
6	-2.370469000	-0.005149000	-0.158619000
6	-1.027498000	-0.015455000	-0.102672000
6	0.205854000	-0.018722000	-0.049835000
6	1.546201000	-0.019468000	0.010786000
6	2.804519000	-0.020631000	0.067047000
1	3.540081000	1.172470000	2.260286000
1	3.662397000	1.507599000	2.921293000
1	5.185499000	-0.672945000	1.374381000
1	5.843209000	-0.800369000	1.712137000
1	5.728244000	1.971235000	0.234876000
1	5.187893000	1.451477000	0.220741000
1	5.958141000	-0.720938000	-1.390104000
1	5.296293000	-0.599518000	-1.058317000
1	3.158342000	2.716879000	0.221597000
1	3.063759000	3.454069000	0.128375000
1	4.046439000	-3.145183000	0.116954000
1	3.728580000	-2.467821000	0.051710000

$C_6H_{55}^-$

SCF Energy = -260.81355 a. u.

6	3.510785000	0.002060000	0.000078000
6	2.289916000	0.002052000	-0.007385000
6	0.945753000	0.004444000	-0.011723000
6	-0.288778000	0.007317000	-0.012543000
6	-1.630494000	0.010828000	-0.012076000
6	-2.889971000	0.011844000	-0.008787000
1	-3.699617000	1.628000000	1.860108000
1	-3.897913000	2.131773000	2.380543000
1	-5.317628000	1.389933000	-0.218556000
1	-5.981568000	1.730712000	-0.293725000
1	-5.831654000	-0.625218000	1.851329000
1	-5.302059000	-0.439442000	1.353837000
1	-5.960181000	-1.222015000	-1.284116000
1	-5.340177000	-0.921696000	-0.986454000
1	-3.265770000	-0.846350000	2.584408000
1	-3.204245000	-1.167890000	3.258341000
1	-4.080624000	1.070741000	-2.965315000
1	-3.791943000	0.781016000	-2.335445000

1	3.871067000	1.651262000	-2.638652000
1	3.733187000	1.312713000	-1.982682000
1	3.123618000	-1.422657000	2.390429000
1	3.200500000	-1.762871000	3.053742000
1	3.336133000	-1.295805000	-2.282127000
1	3.425840000	-1.632307000	-2.945803000
1	1.127755000	-2.499166000	1.254747000
1	0.635521000	-3.015358000	1.479495000
1	1.112928000	2.411933000	-1.369989000
1	0.880559000	2.922758000	-1.864214000
1	0.567535000	2.753065000	1.913603000
1	0.989756000	2.305614000	1.488722000
1	0.897460000	0.176363000	-3.442523000
1	1.227540000	0.097353000	-2.775915000
1	0.762460000	-2.953722000	-1.669582000
1	1.254912000	-2.437649000	-1.445364000
1	0.591583000	-0.012064000	3.413287000
1	0.927166000	-0.085319000	2.748841000
1	-1.876615000	1.735403000	-3.132654000
1	-1.370039000	1.529197000	-2.624323000
1	-2.066772000	-3.433554000	-0.315312000
1	-1.542310000	-2.902091000	-0.299603000
1	-1.740174000	-1.632748000	-3.303524000
1	-1.443910000	-1.322501000	-2.692097000
1	-1.589743000	2.835482000	-0.057911000
1	-1.919520000	3.501307000	-0.137251000
1	-1.707913000	1.337626000	2.389271000
1	-2.202387000	1.562822000	2.902157000
1	-2.015844000	-1.854335000	2.849055000
1	-1.721782000	-1.537069000	2.239597000
1	-4.229366000	2.393505000	-1.679649000
1	-4.732356000	2.895547000	-1.910208000
1	-4.691652000	-2.628371000	-2.256002000
1	-4.251843000	-2.193297000	-1.836900000
1	-4.286053000	2.428471000	1.203441000
1	-4.792656000	2.934543000	1.416447000
1	-4.410527000	-0.069292000	2.613182000
1	-4.939928000	-0.076624000	3.139867000
1	-4.650110000	0.021768000	-0.253486000
1	-4.392726000	-2.480470000	1.039492000
1	-4.902196000	-2.989090000	1.239207000

1	-3.877543000	-3.137909000	0.615684000
1	-3.748042000	-2.407828000	0.496340000
1	-3.283712000	2.657732000	-0.561929000
1	-3.388105000	3.390035000	-0.681353000
1	-3.344459000	-1.784144000	-2.018794000
1	-3.368399000	-2.308251000	-2.553849000
1	-1.231142000	2.012787000	-1.919622000
1	-0.810285000	2.448781000	-2.358353000
1	-1.170175000	-2.100037000	1.779308000
1	-0.867772000	-2.706553000	2.096134000
1	-0.713055000	0.826403000	3.232865000
1	-1.213449000	0.631046000	2.713031000
1	-0.858798000	-3.265094000	-0.992617000
1	-1.191596000	-2.605729000	-0.874267000
1	-0.754658000	-0.593888000	-3.304624000
1	-1.274973000	-0.571678000	-2.767580000
1	-0.849782000	3.222220000	1.189382000
1	-1.166707000	2.609237000	0.900538000
1	1.895132000	-3.383458000	0.598388000
1	1.367860000	-2.854534000	0.575244000
1	1.902049000	1.051098000	-3.271296000
1	1.393022000	0.861221000	-2.758390000
1	1.880769000	-2.359386000	-2.591752000
1	1.451692000	-1.931525000	-2.154993000
1	1.467208000	-0.891278000	2.664444000
1	1.770953000	-1.185263000	3.280800000
1	4.797641000	-3.231278000	-0.909040000
1	4.271240000	-2.702277000	-0.879280000
1	1.480660000	1.908252000	2.137939000
1	1.904629000	2.336639000	2.579152000
1	1.799825000	3.428447000	-0.711160000
1	1.475318000	2.761914000	-0.616021000
1	4.076784000	-2.139565000	1.937369000
1	4.518227000	-2.569419000	2.359778000
1	4.686911000	-0.750427000	-3.291126000
1	4.178107000	-0.565933000	-2.776427000
1	4.137158000	0.591145000	2.801423000
1	4.645276000	0.775685000	3.317064000
1	4.096465000	2.744752000	0.912172000
1	4.605176000	3.256961000	1.104410000
1	4.572590000	0.002012000	0.010543000
1	4.173436000	2.178899000	-1.888951000
1	4.614630000	2.609358000	-2.310927000

$C_6H_{57}^-$

SCF Energy = -261.98680 a. u.

6	-3.356842000	0.137229000	0.011042000
6	-2.136686000	0.096404000	0.009300000
6	-0.793243000	0.052587000	0.006078000
6	0.440963000	0.021986000	-0.000735000
6	1.782402000	-0.002382000	-0.005365000
6	3.042140000	-0.014878000	-0.010696000
1	3.859159000	-0.003889000	-2.480010000
1	3.983949000	-0.099696000	-3.214456000

$C_6H_{59}^-$

SCF Energy = -263.16016 a. u.

6	3.231034000	0.002150000	0.135228000
6	2.010405000	0.004118000	0.099415000
6	0.667164000	0.004129000	0.058486000
6	-0.567063000	0.000852000	0.024750000
6	-1.907890000	-0.003987000	-0.009039000
6	-3.167276000	-0.009976000	-0.037941000
1	-3.973184000	-2.479328000	-0.083065000
1	-4.097655000	-3.213653000	-0.179958000

1	5.477578000	1.120670000	-0.709989000	1	-5.626700000	-0.745989000	1.077068000
1	6.136280000	1.452715000	-0.847748000	1	-6.283583000	-0.886895000	1.410810000
1	5.977674000	-1.757598000	-0.984575000	1	-6.143838000	-1.047923000	-1.680615000
1	5.446901000	-1.274400000	-0.767828000	1	-5.531872000	-0.767706000	-1.349712000
1	6.132342000	-0.220880000	1.720927000	1	-6.268518000	1.694120000	-0.243732000
1	5.469238000	-0.149722000	1.377553000	1	-5.605540000	1.350807000	-0.170731000
1	3.334980000	-2.354307000	-1.424723000	1	-3.479975000	-1.379444000	-2.411911000
1	3.403806000	-3.017719000	-1.766086000	1	-3.433647000	-1.719407000	-3.077923000
1	4.094659000	2.694973000	1.646845000	1	-4.378252000	1.592770000	2.645180000
1	3.961629000	2.040629000	1.302912000	1	-4.107306000	1.260957000	2.028138000
1	3.988466000	-2.868855000	1.481505000	1	-4.118383000	1.511695000	-2.872635000
1	3.862865000	-2.206295000	1.151152000	1	-3.989853000	1.177696000	-2.212424000
1	3.478574000	2.355395000	-1.276759000	1	-3.632435000	-1.318822000	2.307361000
1	3.566398000	3.020575000	-1.610634000	1	-3.719790000	-1.654869000	2.971410000
1	3.447256000	-0.081716000	2.686668000	1	-3.598683000	2.684435000	-0.051545000
1	3.556532000	-0.177879000	3.421689000	1	-3.707343000	3.419725000	-0.147288000
1	1.375418000	2.750183000	0.182831000	1	-1.544366000	0.120419000	2.752347000
1	1.042402000	3.414527000	0.266866000	1	-1.211181000	0.202305000	3.417107000
1	1.237097000	-2.748482000	-0.026254000	1	-1.343682000	0.062055000	-2.738835000
1	0.901705000	-3.412967000	0.046472000	1	-1.007036000	0.137762000	-3.402482000
1	0.869882000	-1.444911000	-3.026311000	1	-0.943125000	-2.967920000	-1.531339000
1	1.369608000	-1.237050000	-2.510443000	1	-1.446708000	-2.454457000	-1.326840000
1	1.074834000	-1.955697000	2.861365000	1	-1.066453000	2.871212000	-1.815292000
1	1.311545000	-1.462008000	2.351632000	1	-1.490935000	2.425103000	-1.391299000
1	0.872612000	1.539806000	2.964564000	1	-1.048313000	2.930932000	1.606969000
1	1.365871000	1.322639000	2.446004000	1	-1.542460000	2.414881000	1.386004000
1	1.021200000	1.747711000	-2.983047000	1	-1.176302000	-3.029856000	1.697836000
1	1.326762000	1.443157000	-2.372275000	1	-1.486033000	-2.418304000	1.399346000
1	-1.774357000	-2.894450000	1.755048000	1	1.730139000	1.607471000	-2.915987000
1	-1.345269000	-2.449535000	1.335654000	1	1.228640000	1.391966000	-2.406069000
1	-1.715187000	3.010646000	1.812083000	1	1.537195000	1.745193000	3.048944000
1	-1.210108000	2.510007000	1.582728000	1	1.031137000	1.521037000	2.547280000
1	-1.802980000	-0.051946000	3.442123000	1	1.461961000	3.467921000	-0.009398000
1	-1.278095000	-0.038183000	2.911140000	1	1.129896000	2.801986000	0.062888000
1	-1.381650000	-2.297487000	-1.476832000	1	1.317653000	-1.369374000	-2.377916000
1	-1.675897000	-2.906233000	-1.795463000	1	1.615553000	-1.681200000	-2.988287000
1	-4.578844000	-1.790183000	2.727108000	1	4.104557000	3.014108000	-1.725559000
1	-4.134973000	-1.377418000	2.289678000	1	3.669209000	2.572345000	-1.309027000
1	-1.246170000	0.183402000	-2.884676000	1	1.193027000	-2.793612000	0.094512000
1	-1.773099000	0.177664000	-3.413625000	1	1.525963000	-3.458380000	0.171622000
1	-1.579120000	3.203837000	-1.602241000	1	1.404991000	-1.652427000	3.195170000
1	-1.281851000	2.593227000	-1.290434000	1	1.111400000	-1.339610000	2.583309000
1	-3.824740000	-2.796964000	-0.116013000	1	4.125358000	0.011782000	-2.490974000
1	-4.348502000	-3.329606000	-0.128838000	1	4.660456000	0.007684000	-3.013582000
1	-4.558065000	1.697326000	3.011581000	1	4.250022000	3.014112000	1.635389000
1	-4.051787000	1.492906000	2.501835000	1	3.745527000	2.504377000	1.424609000
1	-4.071852000	-1.298105000	-2.345507000	1	3.689016000	-2.570732000	-1.343190000
1	-4.575925000	-1.505158000	-2.857040000	1	4.189247000	-3.080273000	-1.561742000
1	-4.034371000	1.605402000	-2.400724000	1	3.768618000	-2.506064000	1.527483000
1	-4.540727000	1.829283000	-2.902237000	1	4.279179000	-3.008223000	1.740728000
1	-4.416807000	0.192425000	-0.000019000	1	4.291261000	-0.009795000	0.177239000
1	-3.986568000	3.020636000	0.070654000	1	3.868057000	0.021168000	2.882562000
1	-4.511615000	3.551458000	0.084293000	1	4.210100000	0.093897000	3.543278000
1	-6.305856000	-1.364481000	0.110725000	1	6.325521000	-1.628224000	-0.468827000
1	-6.815217000	-1.143060000	-0.386596000	1	6.993190000	-1.715459000	-0.788437000
				1	6.109688000	1.701462000	-0.385582000

				1	6.838353000	1.580843000	-0.487781000
$C_6H_{61}^-$				**$C_6H_{63}^-$**			
SCF Energy = -264.33449 a. u.				SCF Energy = -265.50630 a. u.			
6	3.115728000	-0.011139000	-0.024058000	6	2.942796000	-0.223376000	0.039822000
6	1.894309000	-0.004818000	-0.018888000	6	1.723799000	-0.151768000	0.033890000
6	0.550582000	0.000544000	-0.010202000	6	0.382689000	-0.075705000	0.023235000
6	-0.684358000	0.002666000	-0.003856000	6	-0.850378000	-0.014589000	0.005622000
6	-2.025649000	0.008265000	0.000230000	6	-2.189744000	0.049181000	-0.014297000
6	-3.285622000	0.016266000	-0.000915000	6	-3.448298000	0.106711000	-0.030666000
1	-4.162430000	1.315774000	2.081547000	1	-4.430076000	-2.227129000	0.648349000
1	-4.293206000	1.656862000	2.737784000	1	-4.564592000	-2.954431000	0.777802000
1	-5.727920000	1.411183000	-0.044525000	1	-5.931225000	-0.124088000	1.251003000
1	-6.390816000	1.756403000	-0.107055000	1	-6.594622000	-0.209293000	1.590465000
1	-6.365205000	-0.779550000	1.600543000	1	-6.486783000	-1.122998000	-1.385845000
1	-5.709052000	-0.647498000	1.262236000	1	-5.870924000	-0.826594000	-1.076997000
1	-6.342185000	-1.025326000	-1.482345000	1	-6.459734000	1.889020000	-0.650981000
1	-5.726237000	-0.741674000	-1.161897000	1	-5.804104000	1.543195000	-0.536711000
1	-3.678105000	-1.253315000	2.397332000	1	-3.861955000	-1.860379000	-1.903688000
1	-3.765386000	-1.585963000	3.062919000	1	-3.886824000	-2.391875000	-2.430796000
1	-4.436154000	1.496355000	-2.793342000	1	-4.445836000	2.475938000	2.135037000
1	-4.166321000	1.177731000	-2.169077000	1	-4.249960000	1.957150000	1.628963000
1	-4.282042000	-3.182771000	0.208392000	1	-4.316816000	0.795961000	-3.208494000
1	-4.154416000	-2.449880000	0.106764000	1	-4.190173000	0.675737000	-2.478277000
1	-3.702666000	2.721200000	-0.043523000	1	-3.956198000	-0.496525000	2.589855000
1	-3.813216000	3.455410000	-0.143507000	1	-4.068132000	-0.616432000	3.320900000
1	-3.718765000	-1.397247000	-2.318429000	1	-3.717403000	2.698117000	-0.885434000
1	-3.741028000	-1.914860000	-2.859273000	1	-3.799851000	3.370699000	-1.205052000
1	-1.573764000	2.329760000	-1.483409000	1	-1.758157000	0.850675000	2.622775000
1	-1.253511000	2.932871000	-1.788514000	1	-1.444451000	1.141264000	3.236462000
1	-1.576647000	-2.398587000	1.431407000	1	-1.666317000	-0.779760000	-2.654908000
1	-1.263900000	-3.006717000	1.733627000	1	-1.335390000	-0.892488000	-3.315975000
1	-1.218122000	0.192017000	3.426017000	1	-1.522851000	-3.340986000	-0.624242000
1	-1.552455000	0.114357000	2.761601000	1	-1.855943000	-2.676162000	-0.543175000
1	-1.266941000	-3.138230000	-1.416232000	1	-1.243595000	2.182005000	-2.676020000
1	-1.595733000	-2.478201000	-1.291696000	1	-1.551143000	1.860005000	-2.075184000
1	-1.292363000	-0.025046000	-3.420975000	1	-1.310497000	3.348345000	0.756307000
1	-1.628035000	0.034217000	-2.755089000	1	-1.644119000	2.685818000	0.661027000
1	-1.270559000	3.025794000	1.674571000	1	-1.557046000	-2.258176000	2.523084000
1	-1.582919000	2.416648000	1.373665000	1	-1.854157000	-1.923452000	1.923724000
1	1.505734000	-3.398561000	0.234253000	1	1.528607000	0.552061000	-3.310292000
1	0.998691000	-2.884004000	0.044217000	1	0.999098000	0.537677000	-2.783616000
1	1.458178000	1.604687000	-3.067034000	1	1.313350000	2.422313000	2.427199000
1	0.951761000	1.405004000	-2.555683000	1	0.881613000	1.987463000	2.000390000
1	1.319180000	-1.752832000	-3.052477000	1	1.442477000	3.253765000	-0.895081000
1	1.022012000	-1.438756000	-2.442947000	1	1.111466000	2.593564000	-0.781081000
1	1.104036000	-1.393516000	2.431770000	1	0.860668000	-2.187874000	-1.878495000
1	1.403537000	-1.702514000	3.042827000	1	1.153299000	-2.794790000	-2.201937000
1	3.932452000	-3.164319000	-1.690738000	1	4.267259000	1.935104000	-2.310790000
1	3.436188000	-2.649989000	-1.473425000	1	3.766348000	1.695725000	-1.809247000
1	1.121408000	1.487791000	2.353964000	1	0.674831000	-2.830954000	0.943442000
1	1.416039000	1.807404000	2.962019000	1	1.178400000	-3.342877000	1.149693000
1	1.399400000	3.472483000	-0.092252000	1	1.158188000	-0.889054000	3.471887000
1	1.069574000	2.805724000	-0.019230000	1	0.833040000	-0.784081000	2.807451000
1	3.907728000	-2.260994000	1.365315000	1	3.719709000	-1.164957000	-2.519422000

1	4.420602000	-2.764850000	1.570972000
1	4.354293000	-0.123741000	-3.241956000
1	3.823630000	-0.112586000	-2.715075000
1	3.480932000	0.059521000	2.942442000
1	4.002636000	0.063476000	3.476959000
1	3.860732000	2.315971000	1.244063000
1	4.370942000	2.821836000	1.452534000
1	4.177076000	-0.020202000	-0.029261000
1	3.531545000	2.464793000	-1.414292000
1	3.958175000	2.910124000	-1.836743000
1	5.997071000	0.181370000	1.798127000
1	6.660033000	-0.151005000	1.876502000
1	5.847768000	-1.605156000	-0.942676000
1	6.575144000	-1.484909000	-0.830331000
1	6.011312000	1.663212000	-0.867564000
1	6.742355000	1.762114000	-0.757670000

1	4.326941000	-1.453329000	-2.846990000
1	4.055777000	2.926743000	0.948012000
1	3.549185000	2.411616000	0.754173000
1	3.223420000	-3.130193000	-0.455751000
1	3.742814000	-3.666946000	-0.471071000
1	3.638381000	-1.946181000	2.071889000
1	4.155986000	-2.164646000	2.565781000
1	4.000674000	-0.302147000	0.021586000
1	3.375170000	0.664784000	2.820852000
1	3.701391000	0.946138000	3.431593000
1	5.895295000	-2.109639000	0.034163000
1	6.561070000	-2.432792000	-0.055092000
1	6.335313000	0.298295000	-1.543310000
1	6.999832000	0.206569000	-1.868104000
1	5.710860000	0.683549000	1.337192000
1	6.382248000	0.566722000	1.640768000
1	6.471370000	3.038532000	-0.524925000
1	6.999604000	3.563959000	-0.530472000

$C_2H_8^{2-}$

SCF Energy = -80.63355 a. u.

6	0.634902000	-0.000045000	-0.000083000
6	-0.634901000	-0.000024000	-0.000106000
1	-2.333775000	-1.041094000	-0.325344000
1	-3.037491000	-1.437155000	-0.446814000
1	3.037380000	-1.437199000	0.447129000
1	2.333698000	-1.041092000	0.325616000
1	2.333693000	1.041160000	-0.325365000
1	3.037376000	1.437269000	-0.446846000
1	-3.037268000	1.437316000	0.447213000
1	-2.333619000	1.041211000	0.325546000

$C_2H_{10}^{2-}$

SCF Energy = -81.81425 a. u.

6	0.858192145	0.000393708	-0.002922117
6	-0.411530034	-0.000374128	0.000603262
1	-2.057312025	1.193138589	-0.629407124
1	-2.694378461	1.618106550	-0.851172080
1	3.245028135	1.545752145	0.005198108
1	2.555453028	1.111860139	0.002199790
1	2.555147693	-1.112579820	0.002882958
1	3.244424344	-1.546708897	0.005373795
1	-2.707080831	-0.067489679	1.819138341
1	-2.067308183	-0.049842147	1.344276374
1	-2.695682882	-1.549762779	-0.968371082
1	-2.058265073	-1.142593695	-0.716205952

$C_2H_{12}^{2-}$

SCF Energy = -82.99441 a. u.

