

Table 1

	sto-3g		6-31G*		cc-pVTZ	
1	-20,247082		-20,538623		-20,527635	
2	-20,225704		-20,531303		-20,52034	
3	-15,441403		-15,65172		-15,644625	
4	-15,383062		-15,621789		-15,614929	
5	-15,371284		-15,617914		-15,611217	
6	-15,324515		-15,567039		-15,561269	
7	-11,197704		-11,395854		-11,387789	
8	-11,178067		-11,373261		-11,365704	
9	-11,131189		-11,327974		-11,323234	
10	-11,121618		-11,319236		-11,315672	
11	-11,109928		-11,28896		-11,286354	
12	-11,092803		-11,261658		-11,259641	
13	-11,08744		-11,261321		-11,257507	
14	-11,062376		-11,250889		-11,249157	
15	-1,342119		-1,433511		-1,436026	
16	-1,323132		-1,403855		-1,406707	
17	-1,296137		-1,387146		-1,38847	
18	-1,19477		-1,296141		-1,297892	
19	-1,155515		-1,251008		-1,252354	
20	-1,123412		-1,209589		-1,210155	
21	-0,997154		-1,070588		-1,070935	
22	-0,933926		-0,994734		-0,9945	
23	-0,911819		-0,984269		-0,984827	
24	-0,892134		-0,9589		-0,959233	
25	-0,799811		-0,882499		-0,883126	
26	-0,775238		-0,865898		-0,86728	
27	-0,743325		-0,81792		-0,819079	
28	-0,704387		-0,78792		-0,789648	
29	-0,641065		-0,719995		-0,721245	
30	-0,630467		-0,694511		-0,698702	
31	-0,614435		-0,691164		-0,692889	
32	-0,604755		-0,663318		-0,66551	
33	-0,58114		-0,660167		-0,662743	
34	-0,575397		-0,643282		-0,647009	
35	-0,556841		-0,629102		-0,632207	
36	-0,548858		-0,625557		-0,627751	
37	-0,540913		-0,615587		-0,615825	
38	-0,530721		-0,594091		-0,595686	
39	-0,520947		-0,589097		-0,589028	
40	-0,519478		-0,580572		-0,582204	
41	-0,499174		-0,556603		-0,557252	
42	-0,491098		-0,549383		-0,552703	
43	-0,479078		-0,549155		-0,550781	
44	-0,467578		-0,548297		-0,55014	
45	-0,377965		-0,47616		-0,479443	
46	-0,376771		-0,459772		-0,463106	
47	-0,350653		-0,45962		-0,462963	
48	-0,327115		-0,430382		-0,434222	
49	-0,31279		-0,407392		-0,411991	
50	-0,290231		-0,393566		-0,39652	
51	-0,230436		-0,316145		-0,318846	

