



Supporting Information

Experimentally Based Recommendations of Density Functionals for Predicting Properties in Mechanically Interlocked Molecules

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a) Tetracationic system in acetone

Geometry	SP Energy	Single Point Gas Phase 6-311++G**	Solv 6-31G** Acetone
CBPQT ⁴⁺		E _{scf}	Esolv
B3LYP	B3LYP	-1609.145535	-448.7568
M06-L	M06-L	-1608.934787	-449.2864
B3LYP	M06-L	-1608.933261	-448.0355
B3LYP	M06-2X	-1608.471763	-450.104
M06-L	M06-2X	-1608.473037	-451.3293
M06-L	B3LYP	-1609.144284	-449.9864
M06-L	M06	-1607.900625	-449.999
M06-L	M06-HF	-1608.772614	-454.5968
B3LYP	MO6	-1607.898434	-448.7517
B3LYP	MO6-HF	-1608.771457	-453.4041
M06-L	X3LYP	-1608.383006	-450.064
M06-L	HF	-1598.778199	-453.1094
M06-L	PBE	-1607.097661	-449.7502

Geometry	SP Energy	Single Point Gas Phase 6-311++G**	Solv 6-31G** Acetone
[1 ⊂ CBPQT] ⁴⁺		E _{scf}	Esolv
B3LYP	B3LYP	-2921.377625	-412.2676
M06-L	M06-L	-2921.070358	-413.6445
B3LYP	M06-L	-2921.059593	-411.7853
B3LYP	M06-2X	-2920.213883	-414.0227
M06-L	M06-2X	-2920.227632	-417.9088
M06-L	B3LYP	-2921.361383	-416.106
M06-L	M06	-2919.248409	-415.9611
M06-L	M06-HF	-2920.744647	-421.3955
B3LYP	MO6	-2919.238734	-412.1778
B3LYP	MO6-HF	-2920.732151	-417.5342
M06-L	X3LYP	-2919.985125	-416.194
M06-L	HF	-2902.537783	-420.8745
M06-L	PBE	-2917.644233	-414.9732

Geometry	SP Energy	Single Point Gas Phase 6-311++G**	Solv 6-31G** Acetone
1		E _{scf}	Esolv
B3LYP	B3LYP	-1312.191139	-11.4991
M06-L	M06-L	-1312.014455	-11.0243
B3LYP	M06-L	-1312.012997	-11.251
B3LYP	M06-2X	-1311.631862	-13.2023
M06-L	M06-2X	-1311.632778	-13.0026
M06-L	B3LYP	-1312.186133	-11.379
M06-L	M06	-1311.228589	-11.88
M06-L	M06-HF	-1311.839785	-17.0073
B3LYP	MO6	-1311.226185	-12.0937
B3LYP	MO6-HF	-1311.839954	-17.2378
M06-L	X3LYP	-1311.563626	-11.3846
M06-L	HF	-1303.747493	-15.06
M06-L	PBE	-1310.49623	-11.2481

b) Tetracationic system in acetonitrile

Geometry	SP Energy	Single Point Gas Phase 6-311++G**	Solv 6-31G** Acetonitrile
CBPQT ⁴⁺		E _{SCF}	E _{solv}
B3LYP	B3LYP	-1609.145535	-459.9029
M06-L	M06-L	-1608.934787	-460.5294
B3LYP	M06-L	-1608.933261	-459.1999
B3LYP	M06-2X	-1608.471763	-461.3339
M06-L	M06-2X	-1608.473037	-462.6701
M06-L	B3LYP	-1609.144284	-461.2413
M06-L	M06	-1607.900625	-461.257
M06-L	M06-HF	-1608.772614	-466.075
B3LYP	MO6	-1607.898434	-459.9004
B3LYP	MO6-HF	-1608.771457	-464.7313
MO6-L	X3LYP	-1608.383006	-461.3288
MO6-L	HF	-1598.778199	-464.5335
MO6-L	PBE	-1607.097661	-461.0562

