Table 1

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		-1,433511	-1,436026				
16		-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	-0,954209	-0,959233				
	-0,799811						
25	-0,775238	-0,882499 -0,865898	-0,883126 -0,86728				
27	-0,743325	-0,81792	-0,819079				
28							
29	-0,704387 -0,641065	-0,78792 -0,719995	-0,789648 -0,721245				
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31	-0,614435	-0,694311	-0,692889				
32	-0,604755 -0,58114	-0,663318 -0,660167	-0,66551 -0,662743				
34	-0,575397	-0,643282	-0,647009				
35	-0,556841	-0,629102	-0,632207				
36		-0,625557	-0,627751				
37	-0,540913	-0,625337	-0,615825				
	-0,530721	-0,594091					
38	-0,520947	-0,589097	-0,595686 -0,589028				
40	-0,519478 -0,499174	-0,580572 -0,556603	-0,582204 -0,557252				
42	-0,491098	-0,549383	-0,552703				
43	-0,479078	-0,549155	-0,550781				
44		-0,548297	-0,55014				
45		-0,47616	-0,479443				
46	-0,376771	-0,459772	-0,463106				
47	-0,350653	-0,45962	-0,462963				
48		-0,430382	-0,434222				
49	-0,31279	-0,407392	-0,411991				
50	·	-0,393566	-0,39652				
51	-0,230436	-0,316145	-0,318846				