6	-0.632512000	-0.376520000	-0.000254000
6	0.636922000	-0.386991000	-0.000856000
1	-1.552534000	1.656594000	-0.001477000
1	-1.910174000	2.350166000	-0.002012000
1	2.425475000	-0.432028000	1.118378000
1	3.121762000	-0.426975000	1.515699000
1	-3.118219000	-0.434913000	1.517182000
1	-2.421942000	-0.434084000	1.120383000
1	-2.423602000	-0.436534000	-1.118223000
1	-3.120349000	-0.438111000	-1.514185000
1	1.889211000	2.360720000	0.003309000
1	1.534245000	1.666746000	0.001757000
1	3.123128000	-0.421921000	-1.515468000
1	2.426537000	-0.428594000	-1.118684000

$C_2H_{14}^{2-}$

SCF Energy = -84.17474 a. u.

6	-0.621764000	-0.471562000	-0.303546000
6	0.647829000	-0.457862000	-0.314954000
1	-1.468448000	0.671804000	1.462119000
1	-1.789987000	1.042709000	2.062949000
1	2.470638000	-1.344497000	0.271219000
1	3.163577000	-1.667463000	0.513311000
1	-3.141545000	-1.694790000	0.501006000
1	-2.446755000	-1.369163000	0.267785000
1	-2.369992000	0.615523000	-0.901732000
1	-3.021791000	1.025349000	-1.098350000
1	-0.101835000	2.776019000	-0.487991000
1	-0.038303000	2.011926000	-0.425851000
1	1.760606000	1.072898000	2.072765000
1	1.447853000	0.697391000	1.470480000
1	3.011584000	1.082663000	-1.096306000
1	2.368011000	0.656171000	-0.900404000

$C_2H_{16}^{2-}$

$C_2H_{18}^{2-}$

SCF Energy = -85.35527 a. u.

6	0.630674000	0.001480000	-0.666840000
6	-0.639863000	-0.001284000	-0.681024000
1	1.407728000	0.002067000	1.527235000
1	1.701988000	0.002983000	2.239430000
1	-0.001722000	2.724674000	1.106857000
1	-0.001111000	2.093279000	0.668479000
1	-2.426716000	1.176753000	-0.436294000
1	-3.079300000	1.610048000	-0.305824000
1	3.074854000	1.612826000	-0.325113000
1	2.420038000	1.179653000	-0.445713000
1	2.419831000	-1.180492000	-0.449249000
1	3.074036000	-1.614511000	-0.330138000
1	0.007661000	-2.718438000	1.117026000
1	0.006313000	-2.089248000	0.675587000
1	-1.670681000	0.001839000	2.250543000
1	-1.380641000	-0.000195000	1.537190000
1	-3.074409000	-1.618778000	-0.306196000
1	-2.422739000	-1.183637000	-0.436640000

SCF Energy = -86.53425 a. u.

6	0.577915000	0.005900000	-0.566786000
6	-0.689229000	-0.008958000	-0.663146000
1	1.863666000	-0.016093000	1.330832000
1	2.297539000	-0.023128000	1.971937000
1	0.721130000	2.618643000	1.271899000
1	0.600512000	2.011206000	0.818342000
1	-1.761506000	1.977561000	-0.112246000
1	-2.144985000	2.613903000	0.102226000
1	3.161633000	1.537164000	-0.762741000
1	2.482215000	1.141333000	-0.737376000
1	2.460059000	-1.174034000	-0.740735000
1	3.129761000	-1.584115000	-0.767498000
1	0.654842000	-2.636405000	1.264529000
1	0.541262000	-2.025850000	0.814100000
1	-1.476321000	0.017428000	2.372864000
1	-1.223959000	0.011748000	1.645342000
1	-3.692424000	0.037659000	-0.515383000
1	-2.903299000	0.024980000	-0.583830000
1	-1.821822000	-1.943566000	-0.106147000
1	-2.220418000	-2.570089000	0.113474000

$C_2H_{20}^{2-}$

SCF Energy = -87.71400 a. u.

6	0.708374000	0.035546000	-0.597141000
6	-0.551490000	-0.093998000	-0.490829000
1	1.962468000	2.506463000	0.799751000
1	1.640592000	1.901791000	0.444751000
1	2.938082000	0.220950000	-0.481340000
1	3.720929000	0.276390000	-0.401833000
1	2.453582000	-2.517226000	-0.501584000
1	2.004555000	-1.889991000	-0.553519000
1	-0.332958000	-2.399605000	0.335298000
1	-0.382857000	-3.111927000	0.613905000
1	-3.008597000	-1.781915000	-1.020184000
1	-2.370619000	-1.340097000	-0.908764000
1	1.273135000	-0.489643000	1.657531000
1	1.537383000	-0.647935000	2.362248000
1	-0.637716000	3.157598000	-1.068054000
1	-0.485128000	2.411728000	-0.975375000
1	-3.233466000	1.278676000	-0.221899000
1	-2.545421000	0.916321000	-0.311516000
1	-0.839419000	1.961715000	1.984772000
1	-0.684297000	1.495430000	1.398018000
1	-2.178871000	-0.899242000	2.000767000
1	-1.772677000	-0.698771000	1.374847000

$C_2H_{22}^{2-}$

SCF Energy = -88.89406 a. u.

6	0.740884133	-0.000169866	-0.457521887
6	-0.527375930	-0.000071968	-0.387164067
1	0.402748337	2.989920250	0.955343796
1	0.355365277	2.303113269	0.621496983
1	2.550649157	1.150232898	0.353152787
1	3.161835121	1.531217763	0.642149183
1	3.251701060	0.001364748	-2.146515963
1	2.588568940	0.000949873	-1.726688959
1	3.161727169	-1.531103460	0.640482804
1	2.549864916	-1.150524475	0.352171163
1	0.354776832	-2.304021338	0.621429777
1	0.402782734	-2.990884411	0.955032111
1	-1.883693203	-2.644604049	-1.401957223
1	-1.514298378	-2.004136061	-1.187838350
1	0.611526754	-0.002100834	2.049941115
1	0.722812200	-0.002599848	2.808136223
1	-1.882572935	2.646678423	-1.398323892
1	-1.513232086	2.005944260	-1.184971268
1	-3.570136115	0.002791410	-0.805191869
1	-2.794860224	0.001764277	-0.714321022
1	-2.278077894	1.550284548	1.664694257
1	-1.837845815	1.175177255	1.155962829
1	-2.280564498	-1.552043004	1.660904289
1	-1.840125511	-1.175972079	1.153028012

$C_2H_{24}^{2-}$

SCF Energy = -90.07454 a. u.

6	-0.634685667	-0.053424148	-0.381038312
6	0.635476258	-0.056041987	-0.382228960

$C_2H_{26}^{2-}$

SCF Energy = -91.25406 a. u.

6	-0.597614155	0.029564075	-0.071025112
6	0.661856273	0.106485809	-0.207536967

1	1.552428245	-2.990086412	0.375230062
1	1.285565217	-2.297151029	0.185213096
1	-1.268772835	-2.304400229	0.183332929
1	-1.533183656	-2.998212457	0.372951954
1	-3.023803998	1.805235796	-0.981515845
1	-2.418454330	1.342413141	-0.841797176
1	-3.068697809	-1.224234103	-1.877122409
1	-2.447148967	-0.927176221	-1.520316182
1	-3.245665264	-0.525450254	1.230747216
1	-2.599022837	-0.406608156	0.823830021
1	-1.277135952	1.526584816	1.342315243
1	-1.542842199	2.010214191	1.872266149
1	-0.008328192	3.222805336	-0.765789860
1	-0.007044937	2.460654099	-0.699305089
1	0.000649300	-0.755254999	2.044646167
1	0.000624958	-0.969313017	2.779465929
1	3.077985398	-1.211087223	-1.877898183
1	2.454616187	-0.918766007	-1.520163250
1	3.008149348	1.824322161	-0.977312061
1	2.411852315	1.347976381	-0.844581177
1	3.248128584	-0.508185846	1.234057220
1	2.601539604	-0.394192070	0.825757284
1	1.528931188	2.015913959	1.872441307
1	1.264889203	1.530794950	1.343150285

1	-1.695430988	-0.528992037	1.915618995
1	-2.064335265	-0.710633186	2.566073086
1	1.086044227	-1.271621396	2.730832952
1	0.876831885	-0.957449922	2.067213990
1	2.323906231	-2.532040110	-0.126508288
1	1.907823156	-1.886607382	-0.144574929
1	2.717698244	0.272006631	0.824805823
1	3.402065188	0.325517035	1.183682192
1	-0.696886219	-3.113626015	0.697338137
1	-0.595887979	-2.381507175	0.505260025
1	-2.571713058	-1.107038276	-0.381837369
1	-3.229823285	-1.502117776	-0.493386346
1	-3.132865842	1.600115053	0.689153881
1	-2.500450874	1.197763069	0.494466926
1	0.233970958	2.112157013	2.429428937
1	0.190083114	1.637353256	1.831109918
1	2.303233393	2.715126971	-0.516992943
1	1.892140459	2.067063174	-0.447214043
1	-0.645207828	2.502703052	-0.600988189
1	-0.805709933	3.237958327	-0.730947242
1	-2.404454946	0.815255232	-2.511976355
1	-1.932179068	0.628503289	-1.935716089
1	2.401670415	-0.057866061	-1.656339077
1	2.999364476	-0.128754116	-2.149632288
1	-0.252255090	-2.135406416	-2.562291057
1	-0.193084078	-1.614161005	-2.005208175

$C_2H_{28}^{2-}$

SCF Energy = -92.43480 a. u.

6	-0.643493823	0.024085502	-0.052347801
6	0.623411017	0.004558862	0.022623915
1	-3.089072191	-1.264593922	1.354622319
1	-2.474769902	-0.945853532	1.014152852
1	-2.129834179	1.413568431	1.104401915
1	-2.595122272	1.866208657	1.517080263
1	-3.399258432	0.414394470	-1.421394962
1	-2.711959316	0.313922232	-1.079177094
1	0.130709956	-0.051675217	-2.546146388
1	0.223549341	-0.132386389	-3.300387484
1	1.905690043	2.494277492	-1.444156992
1	1.581473726	1.884568991	-1.113874187
1	-1.211201525	2.811511845	-1.497251992
1	-1.051972091	2.144391845	-1.159111963
1	0.392366409	2.955091920	1.489968925
1	0.319074831	2.276088187	1.150152992
1	2.456485241	0.953527131	1.105091962
1	3.071772858	1.270997496	1.446957928
1	3.379488370	-0.382197739	-1.343241303
1	2.694427145	-0.285603841	-0.997907110
1	-0.080913847	-0.047290454	2.519328214
1	-0.167102004	-0.126968143	3.274269411
1	-1.880555711	-2.465016636	-1.531370166
1	-1.566337669	-1.850445526	-1.198691246
1	1.331280310	-2.789631424	-1.393200927
1	1.091639218	-2.144139957	-1.062967865

$C_2H_{30}^{2-}$

SCF Energy = -93.61378 a. u.

6	-0.635383123	-0.000394766	0.001027133
6	0.634470292	-0.000505893	-0.000468851
1	-1.263921867	-1.731407103	-1.606192124
1	-1.515112782	-2.259895893	-2.096514005
1	-3.185760283	1.360845443	1.258491979
1	-2.570521350	1.021914294	0.946036098
1	-2.564990919	0.309790945	-1.361196287
1	-3.178075042	0.412068207	-1.813707395
1	-3.178702117	-1.777005249	0.547222193
1	-2.565143851	-1.334111938	0.410857979
1	-0.001638862	-2.433047980	0.752004793
1	-0.002062733	-3.162332019	0.977343811
1	1.516201300	-2.260533022	-2.094644421
1	1.266241251	-1.731300210	-1.604406151
1	0.000167220	0.737986358	-3.224104466
1	0.000578920	0.566632944	-2.480227307
1	1.515849397	2.943951151	-0.913643042
1	1.266194154	2.255584157	-0.697718086
1	2.568811050	0.308806146	-1.358743022
1	3.184227256	0.411657036	-1.807884329
1	3.180013418	-1.775068989	0.550399903
1	2.566133413	-1.333225036	0.412534941
1	-1.265128921	2.254835371	-0.693459268
1	-1.515447222	2.944001423	-0.906302295
1	-1.514954029	-0.679251917	3.006291936
1	-1.265287145	-0.521089833	2.302315270

1	-0.415460762	-2.958429441	1.420060377
1	-0.332904878	-2.277639206	1.086716282
1	2.555539284	-1.852867041	1.598338076
1	2.093464356	-1.395679065	1.186080952
1	1.516800328	-0.682904827	3.006076031
1	1.266396300	-0.523256814	2.302803172
1	-0.000193679	2.427465160	2.246637357
1	-0.001035071	1.867127309	1.728230981
1	3.180045169	1.363208219	1.261159033
1	2.565794210	1.023962210	0.946989146

$C_2H_{32}^{2-}$

SCF Energy = -94.79025 a. u.

6	-0.624909118	0.016629924	-0.013200856
6	0.645249104	-0.014369279	0.018713824
1	-3.048909225	-0.094454435	-0.202795010
1	-3.814021209	-0.130222583	-0.265260150
1	-2.100574911	1.925851167	1.994165304
1	-1.735855896	1.461988149	1.504830868
1	-0.011901726	-0.233124274	3.421820433
1	0.000595854	-0.183303824	2.663736981
1	0.159520482	2.626872906	-0.059574246
1	0.193500540	3.386501026	-0.079904177
1	-2.502362262	-1.435961095	2.136757405
1	-2.054946073	-1.089076942	1.623470291
1	-1.404819543	-2.193092028	-0.606291074
1	-1.688732662	-2.878033129	-0.791760821
1	-2.109611142	-0.282888632	-2.847363074
1	-1.748836085	-0.217986630	-2.177692970
1	-2.353420034	2.376486341	-1.316586116
1	-1.940080743	1.814920269	-1.002866030
1	3.020552733	2.104992483	-0.242217127
1	2.459269242	1.588700700	-0.177199764
1	0.607925174	1.294642194	-2.166710954
1	0.732291352	1.680729915	-2.812406154
1	0.590255945	-1.592880141	-2.936618342
1	0.492632797	-1.233481475	-2.273243330
1	1.235311370	1.644711995	1.846850295
1	1.471025438	2.129842646	2.383186254
1	0.200394662	-2.837998224	1.896044200
1	0.180757952	-2.206607215	1.473557022
1	1.915554965	-2.962425788	-0.545248891
1	1.603237728	-2.280618474	-0.411177073
1	3.258264445	-0.493502765	-1.756758927
1	2.638313189	-0.378624205	-1.320489328
1	3.118953243	-0.759152390	1.727476375
1	2.513673955	-0.566371530	1.287190849

$C_2H_{34}^{2-}$

SCF Energy = -95.96886 a. u.

6	0.634170249	-0.000363545	-0.001311830
6	-0.637033098	-0.001444654	-0.000438688
1	3.161510206	-0.002245828	0.003885219
1	3.925491338	-0.002117767	0.005212925
1	2.442928249	-2.562374137	-0.794930063
1	2.016909342	-1.958137858	-0.607517178
1	-0.005038826	-3.166325190	1.071799304
1	-0.004314911	-2.444515251	0.828819104
1	0.001690192	-1.542533160	-2.071972881
1	0.002737963	-2.000526014	-2.680514017
1	2.441031148	-1.552739930	2.187643090
1	2.014492060	-1.186413805	1.672365210
1	2.014142274	1.223372602	1.646645079
1	2.439545219	1.601815299	2.154017050
1	2.449014846	2.538674405	-0.855545201
1	2.021786239	1.940003483	-0.653672018
1	2.445090467	-0.034968562	-2.679328130
1	2.019345145	-0.024769729	-2.046499875
1	-2.436961246	-0.028814760	-2.684755372
1	-2.012892887	-0.020579174	-2.050804203
1	0.004847793	1.495106178	-2.103945241
1	0.006212012	1.935015458	-2.725663949
1	0.003050707	3.195721515	0.989969980
1	0.002768126	2.467836093	0.766325916
1	-2.018803796	-1.955671363	-0.612717932
1	-2.444343798	-2.559509172	-0.802728019
1	-0.003286720	0.035587170	3.342468188
1	-0.003085103	0.029202117	2.580922329
1	-2.440294004	1.606318069	2.149367170
1	-2.015203274	1.227136111	1.642219041
1	-2.441250228	2.542824213	-0.858351957
1	-2.014766174	1.943681265	-0.656405218
1	-3.925701422	0.002001878	-0.002007169
1	-3.161619217	0.000641892	-0.002187090
1	-2.447869177	-1.549312979	2.186159277
1	-2.019984920	-1.182532290	1.672230270

$C_2H_{36}^{2-}$

SCF Energy = -97.14482 a. u.

6	0.634339056	0.003965125	0.001584886
6	-0.638169770	-0.004450910	-0.006050083
1	2.785571576	-1.242770123	-0.655773910
1	3.419140679	-1.615324136	-0.854060858
1	3.521753440	-0.003858760	1.677860187
1	2.867482393	-0.001743639	1.288549247

$C_2H_{38}^{2-}$

SCF Energy = -98.32119 a. u.

6	0.631410060	-0.003584118	0.010185075
6	-0.642089915	-0.007183052	-0.004248764
1	2.482254056	-1.379543392	1.227437213
1	2.948302047	-1.816791969	1.637117243
1	3.079697287	1.346198346	1.639188972
1	2.482868431	1.027205538	1.283695104

1	1.825775282	2.647536220	1.395403892
1	1.526215979	2.028122079	1.065504212
1	0.899291225	0.159614146	2.550937030
1	1.062478376	0.209628805	3.291210492
1	3.514960391	1.375091424	-0.987718331
1	2.864286162	1.056472215	-0.753960102
1	1.366327190	-0.113634993	-2.346281962
1	1.634359171	-0.143278974	-3.059816098
1	0.900016198	-3.016402396	-1.418494012
1	0.760316050	-2.338998895	-1.104752230
1	1.690606479	-2.586605164	1.622523063
1	1.414006060	-1.984133161	1.245815009
1	-1.020976063	-1.840954202	2.742479085
1	-0.859825715	-1.424420268	2.127932316
1	-1.529340771	-2.291342251	-0.086707809
1	-1.831417899	-2.991638488	-0.108921082
1	-1.092821929	-1.451492977	-2.969327317
1	-0.922280802	-1.128710201	-2.303311182
1	-1.379161855	1.094218957	2.084755157
1	-1.646360911	1.425559058	2.717203992
1	1.069097855	2.743582420	-1.854201096
1	0.901639185	2.131695296	-1.436853288
1	-1.675538157	1.656540165	-2.562742974
1	-1.403267995	1.271846826	-1.962811023
1	-3.493538238	-0.844935197	1.496376203
1	-2.846162900	-0.649619049	1.146442930
1	-3.423842419	1.818926141	0.110468926
1	-2.791217368	1.396181783	0.083977254
1	-0.906384317	3.322483280	0.285888009
1	-0.767496986	2.579049042	0.217198156
1	-3.534380138	-0.701323371	-1.503390977
1	-2.876323887	-0.542446369	-1.154610252

1	2.736407305	2.187693891	-1.285195322
1	2.239681322	1.672555714	-1.028536948
1	0.279733148	1.688494004	2.103738332
1	0.297086458	2.206690295	2.656811109
1	3.938717065	-0.425756964	-0.754924263
1	3.198458949	-0.318162529	-0.623388262
1	1.657132843	-2.122043632	-0.873685926
1	1.982074662	-2.751157592	-1.152389295
1	0.317325371	-3.074557388	1.492595232
1	0.245394307	-2.394693213	1.161829288
1	0.897929123	-0.646244486	3.341912022
1	0.774485830	-0.517337437	2.604792986
1	-1.920820279	0.151726230	2.994500279
1	-1.585497060	0.098635993	2.313245955
1	-2.109542349	-1.819408751	0.941242281
1	-2.584881633	-2.334437917	1.239370160
1	-0.909655691	-3.065794213	-1.368452366
1	-0.791489353	-2.390483079	-1.041299115
1	-1.787511004	2.066587444	0.856935878
1	-2.130606778	2.680766434	1.146267244
1	1.882307288	-0.291172373	-3.019927246
1	1.551730260	-0.218762404	-2.338898352
1	-1.023543102	-0.575233133	-3.292478400
1	-0.890369297	-0.467956733	-2.552162075
1	-3.931732455	0.382319450	0.731908228
1	-3.191230388	0.275287530	0.595958889
1	-2.709156794	1.722886820	-1.797537326
1	-2.251563997	1.292337627	-1.364307321
1	0.069597392	2.201111180	-2.649749239
1	0.075005054	1.680927298	-2.097891982
1	-3.380869522	-1.339322746	-1.541474276
1	-2.762610575	-1.042657513	-1.216652051
1	0.392610360	2.815266357	0.040594245
1	0.496361380	3.559429272	-0.045808229

$C_2H_{40}^{2-}$

SCF Energy = -99.49550 a. u.