Geometry	SP Energy	Single Point Gas Phase 6-311++G**	Solv 6-31G** Acetonitrile
[1 ⊂ CBPQT] ⁴⁺		E _{SCF}	E _{solv}
B3LYP	B3LYP	-2921.377625	-423.1268
M06-L	M06-L	-2921.070358	-424.5843
B3LYP	M06-L	-2921.059593	-421.1394
B3LYP	M06-2X	-2920.213883	-424.9472
M06-L	M06-2X	-2920.227632	-429.0169
M06-L	B3LYP	-2921.361383	-427.0456
M06-L	M06	-2919.248409	-426.8899
M06-L	M06-HF	-2920.744647	-432.8068
B3LYP	MO6	-2919.238734	-422.9435
B3LYP	MO6-HF	-2920.732151	-428.6544
MO6-L	X3LYP	-2919.985125	-427.0566
MO6-L	HF	-2902.537783	-432.2076
MO6-L	PBE	-2917.644233	-425.9355

Geometry	SP Energy	Single Point Gas Phase 6-311++G**	Solv 6-31G** Acetonitrile
1		E _{SCF}	E _{solv}
B3LYP	B3LYP	-1312.191139	-12.2461
M06-L	M06-L	-1312.014455	-11.69
B3LYP	M06-L	-1312.012997	-11.9435
B3LYP	M06-2X	-1311.631862	-14.0959
M06-L	M06-2X	-1311.632778	-13.8518
M06-L	B3LYP	-1312.186133	-12.0241
M06-L	M06	-1311.228589	-12.5521
M06-L	M06-HF	-1311.839785	-18.0584
B3LYP	MO6	-1311.226185	-12.8876
B3LYP	MO6-HF	-1311.839954	-18.3835
MO6-L	X3LYP	-1311.563626	-12.1676
MO6-L	HF	-1303.747493	-15.999
MO6-L	PBE	-1310.49623	-11.9966

c) Neutral system in acetonitrile

Geometry	SP Energy	Single Point Gas Phase 6-311++G**	Solv 6-31G** Acetonitrile
CBPQT Cl ₄		E _{SCF}	E _{solv}
B3LYP	B3LYP	-3451.320112	-115.0884
M06-L	M06-L	-3451.059597	-111.609
B3LYP	M06-L	-3451.026327	-112.0222
B3LYP	M06-2X	-3450.521121	-126.011
M06-L	M06-2X	-3450.55665	-125.3472
M06-L	B3LYP	-3451.349334	-114.1628
M06-L	M06	-3449.974984	-115.808
M06-L	M06-HF	-3450.910988	-132.7145
B3LYP	M06	-3449.94029	-116.7185
B3LYP	M06-HF	-3450.871829	-133.6838
M06-L	X3LYP	-3450.38764	-114.8665
M06-L	HF	-3437.975368	-141.3667
M06-L	PBE	-3448.496911	-101.9575

Geometry	SP Energy	Single Point Gas Phase 6-311++G**	Solv 6-31G** Acetonitrile
[1 ⊂ CBPQT]-4Cl		E _{SCF}	E _{solv}
B3LYP	B3LYP	-4763.549869	-93.4732
M06-L	M06-L	-4763.168505	-101.0967
B3LYP	M06-L	-4763.153636	-91.6736
B3LYP	M06-2X	-4762.27845	-99.2013
M06-L	M06-2X	-4762.292925	-108.4047
M06-L	B3LYP	-4763.535483	-103.0655
M06-L	M06	-4761.299437	-103.8434
M06-L	M06-HF	-4762.868413	-111.2348
B3LYP	M06	-4761.28739	-94.35
B3LYP	M06-HF	-4762.853614	-102.7247
M06-L	X3LYP	-4761.960577	-103.3434
M06-L	HF	-4741.721617	-117.902
M06-L	PBE	-4759.009388	-93.7138

Geometry	SP Energy	Single Point Gas Phase 6-311++G**	Solv 6-31G** Acetonitrile
1		E _{SCF}	E _{solv}
B3LYP	B3LYP	-1312.191139	-12.2461
M06-L	M06-L	-1312.014455	-11.69
B3LYP	M06-L	-1312.012997	-11.9435
B3LYP	M06-2X	-1311.631862	-14.0959
M06-L	M06-2X	-1311.632778	-13.8518
M06-L	B3LYP	-1312.186133	-12.0241
M06-L	M06	-1311.228589	-12.5521
M06-L	M06-HF	-1311.839785	-18.0584
B3LYP	M06	-1311.226185	-12.8876
B3LYP	M06-HF	-1311.839954	-18.3835
M06-L	X3LYP	-1311.563626	-12.1676
M06-L	HF	-1303.747493	-15.999
M06-L	PBE	-1310.49623	-11.9966