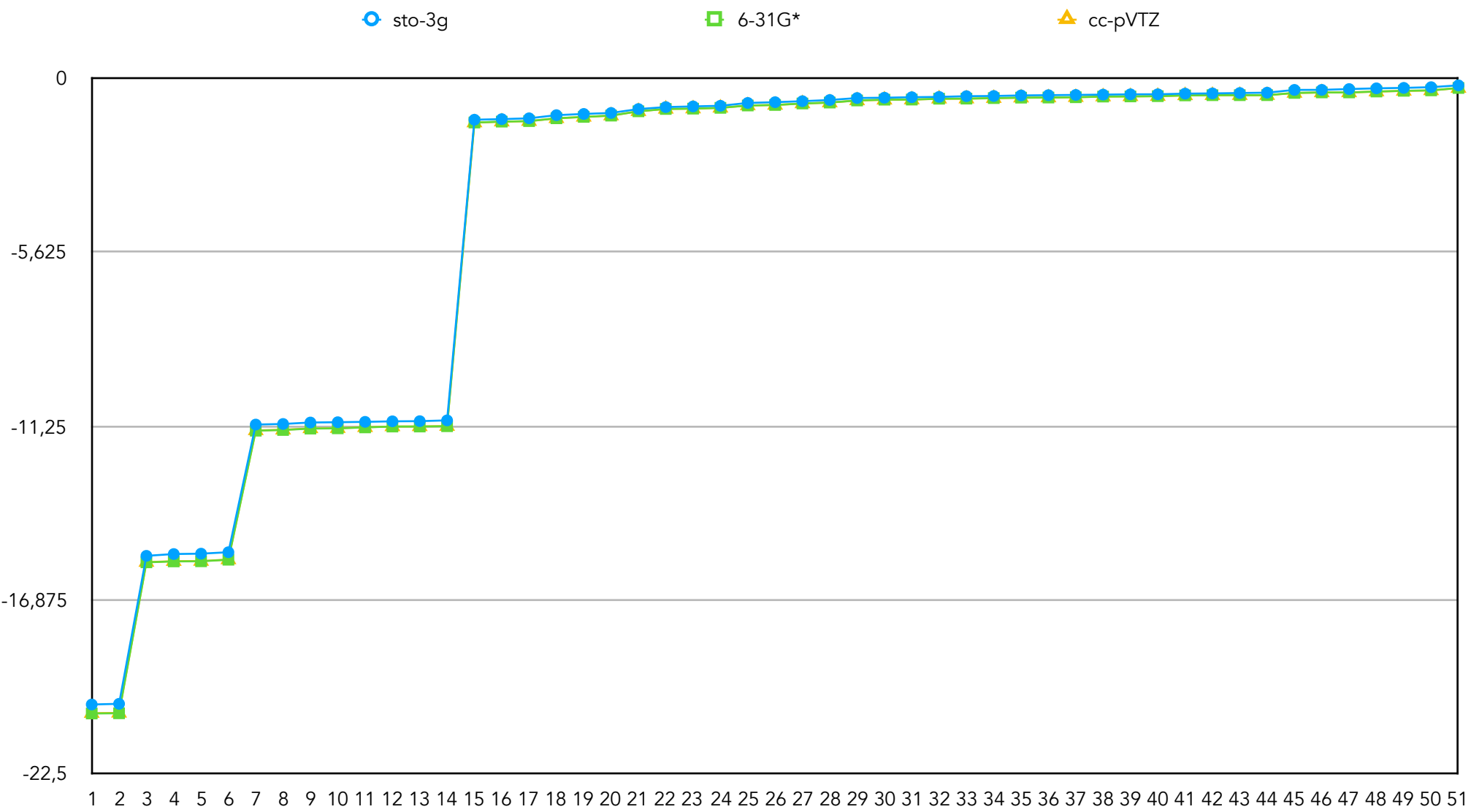


Table 1

	sto-3g		6-31G*		cc-pVTZ	
1	-20,247082	-550,95104219316	-20,538623	-558,88427512974	-20,527635	-558,5852764863
2	-20,225704	-550,36931731152	-20,531303	-558,68508782814	-20,52034	-558,3867694692
3	-15,441403	-420,18188476614	-15,65172	-425,9049005736	-15,644625	-425,7118358325
4	-15,383062	-418,59434564556	-15,621789	-425,09043675882	-15,614929	-424,90376669202
5	-15,371284	-418,27385001192	-15,617914	-424,98499266132	-15,611217	-424,80275804946
6	-15,324515	-417,0012009807	-15,567039	-423,60061370382	-15,561269	-423,44360404122
7	-11,197704	-304,70497867152	-11,395854	-310,09691361852	-11,387789	-309,87745383882
8	-11,178067	-304,17062880246	-11,373261	-309,48212691018	-11,365704	-309,27649051152
9	-11,131189	-302,89501373082	-11,327974	-308,24980514412	-11,323234	-308,12082320292
10	-11,121618	-302,63457361284	-11,319236	-308,01203210568	-11,315672	-307,91505074736
11	-11,109928	-302,31647258064	-11,28896	-307,1881803648	-11,286354	-307,11726750852
12	-11,092803	-301,85047769814	-11,261658	-306,44525526804	-11,259641	-306,39036991458
13	-11,08744	-301,7045430672	-11,261321	-306,43608503298	-11,257507	-306,33230082966
14	-11,062376	-301,02251703888	-11,250889	-306,15221591682	-11,249157	-306,10508580666
15	-1,342119	-36,52091011422	-1,433511	-39,00781255518	-1,436026	-39,07624917588
16	-1,323132	-36,00424764216	-1,403855	-38,2008318699	-1,406707	-38,27843872566
17	-1,296137	-35,26967643906	-1,387146	-37,74615692148	-1,38847	-37,7821847886
18	-1,19477	-32,5113404826	-1,296141	-35,26978528458	-1,297892	-35,31743241096
19	-1,155515	-31,4431577607	-1,251008	-34,04165407104	-1,252354	-34,07828058852
20	-1,123412	-30,56959082856	-1,209589	-32,91458592282	-1,210155	-32,9299875639
21	-0,997154	-27,13393641252	-1,070588	-29,13217689144	-1,070935	-29,1416192403
22	-0,933926	-25,41341527788	-0,994734	-27,06808487292	-0,9945	-27,06171741
23	-0,911819	-24,81185330022	-0,984269	-26,78331778122	-0,984827	-26,79850173126
24	-0,892134	-24,27619728492	-0,9589	-26,092992282	-0,959233	-26,10205367154
25	-0,799811	-21,76396104918	-0,882499	-24,01401563862	-0,883126	-24,03107717388
