

Electronic Supplementary Material (ESI) for RSC Advances.

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Supporting Information

Molecular structures of Pr@C₇₂ and Pr@C₇₂(C₆H₃Cl₂): a combined experimental-theoretical investigation†

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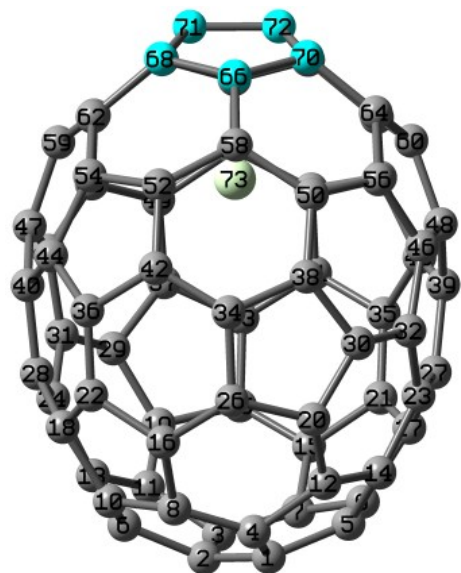
Fig. S1 Optimized twenty-four structures of isomers of $\text{Pr}@C_2(10612)-C_{72}(C_6H_3Cl_2)$ at the BLYP/3-21G~MWB48 level of theory.

Fig. S2 Electron difference densities of $C_2(10612)-C_{72}$ ((a) ~ (d)) and $C_{2v}(11188)-C_{72}$ ((e) ~ (g)). (a) $C_{71}-C_{72}-C_{59}$ plane, (b) $C_{65}-C_{66}-C_{58}$ plane, (c) $C_{70}-C_{56}-C_{55}$ plane, (d) $C_{63}-C_{64}-C_{72}$ plane of $C_2(10612)-C_{72}$; (e) $C_{71}-C_{72}-C_{59}$ plane, (f) $C_{65}-C_{66}-C_{33}$ plane, (g) $C_{69}-C_{70}-C_{43}$ plane and (h) $C_{63}-C_{64}-C_{54}$ plane of $C_{2v}(11188)-C_{72}$. Blue solid lines and brown

dotted lines show the areas in which the electron density is increased and decreased, respectively.

Geometries of stationary points

Table S1 Spin densities and POAV values of all C atoms in Pr@C₂(10612)-C₇₂. Geometries were optimized at the B3LYP/6-31G(d)~MWB48



No.	spin	POA V	No.	spin	POA V
1	0.00	12.13	37	0.06	10.25
2	0.00	12.13	38	0.06	10.25
3	0.00	11.97	39	0.02	7.62
4	0.00	11.97	40	0.02	7.62
5	0.00	11.21	41	0.02	11.78
6	0.00	11.21	42	0.02	11.78
7	0.02	12.26	43	-0.02	11.98
8	0.02	12.26	44	-0.02	11.98
9	0.00	11.19	45	0.05	9.08
10	0.00	11.19	46	0.05	9.08
11	0.02	11.34	47	0.00	9.50
12	0.02	11.34	48	0.00	9.50
13	0.01	10.63	49	-0.02	8.72
14	0.01	10.63	50	-0.02	8.73
15	-0.01	11.97	51	-0.03	10.87
16	-0.01	11.97	52	-0.03	10.87
17	0.05	10.63	53	0.13	10.01
18	0.05	10.63	54	0.13	10.00
19	0.03	11.19	55	0.00	10.31
20	0.03	11.19	56	0.00	10.31
21	0.03	11.45	57	0.03	9.01
22	0.03	11.45	58	0.03	9.00
23	0.01	7.36	59	0.02	10.96
24	0.01	7.36	60	0.02	10.96
25	0.00	12.26	61	-0.04	9.40
26	0.00	12.26	62	-0.04	9.40
27	-0.01	7.28	63	0.00	11.28
28	-0.01	7.27	64	0.00	11.28
29	0.00	10.89	65	-0.02	10.88
30	0.00	10.89	66	-0.02	10.89
31	-0.01	7.44	67	0.06	13.01
32	-0.01	7.45	68	0.06	13.01
33	0.02	11.72	69	0.08	13.11
34	0.02	11.72	70	0.08	13.11
35	0.03	11.05	71	-0.01	15.19
36	0.03	11.05	72	-0.01	15.18

Table S2 Relative energies (kcal/mol) of the optimized twenty-four isomers of Pr@C₂(10612)-C₇₂(C₆H₃Cl₂) at the BLYP or B3LYP level (ECP and MWB48 for Pr atom and 3-21G or 6-31G(d) for the Cl, C, and H atoms)

Addition position	Isomer	BLYP/3-21G~MWB48	B3LYP/6-31G(d)~MWB48
C(70)	1a	0.28	1.35
	1a'	1.61	2.73
	1b	0	1.22
	1b'	1.38	2.69
	1c	0.71	0.00
	1c'	0.75	0.15
C(68)	2a	3.85	
	2a'	5.26	
	2b	3.62	
	2b'	6.65	
	2c	4.65	
	2c'	4.66	
C(71)	3a	10.92	
	3a'	10.68	
	3b	10.79	
	3b'	10.57	
	3c	11.31	
	3c'	13.86	
C(66)	4a	18.90	
	4a'	16.76	
	4b	18.75	
	4b'	16.67	
	4c	16.20	
	4c'	16.59	

Table S3 Relative concentrations (RC, %) and relative Gibbs free energies (ΔG , kcal/mol) for the optimized isomers of Pr@C₂(10612)-C₇₂(C₆H₃Cl₂) with different dichlorophenyl groups at C(70). The temperature is 298.15 K and 486.65 K (the boiling point of TCB) and the computations was performed at the B3LYP/6-31G(d)~MWB48 level of theory

Isomer	298.15 K		486.65 K	
	ΔG	RC (%)	ΔG	RC (%)
1a	2.10	1.59	2.73	3.19
1a'	3.43	0.17	4.01	0.84
1b	2.11	1.57	2.79	2.99
1b'	3.44	0.17	4.05	0.81
1c	0.18	41.15	0.35	37.88
1c'	0.00	55.35	0.00	54.29

Table S4 Orbitals, energies, and occupied electron numbers of Pr@C₇₂(C₆H₃Cl₂) (**1c**, **1c'**) and La@C₇₂(C₆H₃Cl₂) (**C**, **C'**) using the B3LYP functional with the 6-31G(d) (for the Cl, C, and H atoms), MWB48 (for the Pr atom), and MWB46 (for the La atom) basis sets. The structure **C** is given in Figure 4 and **C** and **C'** are two conformational isomers due to different aryl ring orientations. Pink regions and green regions show positive and negative wave function, respectively




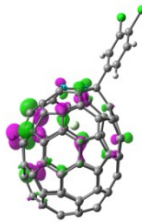

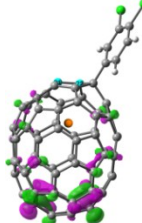

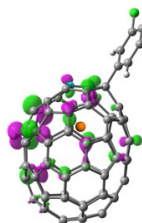

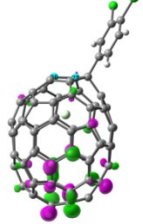

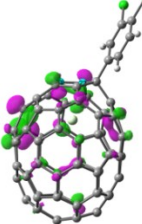

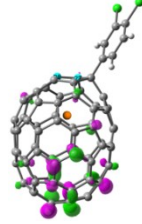

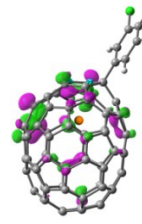

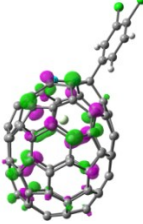

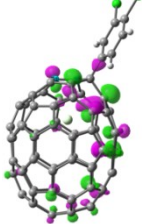

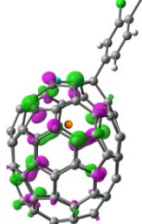

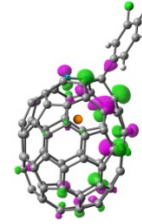
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No. 260 -3.08 eV 		No. 257 -5.69 eV 		No. 260 -3.08 eV 		No. 257 -5.68 eV 	
No. 259 (LUMO) -3.39 eV 		No. 256 -5.85 eV 		No. 259 (LUMO) -3.39 eV 		No. 256 -5.85 eV 	

Table S4 (Continued)


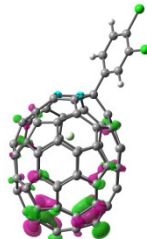

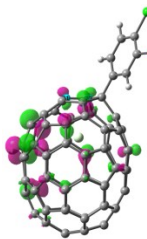

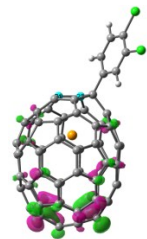

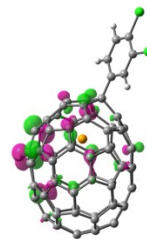

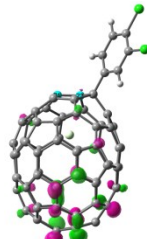

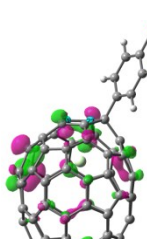

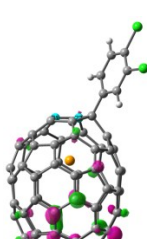

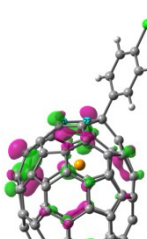

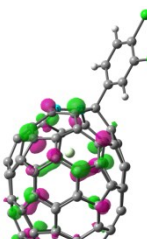

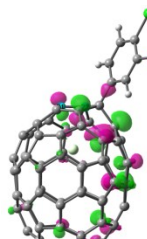

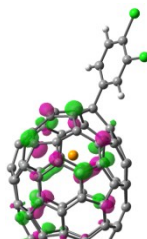

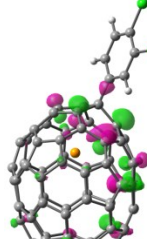
Pr@C ₂ (10612)-C ₇₂ (1c')				La@C ₂ (10612)-C ₇₂ (C')			
No. 261 -2.89 eV 		No. 258 (HOMO) -5.27 eV 		No. 261 -2.90 eV 		No. 258 (HOMO) -5.27 eV 	
No. 260 -3.07 eV 		No. 257 -5.69 eV 		No. 260 -3.07 eV 		No. 257 -5.67 eV 	
No. 259 (LUMO) -3.38 eV 		No. 256 -5.85 eV 		No. 259 (LUMO) -3.38 eV 		No. 256 -5.85 eV 	

Table S5 Relative energies (kcal/mol) of optimized C_{72} , C_{72}^- , C_{72}^{2-} , C_{72}^{3-} and $Pr@C_{72}$ at different levels of computation

Isomer ^a	C_{72}	C_{72}^-	C_{72}^{2-}	C_{72}^{3-}	$Pr@C_{72}$	$Pr@C_{72}$
	B3LYP~ 6-31G(d)	B3LYP~ 6-31G(d)	B3LYP~ 6-31G(d)	B3LYP~ 6-31G(d)	BLYP~3- 21G -MWB48 ^b	B3LYP~6- 31G(d) -MWB48 ^b
11188	0.00	0.00	0.00	0.00	1.62	0.62
10528	32.54	22.06	9.29	0.14	10.07	9.03
10612	18.30	11.08	2.72	5.62	0.00	0.00
10611	43.70	34.97	23.83	8.23	19.57	
10538	25.44	20.34	14.10	10.34	17.14	
10616	47.61	39.76	29.11	10.74	19.57	
10610	39.68	31.31	23.07	10.81	15.28	
10530	38.30	25.91	11.52	11.61	13.86	
10784	27.43	18.79	9.93	11.95	20.47	
10693	34.20	24.61	14.58	12.52	23.66	
10689	31.31	23.45	15.01	13.88	18.11	
10615	36.55	28.43	18.70	14.81	20.78	
10554	34.06	28.21	19.04	15.03	27.86	
11190	11.29	22.58	29.60	36.56	32.01	

^aThe serial numbers of isomers are taken from the Ref [34].

^bThe 6-31G(d) and 3-21G basis sets are employed for the C atom and the MWB48 basis set for the Pr atom.

Table S6 Computed relative energies (RE, kcal/mol), molecular symmetries (MS)^a, and Mulliken charges (Q) of the Pr atoms for the species with different spin multiplicities (m) using the B3LYP functional with the 6-31G(d) (for the Cl, C, and H atoms) and MWB48 (for the Pr atom) basis sets

Species	m	RE	MS	Q
Pr@C ₂ (10612)-C ₇₂ (C ₆ H ₃ Cl ₂)	1	0	C ₁	0.9
	3	23.88	C ₁	0.9
Pr@C ₂ (10612)-C ₇₂	2	0	C ₂	0.9
	4	33.42	C ₂	0.9
Pr@C _{2v} (11188)-C ₇₂	2	0	C _{2v}	1.0
	4	20.78	C _{2v}	1.0

^a The tolerances in symmetry assignment is 0.01.

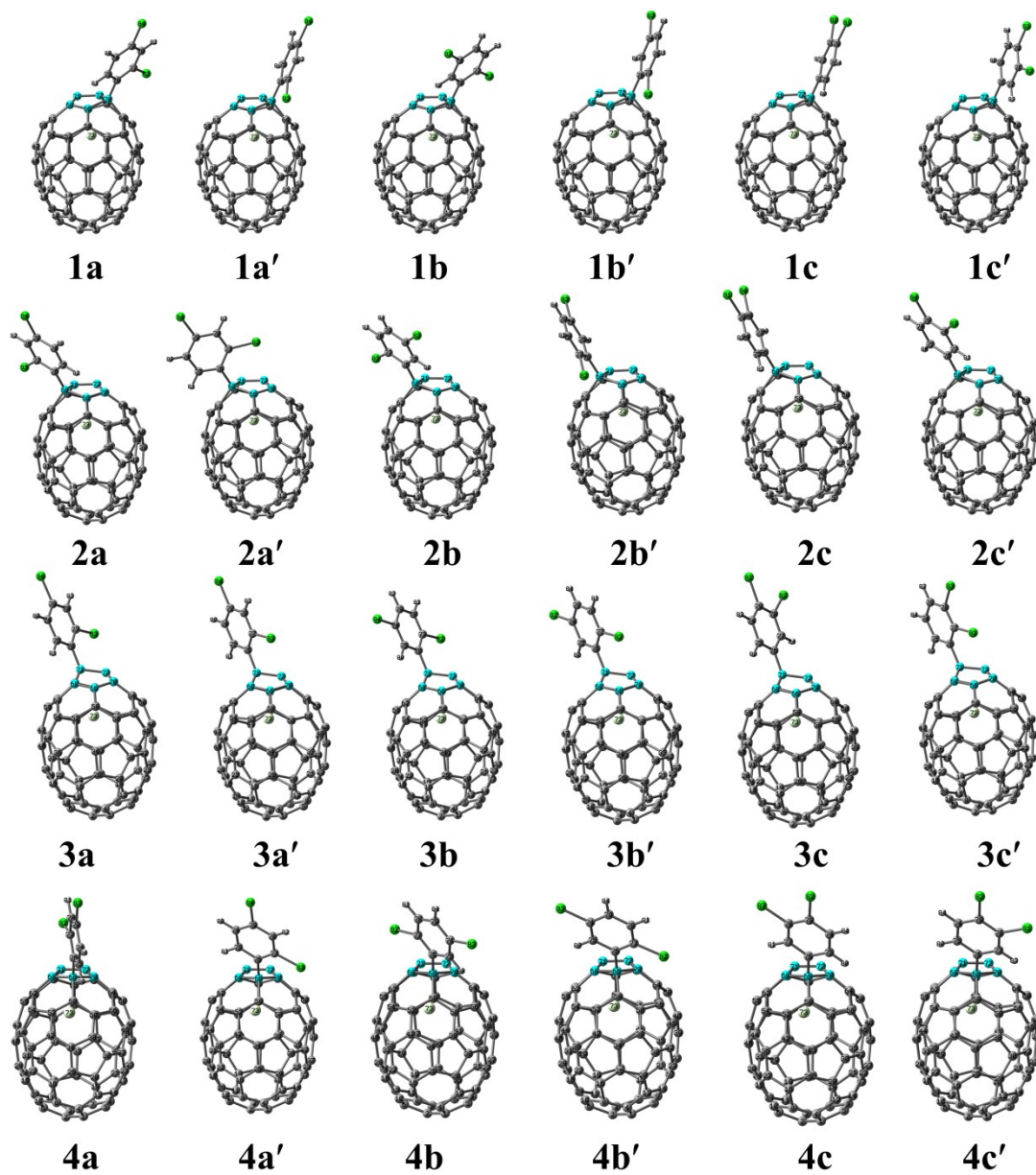


Fig. S1 Optimized twenty-four structures of isomers of $\text{Pr}@C_2(10612)\text{-C}_{72}(\text{C}_6\text{H}_3\text{Cl}_2)$ at the BLYP/3-21G~MWB48 level of theory.