Counterpoise Corrections to BSSE

B3LYP	B3LYP 6-311++G**	B3LYP 6-311++G** Deleted atoms	B3LYP 6-311++G** Ghost atoms	E _{cp}
		E _{SCF}	E _{SCF}	Kcal/mol
CBPQT	-1609.145535	-1609.139969	-1609.14384	4.708
1	-1312.191139	-1312.18382	-1312.18745	

M06	M06 6-311++G**	M06 6-311++G** Deleted atoms	M06 6-311++G** Ghost atoms	E _{cp}
		E _{SCF}	E _{SCF}	Kcal/mol
CBPQT	-1607.900625	-1607.8922	-1607.89865	7.451
1	-1311.228589	-1311.214977	-1311.2204	

M06-L	M06-L 6-311++G**	M06-L 6-311++G** Deleted atoms	M06-L 6-311++G** Ghost atoms	E _{cp}
		E _{SCF}	E _{SCF}	Kcal/mol
CBPQT	-1608.93475	-1608.92685	-1608.93241	6.192
1	-1312.01444	-1312.00220	-1312.006516	

B3LYP Thermodynamic corrections to 298K

6-31G** gas phase Optimization			
	H _{vib}	ZPE	S _{vib}
CBPQT ⁴⁺	16.827	379.572	108.702
1	17.447	335.355	121.139
[1 ⊂ CBPQT] ⁴⁺	37.168	716.425	249.667

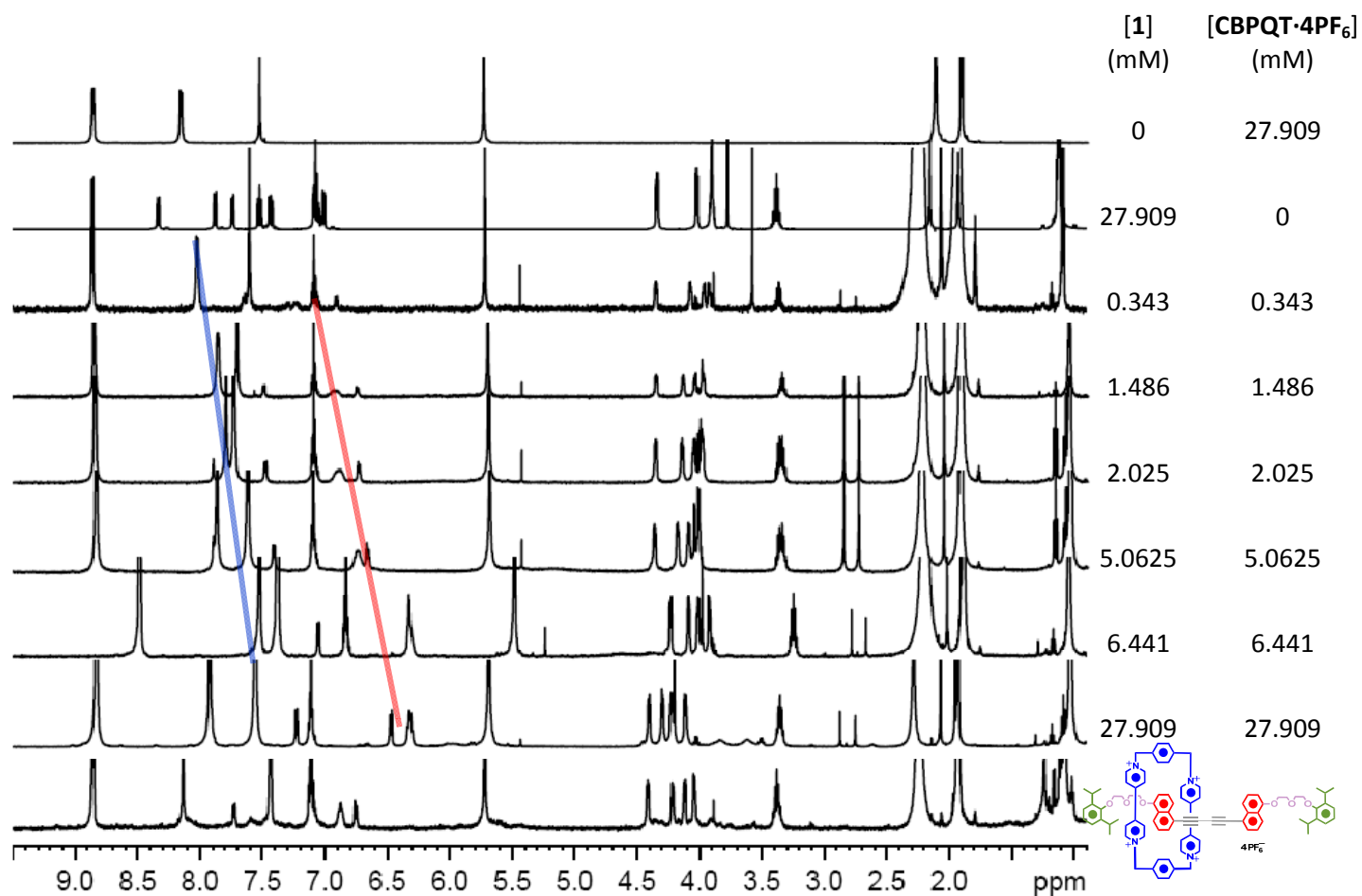
We approximate condensed phase rotational and translational energy components as