26	-0,775238	-21,09529580844	-0,865898	-23,56227951924	-0,86728	-23,5988856464
27	-0,743325	-20,2268990385	-0,81792	-22,2567319296	-0,819079	-22,28826991902
28	-0,704387	-19,16734232406	-0,78792	-21,4403905296	-0,789648	-21,48741179424
29	-0,641065	-17,4442633197	-0,719995	-19,5920575431	-0,721245	-19,6260717681
30	-0,630467	-17,15587711446	-0,694511	-18,89860273518	-0,698702	-19,01264562876
31	-0,614435	-16,7196242703	-0,691164	-18,80752624632	-0,692889	-18,85446587682
32	-0,604755	-16,4562181119	-0,663318	-18,04979815884	-0,66551	-18,1094455038
33	-0,58114	-15,8136213732	-0,660167	-17,96405510046	-0,662743	-18,03415161534
34	-0,575397	-15,65734641786	-0,643282	-17,50459094916	-0,647009	-17,60600776242
35	-0,556841	-15,15241205058	-0,629102	-17,11873358076	-0,632207	-17,20322491566
36	-0,548858	-14,93518360404	-0,625557	-17,02226923866	-0,627751	-17,08197100638
37	-0,540913	-14,71898918994	-0,615587	-16,75097178006	-0,615825	-16,7574480885
38	-0,530721	-14,44165080498	-0,594091	-16,16603595558	-0,595686	-16,20943810668
39	-0,520947	-14,17568677686	-0,589097	-16,03014232386	-0,589028	-16,02826473864
40	-0,519478	-14,13571325964	-0,580572	-15,79816530936	-0,582204	-15,84257428152
41	-0,499174	-13,58321340012	-0,556603	-15,14593574214	-0,557252	-15,16359592776
42	-0,491098	-13,36345429524	-0,549383	-14,94946957854	-0,552703	-15,03981136014
43	-0,479078	-13,03637350764	-0,549155	-14,9432653839	-0,550781	-14,98751108778
44	-0,467578	-12,72344263764	-0,548297	-14,91991801986	-0,55014	-14,9700685932
45	-0,377965	-10,2849492417	-0,47616	-12,9569707008	-0,479443	-13,04630566134
46	-0,376771	-10,25245885398	-0,459772	-12,51103060536	-0,463106	-12,60175334628
47	-0,350653	-9,54175203114	-0,45962	-12,5068944756	-0,462963	-12,59786211894
48	-0,327115	-8,9012505687	-0,430382	-11,71128814716	-0,434222	-11,81577984636
49	-0,31279	-8,5114475502	-0,407392	-11,08569852096	-0,411991	-11,21084365758
50	-0,290231	-7,89758602878	-0,393566	-10,70947398108	-0,39652	-10,7898563976
51	-0,230436	-6,27048156168	-0,316145	-8,6027417301	-0,318846	-8,67623966748
52	0,229422	6,24288922236	0,119634	3,25540623492	0,111866	3,03913018668