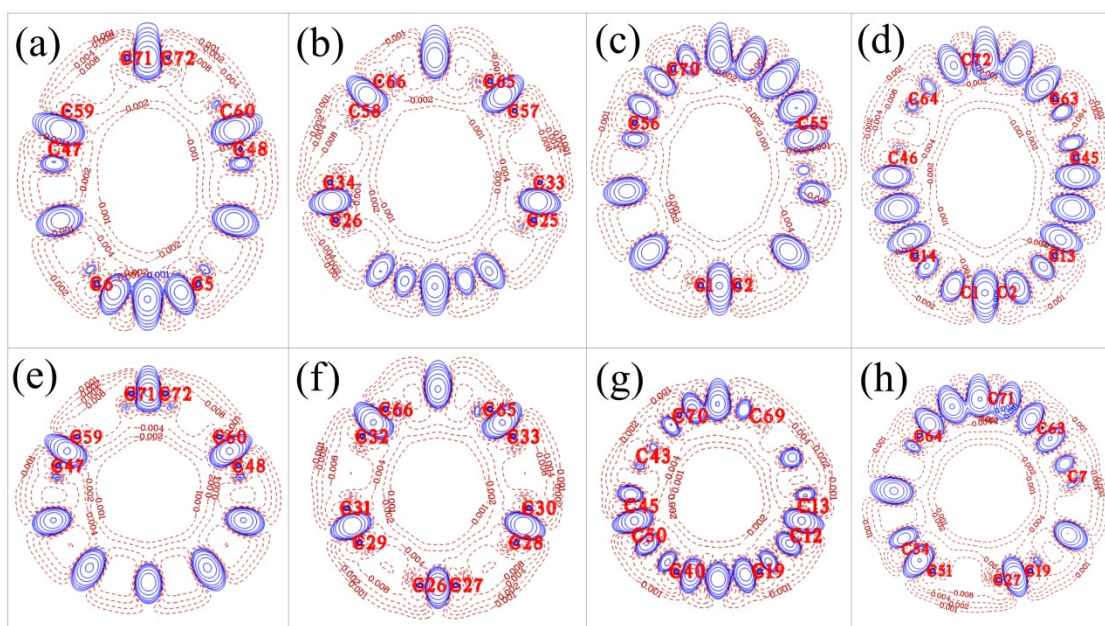


Fig. S2 Electron difference densities of $C_2(10612)-C_{72}$ ((a) ~ (d)) and $C_{2v}(11188)-C_{72}$ ((e) ~ (g)). (a) $C_{71}-C_{72}-C_{59}$ plane, (b) $C_{65}-C_{66}-C_{58}$ plane, (c) $C_{70}-C_{56}-C_{55}$ plane, (d) $C_{63}-C_{64}-C_{72}$ plane of $C_2(10612)-C_{72}$; (e) $C_{71}-C_{72}-C_{59}$ plane, (f) $C_{65}-C_{66}-C_{33}$ plane, (g) $C_{69}-C_{70}-C_{43}$ plane and (h) $C_{63}-C_{64}-C_{54}$ plane of $C_{2v}(11188)-C_{72}$. Blue solid lines and brown dotted lines show the areas in which the electron density is increased and decreased, respectively.

Geometries of stationary points

1. Pr@C₂(10612)-C₇₂ (B3LYP/6-31G(d)~MWB48)

C	4.39565400	-0.33626600	0.61054100
C	4.39553300	0.33628200	-0.61120100
C	3.99979900	1.72703700	-0.68062200
C	3.99994800	-1.72702100	0.68003900
C	3.85955200	0.33129800	1.78346300
C	3.85920800	-0.33128200	-1.78401700
C	3.62617600	2.40859000	0.48170000
C	3.62610600	-2.40857900	-0.48221900
C	3.48964700	1.66312900	1.72137400
C	3.48932400	-1.66311500	-1.72185400
C	3.22437300	1.90776000	-1.89254900
C	3.22476000	-1.90775000	1.89211100
C	3.04639200	0.61374000	-2.51482300
C	3.04688400	-0.61372200	2.51442600
C	2.56178800	3.38589700	0.44444300
C	2.56172400	-3.38588100	-0.44475400
C	2.29247300	2.11184800	2.39653900
C	2.29200700	-2.11184000	-2.39678200
C	2.20396600	2.85386000	-1.92730000
C	2.20436000	-2.85384200	1.92705800
C	1.79248900	3.25251000	1.66374700
C	1.79218100	-3.25249900	-1.66391500
C	1.80105500	-0.22997300	3.08025300
C	1.80044500	0.22998400	-3.08038500
C	1.89912400	3.65709800	-0.76000800
C	1.89929100	-3.65707700	0.75981900
C	1.41104000	1.18978000	3.02936400
C	1.41044500	-1.18976700	-3.02942600
C	0.97541200	2.54943500	-2.60462500
C	0.97593500	-2.54942300	2.60462400
C	0.76327500	1.26369700	-3.16780500
C	0.76389500	-1.26369400	3.16789400
C	0.47704900	3.90834600	-0.76963300
C	0.47721700	-3.90833400	0.76972800
C	0.42959000	3.53637000	1.65735700
C	0.42927700	-3.53637700	-1.65725700
C	-0.09766000	3.26157100	-1.91995500
C	-0.09725000	-3.26154500	1.92015200
C	-0.00869400	1.55615500	3.09483400
C	-0.00928700	-1.55615400	-3.09459000

C	-0.24017900	3.92428700	0.43506700
C	-0.24025400	-3.92429600	-0.43484000
C	-0.47058300	2.73612600	2.43471000
C	-0.47104200	-2.73612100	-2.43441600
C	-0.59564700	0.85608600	-3.29226600
C	-0.59498800	-0.85611100	3.29271700
C	-0.97511000	-0.52278500	-3.29033500
C	-0.97444700	0.52278800	3.29081000
C	-1.42801000	2.77013000	-1.89997600
C	-1.42761000	-2.77007800	1.90045100
C	-1.58600000	3.43139600	0.48684400
C	-1.58607000	-3.43139000	-0.48634500
C	-1.76166000	2.77250700	1.78037200
C	-1.76202100	-2.77249200	-1.77982900
C	-1.68214400	1.62989100	-2.74541000
C	-1.68155700	-1.62990100	2.74597000
C	-2.23780600	2.93307100	-0.67905200
C	-2.23762500	-2.93300600	0.67966400
C	-2.32647400	-0.62091000	-2.78669300
C	-2.32582900	0.62088900	2.78726200
C	-2.72425800	1.74558400	1.96388100
C	-2.72477000	-1.74568300	-1.96325800
C	-2.77370700	0.73361400	-2.50203700
C	-2.77308100	-0.73359100	2.50265900
C	-3.35760400	2.03049200	-0.46134700
C	-3.35745800	-2.03047700	0.46212800
C	-3.65597700	1.50287700	0.87975800
C	-3.65628600	-1.50295900	-0.87893900
C	-3.67517100	0.98331500	-1.42546900
C	-3.67466000	-0.98324600	1.42625800
C	-4.18436900	-0.16126100	-0.70161700
C	-4.18410700	0.16125700	0.70254700
Pr	-1.72250800	-0.00002500	-0.00051000

2. Pr@C_{2v}(11188)-C₇₂ (B3LYP/6-31G(d)~MWB48)

C	-3.87514400	1.44692300	0.71609400
C	-3.87579000	1.43852900	-0.72416300
C	-3.84864100	0.06909000	1.16445100
C	-3.85015200	0.05535400	-1.15679900
C	-3.12312700	2.39484800	-1.43448100
C	-3.12171800	2.41181000	1.41450100
C	-3.15005500	-0.27060600	2.32290100
C	-3.15327700	-0.29775700	-2.31253800
C	-2.32064800	3.36075300	-0.71003300
C	-2.32004700	3.36877100	0.67793200
C	-2.37376500	2.01642800	-2.60055400
C	-2.37066000	2.04652200	2.58366300
C	-2.39753700	0.72948600	3.05024200
C	-2.40155300	0.69379900	-3.05209700
C	-2.44803200	-1.54433400	-2.37807500
C	-2.44487000	-1.51638000	2.40244100
C	-2.42395000	-2.44569400	-1.27080200
C	-1.08153600	3.57480100	-1.43561400
C	-1.07953900	3.59076900	1.39931500
C	-1.11258900	2.72964000	-2.59643100
C	-1.10901100	2.75961300	2.56978500
C	-1.21882000	0.06749200	-3.57326800
C	-1.21415100	0.10893300	3.57787400
C	-1.26545800	-1.29016300	3.23040800
C	-1.26956400	-1.32788400	-3.20997700
C	0.13717600	3.84863500	-0.75687500
C	0.13816000	3.85722300	0.71585100
C	0.07968900	2.18229400	3.10565800
C	0.07554100	2.14644000	-3.12734300
C	0.03104800	0.80703800	3.63083000
C	0.02618600	0.76512900	-3.63608200
C	-0.07424000	-2.07156100	-3.00830600
C	-0.06996100	-2.03497800	3.03450400
C	1.17046700	-1.41459300	-3.21072900
C	1.17535300	-1.37696900	3.22959900
C	1.21857500	-0.01917000	-3.57415000
C	1.22359100	0.02227300	3.57692800
C	1.30262500	2.64412300	-2.59790000
C	1.30596700	2.67420200	2.56920000
C	1.33277800	3.48938300	-1.43702500
C	1.33449200	3.50536500	1.39857700
C	2.24510600	-2.59360300	1.30270800

C	2.33164600	-1.71387400	-2.38023600
C	2.33544000	-1.68627700	2.40116100
C	2.44316600	0.52194600	-3.05409100
C	2.44744100	0.55766600	3.04816900
C	-3.79361800	-0.80095600	0.00847300
C	3.72835600	-1.06704700	0.00530500
C	2.51371800	1.87327900	2.58168400
C	2.50989200	1.84316600	-2.60284600
C	2.55431900	3.18852200	-0.71230600
C	2.55556900	3.19655300	0.67588200
C	3.12381100	-0.52051500	-2.31565500
C	3.28546600	2.16765300	-1.43731100
C	3.84429200	-0.21737800	-1.16024100
C	3.84606900	-0.20360800	1.16134900
C	3.96974400	1.16873400	0.71272000
C	3.96847100	1.16034900	-0.72762500
C	-3.04078700	-2.02007000	0.01502000
C	2.88967600	-2.22852400	0.01267000
C	3.12707800	-0.49341500	2.32084000
C	3.28791400	2.18467400	1.41170300
C	-2.42113200	-2.42878000	1.30467000
C	2.24368500	-2.60990700	-1.27212200
C	-0.10928400	-3.12213200	2.08840300
C	-0.11237600	-3.15098900	-2.05232100
C	1.06847100	-3.44528200	1.28429500
C	-1.31112500	-3.38076800	-1.24395500
C	-1.30815900	-3.36223200	1.28544100
C	1.06738400	-3.46318000	-1.24452600
C	-0.85813400	-3.89342200	0.02417700
C	0.58101000	-3.94274400	0.02357700
Pr	-0.05806000	-1.49627900	-0.00330800

3. 1a (B3LYP/6-31G(d)~MWB48)

C	4.65656700	1.43481700	-1.99553400
C	5.26736800	0.81498200	-0.90490400
C	5.28305700	-0.62763300	-0.79752800
C	3.93066200	2.67499800	-1.81977700
C	3.91567400	0.62144800	-2.94368800
C	5.04579100	1.35432600	0.42606000
C	4.69818400	-1.41582400	-1.79485700
C	3.84756600	3.27016100	-0.55973400
C	3.93709500	-0.76099200	-2.84710300
C	4.36071300	2.54696200	0.59312200
C	5.07055100	-0.96914600	0.59529300
C	2.74726700	2.61944000	-2.66117600
C	4.81323500	0.25528300	1.33032200
C	2.68579100	1.30339200	-3.26656900
C	4.00212600	-2.63170600	-1.44890500
C	2.63617100	3.94533200	-0.14931200
C	2.73158300	-1.51820300	-3.08308600
C	3.41869800	2.68821800	1.67604400
C	4.39661900	-2.13713600	0.92592700
C	1.58539900	3.26763100	-2.26589800
C	2.83288900	-2.73391000	-2.30003000
C	2.41841400	3.65076400	1.24711100
C	1.45976200	0.59750800	-3.37650500
C	3.80736900	0.32144400	2.32916000
C	3.90466300	-3.03014300	-0.10868500
C	1.53429600	4.00634000	-1.01814800
C	1.48261800	-0.87352400	-3.29133200
C	3.08559300	1.59282100	2.51694800
C	3.46669900	-2.14133500	2.02045600
C	0.30855200	2.64113400	-2.48539500
C	3.16389300	-0.94003400	2.71648600
C	0.24322400	1.32606000	-3.00745100
C	2.69658500	-3.63686000	0.38847500
C	0.19600400	3.87998600	-0.50406900
C	1.68490100	-3.35559600	-1.82926600
C	1.12506700	3.56923100	1.74521000
C	2.43145400	-3.11585900	1.71024300
C	-0.58771700	3.06451800	-1.42072800
C	0.27740000	-1.59723300	-2.86688100
C	1.74087100	1.58429000	3.11364500
C	1.61985500	-3.87154400	-0.47579000
C	-0.01860800	3.73567900	0.86537600

C	0.39146500	-2.84301300	-2.18369700
C	0.79816500	2.59081600	2.73633800
C	1.89388500	-0.88967600	3.35266500
C	-0.90786900	0.57499100	-2.63980000
C	1.20649900	0.34739300	3.57296500
C	-0.90841400	-0.84960700	-2.60745300
C	1.11008700	-2.97673000	2.19463500
C	-1.65683300	2.26758300	-0.96704400
C	0.26906700	-3.74803000	-0.01630500
C	-1.08712300	2.90898800	1.35582700
C	-0.52632500	-3.18585000	-1.11572700
C	-0.59911800	2.25771300	2.55079500
C	0.90718600	-1.92323500	3.15776300
C	-1.89457700	1.04727000	-1.70530100
C	-0.02040900	-3.37169500	1.32463900
C	-1.99070400	2.23255100	0.47428800
C	-0.21458400	0.07729600	3.56554500
C	-1.93819300	-1.27601200	-1.68427200
C	-1.73006600	-2.47528800	-0.88845900
C	-1.13873900	1.02100300	2.97869900
C	-0.38015700	-1.33772500	3.36293400
C	-2.57546300	-0.08746300	-1.16315100
C	-1.32575600	-2.79467300	1.57294600
C	-2.70135700	1.10159700	1.00021900
C	-2.24078500	-2.41337800	0.47531300
C	-2.29876100	0.53534200	2.26267200
C	-1.50276000	-1.81695000	2.62807300
C	-3.41257600	-0.01065200	0.10992900
C	-2.51812000	-0.89937600	2.20839800
C	-2.99481200	-1.27188000	0.91166100
Pr	-0.54407500	-0.48931600	0.51201000
C	-6.84873700	1.71821300	0.24351000
C	-5.49427900	1.42614200	0.38818200
C	-4.92025600	0.23395200	-0.07598400
C	-5.78945700	-0.67330200	-0.70666600
C	-7.15039600	-0.41055300	-0.86519300
C	-7.67059000	0.78906000	-0.38702900
H	-7.25648500	2.65164100	0.61518300
H	-4.85876200	2.15332800	0.88240300
H	-7.78932500	-1.13544300	-1.35495400
Cl	-5.22291900	-2.21102100	-1.34061000
Cl	-9.38021300	1.12223600	-0.58573400

4. 1a' (B3LYP/6-31G(d)~MWB48)

C	4.64775400	1.83475300	-1.61151500
C	5.26081700	1.01284300	-0.66535800
C	5.30573200	-0.41988500	-0.86051800
C	3.89427600	2.99763100	-1.19262000
C	3.93423800	1.22331800	-2.71904700
C	5.01395300	1.25886000	0.74537700
C	4.74777300	-0.99323100	-2.00872100
C	3.78512600	3.31500800	0.16238100
C	3.98402400	-0.14810700	-2.91295000
C	4.30152700	2.37747100	1.14667100
C	5.08622400	-1.04795800	0.42790800
C	2.72111000	3.09651500	-2.04460200
C	4.79558600	-0.00835400	1.39787000
C	2.69376000	1.93442000	-2.91140200
C	4.07441000	-2.26726900	-1.93352500
C	2.55579500	3.86764300	0.68730900
C	2.79709600	-0.86214400	-3.31844700
C	3.34501300	2.27226100	2.22141000
C	4.43438900	-2.27148800	0.49857300
C	1.54180300	3.62529700	-1.53869900
C	2.91673700	-2.21216900	-2.80406300
C	2.32896300	3.28432700	1.98850100
C	1.48452900	1.24373400	-3.18316200
C	3.77847700	-0.17039000	2.37441400
C	3.97097500	-2.93715100	-0.70659900
C	1.46214800	4.08693700	-0.16527000
C	1.53656600	-0.21212800	-3.40513400
C	3.02675500	1.02032200	2.81122300
C	3.49377400	-2.52140400	1.55522600
C	0.28184200	3.03292400	-1.90115000
C	3.15758600	-1.49661400	2.48082500
C	0.25023300	1.85532400	-2.68612800
C	2.77134500	-3.65630700	-0.36444700
C	0.12201100	3.83154000	0.29229700
C	1.77783500	-2.94091500	-2.49132600
C	1.03228800	3.07695300	2.44001100
C	2.48244200	-3.42792600	1.03326800
C	-0.63305600	3.20683300	-0.78341400
C	0.34203000	-1.03133900	-3.15963000
C	1.67566800	0.86320400	3.37230300
C	1.70958600	-3.72772500	-1.27526600
C	-0.10572200	3.40188000	1.59794600