$$KE_{\text{rot}} + KE_{\text{trans}} + PE_{\text{rot}} + PE_{\text{trans}} = 6 RT$$

Reported energies are calculated by

$$H_{\text{TOT}} = E_{\text{SCF}} + E_{\text{solv}} + ZPE + H_{\text{VIB}} + 6RT$$

$^1\text{H-NMR}$ 268K CD_3CN

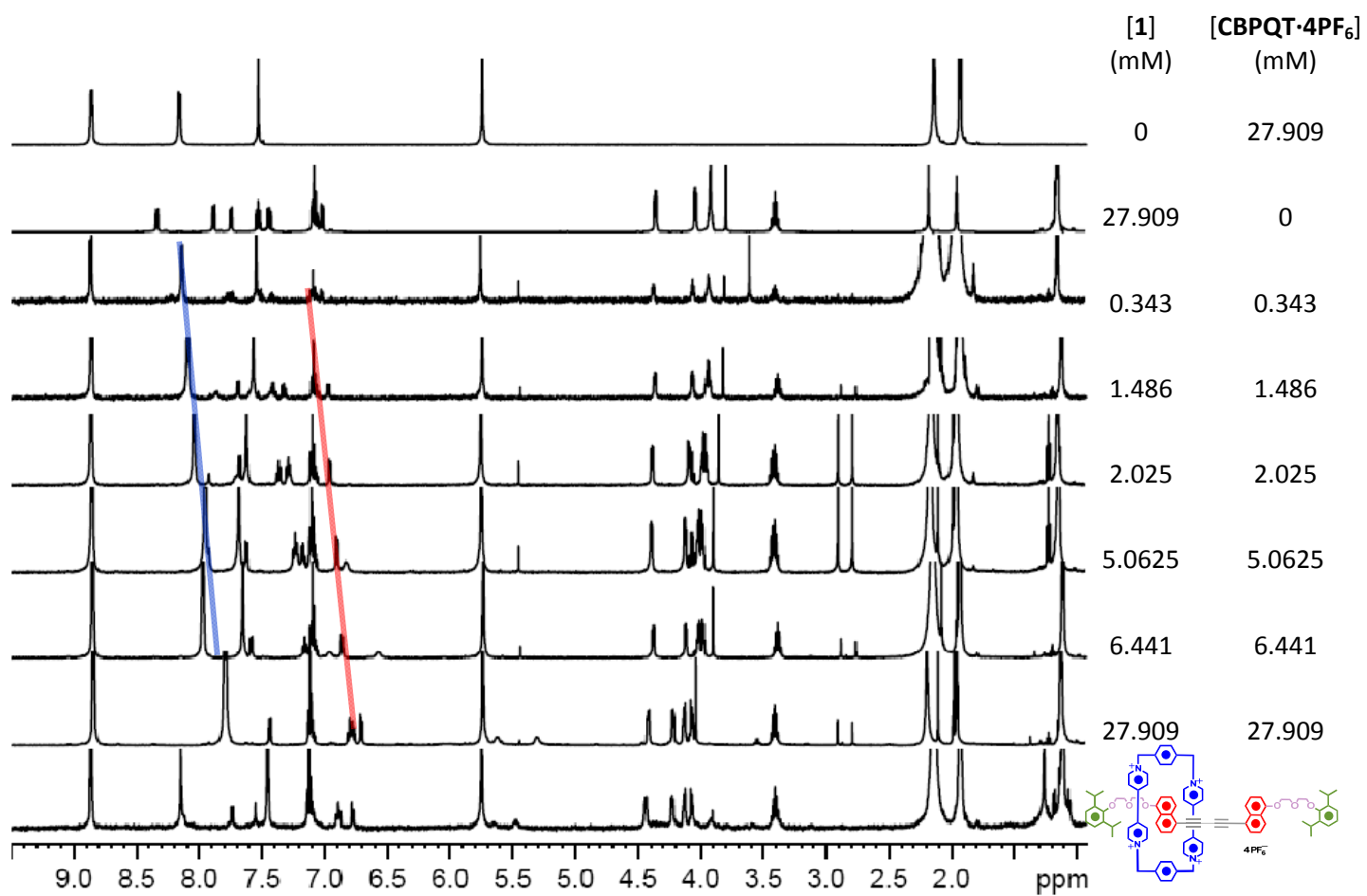