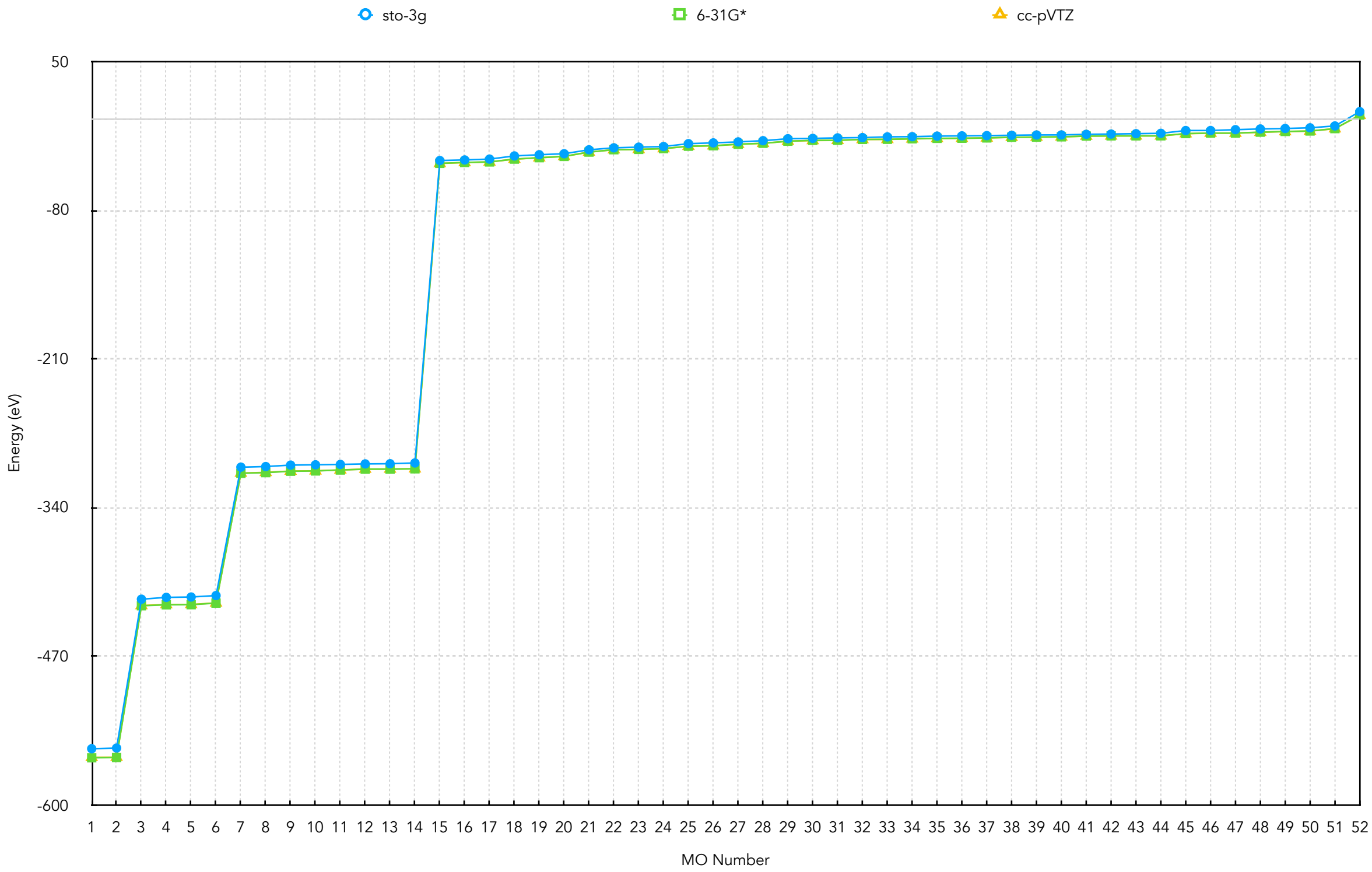


Table 1

	sto-3g		6-31G*		cc-pVTZ	
1	-20,247082		-20,538623		-20,527635	
2	-20,225704		-20,531303		-20,52034	
3	-15,441403		-15,65172		-15,644625	
4	-15,383062		-15,621789		-15,614929	
5	-15,371284		-15,617914		-15,611217	
6	-15,324515		-15,567039		-15,561269	
7	-11,197704		-11,395854		-11,387789	
8	-11,178067		-11,373261		-11,365704	
9	-11,131189		-11,327974		-11,323234	
10	-11,121618		-11,319236		-11,315672	
11	-11,109928		-11,28896		-11,286354	
12	-11,092803		-11,261658		-11,259641	
13	-11,08744		-11,261321		-11,257507	
14	-11,062376		-11,250889		-11,249157	
15	-1,342119		-1,433511		-1,436026	
16	-1,323132		-1,403855		-1,406707	
17	-1,296137		-1,387146		-1,38847	
18	-1,19477		-1,296141		-1,297892	
19	-1,155515		-1,251008		-1,252354	
20	-1,123412		-1,209589		-1,210155	
21	-0,997154		-1,070588		-1,070935	
22	-0,933926		-0,994734		-0,9945	
23	-0,911819		-0,984269		-0,984827	
24	-0,892134		-0,9589		-0,959233	
25	-0,799811		-0,882499		-0,883126	
26	-0,775238		-0,865898		-0,86728	
27	-0,743325		-0,81792		-0,819079	
28	-0,704387		-0,78792		-0,789648	
29	-0,641065		-0,719995		-0,721245	