C	0.47738100	-2.38899400	-2.74885600
C	0.71563700	1.90818800	3.20137100
C	1.87985800	-1.60270500	3.09430000
C	-0.88674200	1.02093200	-2.49688400
C	1.16282100	-0.45140300	3.55560800
C	-0.86398800	-0.37706900	-2.76912700
C	1.15403800	-3.41743500	1.51690900
C	-1.68467600	2.31052300	-0.51910400
C	0.35182100	-3.72728900	-0.81963500
C	-1.16171700	2.46987000	1.88913500
C	-0.44363700	-2.96418300	-1.79029600
C	-0.67350900	1.59572800	2.93105900
C	0.91818700	-2.59112400	2.67377400
C	-1.89077200	1.26937300	-1.49897800
C	0.04221000	-3.64323700	0.56634300
C	-2.04465300	1.97504700	0.87602700
C	-0.25203200	-0.73978200	3.47000500
C	-1.89910200	-1.00499400	-1.97345800
C	-1.66342500	-2.33705900	-1.43798400
C	-1.19418500	0.28821300	3.08315000
C	-0.38295300	-2.08473200	2.97766100
C	-2.56791800	0.04056700	-1.22241500
C	-1.27514000	-3.15216700	0.90976000
C	-2.75731100	0.75695500	1.14735600
C	-2.18428800	-2.56922200	-0.09821500
C	-2.34140600	-0.05587900	2.26827000
C	-1.48544500	-2.41941400	2.14196200
C	-3.42230100	-0.17455300	0.02609900
C	-2.51361300	-1.45262300	1.90917400
C	-2.95770700	-1.55254900	0.55466500
Pr	-0.54731100	-0.63800700	0.36724000
C	-7.08898500	-1.31089800	-0.14525500
C	-5.70542500	-1.26492300	0.00160500
C	-4.95558800	-0.08660300	-0.14232400
C	-5.68647000	1.07384300	-0.45178200
C	-7.07453400	1.06198800	-0.60172700
C	-7.76780700	-0.13439300	-0.44703800
H	-7.62793200	-2.24422800	-0.02611800
H	-5.18117500	-2.18532600	0.23747600
H	-7.60017000	1.97938100	-0.83754000
Cl	-4.91700300	2.63603700	-0.67896200
Cl	-9.51003300	-0.14899800	-0.63698200

5. **1b** (B3LYP/6-31G(d)~MWB48)

C	4.59382900	1.53959500	-1.93111100
C	5.19302400	1.02923700	-0.77907300
C	5.29367300	-0.39994000	-0.57828900
C	3.78532800	2.73848900	-1.86571000
C	3.94827900	0.62323800	-2.85465700
C	4.87885700	1.63426000	0.50399800
C	4.80304500	-1.28404700	-1.54578500
C	3.60945800	3.40377400	-0.65130800
C	4.05099800	-0.74627000	-2.66820600
C	4.11471100	2.78844700	0.56578900
C	5.04018500	-0.66768800	0.82398600
C	2.64674400	2.55481400	-2.74949300
C	4.67519200	0.58077400	1.46738600
C	2.69432200	1.20297400	-3.27117800
C	4.16914100	-2.51857700	-1.15054500
C	2.34176400	4.02366600	-0.33509200
C	2.90670700	-1.59316500	-2.90425300
C	3.11769400	2.93487200	1.59761400
C	4.42690000	-1.85456300	1.20232500
C	1.43069100	3.15042900	-2.44507000
C	3.04787900	-2.74869600	-2.04022400
C	2.07999400	3.80269000	1.06739500
C	1.52044500	0.41415000	-3.38517900
C	3.62275300	0.64337100	2.41738300
C	4.03670900	-2.83868000	0.20756600
C	1.27844000	3.95913200	-1.24991400
C	1.63067900	-1.04424500	-3.20382000
C	2.81558800	1.87448000	2.49290300
C	3.45042800	-1.85107200	2.25613900
C	0.20592700	2.43093900	-2.67592400
C	3.04212700	-0.63062200	2.85897200
C	0.24581700	1.08438600	-3.11334900
C	2.84779700	-3.49062000	0.69348700
C	-0.07132900	3.77911600	-0.78433200
C	1.92108900	-3.41346400	-1.57727300
C	0.77313700	3.66848100	1.51632800
C	2.49215700	-2.90762600	1.96704300
C	-0.76175400	2.86062200	-1.67822800
C	0.45516400	-1.81636300	-2.78236100
C	1.44847400	1.81592300	3.03299100
C	1.82785800	-3.84866300	-0.19714300
C	-0.33827700	3.70663700	0.58156500

C	0.61590600	-3.00606000	-2.01467500
C	0.46320800	2.73444600	2.55425700
C	1.74390800	-0.62290900	3.43789100
C	-0.87189500	0.28466300	-2.74615900
C	0.97200200	0.57840000	3.55034800
C	-0.78519800	-1.13248300	-2.62153100
C	1.14408200	-2.82345100	2.38628800
C	-1.79894700	2.02525600	-1.21858400
C	0.45266800	-3.78429300	0.19842300
C	-1.37438100	2.84396500	1.07973200
C	-0.32538900	-3.34110400	-0.96535900
C	-0.90127500	2.30093000	2.33351700
C	0.83286700	-1.72797600	3.26931500
C	-1.92713900	0.74897300	-1.88534900
C	0.08036200	-3.34468500	1.49907600
C	-2.19398200	2.05743400	0.20751700
C	-0.42813200	0.21690500	3.50218600
C	-1.82494100	-1.56608400	-1.71354800
C	-1.57926800	-2.69708900	-0.83426100
C	-1.38225000	1.06108000	2.81901300
C	-0.49626600	-1.21547000	3.38354300
C	-2.55833800	-0.39222700	-1.29773600
C	-1.26816100	-2.83827200	1.65566800
C	-2.85565100	0.91719400	0.77646800
C	-2.15451800	-2.58461400	0.49965300
C	-2.47734100	0.45805100	2.08955700
C	-1.55396400	-1.81155300	2.63782800
C	-3.45468100	-0.29116300	-0.06800700
C	-2.60454500	-0.98885200	2.11888300
C	-2.99890400	-1.47140600	0.83048700
Pr	-0.58419000	-0.55185500	0.48835900
C	-6.98366500	1.20088700	-0.19794700
C	-5.62189500	1.02437800	0.03370300
C	-4.96581000	-0.15787200	-0.33522100
C	-5.74485500	-1.15557200	-0.94676800
C	-7.10971900	-0.97825700	-1.17670900
C	-7.74274200	0.20463500	-0.80445400
H	-5.06086100	1.81934600	0.51040500
H	-7.67501200	-1.77402400	-1.64970600
Cl	-5.05555000	-2.68885700	-1.45732400
Cl	-7.74861500	2.70487700	0.28524900
H	-8.80291500	0.34579600	-0.98297500

6. **1b'** (B3LYP/6-31G(d)~MWB48)

C	4.79358600	1.48626700	-1.51772900
C	5.30748800	0.61578000	-0.55604000
C	5.22860000	-0.81581800	-0.74901500
C	4.13700500	2.71297000	-1.11811100
C	4.05592700	0.93781300	-2.64221000
C	5.04818500	0.88692500	0.84784400
C	4.64985300	-1.34036300	-1.91010600
C	4.02348000	3.04296100	0.23363700
C	3.98743600	-0.43294300	-2.83361800
C	4.43013500	2.06634700	1.23154900
C	4.92220000	-1.41798400	0.53377500
C	2.99873100	2.91358800	-1.99907600
C	4.70199900	-0.35386000	1.49573300
C	2.88902700	1.75643500	-2.86594700
C	3.86352200	-2.54847400	-1.85066800
C	2.83574000	3.70443500	0.72768500
C	2.75201700	-1.03933800	-3.26845100
C	3.44157800	2.04987100	2.28226300
C	4.16230900	-2.57836100	0.58932100
C	1.85916200	3.54637200	-1.52255600
C	2.73750000	-2.39261600	-2.74986700
C	2.52570400	3.14780800	2.02310000
C	1.62978500	1.17550300	-3.16662600
C	3.65001000	-0.42164700	2.44586700
C	3.67102100	-3.20328000	-0.62658300
C	1.78723200	4.01757800	-0.15215300
C	1.55701000	-0.27954500	-3.38745800
C	2.99771500	0.83260800	2.86383600
C	3.17699200	-2.73996500	1.62198700
C	0.56066100	3.06834600	-1.91621000
C	2.91117200	-1.68691000	2.53864000
C	0.44304300	1.89615500	-2.70098500
C	2.40413300	-3.81185800	-0.31393000
C	0.41858700	3.88484300	0.27203300
C	1.53102900	-3.01658400	-2.46584200
C	1.20471900	3.05773600	2.44191600
C	2.10233600	-3.55515000	1.07617900
C	-0.36224400	3.32627900	-0.82156200
C	0.28833200	-0.98826700	-3.17020700
C	1.62481200	0.79806500	3.39147100
C	1.36316300	-3.79009000	-1.25076200
C	0.12141400	3.47971000	1.57145700

C	0.29189900	-2.35129000	-2.75568200
C	0.76642600	1.92398800	3.19588200
C	1.61437500	-1.67676700	3.12055200
C	-0.76881700	1.16764100	-2.54012700
C	0.99173900	-0.46478300	3.56286600
C	-0.86431400	-0.22798400	-2.81105600
C	0.76855000	-3.42366300	1.52658900
C	-1.49616100	2.52869400	-0.58285400
C	0.00017400	-3.66719600	-0.82922800
C	-1.02087900	2.64751700	1.83760600
C	-0.69985200	-2.83883000	-1.81941500
C	-0.63774500	1.73579000	2.89111800
C	0.57938100	-2.57725100	2.67767300
C	-1.77093000	1.50782600	-1.56780800
C	-0.33481800	-3.55209400	0.54849200
C	-1.92008300	2.23145700	0.80309200
C	-0.44084800	-0.62640700	3.44357400
C	-1.97076000	-0.75893600	-2.04086400
C	-1.86834600	-2.10571200	-1.49926400
C	-1.27673500	0.48055500	3.03133600
C	-0.67855200	-1.95570000	2.94843500
C	-2.56197700	0.34486800	-1.30770000
C	-1.61039900	-2.94388400	0.85823400
C	-2.74415600	1.08172200	1.05736600
C	-2.43947700	-2.28597300	-0.17209700
C	-2.42913700	0.23788300	2.18829800
C	-1.78412100	-2.19197200	2.08439600
C	-3.46092900	0.20962100	-0.07926600
C	-2.71591300	-1.13847500	1.82567400
C	-3.13429300	-1.20227800	0.46091100
Pr	-0.64858400	-0.50549200	0.32572300
C	-7.20394700	-0.56021400	-0.31634500
C	-5.82814800	-0.66469400	-0.13448900
C	-4.97658600	0.44059800	-0.28467500
C	-5.58480200	1.66039700	-0.63002900
C	-6.96578200	1.76546000	-0.80923400
C	-7.79033500	0.65560000	-0.65426100
H	-5.40420100	-1.62686700	0.12909500
H	-7.39151300	2.72744100	-1.07330700
Cl	-4.66644700	3.13829200	-0.86450900
Cl	-8.20826800	-1.98501200	-0.11435600
H	-8.86256800	0.73655600	-0.79446000

7. 1c (B3LYP/6-31G(d)~MWB48)

C	4.83053900	1.61564000	-1.66282800
C	5.39696300	0.78870500	-0.69230100
C	5.36320000	-0.64934000	-0.84630800
C	4.14141700	2.82953900	-1.27889700
C	4.08564900	1.01298000	-2.75425500
C	5.16239100	1.08806100	0.71016400
C	4.77575400	-1.22370400	-1.97932100
C	4.04900100	3.19103200	0.06617700
C	4.06046100	-0.36394700	-2.90870800
C	4.51271400	2.25522400	1.07806300
C	5.10870200	-1.22746900	0.45864600
C	2.97611500	2.96819900	-2.13629400
C	4.87456700	-0.14641100	1.39790300
C	2.88608500	1.78547200	-2.96995300
C	4.03279600	-2.45569700	-1.86929900
C	2.85090900	3.82417500	0.57220200
C	2.83662500	-1.02324300	-3.29732000
C	3.55047800	2.23295500	2.15278000
C	4.39014500	-2.41106500	0.56231900
C	1.82672100	3.57429400	-1.64804900
C	2.88085000	-2.36182200	-2.74426300
C	2.59185300	3.29168500	1.88881400
C	1.64097600	1.15516700	-3.22596400
C	3.84851700	-0.22473400	2.37533300
C	3.89221000	-3.08430500	-0.62462100
C	1.77145200	4.07842100	-0.28878000
C	1.61393300	-0.30721000	-3.40713200
C	3.16305100	1.01725000	2.77632500
C	3.43615400	-2.57883200	1.62267900
C	0.53608400	3.04408300	-1.99807900
C	3.15603800	-1.51132300	2.51790900
C	0.44088800	1.84821600	-2.75084600
C	2.65442200	-3.72712500	-0.26535800
C	0.41842100	3.91156800	0.17235400
C	1.70322500	-3.01778600	-2.41360200
C	1.28525600	3.16927000	2.34339100
C	2.37686300	-3.44392500	1.12409800
C	-0.36996300	3.30118600	-0.88808400
C	0.37652100	-1.05204700	-3.14087100
C	1.80537000	0.95059700	3.33869400
C	1.59110500	-3.76595500	-1.17630200
C	0.16746200	3.53208100	1.48972800

C	0.43608900	-2.40226000	-2.68918600
C	0.90454600	2.04130000	3.13584200
C	1.87356100	-1.52964100	3.13103100
C	-0.74114000	1.08404200	-2.54376900
C	1.22109000	-0.32878400	3.55854800
C	-0.79170300	-0.32130500	-2.77295000
C	1.05034200	-3.34621600	1.60348300
C	-1.47283600	2.47425800	-0.60234200
C	0.23518400	-3.67866100	-0.72383700
C	-0.93908200	2.66993000	1.80600800
C	-0.51626700	-2.89921100	-1.71632000
C	-0.49987400	1.79798600	2.87158000
C	0.85923500	-2.47545100	2.73594600
C	-1.72986000	1.41512100	-1.55290900
C	-0.07226400	-3.54000500	0.65825400
C	-1.84754900	2.19637600	0.80406200
C	-0.20738900	-0.54209300	3.47947400
C	-1.85552700	-0.87051800	-1.95718600
C	-1.70115500	-2.19946000	-1.38516400
C	-1.08925800	0.52452500	3.06078600
C	-0.41263700	-1.89142000	3.02262600
C	-2.45807600	0.22756900	-1.23492200
C	-1.36319500	-2.96989700	0.98497700
C	-2.60919400	1.01793200	1.10729200
C	-2.24037700	-2.36616600	-0.04103300
C	-2.25052100	0.21791100	2.25217200
C	-1.53338600	-2.19179400	2.19608400
C	-3.32012100	0.09916500	0.01507800
C	-2.50724500	-1.17719000	1.93309500
C	-2.96439100	-1.29347000	0.58231400
Pr	-0.48514400	-0.53787600	0.38063900
C	-6.58573000	1.95422200	-0.72019000
C	-5.23648100	1.68607700	-0.51985500
C	-4.80848900	0.39525900	-0.18227500
C	-5.75969900	-0.61574100	-0.04995800
C	-7.11783900	-0.35395800	-0.25046600
C	-7.53703600	0.93797200	-0.58746500
H	-4.51548200	2.49068400	-0.62914300
Cl	-9.22035900	1.31839000	-0.84736600
Cl	-8.25680900	-1.66566300	-0.06981800
H	-5.45410200	-1.62367600	0.21060100
H	-6.91692400	2.95374600	-0.98081000

8. 1c' (B3LYP/6-31G(d)~MWB48)