If we assume the [2] rotaxane shifts (bottom spectra, see ref 3 in the manuscript) are the time averaged 50% superstructure [1 \subset CBPQT 4PF₆] chemical shifts then,

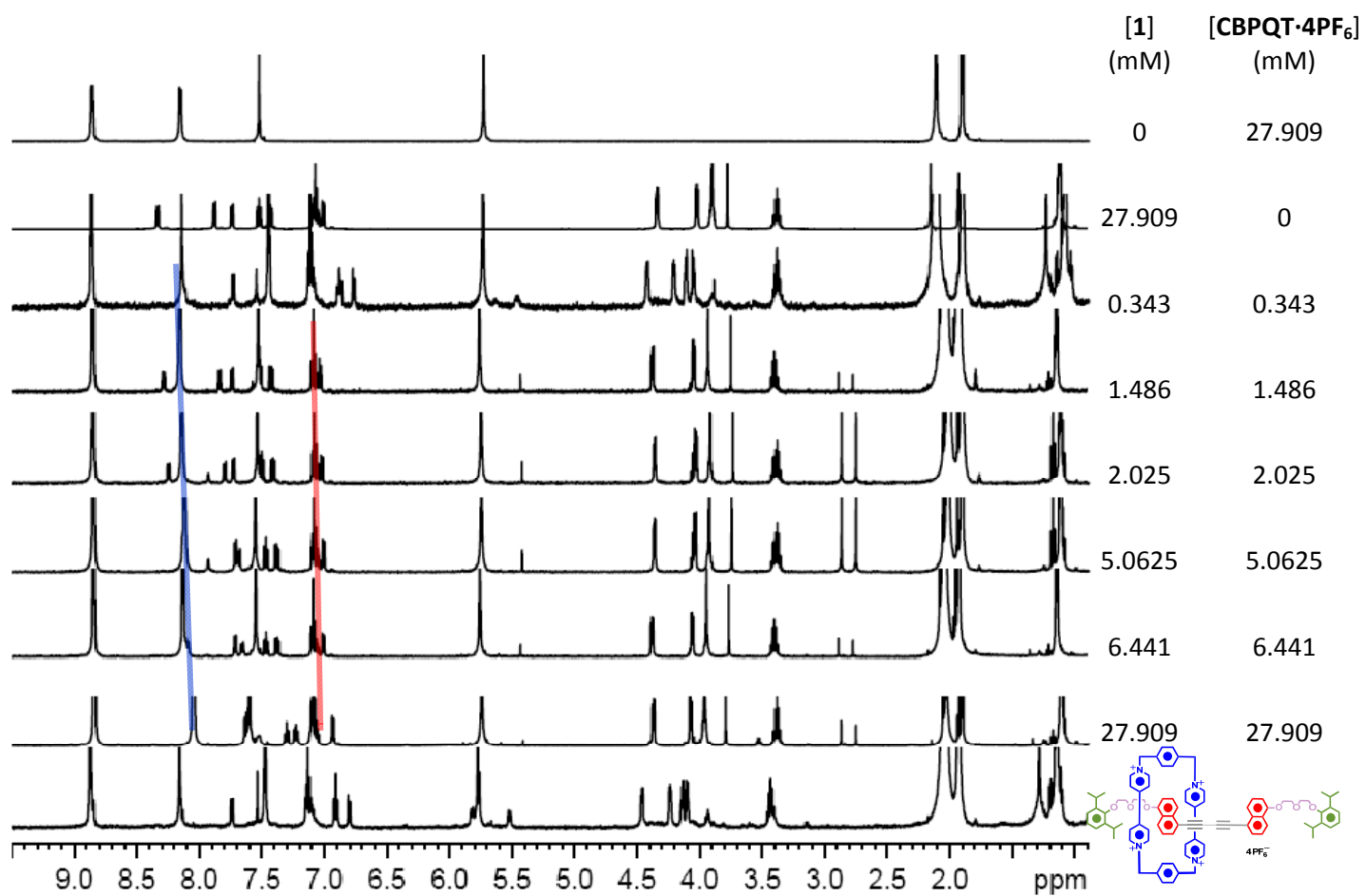
$$[1 \subset \text{CBPQT } 4\text{PF}_6] = C \Delta\delta/2[\Delta\delta_{(\text{mon})} - \Delta\delta_{(\text{rot})}]$$