6	0.635606965	0.027146264	-0.000215904
6	-0.637994083	-0.015990678	0.010930156
1	0.328553983	2.646249261	0.523071073
1	0.427756196	3.389710486	0.635996968
1	3.641460213	1.311593329	0.001625103
1	2.953994406	0.975957896	0.002644828
1	3.211296260	-0.895036111	2.168287902
1	2.678546006	-0.697222247	1.668772097
1	2.354005304	0.007666191	-2.097672374
1	2.738457338	-0.001318181	-2.749532489
1	1.969347420	1.722171373	2.598358190
1	1.650992270	1.377564269	2.002608856
1	-0.798108831	1.331830125	2.273307361
1	-0.924851016	1.688960209	2.930496291
1	-2.464948902	2.862195383	0.651652148
1	-2.105334860	2.206879212	0.536435973
1	1.687887037	2.583617429	-1.976627311

$C_2H_{42}^{2-}$

SCF Energy = -100.67056 a. u.

6	-0.689153000	0.248932000	0.019873000
6	0.393040000	-0.425960000	-0.005882000
1	-0.343485000	0.314313000	2.689875000
1	-0.437227000	0.429179000	3.434256000
1	-3.310764000	1.784069000	1.223009000
1	-2.690551000	1.445607000	0.929681000
1	-1.603001000	3.547606000	-0.685296000
1	-1.462490000	2.813649000	-0.566354000
1	-3.248124000	-0.566019000	-0.254846000
1	-3.932828000	-0.877079000	-0.342054000
1	-0.539537000	3.033307000	1.933106000
1	-0.559642000	2.369334000	1.567027000
1	1.633172000	1.264372000	1.588382000
1	2.067729000	1.696499000	2.035226000
1	2.068082000	-1.119948000	2.947276000
1	1.719927000	-0.984890000	2.288987000
1	-2.840267000	-0.965106000	2.357382000

1	1.443215057	2.047212148	-1.501294377
1	-0.058502662	0.493604896	-3.419873060
1	0.022715992	0.389671309	-2.673229363
1	-2.798662892	0.650554105	-1.113692150
1	-3.454901948	0.842332174	-1.452044379
1	-3.347664179	0.271787023	1.904025251
1	-2.778740956	0.224827304	1.400159079
1	0.788215863	-1.810264039	-1.798708924
1	0.964804956	-2.337859048	-2.316546434
1	-1.687252025	-2.233370883	2.219285243
1	-1.446555224	-1.723048220	1.709513982
1	-1.956383107	-1.548326063	-2.691229327
1	-1.644180172	-1.220835197	-2.082425190
1	-1.092275289	-3.447314076	-0.498754849
1	-0.968667950	-2.709419266	-0.391578993
1	1.165757371	-2.987763323	1.273555010
1	1.018958310	-2.317582034	0.945741875
1	-3.604647997	-1.821741893	-0.174178162
1	-2.935900249	-1.471708077	-0.108972942
1	2.800218144	-1.447772331	-0.442161988
1	3.351423454	-1.945206354	-0.597822122
1	-1.192681909	2.765674511	-1.969150037
1	-0.983302876	2.217809368	-1.490962191
1	0.583169204	-0.794494021	3.387556206
1	0.477109912	-0.664518035	2.649079301

1	-2.332390000	-0.741319000	1.841146000
1	-1.991698000	-3.016382000	0.155728000
1	-1.635169000	-2.348189000	0.109358000
1	1.532006000	-2.603063000	0.585142000
1	1.867702000	-3.273206000	0.721519000
1	3.647680000	-0.392147000	0.532531000
1	2.896702000	-0.463978000	0.411754000
1	-1.658720000	-1.022986000	-1.996937000
1	-1.999972000	-1.328856000	-2.602971000
1	4.392754000	2.761095000	0.012323000
1	3.853894000	2.242048000	0.025097000
1	2.609325000	0.949365000	-2.002911000
1	2.083390000	0.683572000	-1.520827000
1	0.129222000	-3.299515000	-1.777397000
1	0.184846000	-2.632933000	-1.419083000
1	0.752969000	-0.862667000	-3.465580000
1	0.637678000	-0.739197000	-2.728108000
1	-0.265176000	1.786186000	-2.889510000
1	-0.325073000	1.429214000	-2.220712000
1	2.920217000	-2.019278000	-1.772752000
1	2.331342000	-1.689453000	-1.428225000
1	-2.636722000	1.168017000	-1.539338000
1	-3.158047000	1.395711000	-2.040299000
1	-0.445567000	-2.573445000	2.598394000
1	-0.302653000	-2.055603000	2.064937000
1	1.251788000	3.096215000	-0.502203000
1	0.915358000	2.428068000	-0.380673000

$C_4H_2^{2-}$

SCF Energy = -153.33660 a. u.

6	0.000000000	0.000000000	0.350891084
6	0.000000000	0.000000000	-1.034707683
6	0.000000000	0.000000000	-2.294237379
6	0.000000000	0.000000000	1.608688253
1	0.000000000	0.000000000	4.512486494
1	0.000000000	0.000000000	3.703706803

$C_4H_4^{2-}$

SCF Energy = -154.51697 a. u.

6	-0.691961167	-0.031596115	-0.002706212
6	0.692134208	-0.031640037	0.002379710
6	1.949295306	-0.031030954	0.007221153
6	-1.949133907	-0.030599674	-0.006920051
1	4.865577367	0.229402042	-0.014294136
1	4.066345622	0.145814791	-0.005745807
1	-4.866536236	0.228596105	0.014351816
1	-4.067393922	0.145387216	0.005838942

$C_4H_6^{2-}$

SCF Energy = -155.69614 a. u.

6	0.438354029	-0.009777079	-0.042994064
6	-0.944125239	-0.033174122	-0.038833143
6	-2.201041328	-0.054173992	-0.034209192
6	1.694672148	0.011841928	-0.046905213
1	-5.125786521	0.208649298	0.273263956
1	-4.337406084	0.123435356	0.177779743
1	3.558114267	-1.132386395	0.118354725
1	4.244580457	-1.511010071	0.188329950
1	4.205841507	1.608972951	0.138256023
1	3.527495542	1.214036857	0.081663691

$C_4H_8^{2-}$

SCF Energy = -156.87525 a. u.

6	-0.690653041	-0.000175687	-0.000123827
6	0.690853070	-0.000008996	-0.000351903
6	1.947138380	0.000111127	-0.000900660
6	-1.946944172	-0.000420167	0.000386299
1	4.507539215	-1.509569121	0.424731419
1	3.825688509	-1.137852796	0.316721050
1	4.506366559	1.509827360	-0.421872803
1	3.824063406	1.138405257	-0.314943015
1	-3.824990524	1.138892100	0.316152185
1	-4.507081477	1.510323199	0.423565112
1	-4.508127131	-1.509081220	-0.422921632
1	-3.825823449	-1.137981915	-0.315492830

$C_4H_{10}^{2-}$

$C_4H_{12}^{2-}$

SCF Energy = -158.05407 a. u.

6	0.914880258	0.001102805	-0.002670758
6	-0.466094029	0.002630011	-0.007349214
6	-1.721767081	0.004974795	-0.013119892
6	2.171074550	-0.000717564	0.001841008
1	-3.519114962	1.348505030	-0.343766241
1	-4.152315228	1.785339261	-0.450125047
1	-4.101966130	-0.497355175	1.813325329
1	-3.480455918	-0.374257963	1.364214185
1	-4.149016337	-1.312181245	-1.296696989
1	-3.516597136	-0.988821137	-0.983002304
1	4.050276625	-1.203213595	0.004480015
1	4.716325570	-1.614040352	0.005122965
1	4.715400568	1.609357663	0.007883153
1	4.048901294	1.198726701	0.006358065

SCF Energy = -159.23291 a. u.

6	-0.690085233	-0.003767213	-0.000532881
6	0.690114867	-0.003782030	-0.000849329
6	1.945552965	-0.003794201	-0.001128206
6	-1.945522273	-0.003735991	-0.000198971
1	3.745680084	-0.386062320	1.346832829
1	4.375461337	-0.508400163	1.781923951
1	4.365299017	1.810119044	-0.439422967
1	3.738120258	1.367180753	-0.333131895
1	4.383216958	-1.273505267	-1.335744449
1	3.751586231	-0.963869371	-1.009889270
1	-3.750269638	-0.920701208	-1.050527437
1	-4.381423577	-1.216242997	-1.390085132
1	-4.377694465	-0.582830001	1.756956839
1	-3.747341701	-0.442341908	1.328203144
1	-4.365055595	1.827050070	-0.363527307
1	-3.737941396	1.380078919	-0.275331981

$C_4H_{14}^{2-}$

SCF Energy = -160.41120 a. u.

6	0.844340931	-0.105465026	-0.016573831
6	-0.534084839	-0.087147026	-0.047260291
6	-1.789073136	-0.065498914	-0.077621306
6	2.099251968	-0.124513290	0.012491758
1	-3.607676479	0.136771152	1.346952953
1	-4.191610343	0.193555046	1.847094246
1	-4.539988364	0.262090908	-1.472632020
1	-3.849980391	0.173918865	-1.138915384
1	-3.132380057	2.747645972	0.028496724
1	-2.779719934	2.067116092	-0.008761059
1	-3.779592408	-2.441719079	0.022257724
1	-3.249869048	-1.883847193	0.001283784
1	3.715464592	1.516861713	-0.100075885
1	4.267622422	2.055485834	-0.125041938
1	4.673544235	-0.569902201	1.656340136
1	4.002628448	-0.471069354	1.284923854
1	4.711533341	-0.819317197	-1.459127946
1	4.037413385	-0.671842377	-1.109016340

$C_4H_{16}^{2-}$

SCF Energy = -161.58911 a. u.

6	-0.690693258	-0.080280951	-0.073343967
6	0.686150271	-0.073966279	-0.129836284
6	1.940579228	-0.071690288	-0.181833240
6	-1.944833284	-0.081607069	-0.017767126
1	3.621958443	0.711249148	1.229669282
1	4.171348147	0.949801194	1.711954018
1	4.916200579	-0.640405015	-0.949376265
1	4.169998215	-0.516002323	-0.804569027
1	3.570137174	-2.173837384	1.464203285
1	3.136300202	-1.698885457	1.047079848
1	3.735922585	2.258153841	-1.213893979
1	3.249383264	1.711268205	-0.981097266
1	-3.222824387	2.422506240	1.370020318
1	-2.891259914	1.812227815	1.046835897
1	-3.440639034	-1.656813220	-0.858648296
1	-3.959735986	-2.167615318	-1.107419283
1	-4.616655564	-0.531755401	1.521749194
1	-3.939613492	-0.431659936	1.169231949
1	-4.546829039	1.042905697	-1.267049305
1	-3.900909997	0.754129968	-0.962009313

$C_4H_{18}^{2-}$

SCF Energy = -162.76694 a. u.

6	0.805151122	-0.056008120	-0.017115180
6	-0.571196039	-0.018648206	-0.042700900
6	-1.826053100	0.015024930	-0.073691107
6	2.059906052	-0.084640843	0.006838028
1	-2.757640013	1.967533400	-1.077133940
1	-3.083471379	2.589729426	-1.380703878
1	-3.230645097	-1.195629956	1.384620318
1	-3.692278162	-1.609175096	1.835296239
1	-4.911793591	-0.089366925	-0.704758789

$C_4H_{20}^{2-}$

SCF Energy = -163.94406 a. u.

6	-0.680165277	-0.044055064	-0.140270072
6	0.695241007	-0.046440066	-0.193501070
6	1.950054147	-0.043584097	-0.240707384
6	-1.934342345	-0.040949852	-0.082475978
1	3.264835239	-1.795783103	-1.163100372
1	3.743747529	-2.339388899	-1.412645016
1	3.005933153	1.139296392	1.556182758
1	3.355345187	1.481570353	2.142710120
1	5.097514168	0.300398049	-0.233660331

1	-4.157700136	-0.024837993	-0.576783093
1	-3.698617176	1.726201058	1.744194142
1	-3.236919023	1.298571864	1.306054431
1	-3.057844383	-2.655912037	-1.232299822
1	-2.729104130	-2.024097156	-0.954935801
1	3.114918266	2.043819063	0.079303032
1	3.471752540	2.719622332	0.118860089
1	4.726096299	0.151271138	1.615880301
1	4.050200424	0.081470013	1.256010138
1	4.034496031	-2.497098007	0.017480312
1	3.509247394	-1.936922084	0.015938290
1	4.761615205	0.199130986	-1.518452949
1	4.080839257	0.121323939	-1.168555131

1	4.340053029	0.200053342	-0.296038158
1	3.703218373	-1.766151823	1.732860224
1	3.257977102	-1.343697983	1.277276713
1	3.199644306	2.783096614	-0.926889406
1	2.865224923	2.108513099	-0.797031955
1	-2.890449215	2.764435178	1.103362081
1	-2.596326150	2.124249243	0.812325707
1	-2.694650987	-1.944711044	1.204485737
1	-2.991456981	-2.550775101	1.560573870
1	-4.737773653	0.195325673	1.334667044
1	-4.053410413	0.126307730	0.995858665
1	-4.283906264	1.441048076	-1.531440017
1	-3.680504497	1.099809185	-1.203624236
1	-4.351636189	-1.670032068	-1.245858402
1	-3.738105441	-1.303388965	-0.968287472

$C_4H_{22}^{2-}$

SCF Energy = -165.12243 a. u.

6	-0.822265243	-0.052388018	-0.116133768
6	0.553370174	-0.067503967	-0.110702822
6	1.808777051	-0.076276667	-0.100125098
6	-2.077453040	-0.038192839	-0.113418031
1	3.245617109	-1.766415883	-1.017676114
1	3.746108189	-2.286252095	-1.269333234
1	2.636683853	0.868090406	1.984634292
1	2.948334327	1.167109948	2.612178183
1	4.949712316	0.257555859	0.315534106
1	4.200025320	0.156199894	0.205202766
1	3.376076235	-2.020317243	1.876120147
1	2.955295124	-1.573428115	1.423722284
1	3.680643142	0.699234179	-2.538602966
1	3.184605089	0.503250210	-1.992123209
1	3.119182906	2.829922450	-0.210008225
1	2.774764189	2.151292317	-0.171045962
1	-3.006517365	2.688915235	1.275236206
1	-2.722370350	2.058570408	0.955608914
1	-2.911232122	-2.048793859	0.947555895
1	-3.222525401	-2.669698163	1.262361853
1	-4.900761304	0.121886983	1.277766202
1	-4.214826408	0.067578051	0.940444282
1	-4.396250594	1.613111117	-1.464105387
1	-3.801971314	1.242487014	-1.154490129
1	-4.514617490	-1.495344837	-1.463940284
1	-3.900546452	-1.158784931	-1.152759190

$C_4H_{24}^{2-}$

SCF Energy = -166.29953 a. u.

6	-0.741850939	-0.002615723	-0.059421842
6	0.633180158	-0.018710120	-0.060563278
6	1.888366367	-0.032539109	-0.055006917
6	-1.997389052	0.009972345	-0.059819255
1	3.055058265	-2.124542407	0.275218208
1	3.414191284	-2.789586444	0.376151889
1	2.873642545	1.878571296	1.076443893
1	3.203783531	2.482672106	1.402339289
1	5.051477335	0.138569825	0.275211858
1	4.298013600	0.058058153	0.174000888
1	3.187822487	-0.536426977	2.807850996
1	2.849042153	-0.426974072	2.133918898
1	3.765068080	-1.093764394	-2.388001238
1	3.272765489	-0.858088956	-1.854563054
1	3.536415354	2.031532097	-1.833253086
1	3.105806363	1.570001163	-1.405886894
1	-2.194417087	3.193209511	0.619428958
1	-2.075854925	2.454651112	0.489298981
1	-3.208046054	-1.398633990	1.489419110
1	-3.636137219	-1.840779045	1.939656343
1	-4.642055014	1.156912173	1.241327057
1	-4.007933449	0.864023149	0.929073850
1	-3.880752048	1.818575297	-1.841472267
1	-3.424960041	1.377823037	-1.415217876
1	-2.221879270	-3.168304313	-0.763285264
1	-2.101063341	-2.430342297	-0.631606914
1	-4.793492313	-1.206801946	-0.930033249
1	-4.120331226	-0.886998967	-0.757154216

$C_4H_{26}^{2-}$

SCF Energy = -167.47710 a. u.

6	-0.628801745	0.061375036	-0.062860965
6	0.745048228	0.018260849	-0.064722082
6	1.999569262	-0.020789257	-0.059844126
6	-1.884055160	0.095814949	-0.058763017
1	3.141191387	-2.120111077	0.350652954

$C_4H_{28}^{2-}$

SCF Energy = -168.65392 a. u.

6	-0.689188807	-0.207663969	-0.042679203
6	0.682240181	-0.168687948	0.036030091
6	1.935200141	-0.119161720	0.099476856
6	-1.942550942	-0.226600048	-0.113617001
1	3.198040370	1.941870950	0.358014868

1	3.496310597	-2.784319013	0.466691999
1	3.037081585	1.906434066	1.003035896
1	3.374255336	2.512790229	1.316496156
1	5.174986775	0.099967932	0.255798990
1	4.421097583	0.026810765	0.156487767
1	3.306664584	-0.449921843	2.818828249
1	2.967188383	-0.351593831	2.144179116
1	3.857048611	-1.201296386	-2.361149197
1	3.369005368	-0.948452850	-1.832474137
1	3.690553573	1.949176242	-1.905636067
1	3.256777457	1.498451107	-1.470517957
1	-2.078641043	3.347504367	0.120723852
1	-1.961861149	2.602359300	0.036748714
1	-2.621373167	-0.899351022	2.068614193
1	-2.918352202	-1.209950021	2.695734213
1	-4.284216362	1.482566265	1.545134066
1	-3.686283113	1.161233964	1.198066817
1	-4.324837066	1.454754296	-1.570435088
1	-3.718371363	1.134671382	-1.234145063
1	-2.736210980	-1.029874178	-2.051166160
1	-3.046741186	-1.358100071	-2.663574524
1	-2.176942067	-3.156098311	0.169874893
1	-2.050542260	-2.413768995	0.079496181
1	-4.780263411	-1.259530225	0.097132072
1	-4.098089377	-0.922324194	0.042544792

1	3.561210483	2.606970021	0.434430179
1	2.984495125	-1.709085349	-1.436034122
1	3.393213111	-2.166096050	-1.886017349
1	5.122457467	-0.322254128	-0.124283098
1	4.369248267	-0.234040809	-0.037719225
1	0.776141096	2.871576108	-1.415269206
1	0.872291015	2.202153130	-1.081185321
1	3.391833546	1.068208308	-2.500170410
1	3.048192190	0.778619233	-1.886404178
1	3.787469212	0.228418301	2.686091016
1	3.278964272	0.172583222	2.121825082
1	3.384876452	-2.668318069	1.358145051
1	3.043617982	-2.055840912	1.061009909
1	-2.594686229	-3.081037164	-1.453902321
1	-2.427432351	-2.414944827	-1.127766149
1	-2.718335902	1.725791474	-1.404082928
1	-3.014827035	2.338002455	-1.743249032
1	-4.679670520	-0.548452001	-1.696607349
1	-4.007610122	-0.461338842	-1.343374127
1	-4.353164453	-1.858971100	1.155328346
1	-3.750767065	-1.499777225	0.854040221
1	-2.291035328	0.054802125	2.354709110
1	-2.432828901	0.161930884	3.092214446
1	-1.697138114	2.841810417	1.276641172
1	-1.624046036	2.164831317	0.947601933
1	-4.580784226	1.268768072	0.913565253
1	-3.953925090	0.926503107	0.647181130

$C_4H_{30}^{2-}$

SCF Energy = -169.83161 a. u.

6	0.702489148	-0.247161230	-0.046816840
6	-0.671322196	-0.245908138	-0.070339827
6	-1.926505230	-0.215811182	-0.084070919
6	1.957259424	-0.230538185	-0.018637094
1	-3.171879434	1.841740031	0.400827953
1	-3.525728090	2.502563350	0.528359141
1	-2.922307273	-2.215184119	0.914664883
1	-3.248291042	-2.831765045	1.217762265
1	-5.106810225	-0.427311158	0.247591980
1	-4.355695508	-0.338102986	0.147381156
1	-0.642388900	2.306403164	2.158927286
1	-0.681363863	1.767652041	1.634259156
1	-3.211152324	0.104519915	2.829637224
1	-2.875261299	0.017756013	2.152807880
1	-3.807640390	1.023297034	-2.355087471
1	-3.319511420	0.759579965	-1.833549425
1	-3.605147011	-2.142070345	-2.002478149
1	-3.176154128	-1.696225283	-1.558960409
1	-0.932696068	2.138532266	-1.205631935
1	-0.846868281	2.810721254	-1.536734435
1	2.249461047	-3.480298223	0.193557692
1	2.124751961	-2.737313257	0.106383677
1	2.700341230	0.860968738	2.054721173
1	2.995976154	1.185081866	2.675463020
1	4.478243434	-1.495695152	1.490238806

$C_4H_{32}^{2-}$

SCF Energy = -171.00860 a. u.