C	4.50391900	2.31665700	-1.46338000
C	5.20481500	1.45256600	-0.62141200
C	5.35976600	0.05700900	-0.97066500
C	3.66933700	3.36166100	-0.90843800
C	3.81403100	1.76913700	-2.61822900
C	4.97398100	1.52584000	0.81141500
C	4.82155600	-0.43554300	-2.16500700
C	3.56931900	3.52322200	0.47441800
C	3.96902600	0.43475600	-2.95904300
C	4.18496100	2.53291600	1.34335900
C	5.22435200	-0.72029700	0.24565600
C	2.47059600	3.45254100	-1.72484400
C	4.87499300	0.18246600	1.32648100
C	2.51541700	2.39141000	-2.71173100
C	4.25394000	-1.76131200	-2.21593900
C	2.31287900	3.91263900	1.07630200
C	2.83359800	-0.32799100	-3.41960500
C	3.26763400	2.23513700	2.41631500
C	4.67495400	-1.99447000	0.19444800
C	1.26539200	3.82506100	-1.14540400
C	3.07368200	-1.70991200	-3.05608200
C	2.16794500	3.17833000	2.31100000
C	1.35910500	1.63593500	-3.03670200
C	3.89971300	-0.16637800	2.29631900
C	4.23642200	-2.56429600	-1.06760600
C	1.18356500	4.12997900	0.27089700
C	1.52311100	0.22165500	-3.41662800
C	3.06619900	0.90501000	2.87177900
C	3.78493200	-2.43242800	1.23306000
C	0.04800800	3.17370100	-1.54953500
C	3.39110700	-1.54338200	2.26955200
C	0.09150200	2.08826200	-2.45832500
C	3.10763300	-3.41304200	-0.78516100
C	-0.12016800	3.71826600	0.72045200
C	2.00530400	-2.55945900	-2.80429100
C	0.90387500	2.81703700	2.75864200
C	2.83668100	-3.35972600	0.63306100
C	-0.85071100	3.15299200	-0.40472600
C	0.40583500	-0.71483800	-3.24016200
C	1.74713500	0.57755500	3.43429900
C	2.03209600	-3.47510000	-1.68024200
C	-0.27772600	3.13425500	1.97594700

C	0.65929800	-2.09251100	-2.97882000
C	0.70232000	1.55139200	3.39337400
C	2.14199500	-1.81993500	2.88967600
C	-0.96935000	1.14741700	-2.34217000
C	1.34713400	-0.78792500	3.48434300
C	-0.83820400	-0.20754500	-2.76193600
C	1.52405000	-3.51031500	1.13650000
C	-1.82268500	2.15156500	-0.22134500
C	0.69077700	-3.63707200	-1.20514200
C	-1.24862200	2.09409300	2.18427200
C	-0.18821600	-2.84168200	-2.07293300
C	-0.66418100	1.15577200	3.11497500
C	1.25213800	-2.83436600	2.38027100
C	-1.96312900	1.20366000	-1.30437100
C	0.40961000	-3.72770500	0.18649900
C	-2.11572700	1.63981500	1.13767500
C	-0.04141700	-1.18215300	3.39264600
C	-1.79429000	-1.00187600	-2.01806500
C	-1.44570600	-2.36166700	-1.63539000
C	-1.07098900	-0.20007500	3.13432000
C	-0.07734500	-2.47323200	2.75779300
C	-2.51737500	-0.10377800	-1.14544100
C	-0.93612500	-3.38964000	0.60319800
C	-2.70101700	0.33758600	1.28423200
C	-1.91695500	-2.77975100	-0.32065900
C	-2.20431400	-0.55148600	2.30442700
C	-1.17226200	-2.81069900	1.91114900
C	-3.31619000	-0.51609600	0.08288100
C	-2.28079800	-1.91333500	1.80027300
C	-2.75925400	-1.90944000	0.45170500
Pr	-0.41089600	-0.80074700	0.32938100
C	-7.05839000	-1.36053000	0.13815300
C	-5.67486200	-1.48342000	0.25067400
C	-4.83771800	-0.40387400	-0.04293200
C	-5.41323400	0.80300300	-0.45327900
C	-6.79662300	0.93423500	-0.56629400
C	-7.62955900	-0.15446500	-0.26863900
H	-5.24762300	-2.43101100	0.56423300
Cl	-9.36627400	-0.04031900	-0.39799100
Cl	-7.45299800	2.46784300	-1.08409700
H	-4.79075500	1.65761900	-0.69644100
H	-7.70612900	-2.20113300	0.36306700

9. 2a (BLYP/3-21G~MWB48)

C	-4.95906500	2.07637500	-0.38822300
C	-4.94917400	1.35296700	-1.59115100
C	-5.14093200	-0.10138500	-1.58579100
C	-4.05965400	3.21768600	-0.19909200
C	-5.01576200	1.33892700	0.88188400
C	-3.92414000	1.66167300	-2.59663000
C	-5.34987900	-0.78532500	-0.37373500
C	-3.17731800	3.60471300	-1.22633700
C	-5.20472200	-0.04229900	0.89002700
C	-3.06775800	2.74819100	-2.42122400
C	-4.23972800	-0.67751500	-2.58830000
C	-3.56660000	3.17635600	1.18055800
C	-3.40817900	0.40417200	-3.12576400
C	-4.07321400	1.94887900	1.81008400
C	-4.78326900	-2.11452000	-0.17121200
C	-1.84322400	4.10119600	-0.91156900
C	-4.46925000	-0.87048300	1.83441100
C	-1.66193100	2.63072500	-2.77533100
C	-3.69569200	-1.95121200	-2.39329900
C	-2.28721000	3.64714700	1.48177600
C	-4.30851300	-2.19306400	1.21441300
C	-0.91545100	3.55476400	-1.91047300
C	-3.24535200	1.15291300	2.65793800
C	-2.01108600	0.21748300	-3.35753400
C	-4.02027200	-2.72696500	-1.18673400
C	-1.41427900	4.18609300	0.42955900
C	-3.45600500	-0.31918900	2.67895500
C	-1.10329800	1.37974900	-3.18076400
C	-2.32129500	-2.22063000	-2.76285300
C	-1.46538000	2.93640900	2.44570700
C	-1.47718800	-1.15615600	-3.21424200
C	-1.92177600	1.70604500	3.02207000
C	-2.84756500	-3.52455300	-0.85313700
C	-0.03832000	3.87142400	0.79773500
C	-3.21386000	-2.98930700	1.53729600
C	0.40525000	3.27787300	-1.56413800
C	-1.79860400	-3.23321000	-1.82745300
C	-0.06486100	3.10885200	2.04282800
C	-2.35327300	-1.21553700	3.09765300
C	0.32681800	1.14958800	-2.88059200
C	-2.48342900	-3.72559500	0.49404700
C	0.89363000	3.48668000	-0.19000000

C	-2.26317400	-2.54243600	2.53983000
C	1.06441700	2.10615700	-2.10425300
C	-0.07609600	-1.32199800	-2.99505800
C	-0.90912900	0.80918300	3.47485100
C	0.80809300	-0.19360200	-2.84302700
C	-1.12596200	-0.62729600	3.54133600
C	-0.41988400	-3.30392900	-1.47410900
C	0.92123600	2.11706400	2.32745900
C	-1.09421700	-3.80370800	0.88385700
C	1.93269800	2.52015700	0.07589800
C	-0.97356900	-3.12491400	2.20274500
C	2.08310600	1.67724400	-1.14622800
C	0.47217400	-2.42262700	-2.21001500
C	0.49351000	1.04249400	3.19429000
C	-0.04108700	-3.66809800	-0.07972000
C	2.00522000	1.84705500	1.34157100
C	1.95592900	-0.59657900	-2.02931400
C	0.15528000	-1.29096600	3.36762000
C	0.24739200	-2.53942700	2.63162600
C	2.58506600	0.35173500	-1.12189900
C	1.76772400	-2.01390900	-1.70732400
C	1.16493500	-0.24121700	3.18788200
C	1.27324200	-3.25316200	0.41411800
C	2.69252900	0.56778400	1.39171600
C	1.43177200	-2.75557800	1.80110300
C	3.40830900	-0.12236200	0.13316400
C	2.24032300	-2.50235000	-0.42753500
C	2.30422300	-0.44114300	2.35982700
C	2.99960900	-1.61727400	0.42155600
C	2.50430200	-1.77208500	1.78420400
Pr	0.53482600	-0.70577200	0.35942300
C	6.87614300	1.38571400	0.95802100
C	5.50498900	1.07982800	0.97328700
C	4.92624600	0.17061600	0.05557000
C	5.79709500	-0.41845300	-0.88003100
C	7.16875800	-0.14266200	-0.92756700
C	7.68297900	0.76428400	0.00275300
H	7.30190800	2.08857700	1.67122200
H	4.85978900	1.55073300	1.71455300
H	7.80829600	-0.62253500	-1.66388400
Cl	5.17832100	-1.63075400	-2.13391300
Cl	9.48962400	1.14504200	-0.04051400

10. **2a'** (BLYP/3-21G~MWB48)

C	-4.94029700	2.08579700	-0.35823300
C	-4.94074500	1.39716300	-1.58144200
C	-5.14901500	-0.05427200	-1.61740000
C	-4.02748100	3.21063800	-0.13847400
C	-5.00283100	1.31302100	0.89061600
C	-3.91457600	1.72279600	-2.58036400
C	-5.36342700	-0.77015800	-0.42496200
C	-3.14278100	3.61657800	-1.15638500
C	-5.20713100	-0.06558500	0.85936800
C	-3.04562800	2.79403800	-2.37628900
C	-4.25663900	-0.61143000	-2.63839200
C	-3.53236600	3.12454000	1.23830000
C	-3.41394700	0.47530800	-3.14689400
C	-4.05113200	1.88544600	1.83369900
C	-4.81148100	-2.11092500	-0.26184500
C	-1.80280300	4.08822900	-0.83044700
C	-4.47912300	-0.92877700	1.77783700
C	-1.64222600	2.67088000	-2.73814000
C	-3.72606500	-1.89572000	-2.48063500
C	-2.24747200	3.57306900	1.55036400
C	-4.33537900	-2.23484500	1.12037000
C	-0.88370000	3.56078800	-1.84823700
C	-3.22993000	1.05603000	2.65566200
C	-2.01960700	0.27957100	-3.38875900
C	-4.05713500	-2.70200400	-1.29611000
C	-1.37078600	4.13181000	0.51180200
C	-3.45721500	-0.41348500	2.63503900
C	-1.09835700	1.42575900	-3.18141500
C	-2.35531000	-2.16921500	-2.86063200
C	-1.43124100	2.82499900	2.49086300
C	-1.49980500	-1.10336400	-3.28722400
C	-1.89965900	1.58392900	3.03202500
C	-2.89296400	-3.52207700	-0.98818200
C	0.00167900	3.79011600	0.86800200
C	-3.24943300	-3.05252500	1.41794300
C	0.43308700	3.25681600	-1.51288000
C	-1.84264800	-3.21359700	-1.95576900
C	-0.02918100	2.99335200	2.08976500
C	-2.36355100	-1.33370700	3.02484700
C	0.33063100	1.17016000	-2.89358700
C	-2.52948800	-3.76609400	0.35216900
C	0.92417900	3.41836000	-0.13332000

C	-2.29141800	-2.64588500	2.43136600
C	1.07841200	2.09483000	-2.08915500
C	-0.09923500	-1.29191800	-3.07990600
C	-0.89490200	0.66300500	3.45500900
C	0.79888300	-0.17819300	-2.89931200
C	-1.12711300	-0.77136200	3.47886200
C	-0.46423300	-3.30838200	-1.60861400
C	0.94742100	1.98191100	2.34260900
C	-1.14086400	-3.87097600	0.73661100
C	1.94484200	2.42936300	0.10358300
C	-1.00910600	-3.23313900	2.07467000
C	2.09195000	1.62666400	-1.14436500
C	0.43556400	-2.41988400	-2.32567800
C	0.51010400	0.88894800	3.18094700
C	-0.08961900	-3.71480200	-0.22523200
C	2.02402900	1.72450500	1.34848900
C	1.94299300	-0.61684600	-2.09506500
C	0.14690500	-1.44331000	3.28559300
C	0.21961900	-2.67404800	2.51750700
C	2.58049000	0.29738300	-1.15647500
C	1.73324000	-2.03827300	-1.81116400
C	1.17173900	-0.39953000	3.13629900
C	1.22732100	-3.32883900	0.27838400
C	2.72868900	0.44861300	1.37104900
C	1.39878700	-2.87596200	1.67787300
C	3.41072700	-0.22641300	0.07672400
C	2.19323500	-2.56221300	-0.54359900
C	2.31955700	-0.58558400	2.30849700
C	2.96057000	-1.71069000	0.32789600
C	2.48467200	-1.90510900	1.68916200
Pr	0.53206600	-0.74139400	0.34929900
C	6.93606200	-1.21676200	-1.12474500
C	5.56546000	-1.19724500	-0.82918300
C	4.94612400	-0.11710500	-0.14609800
C	5.78741500	0.94681100	0.22661200
C	7.16489700	0.95904300	-0.04065700
C	7.71378900	-0.12952200	-0.71815100
H	7.38606500	-2.05690700	-1.64969300
H	4.94787900	-2.04466300	-1.12674300
H	7.78062900	1.79772900	0.27354800
Cl	5.16554400	2.44746100	1.11397300
Cl	9.52441600	-0.12727900	-1.07889800

11. **2b** (BLYP/3-21G~MWB48)

C	-4.82715300	2.20110300	-0.45289700
C	-4.91875700	1.32870800	-1.54815500
C	-5.17399200	-0.10053900	-1.34180800
C	-3.87075200	3.31115200	-0.46328800
C	-4.84180400	1.63875600	0.90486400
C	-3.94270000	1.45261900	-2.63834800
C	-5.33934200	-0.61036000	-0.04046200
C	-3.03457300	3.51752300	-1.57781400
C	-5.08920200	0.28136300	1.10495000
C	-3.03204200	2.50849600	-2.65331500
C	-4.35941100	-0.84677200	-2.30492400
C	-3.30028200	3.42450400	0.88172400
C	-3.51450600	0.11255900	-3.02438300
C	-3.82161700	2.31631800	1.69436000
C	-4.82156000	-1.92965500	0.30598400
C	-1.66350000	3.98156000	-1.40139200
C	-4.33708500	-0.45372100	2.11085500
C	-1.65579500	2.27460900	-3.06182000
C	-3.86043700	-2.11021600	-1.97214200
C	-1.98571300	3.86380800	1.04985300
C	-4.27030600	-1.85204600	1.66347300
C	-0.82102900	3.26325000	-2.36634900
C	-2.98037100	1.59547500	2.59468600
C	-2.14273700	-0.17313100	-3.30308700
C	-4.14696900	-2.70665400	-0.65837800
C	-1.15312800	4.21869700	-0.10797000
C	-3.25350100	0.15090100	2.82104200
C	-1.17694100	0.95504000	-3.32876900
C	-2.52203500	-2.49303500	-2.37363300
C	-1.14048700	3.24266700	2.05435700
C	-1.66081500	-1.54094500	-3.00505000
C	-1.61461300	2.12264600	2.81156100
C	-2.99141500	-3.51133600	-0.28396100
C	0.22709700	3.88387600	0.22591500
C	-3.19398500	-2.65440000	2.03051300
C	0.50392700	2.96662000	-2.05612900
C	-1.99039300	-3.40259700	-1.34189400
C	0.24011200	3.29079600	1.55979100
C	-2.16734700	-0.73865500	3.29481800
C	0.25701400	0.69281600	-3.07539400
C	-2.55833900	-3.55548900	1.05716600
C	1.08222700	3.32821700	-0.75029400

C	-2.16732300	-2.12905600	2.91327300
C	1.07836200	1.70322200	-2.46979700
C	-0.25758400	-1.74910700	-2.84153000
C	-0.61721800	1.24216300	3.32676100
C	0.68215400	-0.65676100	-2.88778700
C	-0.89220900	-0.16091900	3.59434900
C	-0.59760700	-3.49496500	-1.05419900
C	1.19797800	2.29676000	1.92158100
C	-1.15308100	-3.65175800	1.38026000
C	2.09148400	2.35257300	-0.41342500
C	-0.92613800	-2.81376800	2.58887200
C	2.13128400	1.35113500	-1.51888900
C	0.28682900	-2.76358200	-1.94552600
C	0.77502700	1.36539000	2.94288800
C	-0.15344500	-3.69452700	0.35336900
C	2.21051100	1.84822200	0.92488700
C	1.85684600	-1.00857000	-2.08808600
C	0.34744200	-0.90512600	3.44170100
C	0.34277600	-2.24193300	2.87424000
C	2.57453400	0.01616000	-1.34542300
C	1.62627000	-2.36013500	-1.56992700
C	1.38917900	0.06012900	3.07157200
C	1.20496200	-3.28719800	0.71930900
C	2.84482800	0.55319600	1.10784800
C	1.46691300	-2.62314200	2.01826800
C	3.45078400	-0.33026000	-0.08639800
C	2.15210400	-2.70105100	-0.26390300
C	2.47042400	-0.30206000	2.21955400
C	2.99945300	-1.75379000	0.41949600
C	2.57785600	-1.70481100	1.81477800
Pr	0.57784000	-0.73342800	0.37259800
C	6.99601900	1.11610100	0.25359700
C	5.63039700	0.89513300	0.43410300
C	4.97086400	-0.11998700	-0.29915300
C	5.75755200	-0.87128000	-1.19273200
C	7.12776100	-0.64856400	-1.37030400
C	7.76790300	0.36613300	-0.63663800
H	5.06387800	1.49921100	1.13987700
H	7.68879900	-1.26180500	-2.07329000
Cl	5.01680100	-2.23089000	-2.20586400
Cl	7.80939600	2.45697200	1.23415700
H	8.83162600	0.56040600	-0.75832000