Where [1 \subset CBPQT 4PF₆] is the concentration of the complex, C is the total concentration of 1 which is the same as the concentration of CBPQT 4PF₆, $\Delta\delta_{(\text{mon})}$ is the chemical shift of protons in the monomeric species 1 or CBPQT 4PF₆ and $\Delta\delta_{(\text{rot})}$ is the chemical shift of protons in the rotaxane.

$^1\text{H-NMR}$ 298K CD_3CN



$^1\text{H-NMR}$ 328K CD_3CN



O2	-5.0776827860	3.1757064949	7.8433989239
O3	-4.2053023728	2.1635871536	10.3688225256
O4	-2.0597026623	3.6053598336	11.8670280408
H4	-3.9877123748	4.0210996074	-0.3282302661
C26	-3.8765648793	4.0350288853	0.7304514670
C27	-3.7468848699	4.0512705107	1.9341954851
C28	-3.5741348809	4.0796742457	3.3535951027
C29	-2.4227676784	4.6418866356	3.8914773533
H30	-1.6748282631	5.0508055644	3.2210029333
C31	-2.2174199578	4.6773299217	5.2833780957
H32	-1.3040744405	5.1115176347	5.6785005833
C33	-3.1630955806	4.1605529668	6.1420968758
H34	-3.0057486681	4.1726862573	7.2138220529
C35	-4.3563109095	3.5875734908	5.6358263909
C36	-4.5768783495	3.5297946770	4.2247971276
C37	-5.7647708477	2.9294250397	3.7292380774
H38	-5.9237876405	2.8871550773	2.6581035761
C39	-6.6879579610	2.4072775032	4.6018405355
H40	-7.5923549677	1.9430575583	4.2192139989
C41	-6.4938785477	2.4601339418	6.0023799414
H42	-7.2470289755	2.0403287000	6.6577585838
C43	-5.3542690594	3.0479148262	6.5128566720
C44	-5.9494581716	2.5569104186	8.7799460560
H45	-5.9900794089	1.4741783674	8.6023874293
H46	-6.9658933164	2.9665663029	8.6871777993
C47	-5.4374309820	2.8331887042	10.1795787016
H48	-5.3371528763	3.9190453197	10.3223701840
H49	-6.1944060041	2.4682606211	10.8945787913
C50	-3.8253263787	1.9869966966	11.7225811573
H51	-3.0219505875	1.2440900760	11.7129980231
H52	-4.6658796978	1.5768902809	12.3081131878
C53	-3.3217408581	3.2402450726	12.4252079717
H54	-4.0373780998	4.0677380060	12.3275037104
H55	-3.2182901596	3.0239163890	13.4997128175
C56	-1.5395743780	4.8058720963	12.3409246584
C57	-0.6962703382	4.7861285367	13.4679602926
C58	-0.1624427058	6.0039651000	13.9042239325
H59	0.4935797847	6.0187061863	14.7705920739
C60	-0.4515190626	7.1950631156	13.2439107401
H61	-0.0289322366	8.1301683498	13.6006057603
C62	-1.2713571727	7.1849445244	12.1187615426
H63	-1.4765805021	8.1160408871	11.5975395311
C64	-1.8268725571	5.9923547906	11.6398243022
C65	-0.3424464620	3.4826349999	14.1765667656
H66	-0.8709023816	2.6780879503	13.6576813486
C67	-2.6868315260	5.9804737924	10.3806870844
H68	-2.9623304384	4.9402054798	10.1854393715
C69	1.1636840209	3.1763849093	14.0675121646
H70	1.4823701587	3.135336023	13.0217477040
H71	1.3952302879	2.2113511920	14.5321945493
H72	1.7654967713	3.9405248774	14.5714845246
C73	-0.7978555835	3.4840558671	15.6482555574
H74	-0.2762054339	4.2535864567	16.2282290960
H75	-0.5872370263	2.5170658066	16.1185241997
H76	-1.8719762320	3.6776968348	15.7363879707
C77	-1.8934823130	6.4791750352	9.1576502091
H78	-1.5872835290	7.5246780557	9.2748531569
H79	-2.5029564556	6.4119874236	8.2499836753
H80	-0.9890126679	5.8817528894	9.0071082205
C81	-3.9802862754	6.7973801975	10.5621643045
H82	-4.5639266796	6.4438432546	11.4193113003
H83	-4.6093405489	6.7254354834	9.6681581488
H84	-3.7636018769	7.8582483264	10.7305781533