30	-0,630467		-0,694511		-0,698702	
31	-0,614435		-0,691164		-0,692889	
32	-0,604755		-0,663318		-0,66551	
33	-0,58114		-0,660167		-0,662743	
34	-0,575397		-0,643282		-0,647009	
35	-0,556841		-0,629102		-0,632207	
36	-0,548858		-0,625557		-0,627751	
37	-0,540913		-0,615587		-0,615825	
38	-0,530721		-0,594091		-0,595686	
39	-0,520947		-0,589097		-0,589028	
40	-0,519478		-0,580572		-0,582204	
41	-0,499174		-0,556603		-0,557252	
42	-0,491098		-0,549383		-0,552703	
43	-0,479078		-0,549155		-0,550781	
44	-0,467578		-0,548297		-0,55014	
45	-0,377965		-0,47616		-0,479443	
46	-0,376771		-0,459772		-0,463106	
47	-0,350653		-0,45962		-0,462963	
48	-0,327115		-0,430382		-0,434222	
49	-0,31279		-0,407392		-0,411991	
50	-0,290231		-0,393566		-0,39652	
51	-0,230436		-0,316145		-0,318846	

Table 2

	sto-3g		6-31G*		cc-pVTZ	
3	-15,441403	-420,18188476614	-15,65172	-425,9049005736	-15,644625	-425,7118358325
4	-15,383062	-418,59434564556	-15,621789	-425,09043675882	-15,614929	-424,90376669202
5	-15,371284	-418,27385001192	-15,617914	-424,98499266132	-15,611217	-424,80275804946
6	-15,324515	-417,0012009807	-15,567039	-423,60061370382	-15,561269	-423,44360404122