12. **2b'** (BLYP/3-21G~MWB48)

C	-5.06400100	1.68023800	-0.47794700
C	-4.99034200	0.92976600	-1.66167000
C	-5.06401200	-0.53449700	-1.61964000
C	-4.26148100	2.89539400	-0.31563400
C	-5.06779900	0.97386500	0.81105500
C	-3.98842100	1.29411600	-2.67190500
C	-5.22282500	-1.20148000	-0.39098000
C	-3.40754200	3.32527700	-1.35002200
C	-5.14483000	-0.41734600	0.85431500
C	-3.22347900	2.45017300	-2.52261500
C	-4.11432600	-1.06131800	-2.60434400
C	-3.77362800	2.92901400	1.06608800
C	-3.37018000	0.06962700	-3.16803100
C	-4.18272400	1.68191300	1.72653900
C	-4.55281800	-2.47544300	-0.15270300
C	-2.11948500	3.93501800	-1.04384200
C	-4.34980800	-1.15925100	1.82211600
C	-1.81138600	2.43802700	-2.87122600
C	-3.47001700	-2.28123500	-2.37528600
C	-2.53818500	3.50872200	1.35892700
C	-4.08046700	-2.47970400	1.23638800
C	-1.14634600	3.44023800	-2.02731700
C	-3.29659400	0.97671400	2.59625800
C	-1.96116200	-0.00907000	-3.39170700
C	-3.73741600	-3.04963600	-1.15013200
C	-1.70676400	4.09041600	0.29633500
C	-3.38791300	-0.50621400	2.65484300
C	-1.15074800	1.22644300	-3.24410300
C	-2.07577600	-2.44602300	-2.73338700
C	-1.66604700	2.89085300	2.34263400
C	-1.31788700	-1.32993600	-3.21079000
C	-2.02348800	1.64389700	2.94949900
C	-2.50494300	-3.73947300	-0.79220200
C	-0.31281200	3.89480700	0.67677600
C	-2.92684300	-3.17631500	1.58259400
C	0.18893000	3.27571600	-1.66941000
C	-1.47834700	-3.38936600	-1.77115200
C	-0.28202200	3.16631100	1.94011800
C	-2.21749800	-1.29914100	3.09844100
C	0.29309200	1.11861400	-2.93574000
C	-2.13399900	-3.87743100	0.56095200
C	0.64823100	3.55450300	-0.29852900

C	-2.01952400	-2.62787700	2.57564900
C	0.94477800	2.14977400	-2.17871800
C	0.09238800	-1.37835700	-2.98747000
C	-0.94284800	0.84433200	3.42922900
C	0.88355300	-0.17906000	-2.86399000
C	-1.04278900	-0.60231800	3.53024800
C	-0.10030400	-3.33806600	-1.41255100
C	0.78154800	2.26550800	2.25407200
C	-0.74554500	-3.83069300	0.95606900
C	1.74997100	2.67635900	-0.00297200
C	-0.68609200	-3.11142600	2.25668900
C	1.98611000	1.82712900	-1.20381500
C	0.72177200	-2.41043200	-2.17232300
C	0.43804900	1.18357200	3.14822300
C	0.29593000	-3.63165700	-0.00776400
C	1.88859100	2.05658000	1.28069600
C	2.05887700	-0.46712800	-2.03612900
C	0.28951600	-1.16328300	3.37657700
C	0.48206300	-2.42136100	2.67715700
C	2.60225800	0.55215300	-1.14497200
C	1.97608500	-1.88507300	-1.67521500
C	1.21529000	-0.03904400	3.17467000
C	1.56794400	-3.10084100	0.48063100
C	2.71124100	0.85618300	1.37618700
C	1.68157200	-2.55705600	1.85367200
C	3.46363000	0.17339100	0.11958100
C	2.46846600	-2.29551500	-0.37824100
C	2.38297300	-0.16175100	2.36345600
C	3.14005100	-1.32755500	0.44982100
C	2.67179700	-1.49071400	1.81674100
Pr	0.64374800	-0.58873900	0.39395600
C	7.12365300	-0.61151500	-0.72248600
C	5.75482300	-0.72600400	-0.48972000
C	4.99293000	0.39989200	-0.08145700
C	5.69757000	1.60884400	0.07044000
C	7.07706600	1.71758100	-0.15629600
C	7.81280300	0.59283200	-0.56261200
H	5.26274900	-1.68894200	-0.61263000
H	7.56926700	2.67802800	-0.01431700
Cl	4.86817200	3.17799500	0.58989700
Cl	8.05951200	-2.11534900	-1.25413200
H	8.88366600	0.65640500	-0.74431200

13. 2c (BLYP/3-21G~MWB48)

C	-5.09719100	1.93071500	-0.46202200
C	-5.01706000	1.26497500	-1.69497400
C	-5.15336300	-0.19364800	-1.76215600
C	-4.25041800	3.09450700	-0.18774200
C	-5.17205500	1.13428900	0.77086800
C	-3.96938100	1.65686000	-2.64689100
C	-5.37997700	-0.93987300	-0.59093700
C	-3.34632600	3.55964800	-1.16235000
C	-5.30913600	-0.25167100	0.70998700
C	-3.16107800	2.76349700	-2.38935600
C	-4.19641100	-0.69018500	-2.75524000
C	-3.80617500	3.00806900	1.20607900
C	-3.38756500	0.44439800	-3.21246900
C	-4.28806100	1.73537500	1.76083600
C	-4.77136300	-2.25588700	-0.42694700
C	-2.04471800	4.08941800	-0.77553900
C	-4.57762100	-1.09551600	1.64326300
C	-1.74043600	2.71393600	-2.69597300
C	-3.61109300	-1.95091700	-2.59654600
C	-2.55679200	3.51010900	1.57583600
C	-4.34501300	-2.38149100	0.97154100
C	-1.06161900	3.62290500	-1.76269100
C	-3.46158100	0.93140400	2.60259600
C	-1.97665400	0.31935700	-3.39861600
C	-3.94938200	-2.79257200	-1.43897400
C	-1.66761900	4.12946700	0.58331100
C	-3.61718400	-0.54717800	2.54972500
C	-1.12040600	1.50386400	-3.13621500
C	-2.21483700	-2.15179700	-2.92473400
C	-1.74393100	2.78574200	2.53702100
C	-1.39634700	-1.03873200	-3.29715500
C	-2.17353500	1.51434200	3.03957200
C	-2.75961300	-3.56121600	-1.09719000
C	-0.29494600	3.84861600	0.98939000
C	-3.23265000	-3.15109700	1.29912400
C	0.25460000	3.37792700	-1.37927200
C	-1.68832500	-3.18743400	-2.01677700
C	-0.33698800	3.02871600	2.19664900
C	-2.49638400	-1.42090200	2.96774500
C	0.30594400	1.31175500	-2.79414700
C	-2.43727100	-3.81046800	0.25242600
C	0.68544500	3.54186100	0.02058200

C	-2.33676400	-2.71733400	2.35679700
C	0.97577900	2.25717300	-1.94553200
C	0.00225200	-1.16469200	-3.03489700
C	-1.14460100	0.63563700	3.49055300
C	0.83771600	-0.01327600	-2.80209700
C	-1.30883600	-0.80889500	3.48316000
C	-0.32148100	-3.22494600	-1.61568900
C	0.67694500	2.06265000	2.47612000
C	-1.06134800	-3.85683500	0.69049800
C	1.74859800	2.60254600	0.28312700
C	-1.01462800	-3.23686900	2.04348900
C	1.97220500	1.82098400	-0.96903300
C	0.56250400	-2.28002100	-2.27935000
C	0.25767300	0.93282800	3.27386800
C	0.01967700	-3.63931800	-0.22548900
C	1.80772000	1.87866100	1.52263100
C	1.97111000	-0.41163700	-1.96367000
C	0.00234900	-1.41675500	3.32870500
C	0.16678400	-2.62735400	2.54295700
C	2.51790600	0.51489400	-0.98312500
C	1.82243000	-1.84806400	-1.71022500
C	0.97774700	-0.32351600	3.23494300
C	1.29910600	-3.20144200	0.33582900
C	2.54892800	0.62735200	1.54517400
C	1.38746000	-2.75980000	1.74795300
C	3.31539700	0.01246300	0.27613900
C	2.26509300	-2.37762700	-0.43502700
C	2.15695400	-0.44102100	2.44608800
C	2.95242900	-1.50148300	0.48169100
C	2.42004800	-1.73781400	1.81650900
Pr	0.46543200	-0.68116400	0.37542100
C	6.72977200	1.78788800	0.60118200
C	5.35874100	1.50684800	0.72681400
C	4.82147600	0.32071600	0.18373400
C	5.67434600	-0.58264200	-0.48361000
C	7.03784700	-0.29484800	-0.60381400
C	7.56520900	0.88283200	-0.06614200
H	5.28447700	-1.51045700	-0.90072900
Cl	9.35106300	1.27948300	-0.20583400
H	4.71087900	2.20907400	1.25057600
H	7.15468700	2.69900500	1.01927300
Cl	8.10713000	-1.50769900	-1.47477500

14. **2c'** (BLYP/3-21G~MWB48)

C	-4.88881300	2.34847900	-0.16181600
C	-4.98817800	1.66791900	-1.38550900
C	-5.28545400	0.23179100	-1.41592900
C	-3.90001200	3.41475200	0.01824500
C	-4.94099400	1.57431700	1.08662600
C	-3.99174100	1.93663600	-2.43036800
C	-5.48793000	-0.47636900	-0.21671500
C	-3.04045600	3.77225900	-1.03858100
C	-5.22976500	0.21068000	1.06096600
C	-3.05048100	2.95197100	-2.26375100
C	-4.47686900	-0.37299900	-2.47885000
C	-3.34758500	3.29109100	1.36965900
C	-3.59432900	0.66379200	-3.02245600
C	-3.91303400	2.08268600	1.98606800
C	-5.01039000	-1.84857900	-0.08321900
C	-1.66074800	4.16133300	-0.77478700
C	-4.51375100	-0.70015100	1.94209100
C	-1.67510300	2.74651300	-2.69086900
C	-4.01914900	-1.68873400	-2.34979700
C	-2.02502800	3.65934900	1.62278700
C	-4.47915000	-2.00857400	1.27496900
C	-0.82337300	3.58411100	-1.83532900
C	-3.10657100	1.20036000	2.76559900
C	-2.22711200	0.38529800	-3.32856900
C	-4.34299100	-2.47966300	-1.15285500
C	-1.16443800	4.16941600	0.54597700
C	-3.42444200	-0.25230400	2.75277700
C	-1.22920500	1.47230900	-3.16044000
C	-2.68655800	-2.04253300	-2.79348200
C	-1.21325100	2.85845600	2.52245900
C	-1.78905200	-1.02685100	-3.25279100
C	-1.73100600	1.64501600	3.08173400
C	-3.21696600	-3.36983600	-0.90122200
C	0.19946000	3.74292300	0.83628200
C	-3.43238500	-2.89252700	1.51919200
C	0.48679900	3.19906000	-1.56166700
C	-2.19618300	-3.12145700	-1.91543300
C	0.17579700	2.94287600	2.05657800
C	-2.37186200	-1.23886900	3.08799700
C	0.19259400	1.12925000	-2.93919300
C	-2.80709000	-3.64358200	0.41969800
C	1.05287900	3.32464100	-0.20698300

C	-2.40524300	-2.54925800	2.48700000
C	1.03223400	2.00310200	-2.16959100
C	-0.39446300	-1.30143000	-3.10977500
C	-0.76624800	0.66351400	3.45729500
C	0.57611400	-0.24583000	-2.96919700
C	-1.08483500	-0.75503600	3.48747700
C	-0.81165300	-3.30389700	-1.63319800
C	1.10173900	1.87627400	2.26514500
C	-1.41045200	-3.83410900	0.73859600
C	2.02808700	2.27779000	-0.02098900
C	-1.17896000	-3.21123200	2.07064700
C	2.05912900	1.46977900	-1.27476500
C	0.10704900	-2.46461800	-2.38563800
C	0.63494600	0.80489300	3.11554500
C	-0.39644900	-3.74280300	-0.27067400
C	2.11720200	1.56222200	1.22040600
C	1.72867300	-0.75799900	-2.22436900
C	0.13455600	-1.50239100	3.23196400
C	0.10043600	-2.73107000	2.45829200
C	2.45682900	0.11180400	-1.31226300
C	1.45102700	-2.16845000	-1.93526200
C	1.21099100	-0.52219200	3.03924300
C	0.96630100	-3.44091100	0.17144200
C	2.72052300	0.23861400	1.20281900
C	1.22592400	-3.00305800	1.56404800
C	3.30082500	-0.46202700	-0.11713900
C	1.94452200	-2.73170100	-0.69313200
C	2.29644000	-0.77427800	2.15307900
C	2.79848200	-1.92858500	0.14580400
C	2.36392900	-2.09736500	1.52536000
Pr	0.41409600	-0.84366700	0.24378700
C	6.83037000	-0.94453800	-1.58177900
C	5.44954600	-1.06474200	-1.36471000
C	4.81965500	-0.32515000	-0.33858400
C	5.58975000	0.53615400	0.46484300
C	6.96783000	0.65056700	0.24112000
C	7.58626200	-0.08272300	-0.77327500
H	4.86210800	-1.73458600	-1.99378700
H	5.12335400	1.11303100	1.26183900
H	7.32648900	-1.51159600	-2.36775400
Cl	7.92759700	1.78597800	1.31936800
Cl	9.38966600	0.04861300	-1.08483700

15. 3a (BLYP/3-21G~MWB48)

C	-5.50303300	0.49922200	-0.05361300
C	-5.31644700	-0.01693100	-1.34632200
C	-4.94874700	-1.42142200	-1.53146100
C	-5.08265900	1.86296800	0.26770200
C	-5.19144200	-0.35001400	1.10510800
C	-4.55760600	0.77716300	-2.32258600
C	-4.80373400	-2.27237800	-0.42241700
C	-4.49324000	2.67550300	-0.71496100
C	-4.85697400	-1.69092600	0.92647700
C	-4.16493200	2.08095200	-2.02071400
C	-3.96523100	-1.48336500	-2.62267200
C	-4.50786300	1.84377100	1.62286800
C	-3.64778500	-0.11232900	-3.03128800
C	-4.47990700	0.45362700	2.09052500
C	-3.76346000	-3.30327300	-0.41157500
C	-3.41701400	3.60413500	-0.36488600
C	-3.79858500	-2.29065700	1.73225000
C	-2.84309300	2.55146600	-2.41190400
C	-2.97364600	-2.46618300	-2.61199500
C	-3.48388600	2.72656200	1.95743500
C	-3.20692400	-3.37039800	0.93810300
C	-2.44315700	3.58642100	-1.44690500
C	-3.35723500	-0.06928400	2.80380600
C	-2.30228600	0.28161800	-3.31985800
C	-2.89865900	-3.44621200	-1.51823900
C	-2.95904000	3.68102100	0.97527300
C	-3.00613400	-1.50296500	2.62990200
C	-1.88328400	1.67246500	-3.00507700
C	-1.62368400	-2.13273700	-3.02960700
C	-2.38583500	2.26600900	2.79981900
C	-1.28262300	-0.78466200	-3.36381200
C	-2.31290800	0.89473100	3.21426100
C	-1.49310800	-3.76234300	-1.31454800
C	-1.54446400	3.84820700	1.25463000
C	-1.86759900	-3.72935900	1.12992600
C	-1.08477200	3.79335200	-1.17744300
C	-0.69591100	-2.98056600	-2.26328500
C	-1.18647400	3.00143500	2.40947400
C	-1.62235100	-1.95733900	2.89546600
C	-0.44789200	1.97994500	-2.78744000
C	-0.99410400	-3.98188100	-0.01753900
C	-0.62148200	3.98362900	0.20533000