6	-0.664674142	-0.134502040	-0.130881938
6	0.707243277	-0.168637147	-0.073114304
6	1.961394415	-0.176326093	-0.016147315
6	-1.918963925	-0.095125961	-0.172911312
1	3.438870524	1.768521479	0.195771769
1	3.955213108	2.325786398	0.230986928
1	2.765851257	-1.822264191	-1.659559121
1	3.018875241	-2.327896228	-2.166826315
1	5.123532226	-0.577230777	-0.400403024
1	4.376729245	-0.465788694	-0.293070002
1	0.902347224	2.991752262	-1.259454024
1	0.990357867	2.312423085	-0.944886196
1	3.331238517	1.005770155	-2.673699272
1	2.997558394	0.715831294	-2.055661521
1	3.936691375	0.037385314	2.499121052
1	3.417895525	0.000712273	1.943610884
1	3.334828456	-2.842805270	1.130516812
1	3.000985346	-2.218698915	0.852864918
1	1.149006265	1.655529436	1.853242756
1	1.122745315	2.187120262	2.388019230
1	-2.749154127	-2.972435175	-1.421319290
1	-2.473404096	-2.332442919	-1.121253035
1	-2.487628909	1.719066161	-1.763097412
1	-2.705884361	2.247690419	-2.262415306
1	-4.596828351	-0.446141930	-1.912704287

1	3.865191062	-1.188844316	1.156563974
1	4.343084156	-1.552219220	-1.649038019
1	3.745737235	-1.238561048	-1.292533423
1	2.547963053	0.911923745	-2.130699384
1	2.826628322	1.241495865	-2.755774134
1	2.176975935	3.083279288	-0.043462915
1	2.057567088	2.339560882	0.028596739
1	4.812172270	1.214546984	-0.151714059
1	4.133274373	0.870478053	-0.102888991

1	-3.934820204	-0.356552222	-1.546334240
1	-4.487864405	-1.566131290	1.051769945
1	-3.872884240	-1.228679192	0.754680842
1	-2.243661264	0.280364986	2.282485940
1	-2.380039237	0.395765314	3.019553117
1	-1.862649940	3.050518453	1.010270807
1	-1.774088953	2.366955330	0.700153889
1	-4.621880131	1.509174884	0.484061713
1	-3.962881415	1.152264938	0.347032852
1	-1.578887107	-2.228936378	1.366083769
1	-1.640164245	-2.889083938	1.728781855

$C_4H_{34}^{2-}$

SCF Energy = -172.18567 a. u.

6	-0.704638137	-0.057119921	-0.268899832
6	0.668645088	-0.089239922	-0.253137758
6	1.923811188	-0.102784214	-0.211958772
6	-1.959719040	-0.024452751	-0.269233742
1	3.305958132	1.786871229	0.555540860
1	3.742515075	2.363726290	0.787988316
1	2.820022073	-1.221870797	-2.211214232
1	3.136624059	-1.554133254	-2.816678202
1	5.113977401	-0.239051060	-0.618642071
1	4.360177110	-0.203676090	-0.510993131
1	0.786584938	3.286754290	-0.411208823
1	0.883937148	2.540407990	-0.375505763
1	3.278223424	1.795279326	-2.426079245
1	2.931618146	1.350148125	-1.917103338
1	3.842613185	-0.451616798	2.357469298
1	3.383023274	-0.369680051	1.757661174
1	3.406517156	-2.914048403	0.245750973
1	3.034540476	-2.260356277	0.135769948
1	1.143486946	1.125652085	2.106420203
1	1.100420914	1.460730295	2.780883065
1	-2.831989946	-2.494659029	-2.191030353
1	-2.582238922	-1.923347100	-1.758856056
1	-2.539660262	2.237407976	-1.147173195
1	-2.771990242	2.914871274	-1.397311047
1	-4.613020117	0.238174213	-2.034645247
1	-3.978095261	0.176992856	-1.616903201
1	0.955376076	-1.936121968	2.612308361
1	1.033767335	-1.537584294	1.976978156
1	-4.526307545	-1.771784915	0.520215103
1	-3.921479116	-1.347105885	0.335626966
1	-2.233342308	-0.377056782	2.217057407
1	-2.409368886	-0.475059879	2.947607237
1	-1.819270106	2.684740026	1.760899210
1	-1.746495005	2.080284138	1.313943934
1	-4.583491497	1.371798883	0.946883310
1	-3.964660509	1.034934171	0.657613859
1	-1.632798098	-2.508366307	0.595323876
1	-1.673771234	-3.221673955	0.840785918

$C_4H_{36}^{2-}$

SCF Energy = -173.36338 a. u.

6	0.685883000	-0.000762000	0.000596000
6	-0.686345000	-0.000927000	0.000156000
6	-1.941350000	-0.000486000	-0.000108000
6	1.940877000	-0.000398000	0.000563000
1	-3.826368000	1.148769000	-0.954255000
1	-4.417563000	1.521147000	-1.261085000
1	-2.370037000	-1.902470000	1.582140000
1	-2.571531000	-2.463076000	2.050384000
1	-4.419085000	-1.854679000	-0.684572000
1	-3.829573000	-1.399964000	-0.517441000
1	-2.573786000	3.004707000	1.111723000
1	-2.370180000	2.320506000	0.857703000
1	-4.418716000	0.337175000	1.946439000
1	-3.827846000	0.254279000	1.470741000
1	-2.573389000	-0.541618000	-3.158899000
1	-2.369552000	-0.418699000	-2.439559000
1	-1.026406000	-3.150040000	-1.162965000
1	-1.108161000	-2.445927000	-0.903487000
1	-1.104535000	2.004930000	-1.663937000
1	-1.023791000	2.583430000	-2.142037000
1	1.026159000	-2.581962000	2.145873000
1	1.105759000	-2.003487000	1.667543000
1	1.107829000	2.446469000	0.899896000
1	1.024566000	3.151311000	1.156864000
1	-1.020370000	0.569687000	3.307336000
1	-1.104809000	0.440351000	2.568454000
1	2.571214000	-3.004842000	-1.110420000
1	2.368325000	-2.320395000	-0.856429000
1	4.417623000	-1.521205000	1.258831000
1	3.826429000	-1.148676000	0.952056000
1	1.107190000	-0.437671000	-2.567569000
1	1.024391000	-0.565437000	-3.306925000
1	2.571920000	2.464524000	-2.047594000
1	2.370460000	1.903458000	-1.579919000
1	2.577278000	0.542877000	3.157027000
1	2.372771000	0.419555000	2.437920000
1	3.826173000	-0.253338000	-1.470964000
1	4.416376000	-0.335705000	-1.947608000
1	4.418335000	1.853101000	0.681847000
1	3.828514000	1.398348000	0.515646000

$C_4H_{38}^{2-}$

$C_4H_{40}^{2-}$

SCF Energy = -174.54027 a. u.

6	-0.788029063	0.036392049	0.034054144
6	0.584066159	0.001373744	-0.012415027
6	1.839131187	-0.022558826	-0.050342219
6	-2.043070807	0.084821821	0.066964735
1	4.176743638	0.530577981	-0.549610899
1	4.898941463	0.714537985	-0.708265118
1	0.808773340	-1.726232279	-2.050390916
1	0.693594208	-2.209425083	-2.616365034
1	3.712496437	-2.105235904	-1.619488232
1	3.272552231	-1.608682962	-1.248006861
1	2.698639396	3.092237200	-0.585008095
1	2.449916034	2.386468211	-0.468474268
1	2.339009479	0.857933907	-3.147004400
1	2.169357370	0.656363942	-2.436147372
1	4.070075263	-1.624241302	1.593027253
1	3.545747394	-1.239546905	1.197803816
1	1.261037322	-3.343929246	0.606012198
1	1.261614125	-2.600322496	0.476122996
1	3.151402392	1.172373145	1.674899969
1	3.565433317	1.537289013	2.196042191
1	-2.119750178	-3.100947458	-0.939688087
1	-2.004538236	-2.385508284	-0.723308040
1	-0.606528146	2.346256032	-1.193901134
1	-0.450811919	2.985292066	-1.559685911
1	-1.513823177	0.003422718	-3.326566411
1	-1.519465794	0.000713860	-2.571626272
1	-1.532915892	-2.502671302	2.317921236
1	-1.526868984	-1.940173349	1.815609258
1	-4.446595988	-1.471865242	1.428801856
1	-3.889312019	-1.068582436	1.097150070
1	1.191527244	-0.534113944	2.552293311
1	1.178580394	-0.670657020	3.294178118
1	0.350420116	2.670771334	2.033565196
1	0.484965019	2.092058332	1.572063896
1	-3.707091421	2.102419094	-1.828972042
1	-3.329843077	1.624595851	-1.374355867
1	-2.133370142	0.480250050	2.587132224
1	-2.237659865	0.594714793	3.328186223
1	-2.834056912	3.054561897	1.144134130
1	-2.639731914	2.362329262	0.902719236
1	-3.894340261	-0.733215296	-1.325005855
1	-4.446706057	-0.999989422	-1.775363212

SCF Energy = -175.71769 a. u.

6	0.695841000	0.001233000	-0.113418000
6	-0.677695000	-0.001227000	-0.115923000
6	-1.933720000	-0.000278000	-0.113820000
6	1.951730000	0.000820000	-0.102400000
1	-3.655604000	0.696504000	1.546109000
1	-4.173467000	0.909198000	2.058695000
1	-1.347631000	-2.614875000	0.490056000
1	-1.256276000	-3.351989000	0.615540000
1	-4.075621000	-2.135840000	1.127857000
1	-3.572222000	-1.628871000	0.873433000
1	-1.338360000	2.549150000	2.136630000
1	-1.332782000	2.011003000	1.608521000
1	-1.600670000	-0.834570000	3.183347000
1	-1.503952000	-0.699389000	2.447166000
1	-5.116164000	-0.077757000	-0.853692000
1	-4.372881000	-0.004775000	-0.714256000
1	-2.996378000	-2.328516000	-2.101297000
1	-2.748740000	-1.801411000	-1.615620000
1	-3.205769000	2.122098000	-0.390739000
1	-3.555646000	2.789149000	-0.479819000
1	0.665702000	-2.933245000	-1.806031000
1	0.773840000	-2.274365000	-1.458607000
1	1.472945000	0.657527000	2.466425000
1	1.387358000	0.786082000	3.204805000
1	1.323660000	-2.581370000	2.112760000
1	1.319588000	-2.042059000	1.586013000
1	-2.984420000	0.791469000	-3.089004000
1	-2.667015000	0.646664000	-2.416269000
1	2.999850000	-0.756195000	-3.087460000
1	2.684635000	-0.618864000	-2.412104000
1	-0.773043000	2.292825000	-1.429513000
1	-0.664085000	2.953128000	-1.774102000
1	1.251274000	3.349759000	0.651096000
1	1.341472000	2.612953000	0.523500000
1	4.159289000	-0.922082000	2.086574000
1	3.644788000	-0.707739000	1.570958000
1	4.069980000	2.131046000	1.174539000
1	3.568133000	1.624788000	0.915163000
1	3.220352000	-2.118475000	-0.397056000
1	3.569556000	-2.785243000	-0.491383000
1	2.754969000	1.823074000	-1.590333000
1	3.002622000	2.352377000	-2.073488000
1	4.385140000	0.020603000	-0.693043000
1	5.128636000	0.094949000	-0.832007000

$C_4H_{42}^{2-}$

SCF Energy = -176.89438 a. u.

6	-0.684043088	0.011304814	0.007498971
6	0.689594157	-0.010101994	0.002298217
6	1.945505339	-0.026581102	0.008308083
6	-1.940175995	0.025702668	0.020649025
1	3.699562287	0.609018983	-1.629424064

$C_4H_{44}^{2-}$

SCF Energy = -178.07007 a. u.

6	-0.679250858	0.000527061	0.009444226
6	0.695083313	0.000531294	0.009471214
6	1.951554364	0.000395295	0.007894266
6	-1.935881192	0.000998028	0.007851932
1	3.533565205	1.191892377	-1.561477176

1	4.230744589	0.806311079	-2.134902110
1	1.240075024	-2.636490174	-0.615995127
1	1.198816132	-3.369370501	-0.784280900
1	4.014661409	-2.219584228	-1.237513806
1	3.545041472	-1.703672395	-0.939754764
1	1.509051057	2.600668049	-2.146228090
1	1.472792361	2.026091096	-1.658617185
1	1.501843133	-0.857405259	-3.284966200
1	1.476198146	-0.675528097	-2.552964308
1	5.086915277	-0.186537097	0.865948296
1	4.356174414	-0.147843127	0.660367168
1	2.737624413	-2.395892329	2.091842428
1	2.514621182	-1.848381205	1.617487942
1	3.297359531	2.053068023	0.314722877
1	3.709981258	2.681898344	0.410535181
1	-0.806804801	-2.967229129	1.619990950
1	-0.935300150	-2.327821084	1.243604107
1	-1.356683993	0.812499806	-2.515450932
1	-1.352318810	1.046453831	-3.232483988
1	-1.398068300	-2.456107408	-2.310304259
1	-1.376032830	-1.915398329	-1.785024930
1	2.999274516	0.817014218	3.005636285
1	2.711938149	0.622932111	2.332860439
1	-3.148909967	-1.003481992	2.885548504
1	-2.839021124	-0.769438008	2.235464308
1	0.882752320	2.245572123	1.375724320
1	0.739152136	2.864287221	1.779964408
1	-1.160979959	3.402567906	-0.644484972
1	-1.201965266	2.664930276	-0.499175016
1	-4.117740375	-0.683218100	-2.281151884
1	-3.614030310	-0.515746201	-1.738666886
1	-0.198948949	-0.055958907	2.638815379
1	-0.097417827	-0.082085975	3.382964535
1	-3.960700147	2.284930210	-1.204250782
1	-3.502755976	1.754412026	-0.914760135
1	-3.300860039	-2.070885421	0.121920851
1	-3.714360200	-2.705175264	0.160113160
1	-2.584159306	1.763223885	1.680851097
1	-2.818258325	2.288452943	2.175024329
1	-4.381321446	0.110944656	0.557468123
1	-5.123220540	0.136026070	0.721020935

1	4.001008107	1.552298067	-2.036595265
1	1.327755990	-2.407060086	-1.124648765
1	1.328051270	-3.086508327	-1.450845264
1	4.002162242	-1.554593109	-2.032130067
1	3.534970170	-1.192326831	-1.558156060
1	1.326131945	3.084185239	-1.458771810
1	1.325140796	2.404984123	-1.132087939
1	1.321168262	-0.009009772	-3.394496365
1	1.336820267	-0.006408866	-2.640542084
1	5.210099273	0.001683313	0.459683047
1	4.457795496	0.001175303	0.357637035
1	3.658665352	-2.638883113	0.947806196
1	3.263748309	-2.031168023	0.727767945
1	3.262485163	2.032280353	0.725499362
1	3.657222286	2.640306600	0.945066116
1	0.808516160	-2.574616124	2.251228499
1	0.940147413	-2.016734184	1.763582138
1	-1.487501372	1.413145089	-2.234871101
1	-1.512724076	1.821446083	-2.868724901
1	-1.514185134	-1.835888389	-2.861270911
1	-1.488449128	-1.423605336	-2.230065113
1	3.073161419	0.004994375	3.051151349
1	2.783054280	0.003485161	2.350645028
1	-3.017134248	-1.788733404	2.508893368
1	-2.737474127	-1.375879369	1.938365150
1	0.936108203	2.024149016	1.754388213
1	0.802801046	2.583348078	2.240069209
1	-1.278117047	3.457190111	0.195250000
1	-1.282785449	2.705211248	0.161493254
1	-4.169212387	-0.006236354	-2.396051082
1	-3.661156190	-0.004472077	-1.833489099
1	-0.566313850	0.003594172	2.696900519
1	-0.435937276	0.004337137	3.436896163
1	-4.010040633	2.507237043	-0.604111923
1	-3.539170250	1.931902838	-0.461235124
1	-1.279350030	-2.703607312	0.173528862
1	-1.272809928	-3.455414192	0.210238946
1	-2.738982282	1.381670155	1.934690014
1	-3.019206506	1.795783103	2.504037108
1	-4.396361192	-0.000558282	0.602097874
1	-5.132917184	-0.001547314	0.785810223
1	-3.534801363	-1.935687513	-0.455134768
1	-4.004980111	-2.512068431	-0.595990110

$C_4H_{46}^{2-}$

SCF Energy = -179.24511 a. u.

6	-0.700976230	0.007486800	0.000128061
6	0.674418941	0.016133027	-0.000232838
6	1.931046100	0.016945843	-0.000485785
6	-1.958034140	-0.011304814	0.000876318
1	4.305450128	1.024558064	0.001409199
1	5.000861531	1.324530125	0.001984944
1	1.628093183	-1.611813045	-2.104406154
1	1.655956482	-2.086926371	-2.689425891
1	4.546601492	-1.237819141	-1.616732806

$C_4H_{48}^{2-}$

SCF Energy = -180.41953 a. u.

6	0.645834903	0.032385118	0.008377934
6	-0.729431149	0.021772998	0.005111852
6	-1.986412328	0.005313998	-0.006825857
6	1.903472261	0.022131780	0.006608895
1	-4.558785269	0.489376241	-0.304996070
1	-5.297881312	0.610585348	-0.411350114
1	-1.513108259	-1.524038944	2.183559958
1	-1.567663258	-1.878539016	2.846744466
1	-4.517968241	-1.626391878	1.427338152

1	3.956729201	-0.949958889	-1.239054770
1	2.731975446	3.287696226	0.003805843
1	2.504768960	2.567948491	0.002264349
1	3.030361034	1.386385125	-2.748836091
1	2.747241151	1.068243233	-2.122489199
1	4.545007611	-1.239989826	1.617646166
1	3.955850237	-0.950853198	1.239846948
1	2.892849563	-3.248796935	-0.001627749
1	2.625450478	-2.543477218	-0.001419783
1	2.744491017	1.065248090	2.125563190
1	3.026984354	1.382298289	2.752724486
1	-0.104882931	-3.346180366	-0.003435948
1	-0.181776089	-2.598986324	-0.002705154
1	0.269319998	2.339632321	-1.297938968
1	0.147460003	2.974897437	-1.679438193
1	0.006343248	0.423391013	-3.448528008
1	-0.007294708	0.322305987	-2.705449378
1	1.655537374	-2.090453338	2.686503245
1	1.627478279	-1.614525078	2.102145509
1	-3.158393881	-3.119767117	-0.003539667
1	-2.857133274	-2.426425327	-0.002574976
1	-0.008798101	0.316480804	2.705913466
1	0.005046234	0.418934282	3.448862449
1	0.145357053	2.972545244	1.682123239
1	0.266621194	2.337639968	1.299806964
1	-2.910122967	1.515341916	-2.719454054
1	-2.645695212	1.167168157	-2.100599253
1	-1.798698870	-1.566212254	2.123808438
1	-1.854137066	-2.025307385	2.720678041
1	-2.358620259	3.364311037	0.000173041
1	-2.189389904	2.628959982	-0.000189975
1	-1.797944263	-1.561645984	-2.127009960
1	-1.853695203	-2.019386421	-2.724856953
1	-2.647457372	1.166000792	2.101697296
1	-2.912391020	1.513613094	2.720697091
1	-4.171374076	1.257699801	0.000064030
1	-4.823106130	1.644869160	0.000311156
1	-4.044582149	-0.738981211	-1.237121156
1	-4.664752484	-0.963044913	-1.611883955
1	-4.045237270	-0.740405227	1.237073001
1	-4.665082162	-0.965310321	1.611904064

1	-3.919931273	-1.289784876	1.108009316
1	-3.495582979	2.962068064	-0.339673055
1	-3.157636100	2.291667166	-0.252591118
1	-3.495826400	1.108553310	2.634462367
1	-3.159510445	0.834054254	2.012329313
1	-4.110897054	-1.791333252	-1.812501400
1	-3.656812174	-1.367467038	-1.380188988
1	-2.567376979	-3.428534104	0.151076930
1	-2.255513247	-2.747380325	0.075521002
1	-2.753693409	0.770237065	-2.258314182
1	-3.056316119	1.052918260	-2.892752194
1	0.300121289	-3.294746454	0.337915128
1	0.416321205	-2.559556269	0.235378040
1	-1.314432894	2.436070112	1.337707168
1	-1.364527987	3.105347037	1.676495968
1	-0.070441959	0.940119367	3.280400459
1	0.015257238	0.626272278	2.604023033
1	-1.157583170	-2.392146283	-2.420890133
1	-1.238544114	-1.747167060	-2.041307059
1	3.253280125	-3.095776338	0.425542118
1	2.922124177	-2.424291155	0.333305995
1	0.299075106	0.477632210	-2.620146005
1	0.180088014	0.398868939	-3.357449195
1	-0.599556765	3.022782157	-1.470309990
1	-0.861110029	2.394262992	-1.150762075
1	2.969861257	1.336794337	2.946789129
1	2.672297481	1.035387147	2.322231385
1	1.941503171	-1.789847322	-1.886905309
1	2.091641341	-2.309626383	-2.413423442
1	2.238840459	2.923210049	-1.967565151
1	2.049096019	2.386371372	-1.475673202
1	1.736008300	-1.368259216	2.245785381
1	1.817658232	-1.714753895	2.911449085
1	2.969882424	0.385336818	-2.450140406
1	3.299403214	0.482292145	-3.121204363
1	3.942776384	1.418042095	-0.009183871
1	4.602436572	1.796630316	-0.019136108
1	4.061357597	-0.605714271	1.385324124
1	4.714612623	-0.752077819	1.736455983
1	4.215404269	-0.863404012	-0.927504310
1	4.845054286	-1.153913326	-1.228391319
1	1.619277090	3.341794016	1.026267306
1	1.516538386	2.608450130	0.888609253

$C_4H_{50}^{2-}$

SCF Energy = -181.59434 a. u.