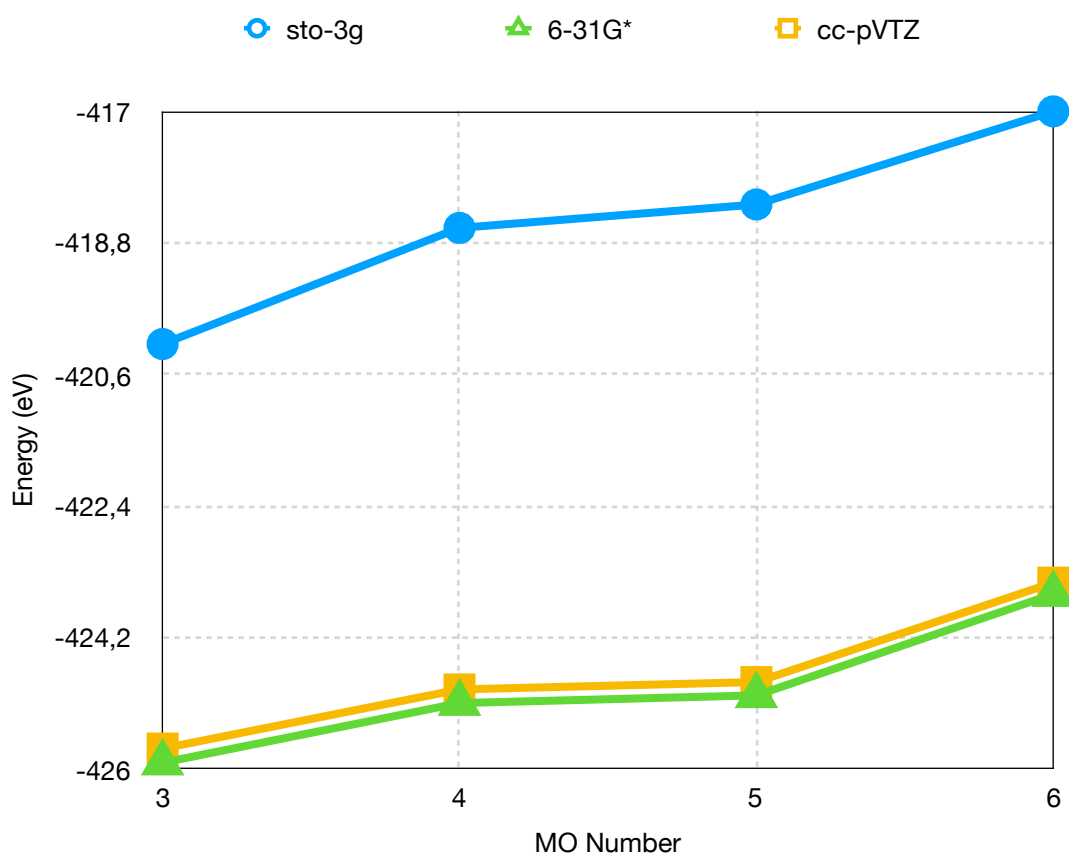


Table 1

	sto-3g		6-31G*		cc-pVTZ	
1	-20,247082		-20,538623		-20,527635	
2	-20,225704		-20,531303		-20,52034	
3	-15,441403		-15,65172		-15,644625	
4	-15,383062		-15,621789		-15,614929	
5	-15,371284		-15,617914		-15,611217	
6	-15,324515		-15,567039		-15,561269	
7	-11,197704		-11,395854		-11,387789	
8	-11,178067		-11,373261		-11,365704	
9	-11,131189		-11,327974		-11,323234	
10	-11,121618		-11,319236		-11,315672	
11	-11,109928		-11,28896		-11,286354	
12	-11,092803		-11,261658		-11,259641	
13	-11,08744		-11,261321		-11,257507	
14	-11,062376		-11,250889		-11,249157	
15	-1,342119		-1,433511		-1,436026	
16	-1,323132		-1,403855		-1,406707	
17	-1,296137		-1,387146		-1,38847	
18	-1,19477		-1,296141		-1,297892	
19	-1,155515		-1,251008		-1,252354	
20	-1,123412		-1,209589		-1,210155	
21	-0,997154		-1,070588		-1,070935	
22	-0,933926		-0,994734		-0,9945	
23	-0,911819		-0,984269		-0,984827	
24	-0,892134		-0,9589		-0,959233	
25	-0,799811		-0,882499		-0,883126	
26	-0,775238		-0,865898		-0,86728	
27	-0,743325		-0,81792		-0,819079	
28	-0,704387		-0,78792		-0,789648	
29	-0,641065		-0,719995		-0,721245	
30	-0,630467		-0,694511		-0,698702	
31	-0,614435		-0,691164		-0,692889	
32	-0,604755		-0,663318		-0,66551	
33	-0,58114		-0,660167		-0,662743	
34	-0,575397		-0,643282		-0,647009	
35	-0,556841		-0,629102		-0,632207	
36	-0,548858		-0,625557		-0,627751	
37	-0,540913		-0,615587		-0,615825	
38	-0,530721		-0,594091		-0,595686	
39	-0,520947		-0,589097		-0,589028	
40	-0,519478		-0,580572		-0,582204	
41	-0,499174		-0,556603		-0,557252	
42	-0,491098		-0,549383		-0,552703	
43	-0,479078		-0,549155		-0,550781	
44	-0,467578		-0,548297		-0,55014	
45	-0,377965		-0,47616		-0,479443	
46	-0,376771		-0,459772		-0,463106	
47	-0,350653		-0,45962		-0,462963	
48	-0,327115		-0,430382		-0,434222	
49	-0,31279		-0,407392		-0,411991	
50	-0,290231		-0,393566		-0,39652	
51	-0,230436		-0,316145		-0,318846	