C	-1.08556600	-3.07639900	2.16438100
C	-0.07689800	3.05600800	-1.89919500
C	0.09287500	-0.42023000	-3.19116000
C	-1.00739200	0.40092200	3.51404000
C	0.51527900	0.93846600	-2.96341600
C	-0.67006900	-1.00819700	3.39516900
C	0.61757300	-2.54446700	-1.94065000
C	0.11036500	2.43832300	2.54504100
C	0.34936100	-3.55115000	0.33826300
C	0.71282500	3.42300900	0.31317400
C	0.30253400	-3.06538000	1.71332000
C	1.07185600	2.90114600	-1.00050900
C	1.05362300	-1.31170200	-2.55644600
C	0.18755200	1.18520600	3.26134000
C	1.20928300	-2.89134500	-0.61414700
C	1.12987700	2.69032000	1.48908600
C	1.79218100	0.90266300	-2.23183900
C	0.74918500	-1.10296900	3.10743500
C	1.25623900	-2.10124600	2.18604200
C	2.05536000	1.86403300	-1.16718900
C	2.14391300	-0.50410200	-2.01939000
C	1.28570200	0.26285000	3.06348700
C	2.31495100	-2.09657100	-0.10788700
C	2.24747100	1.79435000	1.34037200
C	2.38642200	-1.76706000	1.33323900
C	2.77820500	1.43571000	0.01590000
C	2.85379300	-0.93999300	-0.85388000
C	2.36737700	0.57607400	2.19301800
C	3.57209600	0.07682300	0.08727600
C	3.03415000	-0.46117700	1.46332300
Pr	0.62780200	-0.09925200	0.17119800
C	6.98770700	1.74754000	-0.62358100
C	5.61489700	1.51932700	-0.43202700
C	5.09964900	0.24574400	-0.08857800
C	6.04141300	-0.79064400	0.05405800
C	7.41740100	-0.60671700	-0.12674700
C	7.86477000	0.67251000	-0.46632000
H	7.36124100	2.73440700	-0.88904900
H	4.91546800	2.34742000	-0.55023000
H	8.11055700	-1.43499800	-0.00472500
Cl	5.52610800	-2.51297800	0.50660400
Cl	9.67577100	0.93798300	-0.71342600

16. 3a' (BLYP/3-21G~MWB48)

C	-5.48031300	0.62995200	-0.18775300
C	-5.33266800	-0.23229200	-1.28638400
C	-5.03029300	-1.64836500	-1.07507200
C	-4.99328300	2.00726400	-0.25880900
C	-5.18868300	0.12160700	1.16074700
C	-4.55416600	0.22395200	-2.44674000
C	-4.90786500	-2.16466400	0.22669200
C	-4.38350700	2.48709200	-1.42952400
C	-4.91578300	-1.23000200	1.36062200
C	-4.10055300	1.54037500	-2.51932100
C	-4.06577100	-2.05539200	-2.10691000
C	-4.40102600	2.33836400	1.04731000
C	-3.69408500	-0.86838900	-2.88024600
C	-4.42800700	1.13325900	1.88244300
C	-3.91392100	-3.19922500	0.52220200
C	-3.26114000	3.42507700	-1.35281800
C	-3.87366900	-1.63144300	2.30032300
C	-2.76404600	1.82313000	-3.02844500
C	-3.11797300	-3.04128100	-1.82469300
C	-3.33402100	3.23100900	1.12151500
C	-3.34101500	-2.91376700	1.83605000
C	-2.30508400	3.06451500	-2.39031900
C	-3.31905000	0.77700800	2.71137200
C	-2.33657500	-0.63211000	-3.26752500
C	-3.07138800	-3.68281200	-0.50260100
C	-2.78194400	3.84924600	-0.08803200
C	-3.03460300	-0.66320300	2.94286600
C	-1.85207500	0.77041700	-3.35266200
C	-1.76160200	-2.90060200	-2.32104400
C	-2.24486800	2.97034300	2.05602300
C	-1.36660600	-1.71441700	-3.01475300
C	-2.22715100	1.76645700	2.83552100
C	-1.67845600	-3.99420500	-0.21972900
C	-1.35593300	4.01959700	0.13126200
C	-2.01673800	-3.26878500	2.12019700
C	-0.93398800	3.27526400	-2.19044800
C	-0.86084600	-3.54472300	-1.34894100
C	-1.01966200	3.51204500	1.47545000
C	-1.66894900	-1.09023000	3.32449600
C	-0.40111900	1.06132100	-3.23087500
C	-1.17172300	-3.87055200	1.08743200
C	-0.44422100	3.81769500	-0.91573700

C	-1.19164800	-2.39166300	2.93089800
C	0.03073000	2.32174000	-2.67991100
C	0.02560800	-1.37861400	-2.95063400
C	-0.94070100	1.31557300	3.25999000
C	0.51215000	-0.03295400	-3.11117200
C	-0.66818300	-0.08542300	3.53966800
C	0.47465800	-3.09839000	-1.16153600
C	0.25208900	2.94833700	1.75979100
C	0.19392400	-3.42026200	1.30715000
C	0.86677300	3.24631000	-0.65846500
C	0.19009800	-2.57254900	2.49501100
C	1.18987600	2.37172100	-1.77706800
C	0.95377400	-2.10223400	-2.09397700
C	0.28342600	1.94230100	2.79661100
C	1.07002800	-3.09316600	0.20910900
C	1.26667300	2.84976700	0.67349300
C	1.79767600	0.07651800	-2.40028700
C	0.74098100	-0.32361200	3.28553200
C	1.19261700	-1.56162800	2.68080100
C	2.12799700	1.28573900	-1.64966600
C	2.08347500	-1.22921000	-1.80424600
C	1.33429800	0.94905900	2.85744200
C	2.22160400	-2.24607600	0.47584500
C	2.33723500	1.89332100	0.77468700
C	2.33082500	-1.53275600	1.77098900
C	2.84660000	1.16863700	-0.39422700
C	2.78838900	-1.35688600	-0.56150900
C	2.41353300	0.95713000	1.93457700
C	3.57058400	-0.16125900	0.05578500
C	3.02686300	-0.26861800	1.52502400
Pr	0.62278200	-0.17184500	0.17938600
C	6.98933600	-1.34263200	-1.30307300
C	5.61709900	-1.22255400	-1.02902100
C	5.09976500	-0.21757600	-0.17629100
C	6.03904300	0.66376400	0.39173500
C	7.41492700	0.57848700	0.14703100
C	7.86436400	-0.43321600	-0.70547200
H	7.36429000	-2.12185600	-1.96354000
H	4.91724000	-1.92361200	-1.48470000
H	8.10683900	1.27799600	0.60896400
Cl	5.52482400	2.03031000	1.53596800
Cl	9.67486900	-0.56369800	-1.04485400

17. **3b** (BLYP/3-21G~MWB48)

C	-5.40207900	0.80047700	-0.02544200
C	-5.24141600	0.35874600	-1.34903400
C	-4.96793400	-1.05218300	-1.62516000
C	-4.89094600	2.10784100	0.38563700
C	-5.15520100	-0.14236100	1.07515100
C	-4.42393800	1.16208000	-2.26917400
C	-4.88918800	-1.98258200	-0.57486700
C	-4.24138100	2.94125000	-0.53962900
C	-4.91069000	-1.48796600	0.80919900
C	-3.94547400	2.41302700	-1.88084200
C	-3.98354400	-1.10882600	-2.71549500
C	-4.32832600	1.96105300	1.73815700
C	-3.57125800	0.26131600	-3.03228800
C	-4.39791000	0.54450700	2.11298700
C	-3.92172600	-3.08072800	-0.62993600
C	-3.10678100	3.76965500	-0.12690900
C	-3.90164900	-2.21040500	1.57653800
C	-2.59175000	2.81691100	-2.23731000
C	-3.06187000	-2.15554200	-2.76869800
C	-3.24854700	2.74764600	2.13199400
C	-3.37939300	-3.27296100	0.71359700
C	-2.12897000	3.75700300	-1.20552000
C	-3.31775700	-0.09963200	2.79283200
C	-2.20023800	0.58082200	-3.29100200
C	-3.06097500	-3.20854500	-1.74203500
C	-2.65388600	3.72690300	1.21629000
C	-3.06292700	-1.53877700	2.52492300
C	-1.68973000	1.91602800	-2.88471300
C	-1.68941500	-1.88791900	-3.16098000
C	-2.19023900	2.15883500	2.94486200
C	-1.25538700	-0.54700700	-3.40314100
C	-2.21315200	0.76153000	3.26837600
C	-1.68132800	-3.63039400	-1.55577700
C	-1.23309400	3.77879500	1.50990200
C	-2.06919900	-3.73428200	0.88409500
C	-0.76151300	3.85228400	-0.91877800
C	-0.82685100	-2.84453100	-2.44989600
C	-0.94121000	2.83420400	2.60590100
C	-1.71578500	-2.10485900	2.76538300
C	-0.23791900	2.11121600	-2.64426200
C	-1.20732200	-3.97050100	-0.27565100
C	-0.29581300	3.91968200	0.47398400
C	-1.25139500	-3.20658700	1.96096000

C	0.19949000	3.09775800	-1.68526800
C	0.14087200	-0.28868400	-3.20584700
C	-0.94631300	0.16093400	3.53869600
C	0.65314100	1.02042000	-2.88783000
C	-0.70428000	-1.25756700	3.32899900
C	0.51129200	-2.52111700	-2.09716000
C	0.31346500	2.17643300	2.70670000
C	0.15873800	-3.65407200	0.10980700
C	0.99773900	3.26508100	0.54773800
C	0.13703600	-3.26000900	1.51415500
C	1.32989700	2.80766000	-0.79732400
C	1.03375300	-1.28263800	-2.62717900
C	0.30102800	0.87683900	3.33907300
C	1.06746200	-2.99413500	-0.79517700
C	1.35503800	2.42801500	1.67234000
C	1.91969500	0.84923300	-2.15651600
C	0.70729500	-1.43012600	3.03830900
C	1.15134800	-2.39789700	2.05272100
C	2.24162600	1.71855700	-1.03027900
C	2.17233400	-0.58939600	-2.03533300
C	1.33449600	-0.10360800	3.08207300
C	2.22215000	-2.31454700	-0.23448700
C	2.41100000	1.46985800	1.46721900
C	2.30645000	-2.08617600	1.22543000
C	2.92538700	1.16348800	0.12347400
C	2.84275500	-1.15011800	-0.90012200
C	2.44228600	0.19214500	2.23869800
C	3.62190000	-0.24901100	0.10688200
C	3.04094800	-0.83842200	1.44280800
Pr	0.67594300	-0.22503100	0.17917500
C	7.12954100	1.18889200	-0.50987400
C	5.75029700	1.08041800	-0.33428600
C	5.15967700	-0.17726800	-0.06172000
C	6.03203700	-1.27894600	0.02042100
C	7.41634200	-1.16842500	-0.15508900
C	7.98532100	0.08828600	-0.42780600
H	5.11802600	1.96383600	-0.40453900
H	8.04328500	-2.05512200	-0.07911700
Cl	5.40094000	-2.98435300	0.37820500
H	9.05830100	0.19933600	-0.57068000
Cl	7.84629300	2.85648900	-0.86689900

18. **3b'** (BLYP/3-21G~MWB48)

C	5.44642700	-0.30856700	-0.36065400
C	5.21507500	0.70777300	-1.30239000
C	4.83360500	2.04921700	-0.85883400
C	5.04127100	-1.68522500	-0.64533700
C	5.16309900	-0.04340700	1.05775100
C	4.43206400	0.39444800	-2.50570200
C	4.71726600	2.34003800	0.51146000
C	4.42778100	-2.00897400	-1.86682100
C	4.81352900	1.23801200	1.47855000
C	4.05745100	-0.91945500	-2.78355500
C	3.81839600	2.55517300	-1.79416000
C	4.50732500	-2.25917500	0.60050700
C	3.49666800	1.48531900	-2.74235200
C	4.48544300	-1.20442900	1.61989200
C	3.67185500	3.24785600	0.98899000
C	3.36668100	-3.01718400	-1.92282500
C	3.77639800	1.41585200	2.48992500
C	2.72646700	-1.20203300	-3.30808100
C	2.82121300	3.41993200	-1.33821000
C	3.49856200	-3.21825000	0.54871800
C	3.15495900	2.72021100	2.24988600
C	2.36110000	-2.55648000	-2.87006000
C	3.38102600	-1.05755200	2.51560300
C	2.14551500	1.22753400	-3.13772200
C	2.77328900	3.83540100	0.07185200
C	2.94990400	-3.66841400	-0.73466200
C	3.01552300	0.30560500	2.98121000
C	1.74394100	-0.17138200	-3.44128900
C	1.46234400	3.27412700	-1.82629400
C	2.42289300	-3.18179400	1.53318100
C	1.11967100	2.19183400	-2.69617800
C	2.35507400	-2.12264400	2.49819100
C	1.37287200	4.00713900	0.42590200
C	1.54421200	-3.96472400	-0.51966600
C	1.82022000	2.93937200	2.61108200
C	1.01187800	-2.88341100	-2.68114400
C	0.55228400	3.69549400	-0.74642700
C	1.21649200	-3.70050500	0.89503300
C	1.63863900	0.57825100	3.45185100
C	0.31735400	-0.56979900	-3.34009900
C	0.91160100	3.64308300	1.70484200
C	0.59201100	-3.65523400	-1.50287400

C	1.07310300	1.89321300	3.28573600
C	-0.02224000	-1.92743800	-2.99187100
C	-0.24767300	1.76275600	-2.66269000
C	1.05578800	-1.82694300	3.01112800
C	-0.65572400	0.43029400	-3.02691000
C	0.70655100	-0.50957500	3.51847600
C	-0.74737000	3.13810000	-0.60896200
C	-0.07811000	-3.27111700	1.28921000
C	-0.41794100	3.07813800	1.87474600
C	-0.74275800	-3.21791200	-1.13241600
C	-0.32920700	2.05309500	2.91084800
C	-1.14879200	-2.19569100	-2.08716600
C	-1.19209000	2.27745100	-1.68136300
C	-0.14053900	-2.44758200	2.47470500
C	-1.30094700	2.87274300	0.75380400
C	-1.12827600	-3.06666500	0.25295600
C	-1.90920700	0.12523800	-2.31784100
C	-0.72118500	-0.32533700	3.33529900
C	-1.26480700	0.96373400	2.95109900
C	-2.14576300	-1.20651700	-1.76805600
C	-2.25639900	1.29691300	-1.51438900
C	-1.24849700	-1.54921800	2.71801400
C	-2.39118700	1.92252800	0.90128100
C	-2.25226500	-2.21056800	0.52822300
C	-2.42421300	1.00765200	2.06728900
C	-2.83732900	-1.34021900	-0.49889300
C	-2.93124200	1.17783700	-0.25555000
C	-2.35172900	-1.47940100	1.82557100
C	-3.62355500	-0.14808900	0.17321300
C	-3.04754800	-0.24433300	1.63048500
Pr	-0.68281300	0.02168100	0.25815400
C	-7.13372400	1.00448300	-0.86421800
C	-5.75455500	0.95871000	-0.66372200
C	-5.16157200	-0.15078500	-0.01426300
C	-6.03118700	-1.17486200	0.40624700
C	-7.41558400	-1.12710800	0.20519300
C	-7.98702700	-0.01830200	-0.44416300
H	-5.12106500	1.77603300	-1.00448000
H	-8.04104700	-1.94695300	0.55394900
Cl	-5.40089300	-2.68489000	1.27975600
Cl	-7.85434600	2.47672800	-1.72140800
H	-9.06031900	0.04095400	-0.61327500

19. 3c (BLYP/3-21G~MWB48)

C	5.60198900	-0.26639900	-0.02335100
C	5.40055300	0.28565000	-1.29878000
C	4.96977500	1.67739100	-1.43919000
C	5.24277300	-1.65865800	0.24594200
C	5.24063100	0.52597600	1.16098500
C	4.68770000	-0.50790200	-2.30957700
C	4.77477700	2.48026800	-0.30211500
C	4.70038600	-2.46251200	-0.77027200
C	4.84487100	1.85521400	1.02599400
C	4.35459700	-1.83824700	-2.05733700
C	3.99278400	1.73160000	-2.53687600
C	4.65636000	-1.71413900	1.59496300
C	3.74267100	0.36234500	-2.99483200
C	4.55918800	-0.34432100	2.11026800
C	3.68664500	3.45967500	-0.26545500
C	3.66579600	-3.45217500	-0.46338600
C	3.75234300	2.37584100	1.84204200
C	3.05960400	-2.35674700	-2.47754300
C	2.95584500	2.66604400	-2.50174300
C	3.67258800	-2.65504200	1.88827900
C	3.11659800	3.45286700	1.07987600
C	2.70124200	-3.44268000	-1.55352900
C	3.40712300	0.10002000	2.83042700
C	2.41983300	-0.08368000	-3.30980600
C	2.82520800	3.60104900	-1.37445100
C	3.20119600	-3.59768700	0.86844100
C	2.99047800	1.52059600	2.70337300
C	2.06419300	-1.50313600	-3.04870000
C	1.62651500	2.28433400	-2.94308900
C	2.54683800	-2.27568300	2.73445400
C	1.35216900	0.93470200	-3.32683800
C	2.40634600	-0.92515700	3.19654500
C	1.40507700	3.84417400	-1.17382000
C	1.79371500	-3.84061000	1.12780600
C	1.76057000	3.74283000	1.27148200
C	1.35160400	-3.72333100	-1.30482400
C	0.65340800	3.06084400	-2.15706000
C	1.38699300	-3.05268100	2.30784000
C	1.58520600	1.90087100	2.97167700
C	0.64343100	-1.88556000	-2.85483800
C	0.88568300	3.99376300	0.12551400
C	0.88697000	-3.98237400	0.06578600