6	-0.680482254	0.020733165	-0.000859913
6	0.695361131	0.022630265	0.004814984
6	1.952932342	0.020436825	0.003734933
6	-1.938268311	0.013796180	-0.018103154
1	4.930148633	-0.337242015	1.303456170
1	4.248857267	-0.248294199	0.979295946
1	4.749155726	1.548912921	-1.230392138
1	4.130962397	1.217342098	-0.950343071
1	4.485930263	-1.287518410	-1.886166048

$C_4H_{52}^{2-}$

SCF Energy = -182.76893 a. u.

6	0.567265000	-0.145914000	0.012260000
6	-0.804352000	-0.029560000	0.013538000
6	-2.057443000	0.079515000	0.006029000
6	1.820498000	-0.254075000	0.005086000
1	-5.085824000	0.742392000	1.301077000
1	-4.407104000	0.589594000	1.002739000
1	-5.131773000	-0.914071000	-1.210269000
1	-4.461081000	-0.696751000	-0.940501000
1	-4.450562000	1.964584000	-1.545833000

1	3.957647323	-1.037558361	-1.408181935	1	-3.927434000	1.547232000	-1.195838000
1	3.212975340	-2.355136156	0.339233309	1	-2.985333000	2.474988000	0.751841000
1	3.555890135	-3.020134154	0.431422336	1	-3.259112000	3.147842000	0.954658000
1	-0.441768809	2.332876315	-2.480497188	1	-0.332071000	-2.188644000	-2.607250000
1	-0.626682920	1.820815304	-1.962507275	1	-0.319473000	-1.705885000	-2.032549000
1	3.208499558	1.951741164	1.115689265	1	-3.506345000	-1.658613000	1.096065000
1	3.548563146	2.554567185	1.421244147	1	-3.941011000	-2.186011000	1.423511000
1	1.610358337	1.148579219	3.367606224	1	-1.375508000	-1.825609000	3.064806000
1	1.515791187	1.002290285	2.635803302	1	-1.373405000	-1.435453000	2.422932000
1	2.423594229	0.586567051	-3.235851143	1	-2.725137000	-0.067331000	-3.229836000
1	2.294832175	0.466161764	-2.500733984	1	-2.508789000	-0.027763000	-2.506308000
1	-3.635595341	2.095953077	-1.959043281	1	4.678551000	-1.442488000	-1.540148000
1	-3.213671208	1.648583455	-1.518631282	1	4.058892000	-1.181780000	-1.197187000
1	-1.399814056	-2.423496331	-1.169927288	1	1.415733000	2.422796000	-0.788487000
1	-1.333851053	-3.094737033	-1.505074290	1	1.459926000	3.136545000	-1.022650000
1	0.645832257	-3.219001081	1.047244951	1	-0.313259000	2.987542000	1.486465000
1	0.753397058	-2.542508294	0.738273172	1	-0.528624000	2.339859000	1.172156000
1	-1.754226285	1.774234476	2.941905352	1	1.461562000	-2.619016000	2.462388000
1	-1.679513866	1.431435042	2.274662055	1	1.428484000	-2.101990000	1.914703000
1	-3.012410283	-0.667159158	-2.207689911	1	3.187742000	0.977348000	-1.729303000
1	-3.348401323	-0.819982902	-2.868638116	1	3.599803000	1.348577000	-2.245258000
1	-2.122042044	-3.092630908	1.619724245	1	2.646089000	2.494919000	1.803086000
1	-2.000388957	-2.430180898	1.284047007	1	2.388382000	1.903755000	1.410774000
1	-1.741991178	2.874966547	0.028168105	1	2.033839000	-2.720216000	-0.677156000
1	-2.040554040	3.561213129	0.098447077	1	2.176855000	-3.433381000	-0.883304000
1	-3.732645390	-2.072956092	-0.359127198	1	4.173082000	3.270623000	-0.371557000
1	-4.094978344	-2.726507986	-0.453266773	1	4.619234000	3.868326000	-0.423469000
1	-3.557858145	-0.573947761	1.777528076	1	2.999568000	-0.187648000	2.415100000
1	-4.066042403	-0.765677674	2.307605455	1	3.339977000	-0.169563000	3.087774000
1	-3.752268341	1.675638171	0.915541200	1	3.716526000	-1.885835000	0.973961000
1	-4.270178348	2.172638269	1.151103924	1	4.250573000	-2.346128000	1.243737000
1	-4.562345045	0.041216028	-0.453839872	1	4.206986000	0.499545000	0.446568000
1	-5.304555296	-0.039842813	-0.571332038	1	4.914006000	0.738924000	0.582701000
1	-0.512353117	-1.145107287	3.228427315	1	0.404569000	0.588246000	3.321684000
1	-0.633227784	-0.827959191	2.558339161	1	0.582128000	0.434767000	2.607781000
1	-0.309722152	-0.711174005	-3.358091087	1	0.331932000	1.033158000	-3.176899000
1	-0.424618175	-0.587366108	-2.626788238	1	0.460913000	0.768816000	-2.485503000
1	0.712545103	2.504502255	0.916186267	1	-0.823641000	-2.690154000	0.315876000
1	0.608732169	3.175941399	1.237467238	1	-0.741142000	-3.427617000	0.432283000
1	2.402072061	-1.275656373	2.304502360	1	-2.456029000	0.805646000	2.464717000
1	2.548268389	-1.616987340	2.960660452	1	-2.642156000	1.032659000	3.160729000
1	1.732331047	-2.081332439	-1.690956265	1	-1.592329000	2.347951000	-1.361489000
1	1.798558109	-2.741957316	-2.047576222	1	-1.591292000	3.008064000	-1.725568000
1	2.102860427	2.508998145	-1.077983270	1	-2.725134000	-2.233582000	-1.227508000
1	2.216642532	3.181301965	-1.398469945	1	-2.979981000	-2.864136000	-1.551806000
				1	2.331399000	-1.292122000	-3.282964000
				1	2.160993000	-1.072715000	-2.582950000
$C_6H_2^{2-}$				**$C_6H_4^{2-}$**			
SCF Energy = -229.562777 a. u.				SCF Energy = -230.741051 a. u.			
6	3.553921000	0.037988000	0.001673000	6	-3.239638000	-0.025415000	0.056340000
6	2.293866000	0.018342000	-0.000580000	6	-1.981176000	-0.028805000	0.036473000
6	0.931593000	-0.003745000	-0.001060000	6	-0.619381000	-0.029732000	0.011298000
6	-0.307607000	-0.023351000	-0.001285000	6	0.619343000	-0.029696000	-0.011272000
6	-1.670166000	-0.044347000	-0.000227000	6	1.981133000	-0.028661000	-0.036538000

6	-2.928802000	-0.060740000	0.001231000
1	-5.233107000	0.176482000	0.005349000
1	-6.003731000	0.278636000	-0.003866000

6	3.239597000	-0.025113000	-0.056486000
1	5.555694000	0.201252000	0.088693000
1	6.320571000	0.300361000	0.171358000
1	-5.555321000	0.201625000	-0.088343000
1	-6.320205000	0.301287000	-0.170599000

$C_6H_6^{2-}$

SCF Energy = -231.91824 a. u.

6	-3.487480000	-0.089116000	-0.020442000
6	-2.228935000	-0.102031000	-0.025719000
6	-0.867632000	-0.107686000	-0.028952000
6	0.371056000	-0.109615000	-0.030271000
6	1.732558000	-0.105661000	-0.030090000
6	2.990353000	-0.101957000	-0.026444000
1	5.251368000	-0.741930000	0.212218000
1	5.999388000	-0.897970000	0.313229000
1	5.159418000	2.142983000	-0.012658000
1	4.620694000	1.595655000	-0.017980000
1	-5.690732000	0.649176000	0.194290000
1	-6.399655000	0.948488000	0.282412000

$C_6H_8^{2-}$

SCF Energy = -233.095534 a. u.

6	-3.238333000	-0.047636000	-0.062861000
6	-1.980859000	-0.064039000	-0.075606000
6	-0.620073000	-0.081394000	-0.082369000
6	0.618229000	-0.095476000	-0.084983000
6	1.979081000	-0.106963000	-0.083511000
6	3.236757000	-0.120444000	-0.078321000
1	5.514857000	-0.767310000	0.068646000
1	6.262935000	-0.925148000	0.159219000
1	5.346989000	2.032238000	0.740176000
1	4.827560000	1.506942000	0.533021000
1	-5.061810000	1.433841000	-0.158445000
1	-5.626526000	1.955352000	-0.171579000
1	-5.289689000	-0.920516000	0.678979000
1	-5.943124000	-1.219700000	0.955892000

$C_6H_{10}^{2-}$

SCF Energy = -234.27332 a. u.

6	-3.011466000	-0.083604000	-0.072165000
6	-1.755472000	-0.047012000	-0.048486000
6	-0.395573000	-0.011087000	-0.027358000
6	0.841879000	0.022573000	-0.007561000
6	2.201628000	0.057697000	0.013605000
6	3.458571000	0.092352000	0.031085000
1	5.583265000	1.122787000	-0.032876000
1	6.272849000	1.462482000	-0.069929000
1	5.869561000	-1.886625000	0.063961000
1	5.301786000	-1.369200000	0.059035000
1	-5.367943000	-0.386568000	1.983733000
1	-4.808648000	-0.337557000	1.463350000
1	-5.029663000	-0.962846000	-0.967392000
1	-5.674311000	-1.254582000	-1.263428000
1	-4.812238000	1.452801000	-0.268208000
1	-5.372060000	1.973792000	-0.302960000

$C_6H_{12}^{2-}$

SCF Energy = -235.450842 a. u.

6	3.238552064	-0.103663706	-0.077158276
6	1.982374176	-0.094332195	-0.043276115
6	0.622773887	-0.089693956	-0.009520957
6	-0.614616091	-0.082117196	0.021966677
6	-1.974232255	-0.073148700	0.054474035
6	-3.230464119	-0.067353151	0.086858095
1	-5.215579433	-1.068367061	-0.759374115
1	-5.852578663	-1.380994925	-1.048026016
1	-5.260750532	0.219815996	1.326796062
1	-5.932684457	0.318531366	1.680235134
1	-5.422371318	1.901405295	-1.037026009
1	-4.892327277	1.410929424	-0.786892390
1	5.515021259	0.720502342	1.929046868
1	4.973480312	0.510438024	1.431575803
1	4.984338500	1.277791074	-0.926686202
1	5.530329298	1.754926915	-1.170748041
1	5.370052622	-1.137510948	-0.373971149
1	6.056740538	-1.465615130	-0.464988049

$C_6H_{14}^{2-}$

SCF Energy = -236.627811 a. u.

6	3.411267051	-0.133527824	-0.092383235
6	2.154709214	-0.117192123	-0.106394261
6	0.795423257	-0.104371746	-0.124563033
6	-0.442103779	-0.087416906	-0.137283925
6	-1.801522030	-0.068300908	-0.147313950
6	-3.057800991	-0.044420726	-0.159163287
1	-4.760676444	0.191434103	1.532823286

$C_6H_{16}^{2-}$

SCF Energy = -237.803696 a. u.

6	3.260519799	-0.047606902	-0.026644074
6	2.004256714	-0.056584923	-0.056111839
6	0.645311546	-0.065188287	-0.083814797
6	-0.591896395	-0.073293166	-0.108090274
6	-1.951104563	-0.078279074	-0.126997248
6	-3.207262342	-0.075978211	-0.144765962
1	-4.982657833	0.111430970	1.478817044

1	-5.301562269	0.242277983	2.067711945
1	-5.380945207	0.200880975	-0.847155095
1	-6.123418459	0.304924102	-0.993175207
1	-5.106007463	-2.424145102	0.355687017
1	-4.589754310	-1.882197219	0.211440178
1	-4.109087268	2.135691113	0.052135072
1	-4.450742092	2.810615418	0.134290898
1	6.409131310	-0.894921809	-0.790517254
1	5.669664314	-0.750290787	-0.653658259
1	5.063014457	-0.153034885	1.649983129
1	5.601042725	-0.148296103	2.191846874
1	5.089355313	1.579672936	-0.152790935
1	5.630151707	2.118772258	-0.156013095

1	-5.530182716	0.163304628	2.007783151
1	-5.507994843	0.199467543	-0.910661128
1	-6.243594612	0.302285624	-1.085347300
1	-5.281697484	-2.481277195	0.112527954
1	-4.757204512	-1.931220199	0.058761958
1	-4.254430562	2.121235049	0.026882733
1	-4.599181602	2.794978231	0.098050723
1	5.597781934	0.055748823	-2.177274391
1	5.054132217	0.048645148	-1.641028921
1	5.021151245	-1.679555141	0.210918939
1	5.558521216	-2.216656291	0.282557896
1	4.954853273	2.622763316	0.064633709
1	4.583659246	1.956593190	0.052417123
1	4.532176121	0.129437813	2.016039904
1	4.895716128	0.184401338	2.683465238

$C_6H_{18}^{2-}$

SCF Energy = -238.980987 a. u.

6	3.379667231	-0.006554919	0.015886959
6	2.123321066	0.001941022	0.003502624
6	0.764786011	0.010844959	-0.009803009
6	-0.472348904	0.018675194	-0.022230207
6	-1.831012020	0.027140972	-0.035066989
6	-3.087326964	0.038591309	-0.055686380
1	-4.582629467	-1.755016346	0.627588871
1	-5.062223337	-2.308348949	0.834255871
1	-5.491850174	0.254008255	-0.532986267
1	-6.239727384	0.312212989	-0.666633156
1	-4.384540431	-1.782455245	-2.366813510
1	-4.057762367	-1.349806806	-1.834902531
1	-4.454074321	2.940395080	0.098828085
1	-4.110933038	2.263979024	0.054876739
1	-4.616463473	0.472020285	1.784689961
1	-5.104329442	0.608959186	2.352447935
1	5.167598403	2.289998141	-1.272876075
1	4.728451137	1.747446466	-0.968776432
1	5.463536546	-0.637523116	-1.049321442
1	6.126921612	-0.830201844	-1.373301217
1	6.118558495	0.765363343	1.451034180
1	5.456547702	0.585316076	1.117110106
1	4.677874493	-1.785154049	1.026935128
1	5.102527593	-2.335023187	1.338224174

$C_6H_{20}^{2-}$

SCF Energy = -240.157664 a. u.

6	3.225069000	0.118329000	-0.000542000
6	1.968843000	0.121373000	0.019277000
6	0.610553000	0.121014000	0.026789000
6	-0.626678000	0.118202000	0.033906000
6	-1.984946000	0.112501000	0.038365000
6	-3.241212000	0.105769000	0.050706000
1	-4.835452000	0.172578000	-1.802206000
1	-5.363188000	0.183472000	-2.349543000
1	-5.672249000	0.038691000	0.495127000
1	-6.419546000	-0.045626000	0.613943000
1	-4.871212000	2.826587000	-0.345863000
1	-4.511021000	2.164344000	-0.245797000
1	-4.370352000	-1.497327000	2.612700000
1	-4.078047000	-1.147580000	2.006098000
1	-4.459462000	-1.950401000	-0.430380000
1	-4.813866000	-2.610962000	-0.554903000
1	5.586775000	0.331916000	2.156666000
1	5.039680000	0.299347000	1.628975000
1	3.997451000	-1.960868000	-2.368756000
1	3.785378000	-1.457345000	-1.843722000
1	4.642352000	2.125092000	0.033931000
1	5.154691000	2.686345000	0.045719000
1	5.088376000	-2.410193000	0.719196000
1	4.596611000	-1.860112000	0.540318000
1	5.549583000	0.001616000	-0.809328000
1	6.243720000	-0.072697000	-1.113186000

$C_6H_{22}^{2-}$

SCF Energy = -241.333074 a. u.

6	-3.445564087	-0.087470883	0.017745959
6	-2.188737957	-0.108382909	0.008311258
6	-0.831028948	-0.115254805	-0.003222160
6	0.406083212	-0.115402974	-0.012873824
6	1.763880065	-0.113332833	-0.023451019
6	3.019954234	-0.101796240	-0.030955811
1	4.177273344	0.782936261	-2.019779070

$C_6H_{24}^{2-}$

SCF Energy = -242.51064 a. u.

6	-3.258626000	-0.046764000	-0.004300000
6	-2.002201000	-0.038852000	-0.004514000
6	-0.644637000	-0.030267000	-0.004419000
6	0.592132000	-0.022543000	-0.004292000
6	1.949680000	-0.014092000	-0.003722000
6	3.205841000	-0.005430000	-0.002167000
1	4.432951000	-2.124762000	-0.344398000

1	4.518339194	1.071810946	-2.632785404
1	5.483393393	0.226788964	0.067859045
1	6.230212248	0.338509924	0.154484831
1	4.939067387	-2.054809016	-1.720282210
1	4.489768385	-1.609806934	-1.300232952
1	4.861786341	-2.149313194	1.626247942
1	4.420538242	-1.690990133	1.211898981
1	4.379514305	0.906612922	2.717696127
1	4.050085063	0.646313279	2.085791286
1	3.930762473	2.205400161	0.066140277
1	4.263152462	2.884970114	0.109715907
1	-5.431817661	-1.948977800	1.701922935
1	-4.984041632	-1.502961285	1.278468950
1	-4.087209493	3.107177461	-0.165120765
1	-3.950999269	2.367510436	-0.078309766
1	-4.913881196	-1.601076039	-1.224110804
1	-5.354029664	-2.056839999	-1.643997076
1	-4.980029410	1.189885207	2.530394369
1	-4.647289106	0.887668906	1.917742055
1	-4.701421293	0.783201908	-1.899351029
1	-5.040690586	1.065833360	-2.517718986

1	4.827407000	-2.764664000	-0.446132000
1	5.693606000	0.029862000	0.009649000
1	6.453796000	0.040903000	0.013380000
1	4.793582000	-1.269749000	2.510199000
1	4.405627000	-0.978099000	1.927240000
1	4.748101000	2.004211000	2.005282000
1	4.372136000	1.537705000	1.540291000
1	4.758207000	2.531857000	-1.264385000
1	4.378963000	1.943166000	-0.972990000
1	4.416699000	-0.321617000	-2.136668000
1	4.808360000	-0.415986000	-2.779355000
1	-3.845095000	3.172779000	-0.041574000
1	-3.659633000	2.439246000	-0.031735000
1	-5.791724000	1.096254000	1.631565000
1	-5.195611000	0.824380000	1.246416000
1	-4.197353000	-1.610604000	-2.694991000
1	-3.942702000	-1.253898000	-2.077148000
1	-3.910339000	-1.206569000	2.108777000
1	-4.156802000	-1.549481000	2.737465000
1	-5.820896000	1.057943000	-1.622433000
1	-5.217855000	0.794704000	-1.242054000
1	-5.375305000	-1.321085000	0.027064000
1	-6.029249000	-1.708803000	0.037018000

$C_6H_{26}^{2-}$

SCF Energy = -243.686785 a. u.

6	-3.370047000	-0.054299000	-0.112278000
6	-2.113817000	-0.043025000	-0.108858000
6	-0.756738000	-0.025532000	-0.103893000
6	0.479904000	-0.005965000	-0.096663000
6	1.837038000	0.017283000	-0.087379000
6	3.093226000	0.038772000	-0.074229000
1	4.414325000	1.147413000	-1.857046000
1	4.845671000	1.545311000	-2.337072000
1	5.527546000	0.575047000	0.284875000
1	6.265499000	0.708782000	0.400227000
1	5.489594000	-1.565516000	-1.565172000
1	4.899010000	-1.217159000	-1.240316000
1	5.002772000	-1.937526000	1.645710000
1	4.560050000	-1.488206000	1.225434000
1	4.238892000	0.912520000	2.844694000
1	3.918531000	0.749107000	2.178535000
1	2.903619000	-3.327613000	-0.485320000
1	2.807866000	-2.587112000	-0.379256000
1	3.845322000	2.405777000	0.258447000
1	4.157003000	3.088070000	0.359632000
1	-3.633305000	-1.072650000	3.012261000
1	-3.520275000	-0.783740000	2.322958000
1	-6.098240000	-1.427759000	0.970098000
1	-5.468183000	-1.107703000	0.691431000
1	-3.843851000	3.083481000	-0.923938000
1	-3.710503000	2.351978000	-0.785067000
1	-4.537930000	-1.677163000	-1.555602000
1	-4.951980000	-2.138108000	-1.993300000
1	-5.403295000	1.673009000	1.689608000

$C_6H_{28}^{2-}$

SCF Energy = -244.863086 a. u.

6	-3.231419000	-0.048909000	0.030048000
6	-1.975051000	-0.033782000	0.030096000
6	-0.618234000	-0.012588000	0.029170000
6	0.618055000	0.010944000	0.029153000
6	1.974874000	0.032089000	0.030115000
6	3.231245000	0.047186000	0.030119000
1	4.304628000	1.478830000	-1.700955000
1	4.655115000	1.908960000	-2.216788000
1	5.701230000	0.443344000	0.137815000
1	6.448060000	0.576158000	0.174437000
1	5.196564000	-1.355417000	-2.138488000
1	4.734238000	-1.021709000	-1.638788000
1	5.211991000	-2.327123000	1.011942000
1	4.744769000	-1.772502000	0.790703000
1	4.686399000	0.328229000	2.918887000
1	4.326376000	0.263822000	2.255368000
1	2.703613000	-3.198407000	-1.001015000
1	2.720908000	-2.482207000	-0.767032000
1	4.070666000	2.299155000	0.718530000
1	4.355072000	2.971008000	0.920603000
1	-4.363335000	-2.970345000	0.916852000
1	-4.077210000	-2.299118000	0.715065000
1	-4.686991000	-0.330343000	2.918280000
1	-4.326970000	-0.265952000	2.254751000
1	-6.449847000	-0.567133000	0.175135000
1	-5.702677000	-0.436237000	0.138445000
1	-2.694235000	3.197355000	-1.002563000
1	-2.714207000	2.481100000	-0.769054000
1	-4.308919000	-1.475882000	-1.702155000

1	-4.946383000	1.247790000	1.257686000
1	-5.554560000	0.562512000	-1.097591000
1	-6.224594000	0.716056000	-1.422112000

1	-4.660700000	-1.905082000	-2.217894000
1	-5.203164000	2.330439000	1.015301000
1	-4.737925000	1.774595000	0.792923000
1	-4.734108000	1.024689000	-1.636870000
1	-5.196157000	1.360128000	-2.135641000

$C_6H_{30}^{2-}$

SCF Energy = -246.039926 a. u.