Table 2

	sto-3g		6-31G*		cc-pVTZ	
15	-1,342119	-36,52091011422	-1,433511	-39,00781255518	-1,436026	-39,07624917588
16	-1,323132	-36,00424764216	-1,403855	-38,2008318699	-1,406707	-38,27843872566
17	-1,296137	-35,26967643906	-1,387146	-37,74615692148	-1,38847	-37,7821847886
18	-1,19477	-32,5113404826	-1,296141	-35,26978528458	-1,297892	-35,31743241096
19	-1,155515	-31,4431577607	-1,251008	-34,04165407104	-1,252354	-34,07828058852
20	-1,123412	-30,56959082856	-1,209589	-32,91458592282	-1,210155	-32,9299875639
21	-0,997154	-27,13393641252	-1,070588	-29,13217689144	-1,070935	-29,1416192403
22	-0,933926	-25,41341527788	-0,994734	-27,06808487292	-0,9945	-27,06171741
23	-0,911819	-24,81185330022	-0,984269	-26,78331778122	-0,984827	-26,79850173126
24	-0,892134	-24,27619728492	-0,9589	-26,092992282	-0,959233	-26,10205367154
25	-0,799811	-21,76396104918	-0,882499	-24,01401563862	-0,883126	-24,03107717388
26	-0,775238	-21,09529580844	-0,865898	-23,56227951924	-0,86728	-23,5989856464
27	-0,743325	-20,2268990385	-0,81792	-22,2567319296	-0,819079	-22,28826991902
28	-0,704387	-19,16734232406	-0,78792	-21,4403905296	-0,789648	-21,48741179424
29	-0,641065	-17,4442633197	-0,719995	-19,5920575431	-0,721245	-19,6260717681
30	-0,630467	-17,15587711446	-0,694511	-18,89860273518	-0,698702	-19,01264562876
31	-0,614435	-16,7196242703	-0,691164	-18,80752624632	-0,692889	-18,85446587682
32	-0,604755	-16,4562181119	-0,663318	-18,04979815884	-0,66551	-18,1094455038
33	-0,58114	-15,8136213732	-0,660167	-17,96405510046	-0,662743	-18,03415161534
34	-0,575397	-15,65734641786	-0,643282	-17,50459094916	-0,647009	-17,60600776242
35	-0,556841	-15,15241205058	-0,629102	-17,11873358076	-0,632207	-17,20322491566
36	-0,548858	-14,93518360404	-0,625557	-17,02226923866	-0,627751	-17,08197100638
37	-0,540913	-14,71898918994	-0,615587	-16,75097178006	-0,615825	-16,7574480885
38	-0,530721	-14,44165080498	-0,594091	-16,16603595558	-0,595686	-16,20943810668
39	-0,520947	-14,17568677686	-0,589097	-16,03014232386	-0,589028	-16,02826473864
40	-0,519478	-14,13571325964	-0,580572	-15,79816530936	-0,582204	-15,84257428152
41	-0,499174	-13,58321340012	-0,556603	-15,1459374214	-0,557252	-15,16359592776
42	-0,491098	-13,36345429524	-0,549383	-14,94946957854	-0,552703	-15,03981136014
43	-0,479078	-13,03637350764	-0,549155	-14,9432653839	-0,550781	-14,98751108778
44	-0,467578	-12,72344263764	-0,548297	-14,91991801986	-0,55014	-14,9700685932
45	-0,377965	-10,2849492417	-0,47616	-12,9569707008	-0,479443	-13,04630566134
46	-0,376771	-10,25245885398	-0,459772	-12,51103060536	-0,463106	-12,60175334628
47	-0,350653	-9,54175203114	-0,45962	-12,5068944756	-0,462963	-12,59786211894
48	-0,327115	-8,9012505687	-0,430382	-11,71128814716	-0,434222	-11,81577984636
49	-0,31279	-8,5114475502	-0,407392	-11,08569852096	-0,411991	-11,21084365758
50	-0,290231	-7,89758602878	-0,393566	-10,70947398108	-0,39652	-10,7898563976
51	-0,230436	-6,27048156168	-0,316145	-8,6027417301	-0,318846	-8,67623966748