C	1.00174100	3.01896800	2.27531200
C	0.31585900	-3.00841000	-2.00917900
C	-0.00602500	0.49993800	-3.18051900
C	1.07663700	-0.50372800	3.50108000
C	-0.36598800	-0.88382000	-3.00306800
C	0.67426600	0.89152400	3.42914700
C	-0.64083000	2.55288300	-1.86268200
C	0.06442700	-2.55578600	2.44979100
C	-0.43845200	3.48883500	0.45246700
C	-0.47380900	-3.48996600	0.18031300
C	-0.38104600	2.96009000	1.81190100
C	-0.84723900	-2.94003800	-1.11723200
C	-1.01284100	1.32319600	-2.52601800
C	-0.07731300	-1.33416300	3.20846700
C	-1.25915200	2.82543400	-0.53101300
C	-0.93464800	-2.81950000	1.37713300
C	-1.64853400	-0.93342400	-2.28243600
C	-0.74536800	0.93006500	3.13078800
C	-1.29176700	1.93643900	2.24148600
C	-1.87944100	-1.94655800	-1.25736200
C	-2.06772900	0.44740600	-2.02795400
C	-1.21542700	-0.45831100	3.03296100
C	-2.33384900	1.96476200	-0.06378900
C	-2.09218100	-1.97249400	1.24802000
C	-2.40077600	1.58175600	1.36727900
C	-2.63412900	-1.59716400	-0.06758000
C	-2.80466900	0.80711900	-0.85398600
C	-2.27404200	-0.79155500	2.14359500
C	-3.47713400	-0.27491500	0.04503600
C	-2.97684500	0.23885000	1.44096600
Pr	-0.55469500	0.03176300	0.15950500
C	-6.96674500	-1.77086300	-0.67445600
C	-5.57377800	-1.65235200	-0.52257500
C	-4.99837200	-0.42975300	-0.12341400
C	-5.83693700	0.67955600	0.12201200
C	-7.22045100	0.55364300	-0.02965000
C	-7.78558200	-0.66364600	-0.42506400
H	-4.93434700	-2.51413600	-0.71467600
Cl	-9.59944700	-0.85108500	-0.63083700
Cl	-8.26906900	2.02436700	0.30582200
H	-7.41852200	-2.71163100	-0.98466400
H	-5.42000100	1.63786500	0.42943800

20. 3c' (BLYP/3-21G~MWB48)

C	-5.40064000	0.94886600	0.08440700
C	-5.37929800	0.09553600	-1.03080900
C	-5.16474800	-1.34133000	-0.85394300
C	-4.82316400	2.28988500	0.00043000
C	-5.06802900	0.40071600	1.40758200
C	-4.63984500	0.51472400	-2.23036100
C	-5.00223000	-1.88435800	0.43246900
C	-4.25129800	2.74510000	-1.19897600
C	-4.87888300	-0.96937000	1.57542300
C	-4.09961200	1.79753000	-2.31445300
C	-4.29330400	-1.79847000	-1.94610100
C	-4.13394000	2.55833600	1.27255500
C	-3.88532000	-0.62802300	-2.72723000
C	-4.19695900	1.34567100	2.09433400
C	-4.06824200	-2.99010900	0.65715600
C	-3.06283200	3.60128800	-1.17796500
C	-3.81465800	-1.45665800	2.44739700
C	-2.77806100	1.99485000	-2.89805100
C	-3.40179200	-2.85201400	-1.73116800
C	-3.00487500	3.37352200	1.29390600
C	-3.40149800	-2.76609000	1.93827400
C	-2.19663600	3.19147400	-2.27459200
C	-3.06962300	0.90055100	2.85200500
C	-2.53866400	-0.47981900	-3.19019500
C	-3.32278200	-3.51501300	-0.42098100
C	-2.48205400	3.97067200	0.06112000
C	-2.87337100	-0.55924700	3.04876000
C	-1.96238400	0.88664000	-3.28811600
C	-2.07005000	-2.79692200	-2.30421900
C	-1.88439800	3.02424700	2.15977900
C	-1.63405400	-1.63060600	-3.00641900
C	-1.90577700	1.81017200	2.92324100
C	-1.94138600	-3.92704000	-0.22508100
C	-1.03758100	4.03949500	0.19787800
C	-2.09134400	-3.21712100	2.13969300
C	-0.80486200	3.30240600	-2.15305100
C	-1.16148400	-3.51863100	-1.39555300
C	-0.66002100	3.48934800	1.51426400
C	-1.52186300	-1.08611000	3.34466600
C	-0.48999700	1.07403100	-3.24892800
C	-1.35201400	-3.85983400	1.05164200
C	-0.20501700	3.79004900	-0.90330100

C	-1.16081700	-2.41181800	2.91011000
C	0.06085900	2.29255400	-2.71000000
C	-0.22042900	-1.39403600	-3.02121100
C	-0.63163300	1.26379500	3.26399100
C	0.34938400	-0.08295900	-3.19411900
C	-0.44218300	-0.15699900	3.50989200
C	0.21071100	-3.16841500	-1.28192700
C	0.58326100	2.83391400	1.71556400
C	0.05231400	-3.50835800	1.19540100
C	1.07553100	3.12555500	-0.73105300
C	0.17725100	-2.68076200	2.39116900
C	1.27105300	2.24824600	-1.87661000
C	0.70311800	-2.19343400	-2.22944800
C	0.60359100	1.81071500	2.73578100
C	0.88371900	-3.22569000	0.05154600
C	1.52262200	2.68077000	0.56972800
C	1.67744000	-0.07362800	-2.55827700
C	0.92993900	-0.48811600	3.17369500
C	1.25889200	-1.74610200	2.53084900
C	2.13589600	1.09777500	-1.81659000
C	1.90606500	-1.40476200	-1.99619500
C	1.58573300	0.74778200	2.72700300
C	2.10585100	-2.46506900	0.25942200
C	2.52689600	1.65081000	0.59739500
C	2.34231300	-1.78268900	1.55530500
C	2.91568400	0.91054900	-0.60700000
C	2.67061100	-1.60042900	-0.79893200
C	2.60548600	0.69437100	1.74055400
C	3.57036500	-0.47192400	-0.21528000
C	3.10720200	-0.56448100	1.28118600
Pr	0.64194700	-0.28398500	0.09120100
C	6.79952700	-1.86658100	-1.80188800
C	5.45789300	-1.65411100	-1.44745200
C	5.07934500	-0.63547000	-0.54323700
C	6.10694000	0.16721700	-0.00357400
C	7.44458000	-0.04727300	-0.35607400
C	7.80696400	-1.05793600	-1.25370000
H	4.67611500	-2.28426700	-1.87079400
Cl	5.72458800	1.52007500	1.18545400
H	8.85540500	-1.19959100	-1.50949600
Cl	8.79471700	0.98756500	0.34639800
H	7.06107900	-2.65900600	-2.50317900

21. 4a (BLYP/3-21G~MWB48)

C	-4.54905400	2.63238600	0.72043600
C	-5.03883600	1.90788000	-0.37874500
C	-5.42395000	0.50393000	-0.22614000
C	-3.48269900	3.61531200	0.53493000
C	-4.28843200	1.91990600	1.98099800
C	-4.37688800	2.05266900	-1.68229700
C	-5.32109300	-0.12807900	1.02655400
C	-2.95204800	3.85580500	-0.74508100
C	-4.67088000	0.58840900	2.13201500
C	-3.36974400	2.99474300	-1.86128700
C	-4.99091400	-0.21186300	-1.43205700
C	-2.57004700	3.50318300	1.68363300
C	-4.24474500	0.72371100	-2.27614600
C	-3.01432200	2.37830400	2.51586800
C	-4.92037300	-1.53313000	1.11402200
C	-1.52431000	4.12730700	-0.91488700
C	-3.78979000	-0.34378500	2.83058800
C	-2.18913300	2.66804300	-2.66005600
C	-4.60642700	-1.55346000	-1.35006500
C	-1.21296800	3.76898100	1.52158800
C	-4.04368300	-1.67892000	2.27393400
C	-1.07929700	3.46057100	-2.14049900
C	-2.07715700	1.46348500	3.09107500
C	-3.04269800	0.32558700	-2.93703600
C	-4.62638500	-2.26001100	-0.06036500
C	-0.67545000	4.15229000	0.21167900
C	-2.48560700	0.04450900	3.26535600
C	-1.97099400	1.33794900	-3.15324600
C	-3.47975900	-2.02986300	-2.12433500
C	-0.23092500	2.93043800	2.20163200
C	-2.69245000	-1.10983400	-2.88513400
C	-0.64383000	1.80039800	2.97700000
C	-3.53883400	-3.22587200	-0.07691400
C	0.66320400	3.58238500	0.12224900
C	-3.02977100	-2.63784100	2.27028600
C	0.23523400	2.97721200	-2.24032100
C	-2.83983200	-3.12367600	-1.36131600
C	0.95543800	2.85900500	1.35761200
C	-1.44614600	-1.01101900	3.34862400
C	-0.57276900	0.89953600	-3.34825000
C	-2.79691300	-3.47728300	1.09335800
C	1.13263800	3.06515900	-1.08941500

C	-1.74590200	-2.34228200	2.88308600
C	0.51353200	1.73446100	-2.92592600
C	-1.33119400	-1.48436300	-3.11787200
C	0.33095200	0.76140300	3.12674500
C	-0.29493800	-0.51633700	-3.36708600
C	-0.06710100	-0.62497200	3.34166500
C	-1.45453900	-3.39398200	-1.46622800
C	1.82792900	1.72815000	1.36652300
C	-1.37655500	-3.76515900	1.02033500
C	2.01244500	1.90074100	-1.10427800
C	-0.73998700	-3.12515400	2.18283400
C	1.72569700	1.14675800	-2.31537100
C	-0.73326100	-2.65888600	-2.49590500
C	1.60314100	0.77689500	2.43723100
C	-0.69111000	-3.79055200	-0.24207800
C	2.44263500	1.26943600	0.11153900
C	0.98565700	-1.09500000	-2.96037800
C	0.97085300	-1.47433100	2.79562500
C	0.63220200	-2.72097700	2.14795200
C	2.03913300	-0.26006600	-2.35302800
C	0.69525100	-2.45656700	-2.46623800
C	2.03884800	-0.59885300	2.26371600
C	0.74252900	-3.58986100	-0.22166900
C	3.33745700	-0.00323100	0.01960400
C	1.41898200	-3.12005200	0.99842900
C	2.85523000	-0.82630400	-1.28940400
C	1.46860600	-2.98840700	-1.37241300
C	2.81882200	-1.00598300	1.15585100
C	2.57202700	-2.20895100	-0.87164400
C	2.55123300	-2.29732700	0.59119200
Pr	0.46379100	-0.82182200	-0.28912400
C	6.55737500	2.09165700	0.54207300
C	5.22152600	1.67665300	0.42388200
C	4.85822400	0.34106100	0.11655500
C	5.92630800	-0.56094000	-0.06799600
C	7.27222700	-0.18623100	0.03880300
C	7.56292700	1.14437900	0.34476800
H	4.42891600	2.40827900	0.57127600
H	8.06297600	-0.91619900	-0.11381200
Cl	5.66831300	-2.35284600	-0.47484900
Cl	9.33128200	1.65420100	0.48768200
H	6.80424500	3.12471500	0.77826200

22. 4a' (BLYP/3-21G~MWB48)

C	-4.43694300	2.73503900	0.69567500
C	-4.95523800	2.03012200	-0.40342000
C	-5.39080600	0.64036900	-0.25195900
C	-3.33550600	3.67874100	0.50946100
C	-4.19957200	2.01122400	1.95415200
C	-4.29142700	2.15269200	-1.70806700
C	-5.30869800	0.00284600	0.99944700
C	-2.79883400	3.90234200	-0.77107500
C	-4.62983700	0.69389600	2.10429200
C	-3.24969100	3.05741800	-1.88700900
C	-4.98728600	-0.08912100	-1.45993700
C	-2.42433200	3.53173700	1.65470600
C	-4.20863400	0.82046600	-2.30366900
C	-2.90798300	2.42193700	2.48626700
C	-4.95944300	-1.41597400	1.08328700
C	-1.36270900	4.12358600	-0.94321400
C	-3.78148600	-0.27074900	2.79876600
C	-2.08371200	2.68920600	-2.68795200
C	-4.65269400	-1.44431200	-1.38148300
C	-1.05886900	3.74891500	1.48921700
C	-4.08520700	-1.59589400	2.24046200
C	-0.94396300	3.44030400	-2.16920800
C	-2.00380300	1.47280500	3.05618800
C	-3.02359600	0.37965700	-2.96692600
C	-4.69570200	-2.15190000	-0.09268800
C	-0.50990200	4.11695500	0.17971200
C	-2.46348900	0.06868700	3.23012600
C	-1.91575400	1.35266000	-3.18230300
C	-3.54613600	-1.96080100	-2.15901400
C	-0.10561100	2.87375100	2.16323000
C	-2.72681200	-1.06847500	-2.91871700
C	-0.56019000	1.75737400	2.93443200
C	-3.64455300	-3.15741400	-0.11376500
C	0.81133200	3.50516200	0.08721200
C	-3.10752200	-2.59139600	2.23194400
C	0.35132500	2.91012700	-2.26952100
C	-2.94474800	-3.07855200	-1.39885800
C	1.07928600	2.76726000	1.31885600
C	-1.46332200	-1.02515500	3.30851300
C	-0.53575300	0.86365300	-3.37876000
C	-2.90903100	-3.43828700	1.05405600
C	1.26226200	2.97257300	-1.12563400

C	-1.81161300	-2.34500300	2.84201000
C	0.58087800	1.65724900	-2.95350100
C	-1.38235600	-1.49313800	-3.15667000
C	0.37338900	0.68199700	3.07284600
C	-0.31282400	-0.56138100	-3.40344000
C	-0.07285300	-0.68982800	3.29515700
C	-1.56974900	-3.39981500	-1.50678300
C	1.91598600	1.60882800	1.32112700
C	-1.50075800	-3.77933600	0.97715600
C	2.10811100	1.78165600	-1.14437900
C	-0.83760400	-3.16428000	2.13924500
C	1.77447600	1.02981900	-2.35123800
C	-0.82511800	-2.68932100	-2.53678600
C	1.63565300	0.65138000	2.37370500
C	-0.81851300	-3.82827100	-0.28589700
C	2.53205500	1.14368500	0.06948700
C	0.94291600	-1.18409500	-2.99529900
C	0.93093100	-1.57579800	2.74396300
C	0.54976700	-2.81279400	2.10144900
C	2.01895800	-0.38748600	-2.38611400
C	0.60884900	-2.53715500	-2.50626000
C	2.02173800	-0.73818700	2.20227100
C	0.62448900	-3.68156600	-0.26778100
C	3.34471000	-0.18882300	-0.03201800
C	1.32447600	-3.24209600	0.95261900
C	2.81176700	-0.98672600	-1.32639300
C	1.36591800	-3.10271600	-1.41731200
C	2.80281500	-1.17331700	1.10854500
C	2.50757800	-2.37224300	-0.91977800
C	2.49385200	-2.46356900	0.54445000
Pr	0.45122500	-0.91755500	-0.29228000
C	6.94708700	-0.07665500	-1.44342600
C	5.56191500	-0.25360600	-1.29633100
C	4.88773800	0.01333400	-0.07969300
C	5.68372500	0.47193900	0.98639300
C	7.06812300	0.65854300	0.88362200
C	7.67554700	0.37826000	-0.34232700
H	7.44279900	-0.28767800	-2.38885000
H	4.97404000	-0.61323200	-2.14165100
H	7.64620000	1.00992500	1.73429900
Cl	4.95753500	0.86889100	2.64372200
Cl	9.49951200	0.62104900	-0.50112700

23. 4b (BLYP/3-21G~MWB48)