6	3.328567000	-0.050734000	-0.028845000
6	2.072601000	-0.070960000	-0.038660000
6	0.716140000	-0.087465000	-0.039583000
6	-0.520319000	-0.105893000	-0.035222000
6	-1.876942000	-0.122987000	-0.025098000
6	-3.133428000	-0.130391000	-0.012922000
1	-4.813328000	-0.290646000	-1.864504000
1	-5.343314000	-0.312087000	-2.405346000
1	-5.553972000	-0.653463000	0.465753000
1	-6.289783000	-0.786131000	0.593050000
1	-5.474353000	2.121863000	-0.295597000
1	-4.938885000	1.587550000	-0.253280000
1	-4.519667000	1.062726000	2.667185000
1	-4.194708000	0.773947000	2.047155000
1	-2.960347000	1.578072000	-2.038789000
1	-3.038468000	1.951697000	-2.688837000
1	-3.964099000	-2.266961000	2.316264000
1	-3.751005000	-1.762514000	1.794841000
1	-2.702809000	3.215589000	0.728543000
1	-2.618630000	2.477844000	0.603277000
1	-4.078422000	-2.352202000	-0.644452000
1	-4.406142000	-3.019371000	-0.787902000
1	3.820389000	3.068095000	0.869952000
1	3.691069000	2.338037000	0.723625000
1	4.226032000	0.412072000	3.064110000
1	4.063124000	0.296788000	2.334163000
1	6.351460000	1.056846000	0.475860000
1	5.666812000	0.749787000	0.361370000
1	3.369500000	-3.283252000	-0.924066000
1	3.261251000	-2.550221000	-0.781369000
1	4.380374000	1.541631000	-1.637998000
1	4.782512000	1.996043000	-2.090542000
1	5.597466000	-2.078385000	1.095825000
1	5.076559000	-1.579875000	0.860821000
1	5.155443000	-0.826138000	-1.508165000
1	5.686217000	-1.056767000	-1.998973000

$C_6H_{32}^{2-}$

SCF Energy = -247.214454 a. u.

6	-3.298652000	-0.126981000	0.137720000
6	-2.042012000	-0.147349000	0.100521000
6	-0.686778000	-0.154008000	0.051276000
6	0.548980000	-0.162890000	0.007115000
6	1.904385000	-0.171482000	-0.037031000
6	3.160305000	-0.163771000	-0.072851000
1	4.235864000	0.735206000	1.997579000
1	4.562304000	1.024388000	2.615950000
1	5.601225000	-0.613016000	0.351911000
1	6.339021000	-0.739517000	0.473993000
1	5.419849000	2.174338000	-0.311832000
1	4.889627000	1.634539000	-0.276983000
1	5.310307000	-0.223154000	-2.503838000
1	4.784147000	-0.216556000	-1.958373000
1	2.563186000	2.413157000	0.680884000
1	2.483840000	3.095986000	0.987207000
1	4.486040000	-3.023729000	-0.861515000
1	4.155860000	-2.358241000	-0.715872000
1	2.914739000	2.177981000	-2.511697000
1	2.898423000	1.646527000	-1.977396000
1	3.850077000	-1.776726000	1.729702000
1	4.073631000	-2.276334000	2.251164000
1	-3.892710000	1.538297000	-2.624726000
1	-3.748112000	1.190680000	-1.969479000
1	-3.253186000	-1.761883000	-2.809376000
1	-3.176193000	-1.418464000	-2.142287000
1	-2.767095000	2.540124000	0.144970000
1	-2.670357000	3.281577000	0.232389000
1	-5.991660000	-0.728127000	-1.614065000
1	-5.433887000	-0.555070000	-1.130709000
1	-3.991568000	-1.654625000	2.947634000
1	-3.852236000	-1.314591000	2.286496000
1	-5.206045000	1.491938000	0.196258000
1	-5.746328000	2.024208000	0.198079000
1	-4.604157000	-3.107720000	-0.021483000
1	-4.278597000	-2.427293000	0.041764000
1	-3.675920000	1.215645000	2.258277000
1	-3.797454000	1.569351000	2.914875000

$C_6H_{34}^{2-}$

SCF Energy = -248.392592 a. u.

6	-3.302446000	-0.096692000	-0.085072000
6	-2.046556000	-0.075300000	-0.111961000
6	-0.691107000	-0.043143000	-0.136737000
6	0.544603000	-0.012480000	-0.161525000
6	1.900303000	0.011911000	-0.189301000

$C_6H_{36}^{2-}$

SCF Energy = -249.566118 a. u.

6	-3.333077000	0.016228000	-0.160897000
6	-2.075524000	0.026210000	-0.168998000
6	-0.719857000	0.026715000	-0.159237000
6	0.516439000	0.016860000	-0.160474000
6	1.872282000	0.000850000	-0.161936000

6	3.157017000	0.027864000	-0.195206000
1	4.140631000	-2.010220000	-1.249613000
1	4.448595000	-2.629208000	-1.557062000
1	5.637987000	-0.046470000	-0.689928000
1	6.380040000	-0.132173000	-0.818817000
1	5.182530000	-1.868396000	1.560044000
1	4.735648000	-1.430320000	1.135310000
1	5.356258000	1.283563000	1.880826000
1	4.846427000	1.029830000	1.382139000
1	2.321840000	-2.447523000	0.850265000
1	2.231622000	-3.120942000	1.172808000
1	4.702840000	2.783349000	-0.964991000
1	4.358054000	2.124428000	-0.823334000
1	2.840752000	-0.323550000	3.204499000
1	2.751233000	-0.219512000	2.464027000
1	3.990296000	0.235791000	-2.550211000
1	4.311563000	0.317849000	-3.230139000
1	2.546371000	2.294196000	1.204715000
1	2.475653000	2.958666000	1.551504000
1	-4.952467000	0.224530000	2.711581000
1	-4.600622000	0.142528000	2.046649000
1	-2.986021000	2.655106000	1.916438000
1	-2.974211000	2.102015000	1.405426000
1	-3.795131000	-2.148656000	1.307958000
1	-4.001599000	-2.692632000	1.789793000
1	-5.764862000	2.030799000	0.074006000
1	-5.219588000	1.505010000	0.053066000
1	-5.089561000	0.279625000	-2.753657000
1	-4.723836000	0.185942000	-2.096681000
1	-5.681459000	-0.903880000	0.046980000
1	-6.367945000	-1.218768000	0.116697000
1	-3.169888000	2.925073000	-1.639341000
1	-3.095578000	2.254056000	-1.304206000
1	-3.967720000	-2.195039000	-1.292940000
1	-4.238731000	-2.818031000	-1.625003000

6	3.128861000	-0.017125000	-0.148650000
1	4.054091000	-2.292116000	-0.621375000
1	4.376418000	-2.966652000	-0.736940000
1	5.598696000	-0.303367000	-0.693424000
1	6.336554000	-0.411888000	-0.826238000
1	5.271548000	-1.269972000	1.999032000
1	4.769189000	-1.018615000	1.492062000
1	5.466051000	1.845334000	1.235042000
1	4.943762000	1.370856000	0.962131000
1	2.338866000	-2.050412000	1.578381000
1	2.307899000	-2.590454000	2.100944000
1	4.797699000	2.216849000	-1.849148000
1	4.378840000	1.745352000	-1.431661000
1	2.936060000	0.931552000	3.102044000
1	2.854502000	0.634084000	2.414593000
1	3.892345000	-0.506076000	-2.497584000
1	4.203834000	-0.621172000	-3.176719000
1	2.677384000	2.582210000	0.480029000
1	2.764443000	3.318658000	0.610253000
1	-3.234796000	1.953854000	2.595680000
1	-3.207271000	1.442921000	2.042244000
1	-2.629999000	3.431882000	-0.470591000
1	-2.727043000	2.692062000	-0.372721000
1	-2.893479000	-1.441162000	2.028199000
1	-2.846727000	-1.797883000	2.690354000
1	-5.695907000	2.261152000	0.121584000
1	-5.165334000	1.722163000	0.075945000
1	-2.278604000	-2.647999000	-0.543410000
1	-1.977439000	-3.327925000	-0.649875000
1	-4.258105000	-1.764876000	-2.745099000
1	-4.040174000	-1.292779000	-2.196298000
1	-5.160305000	-0.167344000	1.595455000
1	-5.692314000	-0.198757000	2.132700000
1	-4.451784000	1.595519000	-2.796357000
1	-4.175513000	1.249002000	-2.183354000
1	-4.759479000	-2.038163000	0.104141000
1	-5.108645000	-2.704271000	0.191131000

$C_6H_{38}^{2-}$

SCF Energy = -250.742492 a. u.

6	3.251989000	0.007913000	-0.070792000
6	1.994260000	0.004284000	-0.095043000
6	0.638636000	-0.001226000	-0.113420000
6	-0.597233000	-0.005833000	-0.140097000
6	-1.952408000	-0.008732000	-0.168500000
6	-3.208914000	-0.009600000	-0.167228000
1	-4.256308000	2.047809000	-1.135463000
1	-4.572443000	2.667225000	-1.433005000
1	-5.695816000	0.031940000	-0.621774000
1	-6.438959000	0.113677000	-0.746642000
1	-5.206831000	1.758628000	1.716139000
1	-4.760488000	1.332366000	1.278389000
1	-5.282266000	-1.564752000	1.831412000
1	-4.828113000	-1.159546000	1.382022000
1	-2.358000000	2.436717000	0.932007000

$C_6H_{40}^{2-}$

SCF Energy = -251.91799 a. u.

6	3.311741000	0.007162000	-0.040398000
6	2.054503000	-0.029695000	-0.049517000
6	0.699738000	-0.066998000	-0.055336000
6	-0.536016000	-0.085309000	-0.071053000
6	-1.891209000	-0.087258000	-0.096894000
6	-3.147902000	-0.069991000	-0.109219000
1	-4.362907000	2.149446000	-0.022740000
1	-4.702511000	2.822409000	0.031711000
1	-5.617219000	0.128374000	-0.649390000
1	-6.356842000	0.224470000	-0.782647000
1	-5.347372000	0.634440000	2.227434000
1	-4.833843000	0.453075000	1.702709000
1	-5.349189000	-2.303834000	0.889989000
1	-4.843196000	-1.787012000	0.668986000
1	-2.465305000	1.693014000	1.904274000

1	-2.268835000	3.108979000	1.257018000
1	-4.704472000	-2.731318000	-1.151810000
1	-4.366533000	-2.098712000	-0.910807000
1	-2.628680000	-0.022037000	3.245929000
1	-2.721537000	0.061137000	2.503683000
1	-4.068606000	-0.149543000	-2.522105000
1	-4.391223000	-0.222467000	-3.202046000
1	-2.453850000	-2.371866000	1.110983000
1	-2.371783000	-3.038981000	1.448612000
1	2.557634000	-0.379575000	3.288435000
1	2.657655000	-0.277156000	2.549064000
1	2.243938000	-2.386493000	-2.550996000
1	2.285994000	-1.856690000	-2.019795000
1	2.490122000	-3.289942000	0.811920000
1	2.592312000	-2.556326000	0.678852000
1	2.616363000	2.334576000	1.211257000
1	2.545655000	3.004969000	1.546338000
1	5.230928000	-1.814660000	1.842350000
1	4.797988000	-1.381240000	1.399205000
1	2.273406000	2.241118000	-1.608371000
1	2.168324000	2.898449000	-1.956830000
1	4.163380000	0.345722000	-3.191870000
1	4.017137000	0.243320000	-2.457357000
1	4.867679000	1.035444000	1.619557000
1	5.354945000	1.295894000	2.135929000
1	5.137395000	-2.345668000	-1.294845000
1	4.774018000	-1.748247000	-1.003830000
1	4.740683000	1.933311000	-0.652287000
1	5.101206000	2.583095000	-0.798783000

1	-2.385820000	2.060660000	2.555812000
1	-4.423337000	-2.079863000	-2.333821000
1	-4.164916000	-1.582480000	-1.826182000
1	-2.860384000	-1.453159000	3.012290000
1	-2.793645000	-1.126440000	2.336967000
1	-3.868400000	0.972977000	-2.276465000
1	-4.148725000	1.285780000	-2.904899000
1	-2.459049000	-2.791914000	0.021161000
1	-2.541917000	-3.534523000	-0.060737000
1	-1.557175000	3.177800000	-0.977991000
1	-1.873889000	2.510307000	-0.845539000
1	2.800634000	-1.786371000	2.857536000
1	2.805220000	-1.283042000	2.297934000
1	2.362112000	-1.088737000	-3.306555000
1	2.474955000	-0.942340000	-2.577891000
1	2.736098000	-3.398179000	-0.419930000
1	2.828155000	-2.658385000	-0.315531000
1	2.538309000	1.660409000	2.034649000
1	2.451819000	2.020868000	2.689489000
1	5.517912000	-2.207344000	1.034826000
1	5.018827000	-1.690221000	0.799515000
1	2.068565000	2.597158000	-0.673087000
1	1.754733000	3.268319000	-0.794993000
1	4.402088000	1.509113000	-2.736503000
1	4.129063000	1.184178000	-2.110861000
1	4.923550000	0.465153000	1.882855000
1	5.419124000	0.646632000	2.424407000
1	5.359486000	-1.589671000	-2.024878000
1	4.918727000	-1.169852000	-1.574869000
1	4.581965000	2.163852000	0.152251000
1	4.919170000	2.837470000	0.225215000

$C_6H_{42}^{2-}$

SCF Energy = -253.094873 a. u.

6	-3.372501113	-0.000784241	0.044946199
6	-2.115528931	-0.013208793	0.001332997
6	-0.761248990	-0.026975869	-0.042444249
6	0.474229071	-0.033839298	-0.061415782
6	1.829294311	-0.033559892	-0.065176116
6	3.086213046	-0.030529823	-0.059428193
1	4.250718384	1.939909290	1.003871996
1	4.569858303	2.550412086	1.314530263
1	5.630661305	0.069594217	0.132843069
1	6.376035506	0.157141830	0.232316750
1	4.861990604	1.998536308	-1.919735994
1	4.440951255	1.546198241	-1.484377109
1	5.077207520	-1.184151043	-2.384764261
1	4.590810547	-0.942304869	-1.858384243
1	2.072362355	2.597300365	-0.493921873
1	1.953187934	3.330961228	-0.607345196
1	4.784834444	-2.768845341	0.496804831
1	4.437355495	-2.107067916	0.382370251
1	2.258669260	0.489647179	-3.423140201
1	2.362124470	0.377652106	-2.686212197
1	4.244847162	-0.313883073	2.165187982

$C_6H_{44}^{2-}$

SCF Energy = -254.269788 a. u.

6	-3.352301359	-0.047622248	-0.015671055
6	-2.095247154	-0.025512164	-0.043260769
6	-0.740787822	-0.007922313	-0.073174101
6	0.495019916	-0.001390149	-0.084432876
6	1.849882481	-0.011079913	-0.085626171
6	3.106738244	-0.031254267	-0.072651803
1	4.412240214	0.254244797	2.078109220
1	4.755124317	0.341026161	2.745919266
1	5.628769496	-0.434362974	0.054741270
1	6.370794535	-0.553333132	0.145393037
1	5.288892707	2.404787269	0.283453264
1	4.766499511	1.860240067	0.238539345
1	5.171244434	0.848140953	-2.465514063
1	4.674927505	0.642936070	-1.933199851
1	2.441025327	2.013494032	1.639335025
1	2.416948292	2.550114159	2.166090229
1	4.373115494	-2.478096310	-1.809717928
1	4.075887217	-1.878761271	-1.457556289
1	2.647252051	3.045857989	-1.606726064
1	2.598354486	2.376061941	-1.267094285
1	4.086832190	-2.027643173	1.129327221

1	4.577795433	-0.403938986	2.837617217
1	2.297140446	-2.373498077	-1.311933061
1	2.207750237	-3.040885311	-1.647835199
1	2.045321398	-1.918132058	1.817117942
1	1.862924054	-2.434153961	2.332157163
1	1.762428003	1.553052145	2.941923344
1	1.884263127	1.220299141	2.279368028
1	-3.185688315	-0.265525268	-3.346490464
1	-3.088567356	-0.166835828	-2.606052428
1	-1.942323925	-2.492181421	2.372067182
1	-2.137683995	-1.977858178	1.861450296
1	-2.723970052	-3.180043052	-1.225871377
1	-2.799738180	-2.502568112	-0.906918257
1	-2.730999114	2.359427254	-1.225542229
1	-2.658592320	3.029323317	-1.560424113
1	-5.605270322	-1.709515041	-1.666152140
1	-5.147603440	-1.285450385	-1.238565281
1	-1.950052030	2.227670057	1.529033319
1	-1.667238012	2.840051961	1.857868295
1	-3.912465111	0.325819195	3.275024018
1	-3.791889429	0.226712763	2.536188330
1	-5.115199271	1.138008903	-1.400840130
1	-5.569236526	1.547174044	-1.846652383
1	-5.045976537	-2.426950271	1.427738210
1	-4.711789463	-1.823568084	1.115715195
1	-4.639137130	2.001310255	0.873939931
1	-4.968561081	2.624546114	1.149135913

1	4.381904599	-2.639729268	1.459245952
1	2.263858372	-0.072541205	-2.775682311
1	2.149309490	0.013977159	-3.513469170
1	1.736461275	-2.702355278	0.058677290
1	1.413444074	-3.375703165	0.131025345
1	-0.316958122	2.734628211	0.112132130
1	-0.226495800	3.470865109	0.216965847
1	1.657570473	-1.175874181	3.095015381
1	1.946885433	-0.879270333	2.468711352
1	-3.346916451	2.960627114	-1.512117110
1	-3.253734159	2.290044179	-1.180292811
1	-1.874492927	-3.192833266	-1.441885234
1	-1.988415264	-2.526527141	-1.116305228
1	-2.820127379	-0.418027272	-3.410861172
1	-2.912359270	-0.308498165	-2.671772008
1	-3.007560903	1.948014168	1.725064385
1	-3.013223099	2.484015158	2.253830463
1	-5.710994115	0.663598854	-2.201961038
1	-5.194569509	0.477634856	-1.681492989
1	-1.970668246	-0.519628246	2.623292493
1	-1.651173778	-0.626951213	3.293518234
1	-3.497470025	-3.032649196	1.517378190
1	-3.418622085	-2.362837272	1.180763250
1	-5.273841319	1.529826026	0.507882098
1	-5.799193146	2.042328900	0.691623023
1	-5.086400387	-2.452233302	-1.330173800
1	-4.743958147	-1.854403242	-1.015700166
1	-4.693034362	-0.308503986	2.076998477
1	-5.036959357	-0.383017964	2.747390379

$C_6H_{46}^{2-}$

SCF Energy = -255.447831 a. u.

6	-3.209554000	-0.048574000	-0.059130000
6	-1.953037000	-0.047097000	-0.095668000
6	-0.598771000	-0.054899000	-0.126127000
6	0.636706000	-0.053614000	-0.122507000
6	1.990793000	-0.056520000	-0.097311000
6	3.247269000	-0.061868000	-0.062896000
1	4.363859000	-2.063032000	0.981159000
1	4.688972000	-2.668238000	1.296124000
1	5.774956000	-0.089906000	0.142468000
1	6.530253000	-0.100488000	0.201079000
1	4.652669000	0.222060000	2.888284000
1	4.326853000	0.166325000	2.208885000
1	4.827978000	2.721155000	0.618199000
1	4.469210000	2.074416000	0.462036000
1	1.842069000	-1.294640000	2.247102000
1	1.549436000	-1.603333000	2.866278000
1	5.043510000	1.329611000	-2.410667000
1	4.636722000	1.005765000	-1.861539000
1	1.970221000	2.197953000	2.448643000
1	2.106078000	1.716545000	1.887885000
1	4.617317000	-1.567838000	-1.543492000
1	5.009157000	-2.026965000	-1.998839000
1	2.204828000	2.346250000	-1.205711000

$C_6H_{48}^{2-}$

SCF Energy = -256.622335 a. u.