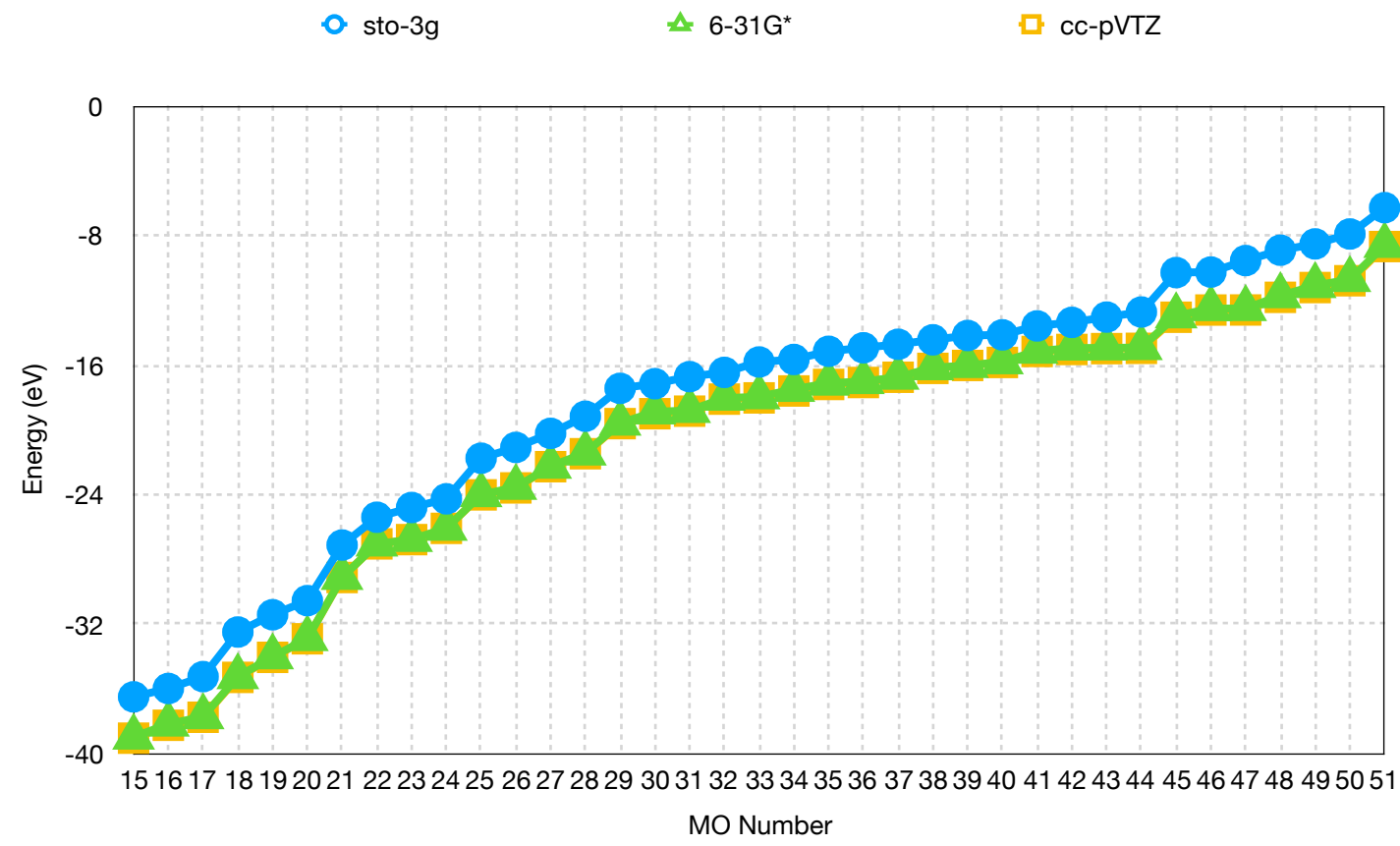




Table 1

	Energy		Time	
sto-3g	-667,737297		5m 15s	
6-31G*	-676,340526		9m 14s	
cc-pVTZ	-676,574796		44m 43s	