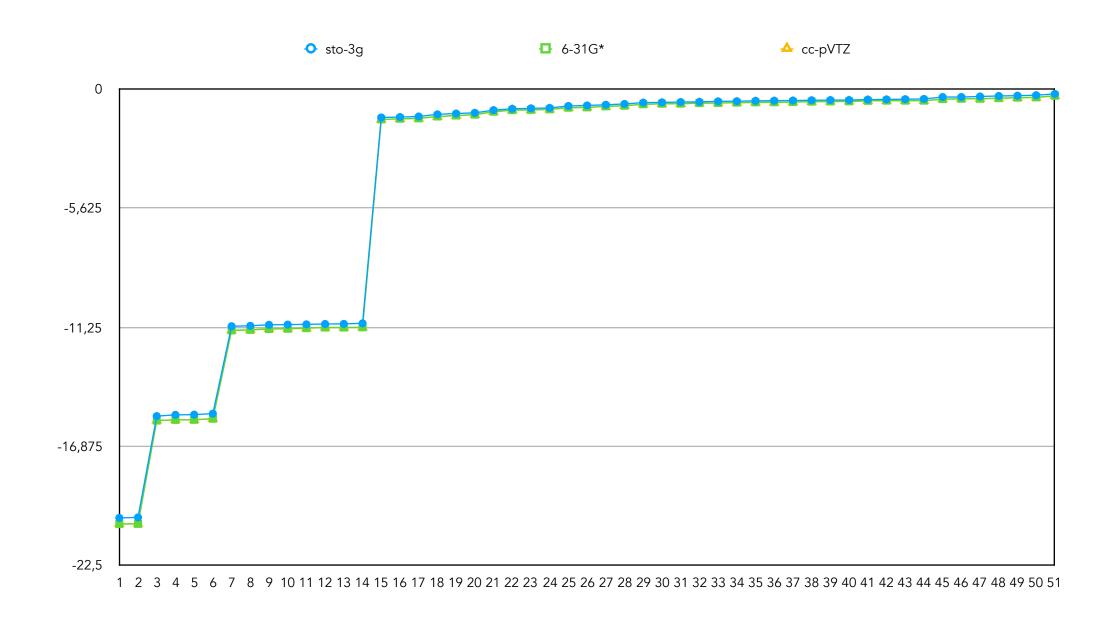


Table 1

Table 1					cc-pVTZ
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-11,121618	-302,63457361284	-11,319236	-308,01203210568	-11,315672	-307,91505074736
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-11,08744	-301,7045430672	-11,261321	-306,43608503298	-11,257507	-306,33230082966
-11,062376	-301,02251703888	-11,250889	-306,15221591682	-11,249157	-306,10508580666
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-1,323132	-36,00424764216	-1,403855	-38,2008318699	-1,406707	-38,27843872566
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-1,19477	-32,5113404826	-1,296141	-35,26978528458	-1,297892	-35,31743241096
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	· ·			-	-26,10205367154
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·	· .			-	-22,28826991902
·				-	-21,48741179424
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·					-12,59786211894
,					-11,81577984636
·	· ·				
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	-11,121618 -11,109928 -11,092803 -11,08744 -11,062376 -1,342119 -1,323132 -1,296137 -1,19477 -1,155515 -1,123412 -0,997154 -0,933926 -0,911819 -0,892134 -0,799811 -0,775238 -0,743325 -0,704387 -0,641065 -0,630467 -0,614435 -0,604755 -0,58114 -0,575397 -0,556841 -0,575397 -0,556841 -0,548858 -0,540913 -0,530721 -0,520947 -0,519478 -0,491098 -0,479078 -0,491098 -0,479078 -0,497578 -0,377965 -0,377965 -0,376771 -0,350653 -0,327115 -0,31279	-20,225704 -550,36931731152 -15,441403 -420,18188476614 -15,383062 -418,59434564556 -15,371284 -418,27385001192 -15,324515 -417,0012009807 -11,197704 -304,70497867152 -11,178067 -304,17062880246 -11,131189 -302,89501373082 -11,121618 -302,63457361284 -11,092803 -301,85047769814 -11,092803 -301,85047769814 -11,08744 -301,7045430672 -11,062376 -301,02251703888 -1,342119 -36,52091011422 -1,323132 -36,00424764216 -1,296137 -35,26967643906 -1,19477 -32,5113404826 -1,155515 -31,4431577607 -1,123412 -30,56959082856 -0,997154 -27,13393641252 -0,933926 -25,41341527788 -0,911819 -24,81185330022 -0,892134 -24,27619728492 -0,799811 -21,76396104918 -0,775238 -21,09529580844 -0,743325 -20,2268990385 -0,704387 -19,16734232406 -0,641065 -17,4442633197 -0,630467 -17,15587711446 -0,614435 -16,7196242703 -0,604755 -16,4562181119 -0,58114 -15,8136213732 -0,575397 -15,65734641786 -0,550841 -15,15241205058 -0,540913 -14,71898918994 -0,530721 -14,44165080498 -0,520947 -14,17568677686 -0,519478 -14,13571325964 -0,499174 -13,58321340012 -0,491098 -13,36345429524 -0,479078 -13,03637350764 -0,467578 -12,72344263764 -0,377965 -10,2849492417 -0,376771 -10,25245885398 -0,350653 -9,54175203114 -0,327115 -8,9012505687 -0,31279 -8,5114475502	-20,247082 -550,95104219316 -20,538623 -20,225704 -550,36931731152 -20,531303 -15,441403 -420,18188476614 -15,65172 -15,383062 -418,59434564556 -15,621789 -15,371284 -418,27385001192 -15,617914 -15,324515 -417,0012009807 -15,567039 -11,197704 -304,70497867152 -11,395854 -11,178067 -304,17062880246 -11,373261 -11,131189 -302,89501373082 -11,327974 -11,121618 -302,63457361284 -11,319236 -11,109280 -302,31647258064 -11,28896 -11,09280 -301,85047769814 -11,261658 -11,08744 -301,7045430672 -11,261321 -11,08744 -301,7045430672 -11,250889 -1,342119 -36,52091011422 -1,433511 -1,323132 -36,00424764216 -1,4038546 -1,19477 -32,5113404826 -1,296141 -1,195515 -31,4431577607 -1,251008 -1,123412 -30,56959082856 -1,209589 -0,997154 -27,13393641252 -1,070589 -0,997154 -24,81185330022 -0,984269 -0,882134 -24,27619728492 -0,9589 -0,799811 -21,76396104918 -0,882499 -0,775238 -21,09529580844 -0,865898 -0,743325 -20,2268990385 -0,81792 -0,743325 -20,2268990385 -0,81792 -0,704387 -19,16734232406 -0,78792 -0,641065 -17,4442633197 -0,719995 -0,641065 -17,1558771446 -0,694511 -0,6814435 -16,7196242703 -0,691164 -0,604755 -16,4562181119 -0,663318 -0,58514 -15,15241205058 -0,629102 -0,548958 -14,93518360404 -0,625557 -0,540913 -14,71898918994 -0,615587 -0,540913 -14,71898918994 -0,615587 -0,540913 -14,71898918994 -0,615587 -0,540913 -14,71898918994 -0,655893 -0,575397 -15,65734641786 -0,643282 -0,549913 -14,71898918994 -0,615587 -0,540913 -14,71898918994 -0,615587 -0,540913 -14,71898918994 -0,6558603 -0,540913 -14,71898918994 -0,6558603 -0,540913 -14,71898918994 -0,655867 -0,540913 -14,71898918994 -0,6558603 -0,540913 -14,71898918994 -0,655867 -0,540913 -14,71898918994 -0,655867 -0,540913 -14,71898918994 -0,655867 -0,540913 -14,71898918994 -0,655867 -0,540913 -14,71898918994 -0,655867 -0,540913 -14,71898918994 -0,655867 -0,540913 -14,71898918994 -0,655867 -0,540913 -14,71898918994 -0,6558603 -0,540977 -14,17568677686 -0,580977 -0,49174 -13,53637350764 -0,549976 -0,49174 -13,53637350764 -0,549976 -0,479078 -13,36345429524 -0,549938 -0,4790	-20,247082 -550,95104219316	-20,247082 -559,95104219316 -20,538623 -558,88427512974 -20,527635 -20,225704 -559,08901731152 -20,53103 -558,6506782814 -20,52034 -15,441403 -420,1818476614 -15,651729 -425,0049005736 -15,544625 -15,343062 -418,59434564556 -15,617914 -424,98498266132 -15,61429 -15,331264 -418,27385001192 -15,617914 -424,98498266132 -15,611291 -15,324515 -417,0012009807 -15,567039 -423,60061370382 -15,561269 -11,197704 -304,70497867152 -11,395854 -310,09691361852 -11,387789 -11,176067 -304,17062890246 -11,372861 -309,48212891018 -11,387789 -11,176067 -304,17062890246 -11,329274 -3004,24960514412 -11,328774 -11,126181 -302,63457361284 -11,319236 -300,01203210568 -11,315672 -11,109928 -302,63457361284 -11,28886 -307,1881803648 -11,286364 -11,2863