C	-4.33613600	2.80645800	0.72956400
C	-4.85924000	2.12537900	-0.38210700
C	-5.32285100	0.74293500	-0.25083000
C	-3.21506600	3.73019700	0.56366700
C	-4.12389700	2.06402300	1.98162700
C	-4.18219100	2.25028400	-1.68009600
C	-5.26352400	0.08965500	0.99352200
C	-2.66394400	3.95782600	-0.70975200
C	-4.58106600	0.75400900	2.11196500
C	-3.12223400	3.13658800	-1.83984100
C	-4.92213800	0.02022300	-1.46408700
C	-2.31742000	3.55186300	1.71583800
C	-4.11954900	0.92403400	-2.29081600
C	-2.82925700	2.44268900	2.53001000
C	-4.94242300	-1.33663800	1.06357900
C	-1.22229400	4.15165400	-0.86762700
C	-3.75782000	-0.23506500	2.80245900
C	-1.95673200	2.75526500	-2.63645800
C	-4.61437000	-1.34163800	-1.39891000
C	-0.94690500	3.74408200	1.56533700
C	-4.08242800	-1.54639600	2.22609900
C	-0.80765700	3.47744400	-2.09959300
C	-1.94853500	1.46952600	3.09770900
C	-2.93720300	0.46848100	-2.94977200
C	-4.68221300	-2.06315500	-0.11911300
C	-0.38066700	4.11438700	0.26399200
C	-2.43717000	0.07340500	3.25066500
C	-1.80973400	1.42205100	-3.14667300
C	-3.51031600	-1.86960000	-2.17306300
C	-0.01700900	2.84319600	2.23953000
C	-2.66772300	-0.98472100	-2.91615200
C	-0.49807000	1.72732900	2.99613700
C	-3.64998900	-3.08782400	-0.14322300
C	0.92434100	3.47178700	0.17425200
C	-3.12356000	-2.56000200	2.21448300
C	0.47800300	2.92273100	-2.19889400
C	-2.93794000	-3.00735500	-1.42205800
C	1.16925200	2.71745000	1.40176700
C	-1.45862000	-1.03941900	3.32554100
C	-0.43688300	0.90844700	-3.34078400
C	-2.93025900	-3.39513100	1.02743500
C	1.37090000	2.94465900	-1.04132800

C	-1.82936700	-2.34530800	2.83906600
C	0.69143500	1.67618600	-2.90066500
C	-1.32906200	-1.43260500	-3.14915100
C	0.41584200	0.63394800	3.13679600
C	-0.23857600	-0.52017700	-3.37836800
C	-0.05996000	-0.73072800	3.33177600
C	-1.56880200	-3.35279400	-1.52286100
C	1.97977700	1.54097200	1.40116100
C	-1.52813400	-3.76064000	0.95806400
C	2.18206100	1.73208900	-1.06662600
C	-0.86462300	-3.17286400	2.13305300
C	1.86395200	1.01325000	-2.29004200
C	-0.80170300	-2.64675600	-2.53947100
C	1.69155600	0.58770900	2.45498000
C	-0.83712500	-3.80854000	-0.30080400
C	2.57408200	1.06444300	0.14267900
C	1.00403800	-1.17424900	-2.96928700
C	0.93206100	-1.62956500	2.77865600
C	0.52799600	-2.84626800	2.11149100
C	2.09700700	-0.40825500	-2.34388200
C	0.63516500	-2.52367900	-2.49658800
C	2.05083300	-0.80742200	2.26477900
C	0.60538000	-3.68877100	-0.26957600
C	3.39569700	-0.25503900	0.03693900
C	1.29951600	-3.27424500	0.96153100
C	2.87673600	-1.03410400	-1.28612200
C	1.37020000	-3.11253800	-1.40699900
C	2.81622300	-1.24308600	1.15723800
C	2.51461800	-2.40463200	-0.88936800
C	2.47643100	-2.50867900	0.57184700
Pr	0.48844800	-0.91371000	-0.27879200
C	6.73461500	1.64873400	0.29403600
C	5.37557400	1.34408700	0.23667700
C	4.93689700	0.00186500	0.11132600
C	5.94885400	-0.97942300	0.05139600
C	7.31360300	-0.66929700	0.11296900
C	7.72577100	0.66798300	0.23580500
H	4.64113300	2.14392600	0.28659200
H	8.04822700	-1.47101700	0.06280900
Cl	5.58022600	-2.78799000	-0.12682700
Cl	7.23595900	3.42153100	0.45142300
H	8.78085800	0.92947700	0.28247300

24. **4b'** (BLYP/3-21G~MWB48)

C	-4.50470000	2.62244900	0.49329100
C	-4.91971600	1.92934900	-0.65576400
C	-5.32667800	0.52562900	-0.56590700
C	-3.41957500	3.59930600	0.41004800
C	-4.34256400	1.87731200	1.75090100
C	-4.16426500	2.09849000	-1.90408700
C	-5.32008800	-0.13749300	0.67424600
C	-2.79488000	3.86483700	-0.82149700
C	-4.74520700	0.54585500	1.84067900
C	-3.13741500	3.03377700	-1.98514100
C	-4.81429100	-0.16542700	-1.75506500
C	-2.59266900	3.45001500	1.61722400
C	-4.00118700	0.78285400	-2.51970000
C	-3.10673200	2.30979900	2.38746800
C	-4.93919000	-1.54816700	0.75479700
C	-1.35655600	4.12811700	-0.88068300
C	-3.92536900	-0.41144700	2.57751500
C	-1.90539700	2.71414800	-2.70306800
C	-4.44937600	-1.51276700	-1.67969200
C	-1.22523100	3.70647700	1.55964600
C	-4.14886000	-1.73066900	1.97025600
C	-0.82873200	3.48317000	-2.08499700
C	-2.22148300	1.37222400	3.00465000
C	-2.75820500	0.38785500	-3.10130600
C	-4.56871800	-2.25025900	-0.41271600
C	-0.59030500	4.11818100	0.30308900
C	-2.65332500	-0.04710400	3.11457300
C	-1.66447700	1.39401300	-3.21058100
C	-3.27438800	-1.98276500	-2.38194300
C	-0.30042100	2.84293600	2.28639900
C	-2.42610700	-1.05330900	-3.06187700
C	-0.78077800	1.69777900	2.99841500
C	-3.49155300	-3.22732200	-0.37511600
C	0.75148000	3.54487500	0.29819200
C	-3.14663600	-2.70008700	2.01524600
C	0.48470600	2.98993800	-2.09893600
C	-2.70008400	-3.10034800	-1.60171400
C	0.94767500	2.78744600	1.53244500
C	-1.63180300	-1.11579900	3.24488200
C	-0.26098400	0.94576100	-3.31151000
C	-2.83796000	-3.51507800	0.83877700
C	1.30446300	3.04928000	-0.88786400

C	-1.90741600	-2.43347300	2.72590400
C	0.79898700	1.75865100	-2.78947500
C	-1.05572400	-1.43656000	-3.20404100
C	0.16882300	0.64354800	3.18216100
C	0.00275600	-0.47159100	-3.34830600
C	-0.25425000	-0.74384900	3.34268200
C	-1.31288100	-3.38423500	-1.61362200
C	1.81494400	1.65209600	1.57468000
C	-1.41902600	-3.81794200	0.86110700
C	2.18121900	1.88160200	-0.86733300
C	-0.86163400	-3.21160600	2.08203200
C	1.96000600	1.14884500	-2.11123800
C	-0.51315500	-2.63167900	-2.56963200
C	1.48135300	0.66220500	2.58179700
C	-0.64339400	-3.81822800	-0.34800800
C	2.53128000	1.22873800	0.36132600
C	1.24139600	-1.07088000	-2.86127100
C	0.81179600	-1.59021800	2.84907200
C	0.51414900	-2.82272700	2.15569400
C	2.24586700	-0.26024200	-2.15586000
C	0.91026900	-2.44322700	-2.42864100
C	1.91544500	-0.71278900	2.40770400
C	0.78938900	-3.63615800	-0.21862200
C	3.38614300	-0.07933100	0.29374000
C	1.38410200	-3.20645900	1.06043600
C	2.97475200	-0.86110900	-1.05187000
C	1.59812300	-3.01135100	-1.29637100
C	2.79095000	-1.10366400	1.36947600
C	2.67890200	-2.26372500	-0.69924100
C	2.55890900	-2.38893700	0.75735900
Pr	0.54158000	-0.88036900	-0.19225600
C	7.03427400	0.33111100	-0.84355400
C	5.66518500	0.06823900	-0.83394700
C	4.92001900	0.18758300	0.36419000
C	5.63134000	0.58327100	1.51255100
C	7.00817500	0.84002900	1.50204200
C	7.73201400	0.71505000	0.30412500
H	5.15730500	-0.23423400	-1.74830800
H	7.50819900	1.13619000	2.42253500
Cl	4.79178700	0.80640600	3.14721300
Cl	7.95684400	0.16409600	-2.43697900
H	8.80155500	0.91235800	0.27116000

25. 4c (BLYP/3-21G~MWB48)

C	-4.58198100	2.69564900	0.60213400
C	-5.02520100	2.01668900	-0.54528900
C	-5.45460000	0.61945800	-0.45796000
C	-3.48171700	3.65365800	0.50911900
C	-4.41422400	1.93971500	1.85279900
C	-4.28504300	2.18063800	-1.80322200
C	-5.44112500	-0.05093700	0.77846900
C	-2.87001400	3.91538200	-0.72988400
C	-4.83868500	0.61533900	1.94050000
C	-3.24311900	3.09766200	-1.89332000
C	-4.97098800	-0.07286700	-1.65804200
C	-2.64048700	3.48290100	1.70411600
C	-4.15303800	0.86523200	-2.42850300
C	-3.16196500	2.34713300	2.47441600
C	-5.08305900	-1.46846400	0.84573300
C	-1.42818100	4.15280500	-0.80795700
C	-4.02406100	-0.36062100	2.66008400
C	-2.02697200	2.76237800	-2.63267500
C	-4.62792900	-1.42755700	-1.59551400
C	-1.26988600	3.71671400	1.62913600
C	-4.27888600	-1.67142200	2.04909500
C	-0.92953600	3.50665600	-2.02500300
C	-2.28331100	1.39060800	3.07261300
C	-2.92509100	0.45266700	-3.03013400
C	-4.74107300	-2.16970400	-0.33086700
C	-0.64636800	4.12191000	0.36482400
C	-2.73814100	-0.02147900	3.18046800
C	-1.81566000	1.44036400	-3.15167300
C	-3.47160600	-1.91256000	-2.31658100
C	-0.34971400	2.83371300	2.33863600
C	-2.61688100	-0.99330600	-3.00071000
C	-0.83753300	1.69182200	3.05004100
C	-3.68055400	-3.16591600	-0.31377600
C	0.68430500	3.52387000	0.33773800
C	-3.29293500	-2.65826500	2.07500500
C	0.37592200	2.99104000	-2.06114200
C	-2.90485700	-3.04655300	-1.55087900
C	0.88668800	2.76100000	1.56641200
C	-1.73330200	-1.10767100	3.29146300
C	-0.42212100	0.96924800	-3.27769700
C	-3.01452500	-3.47040200	0.88907900
C	1.20947600	3.02657700	-0.86075100

C	-2.03946500	-2.41646900	2.76881200
C	0.65904700	1.75849100	-2.76431900
C	-1.25372500	-1.39903100	-3.16257800
C	0.09901100	0.62106100	3.22064900
C	-0.18038800	-0.45457700	-3.32320900
C	-0.34706700	-0.76080900	3.37554700
C	-1.52452700	-3.35490600	-1.58402000
C	1.73087200	1.60764000	1.59027500
C	-1.60065500	-3.79650900	0.88920200
C	2.06091100	1.84068300	-0.85774100
C	-1.01572300	-3.20781900	2.10582400
C	1.81844100	1.12068800	-2.10749400
C	-0.72246300	-2.60830700	-2.54593800
C	1.40536300	0.62165200	2.60624900
C	-0.84399600	-3.80907900	-0.33124600
C	2.40547000	1.17413800	0.35912000
C	1.06161000	-1.08289300	-2.87253200
C	0.69661100	-1.62435200	2.86673000
C	0.36597100	-2.84269700	2.16196400
C	2.09349400	-0.29048000	-2.17487900
C	0.70963400	-2.45399100	-2.43717100
C	1.81027400	-0.76366500	2.41745700
C	0.59311900	-3.65018000	-0.22314100
C	3.23113900	-0.14670300	0.27507700
C	1.20870800	-3.23495300	1.04909700
C	2.82432000	-0.91268800	-1.08022700
C	1.40424200	-3.04376000	-1.31386200
C	2.63254300	-1.16049000	1.34390200
C	2.49725100	-2.30806800	-0.72457400
C	2.38661700	-2.43611000	0.73247300
Pr	0.36236000	-0.89551900	-0.27430000
C	6.63299500	0.75638000	1.85529700
C	5.25961600	0.51498400	1.69771800
C	4.74665000	0.09619800	0.44943400
C	5.62448500	-0.07467100	-0.63677300
C	6.99326300	0.16979000	-0.47153800
C	7.49691800	0.58179700	0.76432900
H	4.58951700	0.65209400	2.54716900
H	5.24437600	-0.39944900	-1.60487300
Cl	9.28610300	0.90687500	1.00722900
Cl	8.09691300	-0.06648700	-1.92023600
H	7.04003900	1.07595700	2.81321800

26. 4c' (BLYP/3-21G~MWB48)

C	-4.36976000	2.87941800	0.80537100
C	-4.97848400	2.14115900	-0.22332600
C	-5.44022600	0.77363000	0.02261000
C	-3.25825300	3.77931300	0.50397500
C	-4.07134000	2.20789700	2.07999200
C	-4.39814500	2.18286800	-1.57195700
C	-5.29394500	0.19277300	1.29577100
C	-2.80042900	3.92703200	-0.81757700
C	-4.52697900	0.91306300	2.32033100
C	-3.34622800	3.04591300	-1.86077100
C	-5.13749500	-0.02284500	-1.17217000
C	-2.27897600	3.65830800	1.59448300
C	-4.39062800	0.82164500	-2.10606600
C	-2.73688800	2.60410900	2.50829900
C	-4.97821900	-1.23051700	1.42579200
C	-1.37291700	4.09566500	-1.09138400
C	-3.66102100	-0.04369400	3.00587100
C	-2.24478900	2.60569400	-2.71615500
C	-4.83515200	-1.38329200	-1.04939100
C	-0.92192900	3.82729200	1.33325600
C	-4.03658300	-1.38298600	2.53353500
C	-1.05457700	3.34362100	-2.30821500
C	-1.82265000	1.65529700	3.06277100
C	-3.26373700	0.31464600	-2.82148600
C	-4.81123200	-2.02721900	0.27237800
C	-0.45007600	4.11502300	-0.02574000
C	-2.30815900	0.27615500	3.33435800
C	-2.14563900	1.24174700	-3.15316200
C	-3.79625000	-1.96796200	-1.86908400
C	0.04987900	2.95720700	1.98760800
C	-3.00472000	-1.13779100	-2.72147400
C	-0.38195900	1.89108700	2.83853900
C	-3.79138500	-3.06391400	0.23348600
C	0.84550900	3.45902200	-0.17216400
C	-3.08910200	-2.40746900	2.51125800
C	0.21738200	2.77048100	-2.46627200
C	-3.17606100	-3.06859600	-1.09564900
C	1.17564300	2.77725100	1.07618200
C	-1.33504700	-0.84186400	3.40219600
C	-0.79675000	0.70254100	-3.41518500
C	-2.99066100	-3.31310200	1.36466800
C	1.19813300	2.85594300	-1.38549700

C	-1.74960900	-2.17019700	3.02256900
C	0.36647800	1.47902300	-3.10221800
C	-1.68796800	-1.61329600	-3.01992800
C	0.53210000	0.79628600	2.97369400
C	-0.61230400	-0.73008000	-3.38262600
C	0.06124600	-0.55052900	3.28539000
C	-1.82231500	-3.43846200	-1.27601800
C	1.97551200	1.59258600	1.08212400
C	-1.59997800	-3.69985800	1.21434200
C	2.00307300	1.63753300	-1.39887100
C	-0.84619000	-3.05113600	2.30086600
C	1.58007500	0.84155500	-2.55221600
C	-1.12424900	-2.79892300	-2.38525000
C	1.74839700	0.69655600	2.20258500
C	-1.00411000	-3.83164900	-0.08598900
C	2.47265900	1.04323800	-0.18628400
C	0.65401700	-1.37752800	-3.04161700
C	1.00099900	-1.49244800	2.71711800
C	0.54309500	-2.74310400	2.15618500
C	1.79070800	-0.58228000	-2.54066000
C	0.31474900	-2.69938100	-2.46648100
C	2.07699400	-0.71509400	2.06924700
C	0.44055100	-3.72991600	-0.16982500
C	3.23525500	-0.31402500	-0.27015200
C	1.22554400	-3.25110500	0.98096800
C	2.63425300	-1.15695800	-1.50322600
C	1.12677400	-3.23837900	-1.39643100
C	2.74392100	-1.22240900	0.93754000
C	2.30929600	-2.50816000	-1.00502200
C	2.38043800	-2.52711100	0.46084400
Pr	0.29494500	-0.98712900	-0.39474400
C	6.88255500	-0.13091300	-1.53363900
C	5.49258500	-0.33731300	-1.49992500
C	4.76788800	-0.12394500	-0.31084900
C	5.44942000	0.30106000	0.84977100
C	6.83245100	0.50246900	0.80818300
C	7.54748100	0.28886000	-0.37507300
H	4.96859100	-0.66740700	-2.39731800
Cl	7.67745100	1.04785400	2.34512400
Cl	9.36215800	0.54679000	-0.45228900
H	4.91352800	0.47492100	1.78229300
H	7.45107700	-0.29294300	-2.44807300