6	-3.382816365	0.112343801	0.047938167
6	-2.125500218	0.097641140	0.029765162
6	-0.771265257	0.082573876	0.012589127
6	0.464720285	0.065912201	-0.002732142
6	1.819343133	0.048806018	0.000122240
6	3.076670393	0.055671034	0.011196861
1	4.264229337	2.262363975	-0.448944982
1	4.597666568	2.930153384	-0.563184825
1	5.570864275	0.375125814	0.502310920
1	6.308479680	0.486861061	0.629473801
1	5.297186502	0.358257760	-2.405501130
1	4.774397481	0.316077042	-1.861243916
1	5.403017190	-2.221781372	-0.651473286
1	4.885376534	-1.702536251	-0.469862830
1	2.355376402	1.549919945	-2.215461937
1	2.278296973	1.902604939	-2.875199385
1	4.156969342	-1.472950056	2.683594357
1	3.870859079	-1.143474246	2.066415990
1	2.732954424	-1.913214414	-2.800667415
1	2.723399070	-1.397105197	-2.253278002
1	3.947132571	1.528027882	1.912611152
1	4.175811227	2.017669240	2.439204958
1	2.669217141	-2.695765434	0.123668194

1	2.032682000	3.005722000	-1.523372000
1	2.419557000	-0.386870000	-2.723815000
1	2.317371000	-0.484404000	-3.462552000
1	-1.168642000	0.680108000	2.495398000
1	-1.081086000	0.889887000	3.209574000
1	2.083900000	-3.388138000	-0.756233000
1	2.215277000	-2.661795000	-0.613707000
1	-0.662451000	3.305995000	0.847645000
1	-0.500802000	2.607157000	0.632473000
1	-3.913469000	2.882293000	1.230977000
1	-3.712305000	2.216583000	0.935990000
1	-2.883379000	-0.378994000	-3.468454000
1	-2.869468000	-0.317040000	-2.718296000
1	-2.002421000	2.751845000	-2.060507000
1	-2.177176000	2.168965000	-1.619909000
1	-3.959226000	-0.019504000	2.377086000
1	-4.211812000	-0.020000000	3.088328000
1	-5.133626000	1.834128000	-1.930577000
1	-4.704932000	1.393770000	-1.490088000
1	-1.980928000	-1.976870000	1.765131000
1	-1.770316000	-2.497596000	2.263779000
1	-2.687900000	-3.249794000	-1.261260000
1	-2.706352000	-2.547004000	-0.992375000
1	-5.645078000	0.343567000	0.538266000
1	-6.370304000	0.459210000	0.723709000
1	-5.574029000	-1.436868000	-1.871690000
1	-5.040142000	-1.111795000	-1.445657000
1	-4.603657000	-1.957519000	0.853001000
1	-5.003816000	-2.535239000	1.131072000

1	2.762997933	-3.434602180	0.223229189
1	1.627471929	0.637832155	2.646351392
1	1.305654902	0.736952875	3.316379220
1	-0.247798889	-0.268584971	-2.743356990
1	-0.152724787	-0.381828902	-3.477737534
1	1.487959110	3.353680395	0.650772126
1	1.806181436	2.683677438	0.535561773
1	-0.135243946	-3.157292134	-1.255840272
1	-0.056563227	-2.487711990	-0.928943143
1	0.649894221	-2.459453925	2.393910031
1	0.656651815	-1.929207209	1.865069339
1	-3.068630074	-2.169254180	-2.490552085
1	-3.046133162	-1.644749037	-1.950907180
1	-1.879086186	-0.436656957	3.444030002
1	-2.002144238	-0.323737941	2.712523419
1	-2.641141113	-3.125716128	1.212120177
1	-2.719866283	-2.448187212	0.894941918
1	-2.951610463	1.333149364	-2.332210081
1	-2.893505213	1.674887269	-3.000223331
1	-5.635201645	-2.280012037	-0.198845231
1	-5.113951471	-1.733600014	-0.160399974
1	-2.115293976	2.806471431	-0.009225147
1	-1.791507880	3.480067502	-0.077405931
1	-4.015441416	2.234678480	2.497848380
1	-3.841552185	1.728090220	1.966350160
1	-5.210801492	0.151889217	-1.707361289
1	-5.740495218	0.160832312	-2.247355979
1	-5.029506424	-0.984636932	2.646669957
1	-4.695823127	-0.701436085	2.029733953
1	-4.733671471	2.181466003	-0.370943197
1	-5.077263084	2.845071207	-0.489919176

$C_6H_{50}^{2-}$

SCF Energy = -257.796498 a. u.

6	-3.389842252	0.057432136	-0.019999196
6	-2.132256224	0.039179225	-0.023100174
6	-0.778292202	0.017796231	-0.025212121
6	0.457852093	0.008131867	-0.022610156
6	1.812636869	-0.002586089	-0.022456166
6	3.070158338	-0.003347046	-0.036217949
1	4.130113597	1.721161173	-1.624621251
1	4.444774560	2.232173884	-2.081739376
1	5.430967274	0.888322969	0.310929205
1	6.128254609	1.160682561	0.421893970
1	5.439336212	-0.773505264	-2.215864112
1	4.910359521	-0.587582013	-1.709167900
1	5.663494107	-1.957764259	0.683213867
1	5.089703512	-1.497162561	0.511029115
1	2.505645278	-0.088309099	-2.708863100
1	2.466227923	-0.093453231	-3.460081006
1	4.236651265	0.116619024	3.014175089
1	3.955737522	0.094810042	2.312910986
1	3.049679178	-3.059816627	-1.519318154
1	2.993625020	-2.388316098	-1.182670934
1	3.377013408	2.445264037	0.720616115

$C_6H_{52}^{2-}$

SCF Energy = -258.977251 a. u.

6	3.245024000	-0.018767000	-0.020694000
6	1.987967000	0.002605000	-0.017564000
6	0.633698000	0.014049000	-0.001372000
6	-0.602836000	0.011750000	0.006563000
6	-1.957329000	-0.007926000	0.023231000
6	-3.214218000	-0.044003000	0.024015000
1	-4.466785000	-0.870196000	-2.035973000
1	-4.800397000	-1.142482000	-2.656114000
1	-5.719247000	-0.597632000	0.119949000
1	-6.459640000	-0.727453000	0.206534000
1	-5.364215000	1.830023000	-1.627427000
1	-4.910308000	1.394372000	-1.209027000
1	-5.407308000	1.814431000	1.681931000
1	-4.950397000	1.380389000	1.266204000
1	-2.446991000	0.973875000	-2.467074000
1	-2.361857000	1.294775000	-3.141697000
1	-4.242246000	-1.420079000	2.803934000
1	-3.956716000	-1.100671000	2.182083000
1	-2.907986000	3.386752000	-0.193671000
1	-2.809324000	2.647146000	-0.095721000
1	-4.084579000	-2.441400000	-0.113488000

1	3.508403356	3.157540848	0.930460824
1	2.907912064	-2.266078271	1.462468113
1	2.972992928	-2.893319472	1.872134913
1	1.562723918	1.434866757	2.316970305
1	1.369371018	1.796801240	2.943914109
1	-0.190066180	-1.667534351	-2.182187272
1	-0.155882917	-2.149889997	-2.754688262
1	1.248705375	2.797156324	-1.938140250
1	1.528957117	2.230204816	-1.535409376
1	0.185690943	-3.456614366	0.414738965
1	0.208985854	-2.712646188	0.330654817
1	0.667431155	-1.278360998	3.246186504
1	0.665679050	-0.983987102	2.557369179
1	-0.427185743	3.416247138	0.828668288
1	-0.375411041	2.691119258	0.646803297
1	-2.978221199	-3.186092077	-1.098948214
1	-2.972830471	-2.471317021	-0.862634059
1	-1.725078143	1.217504026	3.153656158
1	-1.944082911	0.976346312	2.477654977
1	-2.561037436	-2.238237197	2.529330193
1	-2.628634538	-1.744783117	1.965822041
1	-2.955741221	-0.199984020	-2.676065224
1	-2.963495255	-0.246899817	-3.427281013
1	-5.493465753	-2.245893863	1.042710960
1	-5.039625352	-1.696135852	0.790732100
1	-2.208566229	2.234567353	-1.587359235
1	-1.974484143	2.813902138	-2.003751350
1	-3.882584059	3.162460079	1.029586306
1	-3.769337482	2.454842145	0.793552086
1	-5.190422347	-0.937043789	-1.510807925
1	-5.694433513	-1.254550138	-1.976828399
1	-4.990440443	0.452747121	2.796312287
1	-4.639547243	0.367727916	2.131619094
1	-4.864159172	1.527126164	-1.416330207
1	-5.265243247	1.985449225	-1.865787961

1	-4.404402000	-3.121605000	-0.179953000
1	-2.742605000	1.330133000	2.397269000
1	-2.681716000	1.670085000	3.064363000
1	-1.555654000	-2.578438000	0.837284000
1	-1.229811000	-3.242895000	0.958243000
1	0.178404000	2.445311000	-1.304991000
1	0.102529000	3.111697000	-1.638771000
1	-1.783833000	-2.388898000	-2.454219000
1	-1.974734000	-1.874325000	-1.942566000
1	-0.004074000	2.927173000	1.902142000
1	-0.075720000	2.261427000	1.566052000
1	-0.713272000	-0.697371000	3.403186000
1	-0.592375000	-0.575458000	2.673861000
1	1.160491000	-3.096475000	-1.463309000
1	1.247059000	-2.429250000	-1.133543000
1	2.822116000	3.369320000	0.491060000
1	2.907630000	2.628971000	0.387337000
1	1.684157000	-2.603156000	2.178372000
1	1.902328000	-2.088397000	1.677781000
1	2.377699000	0.763028000	3.311081000
1	2.481579000	0.636632000	2.577132000
1	2.853267000	1.628485000	-2.195284000
1	2.854396000	2.141520000	-2.744264000
1	5.400471000	1.603798000	1.844700000
1	4.947951000	1.187668000	1.404962000
1	3.856055000	-0.870825000	-2.308598000
1	4.009734000	-1.188481000	-2.976613000
1	4.086195000	-3.218157000	-0.285422000
1	3.945150000	-2.483590000	-0.189803000
1	5.057134000	1.442328000	-1.048939000
1	5.571964000	1.934862000	-1.301653000
1	4.754912000	-1.487466000	2.508632000
1	4.437207000	-1.170566000	1.901327000
1	5.699336000	-0.731912000	-0.228280000
1	6.388929000	-1.031045000	-0.314883000
1	0.734523000	-0.243531000	-3.456095000
1	0.631134000	-0.128693000	-2.723122000

$C_6H_{54}^{2-}$

SCF Energy = -260.151492 a. u.

6	-3.216601000	-0.027374000	-0.006873000
6	-1.959436000	0.000720000	-0.001717000
6	-0.604621000	0.015356000	0.004394000
6	0.631811000	0.015239000	0.008406000
6	1.986425000	-0.003372000	0.002780000
6	3.243126000	-0.036008000	-0.006135000
1	4.592911000	1.095589000	-1.830674000
1	4.927292000	1.413962000	-2.428401000
1	5.369429000	1.270851000	0.522099000
1	6.026380000	1.621964000	0.652555000
1	6.218795000	-1.126580000	-1.031742000
1	5.581000000	-0.836957000	-0.747744000
1	5.493541000	-1.103330000	2.157872000
1	4.985911000	-0.880762000	1.644305000
1	3.344257000	-1.300333000	-2.260374000

$C_6H_{56}^{2-}$

SCF Energy = -261.327018 a. u.

6	-3.233494000	-0.028710000	-0.005451000
6	-1.975915000	-0.008754000	0.000971000
6	-0.620989000	0.016141000	0.002264000
6	0.615935000	0.026764000	-0.002541000
6	1.971080000	0.012553000	-0.002773000
6	3.228034000	-0.021184000	-0.005233000
1	4.214856000	-1.715019000	1.711700000
1	4.450498000	-2.218173000	2.220750000
1	5.603134000	-1.082866000	-0.152569000
1	6.277934000	-1.415155000	-0.221742000
1	5.701054000	0.744055000	2.095027000
1	5.173780000	0.552059000	1.589873000
1	5.944071000	1.607509000	-0.989609000
1	5.326339000	1.258434000	-0.729135000
1	2.742692000	0.331316000	2.670160000

1	3.446069000	-1.640571000	-2.925333000
1	3.553338000	1.304705000	3.041834000
1	3.441583000	0.984194000	2.368781000
1	4.293965000	-3.197811000	0.140560000
1	3.979643000	-2.516537000	0.068193000
1	3.171540000	2.629605000	-0.112783000
1	3.284866000	3.369766000	-0.035802000
1	2.367235000	-1.684659000	2.113564000
1	2.184384000	-2.189194000	2.639465000
1	0.934058000	2.293006000	1.685019000
1	1.118060000	2.813852000	2.189083000
1	1.287359000	-2.652494000	-0.411121000
1	1.161671000	-3.382339000	-0.525279000
1	1.782305000	1.577288000	-3.018093000
1	2.068128000	1.257508000	-2.402238000
1	-1.031491000	-2.818206000	1.964673000
1	-1.151089000	-2.163158000	1.621602000
1	-0.134157000	0.155769000	3.496783000
1	-0.024999000	0.051026000	2.763008000
1	-0.120183000	3.451546000	-0.683081000
1	-0.011287000	2.715816000	-0.769002000
1	-4.187570000	-2.882957000	1.466286000
1	-3.915094000	-2.258303000	1.145002000
1	-1.935587000	2.707184000	2.100661000
1	-2.128345000	2.182628000	1.599890000
1	-3.501511000	-0.208888000	3.345845000
1	-3.382674000	-0.115908000	2.607743000
1	-3.448929000	-0.392247000	-2.568040000
1	-3.568223000	-0.506290000	-3.303496000
1	-6.222414000	-0.532578000	1.331674000
1	-5.548686000	-0.431007000	1.004060000
1	-1.436065000	1.202089000	-2.470441000
1	-1.148337000	1.515850000	-3.086305000
1	-3.366274000	3.068790000	-1.395392000
1	-3.268805000	2.396513000	-1.070475000
1	-4.949518000	-1.641353000	-1.034553000
1	-5.453732000	-2.146217000	-1.281213000
1	-5.004961000	2.397048000	1.344171000
1	-4.659143000	1.798202000	1.041167000
1	-5.350168000	0.778768000	-1.142766000
1	-5.971633000	1.054576000	-1.474001000
1	0.165490000	-1.368197000	-3.206063000
1	0.060583000	-1.233228000	-2.476912000
1	-2.143649000	-3.177716000	-1.344779000
1	-2.259494000	-2.507640000	-1.024923000

$C_6H_{58}^{2-}$

SCF Energy = -262.500505 a. u.

6	3.249867000	-0.025112000	-0.005857000
6	1.991810000	-0.004168000	-0.013644000
6	0.636196000	0.017978000	-0.009580000
6	-0.600743000	0.032880000	-0.001981000
6	-1.956118000	0.026579000	0.006312000

1	2.833332000	0.439650000	3.408805000
1	4.798699000	-0.673073000	-2.868429000
1	4.461543000	-0.548906000	-2.205201000
1	3.711257000	3.068072000	1.182800000
1	3.585120000	2.395859000	0.866209000
1	3.423314000	-2.494864000	-0.709151000
1	3.541043000	-3.227635000	-0.841305000
1	3.158837000	1.680654000	-2.067843000
1	3.188017000	2.201966000	-2.609557000
1	1.848213000	-0.843450000	-2.579621000
1	1.715838000	-0.974019000	-3.306370000
1	0.524274000	2.063646000	1.844075000
1	0.543083000	2.597499000	2.368736000
1	1.358614000	-2.786458000	1.900362000
1	1.650719000	-2.176902000	1.576142000
1	1.375212000	3.550606000	-0.678766000
1	1.062146000	2.879597000	-0.576736000
1	-0.158445000	1.726317000	-3.069112000
1	-0.070712000	1.387955000	-2.406651000
1	0.302845000	-3.243903000	-1.258150000
1	0.217691000	-2.572621000	-0.937407000
1	-4.692835000	2.962509000	0.154946000
1	-4.354800000	2.290836000	0.096261000
1	-1.528517000	-1.219762000	-3.172577000
1	-1.822493000	-0.917217000	-2.552335000
1	-3.707074000	1.681238000	-2.830028000
1	-3.602794000	1.337689000	-2.167141000
1	-3.469800000	-0.914496000	2.544859000
1	-3.569208000	-1.228900000	3.220635000
1	-6.452448000	0.540507000	-0.827645000
1	-5.720464000	0.418993000	-0.686391000
1	-1.862022000	-2.422908000	1.285753000
1	-1.556708000	-3.039902000	1.583301000
1	-3.022921000	-3.327628000	-1.246488000
1	-2.951769000	-2.651683000	-0.926851000
1	-5.159050000	0.569508000	1.631403000
1	-5.680053000	0.765003000	2.141178000
1	-4.786022000	-1.347071000	-2.671268000
1	-4.460018000	-1.054528000	-2.057612000
1	-4.955406000	-1.757809000	0.536920000
1	-5.470314000	-2.280261000	0.723558000
1	-0.279298000	-0.475558000	3.475122000
1	-0.368601000	-0.368251000	2.739470000
1	-2.716250000	2.198924000	2.649303000
1	-2.725782000	1.677441000	2.108008000
1	-1.789678000	3.403291000	-0.508256000
1	-1.708576000	2.667019000	-0.394832000

$C_6H_{60}^{2-}$

SCF Energy = -263.674357 a. u.

6	3.257891000	-0.033270000	-0.008961000
6	1.999483000	-0.022004000	0.000225000
6	0.643325000	-0.010393000	0.013355000
6	-0.593500000	0.004433000	0.018398000
6	-1.949739000	0.009203000	0.010114000

6	-3.213616000	-0.000959000	0.014092000	6	-3.207978000	0.010253000	-0.018308000
1	-4.525049000	-0.187445000	-2.216097000	1	-4.337959000	-1.413149000	-1.943781000
1	-4.866207000	-0.264140000	-2.884172000	1	-4.585014000	-1.898884000	-2.463579000
1	-5.600028000	-1.153215000	-0.332191000	1	-5.413802000	-1.533306000	0.233993000
1	-6.269430000	-1.486229000	-0.430657000	1	-6.073378000	-1.886749000	0.321434000
1	-6.092510000	1.608385000	-0.514021000	1	-6.343877000	0.484474000	-1.454233000
1	-5.429878000	1.263113000	-0.401720000	1	-5.674038000	0.386156000	-1.123731000
1	-5.866858000	0.112031000	2.129174000	1	-5.721113000	0.884090000	1.873345000
1	-5.216736000	0.056042000	1.751380000	1	-5.184944000	0.672315000	1.382627000
1	-3.444483000	1.984286000	-1.750155000	1	-3.450781000	0.908175000	-2.434345000
1	-3.622230000	2.504215000	-2.264290000	1	-3.555645000	1.221569000	-3.111840000
1	-4.447944000	-2.695186000	1.687375000	1	-4.169599000	-1.937231000	2.651263000
1	-4.152658000	-2.086519000	1.356825000	1	-3.952007000	-1.445977000	2.124930000
1	-4.093392000	2.662550000	1.793176000	1	-3.443308000	2.923048000	1.957774000
1	-3.818699000	2.051318000	1.447356000	1	-3.262665000	2.391236000	1.459446000
1	-3.497617000	-2.288959000	-1.134576000	1	-3.206473000	-2.659159000	-0.056451000
1	-3.605406000	-2.956776000	-1.467105000	1	-3.317718000	-3.398613000	-0.141222000
1	-2.760527000	-0.341024000	2.682396000	1	-2.340315000	0.449688000	2.749859000
1	-2.855993000	-0.454951000	3.419879000	1	-2.428116000	0.366266000	3.490400000
1	-1.585025000	-2.423835000	1.096086000	1	-1.391708000	-1.903997000	1.949196000
1	-1.471769000	-3.091013000	1.418283000	1	-1.096242000	-2.505283000	2.283826000
1	-1.755900000	2.846364000	0.057352000	1	-4.503386000	2.325461000	-0.604423000
1	-1.843543000	3.582749000	-0.045241000	1	-4.840764000	2.985657000	-0.732490000
1	-1.676606000	-0.401658000	-3.367818000	1	-1.547836000	-1.632636000	-2.957607000
1	-1.993552000	-0.312191000	-2.693742000	1	-1.841041000	-1.318855000	-2.342674000
1	-1.127547000	2.077749000	2.690671000	1	-0.489534000	2.779718000	2.126228000
1	-0.710318000	1.644516000	2.245578000	1	-0.309475000	2.260844000	1.617750000
1	0.373510000	-1.231935000	3.264686000	1	0.923112000	-0.161309000	3.492839000
1	0.433609000	-0.908005000	2.592294000	1	0.814336000	-0.066654000	2.758096000
1	-0.434349000	-2.979755000	-1.780568000	1	-0.274902000	-3.398655000	-0.734142000
1	-0.349644000	-2.317390000	-1.441950000	1	-0.181188000	-2.723593000	-0.424581000
1	5.429191000	1.042382000	2.314722000	1	5.619382000	1.795073000	1.569456000
1	4.928722000	0.817763000	1.796898000	1	5.156478000	1.367627000	1.155241000
1	1.427719000	-3.281090000	0.803992000	1	1.751136000	-2.812422000	1.938334000
1	1.758429000	-2.615221000	0.707552000	1	2.030707000	-2.198718000	1.609216000
1	3.745413000	-1.666473000	2.836702000	1	4.145549000	-0.579925000	3.118801000
1	3.625693000	-1.322844000	2.176232000	1	4.002996000	-0.461665000	2.387198000
1	3.133007000	1.902635000	-1.845628000	1	2.972034000	1.195373000	-2.440094000
1	3.158732000	2.434144000	-2.377919000	1	2.979337000	1.702831000	-2.994500000
1	6.470691000	-1.149596000	0.412900000	1	6.632898000	-0.799465000	0.171610000
1	5.789277000	-0.841920000	0.315390000	1	5.892934000	-0.670551000	0.231496000
1	1.645089000	-0.080051000	-2.762206000	1	1.678657000	-1.096775000	-2.501113000
1	1.316552000	-0.147627000	-3.432277000	1	1.352213000	-1.228465000	-3.162877000
1	2.530225000	-2.743132000	-2.295228000	1	2.632314000	-3.365398000	-1.362997000
1	2.544422000	-2.208729000	-1.769189000	1	2.636185000	-2.811275000	-0.858703000
1	5.410413000	1.280448000	-0.674377000	1	5.286457000	1.037274000	-1.337059000
1	6.063243000	1.629362000	-0.822623000	1	5.889173000	1.337187000	-1.676673000
1	4.489841000	-3.243131000	-0.048570000	1	4.700780000	-3.001440000	0.899359000
1	4.163821000	-2.567606000	0.009109000	1	4.370475000	-2.342292000	0.746689000
1	4.632572000	-0.613305000	-2.033832000	1	4.490122000	-1.209139000	-1.875177000
1	5.117930000	-0.808777000	-2.579215000	1	4.813598000	-1.529664000	-2.478176000
1	-0.327703000	2.410823000	-2.576544000	1	-0.255645000	1.531834000	-3.104180000
1	-0.144739000	1.896780000	-2.063829000	1	-0.242631000	1.018186000	-2.559788000
1	3.959183000	3.301814000	0.702827000	1	4.065066000	3.329724000	-0.471058000
1	3.821070000	2.573445000	0.577545000	1	3.755324000	2.651650000	-0.375499000
1	2.280904000	1.566073000	3.041116000	1	2.665415000	2.373669000	2.468904000