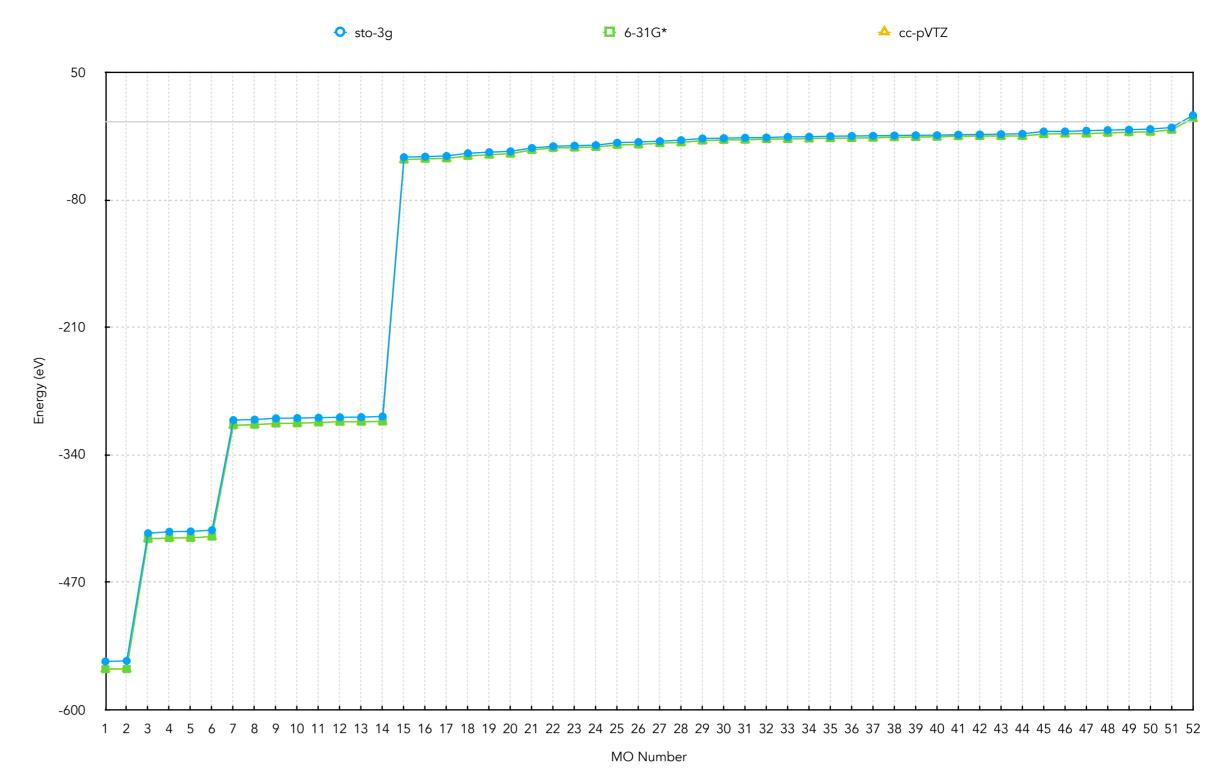


Table 1 Table 2

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		-15,617914	-15,611217				
6	-15,324515	-15,567039	-15,561269				
7	-11,197704	-11,395854	-11,387789				
8		-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		-11,250889	-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	·		-0,692889				
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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				
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		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

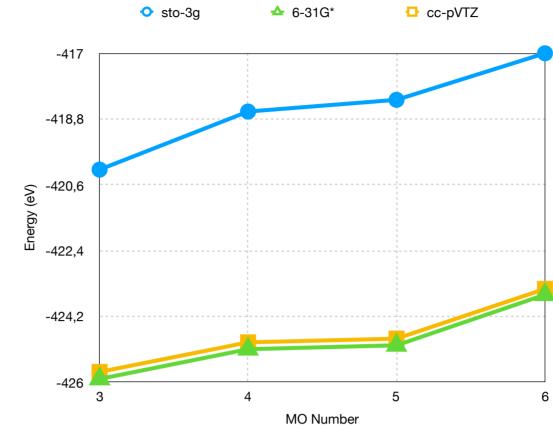


Table 1 Table 2

	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		-0,407392	-0,411991	
50		-0,393566	-0,39652	
51	-0,230436	-0,316145	-0,318846	
	,	3,3 : 3 : 10	2,2.23.0	

		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	-23,5998856464
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

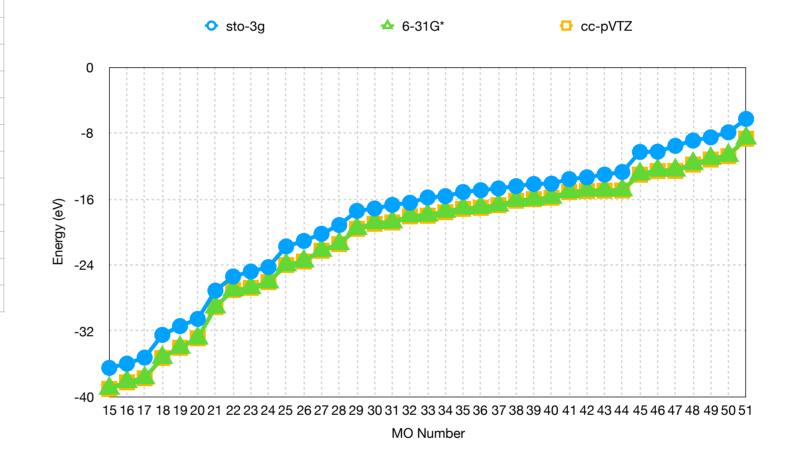


Table 1

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