1	2.381632000	1.233624000	2.374898000	1	2.741302000	2.001303000	1.820824000
1	1.105056000	2.684362000	0.231977000	1	1.213254000	2.588656000	-0.603484000
1	1.206016000	3.419579000	0.135316000	1	1.100722000	3.318696000	-0.725670000
				1	-1.948031000	2.608987000	-0.849655000
				1	-1.825714000	3.345152000	-0.777266000
$C_6H_{62}^{2-}$				**$C_6H_{64}^{2-}$**			
SCF Energy = -264.848168 a. u.				SCF Energy = -266.020744 a. u.			
6	-3.232831000	0.007371000	-0.037882000	6	3.234248000	-0.015075000	-0.025621000
6	-1.974929000	0.006831000	0.010639000	6	1.975750000	0.007770000	0.013795000
6	-0.618548000	0.004906000	0.033871000	6	0.618001000	0.022597000	0.027197000
6	0.618630000	0.002720000	0.034364000	6	-0.619259000	0.026018000	0.015850000
6	1.975098000	-0.005632000	0.013514000	6	-1.976524000	0.012333000	-0.008202000
6	3.233212000	-0.015315000	-0.031108000	6	-3.235226000	-0.013733000	-0.038895000
1	5.011315000	-0.372570000	-2.065754000	1	-4.731782000	-1.140379000	-2.005348000
1	5.485499000	-0.454852000	-2.644494000	1	-5.136265000	-1.462751000	-2.552366000
1	5.643148000	1.222815000	-0.471993000	1	-5.373011000	-1.792885000	0.208492000
1	6.293059000	1.583318000	-0.592639000	1	-5.943221000	-2.278851000	0.280551000
1	6.339737000	-1.309209000	0.348172000	1	-6.645843000	0.429331000	-0.702873000
1	5.649842000	-1.014539000	0.264004000	1	-5.914376000	0.330509000	-0.551446000
1	5.302550000	0.947344000	2.355454000	1	-5.344961000	0.076851000	2.494620000
1	4.843788000	0.717305000	1.800957000	1	-4.879392000	0.045536000	1.900574000
1	4.161387000	-2.342993000	-1.090430000	1	-4.193705000	1.226492000	-2.085812000
1	4.418212000	-2.982570000	-1.391291000	1	-4.468736000	1.580862000	-2.692294000
1	4.136201000	3.296872000	0.472852000	1	-3.825067000	-2.675515000	2.269721000
1	3.919335000	2.585977000	0.359259000	1	-3.651104000	-2.135086000	1.778431000
1	2.844411000	-0.545733000	3.545265000	1	-2.821482000	2.491892000	2.392305000
1	2.827904000	-0.443673000	2.802143000	1	-2.815149000	1.960016000	1.861360000
1	3.556927000	1.656568000	-2.003791000	1	-3.159547000	-2.599638000	-0.721782000
1	3.704578000	2.144548000	-2.558654000	1	-3.234700000	-3.327478000	-0.901165000
1	2.202592000	1.871884000	1.985439000	1	-2.158162000	-0.382692000	2.680677000
1	2.041448000	2.375763000	2.517450000	1	-1.982205000	-0.489560000	3.402926000
1	1.526451000	2.651645000	-0.498438000	1	-1.216977000	-2.454143000	1.088682000
1	1.295225000	3.354300000	-0.617069000	1	-1.030066000	-3.106310000	1.405894000
1	3.761688000	-2.205648000	1.325407000	1	-4.981915000	2.114966000	0.610578000
1	3.951863000	-2.836744000	1.689723000	1	-5.446703000	2.679004000	0.784944000
1	2.509285000	-1.195319000	-3.251166000	1	-2.213778000	-0.942457000	-3.344556000
1	2.575475000	-0.933452000	-2.549801000	1	-2.342675000	-0.751663000	-2.629606000
1	-0.011386000	0.348923000	3.587717000	1	0.117604000	1.746675000	3.184094000
1	-0.000493000	0.276470000	2.842974000	1	0.079559000	1.391764000	2.524213000
1	-0.914417000	3.047912000	1.788959000	1	0.991846000	-1.458179000	3.187714000
1	-0.763428000	2.424068000	1.403870000	1	0.798938000	-1.192976000	2.515158000
1	0.619011000	1.349474000	-3.207731000	1	-0.323210000	-2.961623000	-1.840715000
1	0.493588000	1.079632000	-2.520850000	1	-0.192404000	-2.333880000	-1.452434000
1	-5.292871000	-0.492509000	2.487807000	1	5.322697000	1.801534000	1.804856000
1	-4.832911000	-0.372280000	1.900465000	1	4.856608000	1.381657000	1.383640000
1	-1.458356000	3.081905000	-1.410896000	1	1.616308000	-3.337773000	0.619193000
1	-1.741999000	2.457037000	-1.109124000	1	1.855825000	-2.637289000	0.499121000
1	-3.950588000	3.114153000	1.104400000	1	3.954074000	-1.971229000	2.661026000
1	-3.758714000	2.426549000	0.864584000	1	3.762445000	-1.524490000	2.086070000
1	-3.538461000	-2.019359000	-1.653214000	1	3.710560000	0.738440000	-2.459474000
1	-3.683764000	-2.602612000	-2.107486000	1	3.884991000	0.973222000	-3.154976000
1	-6.340561000	1.338708000	0.090440000	1	6.353194000	-1.029940000	0.926408000
1	-5.651687000	1.030903000	0.064320000	1	5.667043000	-0.796856000	0.716289000
1	-0.503571000	-1.525200000	-2.260705000	1	0.940023000	-0.042184000	-2.747396000

1	-0.610728000	-1.918041000	-2.889050000
1	-2.506949000	0.568804000	-3.421289000
1	-2.573319000	0.439386000	-2.683939000
1	-5.633231000	-1.308100000	-0.233816000
1	-6.283869000	-1.683645000	-0.284194000
1	-4.432994000	2.657429000	-1.934026000
1	-4.172593000	2.082411000	-1.525231000
1	-5.007607000	-0.039909000	-2.106270000
1	-5.484324000	-0.072776000	-2.687799000
1	1.448349000	-3.296648000	-0.801547000
1	1.712830000	-2.613021000	-0.644483000
1	-4.115925000	-3.159105000	1.078708000
1	-3.903838000	-2.480304000	0.834842000
1	-2.865148000	1.247916000	3.376795000
1	-2.830652000	0.997266000	2.670566000
1	-2.221746000	-1.448168000	2.332444000
1	-2.124645000	-1.833365000	2.969011000
1	0.832579000	-2.113053000	1.821916000
1	0.857970000	-2.654478000	2.338268000
1	-1.297382000	-3.421633000	0.035647000
1	-1.461883000	-2.691065000	0.016920000
1	0.817428000	-0.097176000	-3.487146000
1	2.716498000	-2.425785000	-2.480704000
1	2.745938000	-1.896607000	-1.947653000
1	5.713484000	0.953619000	-0.859065000
1	6.379170000	1.228359000	-1.077494000
1	4.550925000	-3.296638000	-0.054504000
1	4.270100000	-2.599817000	-0.038642000
1	5.118675000	-1.140525000	-1.698503000
1	5.622889000	-1.453109000	-2.164294000
1	-1.297950000	2.103588000	-2.777173000
1	-1.414887000	1.655130000	-2.186625000
1	4.238864000	3.235993000	-0.860232000
1	4.008379000	2.542568000	-0.682326000
1	2.950030000	0.852555000	3.522915000
1	2.891742000	0.653925000	2.802328000
1	2.374801000	2.499525000	1.160188000
1	2.323699000	3.174358000	1.484103000
1	-3.005106000	2.822135000	-0.568204000
1	-3.077750000	3.551919000	-0.730250000
1	1.412857000	2.776000000	-1.936765000
1	1.685240000	2.212805000	-1.521924000
1	-0.474913000	3.498609000	0.460375000
1	-0.417335000	2.766186000	0.311558000

$C_6H_{66}^{2-}$

SCF Energy = -267.19437 a. u.

6	3.227789000	0.020692000	0.020397000
6	1.968753000	0.049164000	0.022487000
6	0.611518000	0.056130000	0.010883000
6	-0.626254000	0.054953000	0.006870000
6	-1.983330000	0.047241000	0.008951000
6	-3.242363000	0.033443000	0.016786000
1	-4.975723000	-2.113587000	-0.050466000
1	-5.495815000	-2.656764000	-0.057607000
1	-5.671335000	-0.274961000	1.368112000
1	-6.337253000	-0.358041000	1.708271000
1	-6.579281000	-0.140330000	-1.253319000
1	-5.902874000	-0.070015000	-0.931964000
1	-5.442500000	2.442550000	0.391166000
1	-4.921827000	1.896788000	0.339328000
1	-3.997834000	-1.173473000	-2.124617000
1	-4.266895000	-1.500095000	-2.749178000
1	-4.299537000	1.229281000	3.133010000
1	-4.001079000	0.939251000	2.507276000
1	-2.478698000	3.251471000	-1.365251000
1	-2.571697000	2.576562000	-1.049194000
1	-3.649110000	-1.592228000	1.990366000
1	-3.833202000	-2.097775000	2.518212000
1	-2.289565000	2.419986000	1.413658000
1	-2.256751000	2.962680000	1.930324000
1	-1.763141000	-0.050491000	2.722002000
1	-1.437983000	0.023496000	3.393181000
1	-4.486865000	1.413227000	-2.098011000
1	-4.902552000	1.835683000	-2.559272000
1	-2.573120000	-3.305142000	-0.720172000

1	-2.645622000	-2.623396000	-0.413374000	
1	0.197526000	3.735622000	0.216486000	
1	0.096278000	3.064488000	-0.096654000	
1	0.644607000	2.133956000	2.950015000	
1	0.545265000	1.793694000	2.291333000	
1	-0.945366000	-2.931079000	1.831725000	
1	-0.826963000	-2.206137000	1.688602000	
1	5.522418000	2.406163000	0.067803000	
1	4.994443000	1.865663000	0.061805000	
1	1.171452000	-0.946764000	3.249806000	
1	1.476255000	-0.655030000	2.630809000	
1	3.740564000	1.241706000	3.188147000	
1	3.630161000	0.926934000	2.513618000	
1	4.239456000	-1.332457000	-2.210873000	
1	4.531301000	-1.654933000	-2.823483000	
1	6.227094000	-0.134260000	1.802814000	
1	5.560817000	-0.074863000	1.457275000	
1	2.143292000	-2.268613000	-1.437338000	
1	1.943990000	-2.791253000	-1.936453000	
1	1.941211000	-3.241599000	1.130031000	
1	2.064010000	-2.514312000	0.992835000	
1	5.886004000	-0.243889000	-0.815849000	
1	6.562916000	-0.330817000	-1.132773000	
1	4.086102000	-1.843264000	2.936812000	
1	3.816941000	-1.512555000	2.318653000	
1	4.565111000	-2.147936000	0.067105000	
1	4.911000000	-2.817375000	0.120107000	
1	-0.838533000	-1.737972000	-2.925156000	
1	-0.719786000	-1.587196000	-2.201443000	
1	4.771968000	1.369916000	-2.844309000	
1	4.458512000	1.073613000	-2.228693000	
1	2.845080000	3.423759000	1.376593000	
1	2.900275000	2.752405000	1.047420000	
1	2.691570000	2.434148000	-1.348174000	
1	2.627010000	3.104162000	-1.680607000	
1	-2.318141000	0.521690000	-2.734896000	
1	-2.220565000	0.826194000	-3.413055000	
1	1.954252000	0.053875000	-3.434950000	
1	2.078723000	-0.045582000	-2.701528000	
1	0.016300000	2.433562000	-2.739660000	
1	0.100037000	1.774391000	-2.397176000	
1	0.025789000	-4.596986000	-0.857108000	
1	-0.054793000	-3.925490000	-0.540342000	

25. Cartesian coordinates in Å unit of optimized geometry of $(HC_n)^-(H_2)_m$ and $(C_n)^{2-}(H_2)_m$ complexes at CCSD/aug-cc-pVDZ level

$C_2H_3^-$	**$C_2H_5^-$**

CCSD(T) Energy = -77.75680 a. u.

6	-0.254656000	0.000087000	-0.000099000
6	1.012328000	-0.000214000	-0.000114000
1	2.096144000	0.000841000	0.000814000
1	-3.707280000	0.000754000	-0.000245000
1	-2.934897000	-0.000839000	0.000707000

CCSD(T) Energy = -78.93302 a. u.

6	0.027530000	-0.214063000	-0.000425000
6	1.271529000	0.023056000	0.000129000
1	2.337995000	0.215839000	0.000802000
1	-2.452009000	-1.208819000	0.000241000
1	-3.167915000	-1.496816000	0.000548000
1	-2.539739000	2.078495000	0.000161000
1	-1.972687000	1.557344000	0.000026000

$C_2H_7^-$

CCSD(T) Energy = -80.10944 a. u.

6	0.235355000	-0.025259000	0.021087000
6	1.500589000	0.000428000	-0.000971000
1	2.583980000	0.021155000	-0.018466000
1	-1.866535000	-1.045196000	-1.244833000
1	-2.472000000	-1.343016000	-1.616259000
1	-2.410158000	2.106201000	-0.400138000
1	-1.818525000	1.622563000	-0.304016000
1	-2.524783000	-0.680299000	1.949795000
1	-1.907641000	-0.532420000	1.513220000

$C_4H_3^-$

CCSD(T) Energy = -153.79122 a. u.

6	-0.966101000	-0.000186000	0.000081000
6	0.427205000	-0.000571000	-0.000092000
6	1.697354000	-0.001483000	0.000013000
6	-2.204936000	0.000991000	-0.000064000
1	-3.278478000	0.000975000	0.000231000
1	4.393627000	0.002452000	0.000321000
1	5.163725000	0.004072000	-0.000181000

$C_4H_5^-$

CCSD(T) Energy = -154.96667 a. u.

6	-1.225700000	-0.024560000	-0.000219000
6	0.167146000	-0.062580000	0.000024000
6	1.429513000	-0.198009000	0.000168000
6	-2.460453000	0.076510000	-0.000267000
1	-3.534095000	0.072106000	-0.000128000
1	3.454413000	1.621824000	0.000374000
1	4.009599000	2.152988000	0.000420000
1	3.946346000	-1.154425000	0.000502000
1	4.660699000	-1.440666000	0.000599000

$C_4H_7^-$

CCSD(T) Energy = -156.14247 a. u.

6	-1.453927000	0.000981000	-0.022422000
6	-0.060394000	0.001240000	-0.039435000
6	1.202585000	0.005463000	-0.162825000
6	-2.689735000	-0.001965000	0.058918000
1	-3.763208000	-0.001339000	0.042200000
1	3.213730000	-1.472300000	0.882001000
1	3.777036000	-1.896287000	1.186599000
1	3.558086000	0.034299000	-1.474584000
1	4.220759000	0.043221000	-1.864005000
1	3.783565000	1.832738000	1.273226000
1	3.218863000	1.425352000	0.949145000

$C_6H_3^-$

CCSD(T) Energy = -229.81803 a. u.

6	-3.460474000	-0.020366000	-0.001078000
6	-2.226142000	-0.005262000	0.003036000
6	-0.842846000	0.062987000	-0.001533000
1	-4.533305000	-0.070024000	0.000051000
6	0.399492000	0.000140000	0.003070000
6	1.778423000	0.003720000	-0.002701000
6	3.050793000	-0.029985000	-0.003241000
1	5.784526000	0.000515000	0.005752000
1	6.553298000	0.002107000	0.008875000

$C_6H_5^-$

CCSD(T) Energy = -230.99336 a. u.

6	3.707204000	0.045132000	0.000906000
6	2.473223000	0.019482000	0.001102000
6	1.088358000	0.043295000	-0.001201000
6	-0.151017000	-0.058103000	-0.000511000
6	-1.529640000	-0.101717000	-0.001272000
6	-2.796874000	-0.212640000	-0.001940000
1	-5.300315000	2.263033000	0.002920000
1	-4.768763000	1.709701000	0.001583000
1	-6.091462000	-1.334369000	0.005210000
1	-5.367882000	-1.075443000	0.005497000
1	4.780898000	0.024382000	0.002279000

$C_6H_7^-$

CCSD(T) Energy = -232.16884 a. u.

6	3.936395000	0.034238000	-0.028435000
6	2.702766000	0.015173000	-0.014771000
6	1.318826000	-0.034420000	-0.040697000
6	0.078685000	-0.030064000	0.042490000
6	-1.300470000	-0.044699000	0.071032000
6	-2.567889000	-0.057824000	0.170056000
1	-4.972683000	-0.185226000	1.425215000
1	-5.644758000	-0.222256000	1.793561000
1	-5.211784000	-1.563360000	-1.584018000
1	-4.643720000	-1.233719000	-1.189290000
1	-5.037583000	2.165193000	-0.942305000
1	-4.508508000	1.669922000	-0.691987000
1	5.009159000	0.075019000	-0.009233000

$C_4H_2^-$

CCSD(T) Energy = -153.04727 a. u.

6	0.000000000	0.000000000	-0.334962000
6	0.000000000	0.000000000	1.087917000
6	0.000000000	0.000000000	2.362514000
6	0.000000000	0.000000000	-1.609261000
1	0.000000000	0.000000000	-4.909582000
1	0.000000000	0.000000000	-4.127668000

$C_4H_4^-$

CCSD(T) Energy = -154.22554 a. u.

6	0.711003000	0.002965000	-0.001196000
6	-0.711017000	-0.003050000	-0.000525000
6	-1.985053000	-0.006590000	-0.001082000
6	1.985040000	0.006501000	-0.000893000
1	-5.286214000	0.012690000	0.006397000
1	-4.504673000	0.005833000	0.004649000
1	5.286293000	-0.012093000	0.006647000
1	4.504753000	-0.005393000	0.004489000

$C_4H_6^-$

CCSD(T) Energy = -155.40368 a. u.

6	-0.450966000	-0.109221000	-0.000821000
6	0.968808000	-0.038362000	0.000116000
6	2.240068000	0.041589000	-0.000744000
6	-1.721254000	-0.196404000	-0.000310000
1	5.543659000	0.173406000	0.003189000
1	4.763186000	0.141589000	0.002006000
1	-3.512956000	1.564237000	0.000545000
1	-4.076739000	2.100800000	0.000915000
1	-4.841279000	-1.199001000	0.002285000
1	-4.095809000	-0.966650000	0.001616000

$C_6H_2^-$

CCSD(T) Energy = -229.11706 a. u.

6	-3.627536000	0.012768000	-0.004992000
6	-2.355122000	0.018010000	0.003736000
6	-0.951931000	-0.025842000	-0.010885000
6	0.292874000	0.016486000	0.014986000
6	1.696096000	-0.029040000	-0.000926000
6	2.967504000	-0.020688000	0.003676000
1	5.546559000	0.069652000	-0.015282000
1	6.322126000	0.100184000	-0.018287000

$C_6H_4^-$

CCSD(T) Energy = -230.29447 a. u.

6	3.296472000	0.026467000	0.000339000
6	2.025084000	0.030919000	-0.000597000
6	0.622406000	-0.021373000	0.000083000
6	-0.622421000	0.020873000	-0.000410000
6	-2.025100000	-0.031375000	-0.000409000
6	-3.296487000	-0.026681000	0.000083000
1	-5.878206000	0.053341000	0.001714000
1	-6.653755000	0.080219000	0.001395000
1	5.878343000	-0.050258000	0.001214000
1	6.653894000	-0.076287000	0.001143000

$C_6H_6^-$

CCSD(T) Energy = -231.47149 a. u.

6	-3.546164000	0.033607000	-0.001222000
6	-2.275844000	-0.016963000	-0.003758000
6	-0.872589000	-0.016050000	-0.001105000
6	0.369757000	-0.102200000	-0.007597000

6	1.773309000	-0.102136000	-0.001302000	
6	3.042578000	-0.162726000	0.005482000	
1	5.495137000	-0.947770000	0.006545000	
1	6.232396000	-1.187081000	0.008119000	
1	5.453451000	2.212021000	0.001149000	
1	4.902077000	1.670282000	0.002352000	
1	-6.127682000	0.199071000	0.014596000	
1	-6.901660000	0.252284000	0.024254000	