[1 ⊂ CBPQT]⁴⁺

N1	-0.4741605364	3.6574322279	9.0594728056
N2	-2.9313697414	-0.8750594224	4.2651787360
N3	-6.0874734324	3.8041305061	0.7284291009
N4	-3.4422244465	8.4055350731	5.3847790465
C5	-2.7624734098	9.1032534894	6.5586002946
H6	-3.5475154769	9.6622530136	7.0706285612
H7	-2.0685567278	9.8249233508	6.1227338681
C8	-2.0563716940	8.1238757526	7.4824580191
C9	-2.7596381939	7.4444622071	8.4879450031
H10	-3.8053091266	7.6732783341	8.6751014607
C11	-2.1316947322	6.4700812483	9.2655596402

H12	-2.6896958795	5.9581917103	10.0445067479
C13	-0.7848075702	6.1405664711	9.0453406216
C14	-0.0537497133	6.9002269390	8.1222023735
C15	-0.6817699118	7.8832689776	7.3513976587
H16	-0.0863309421	8.4620777204	6.6496866142
C17	-0.1513901661	4.9599692774	9.7726330924
H18	0.9362637306	5.0379472894	9.8040937558
H19	-0.5203748283	4.8596100254	10.7964611409
C20	0.3966483409	3.1210317137	8.1702057048
H21	1.3786038945	3.5758874750	8.1124452411
C22	0.0308639214	2.0606718949	7.3588907349
H23	0.7726063496	1.6737796495	6.6696254911
C24	-1.2719289630	1.5277901112	7.4258809517
C25	-2.0994303299	2.0235873313	8.4440020102
H26	-3.1105021108	1.6724882183	8.6116423982
C27	-1.6833764711	3.0817762140	9.2444352978
H28	-2.3208706927	3.4957892273	10.0223592778
C29	-1.7901604487	0.5926927851	6.3769135203
C30	-1.2611308413	0.6263261297	5.0725270839
H31	-0.4226979351	1.2623627381	4.8183799594
C32	-1.8443099481	-0.0982946841	4.0485675207
H33	-1.4720584055	-0.0500859290	3.0328719669
C34	-3.4245550704	-0.9853190703	5.5220982924
H35	-4.2664750892	-1.6542014162	5.6576056181
C36	-2.8788953735	-0.2737634647	6.5820213275
H37	-3.3190390046	-0.4127507735	7.5629866097
C38	-3.5936042310	-1.5891511174	3.0915784885
H39	-2.7878000958	-2.0888468544	2.5493394890
H40	-4.2314855105	-2.3595901622	3.5268421600
C41	-4.3777239943	-0.6440006925	2.1934824673
C42	-5.7320111613	-0.3733097113	2.4370271812
H43	-6.2669990547	-0.9085767070	3.2167421253
C44	-6.4128287467	0.5905654489	1.6900647958
H45	-7.4623091428	0.7779776454	1.9026304294
C46	-5.7542253587	1.3145919533	0.6849168223
C47	-4.4434594176	0.9447810357	0.3521885638
H48	-3.9381111631	1.4127164000	-0.4875533075
C49	-3.7649019102	-0.0234337843	1.0953438443
H50	-2.7518466226	-0.2901949493	0.8077212553
C51	-6.4248314899	2.5031403747	0.0074632006
H52	-7.5131372652	2.4210996128	0.0091009101
H53	-6.0974420639	2.6305178785	-1.0260137718
C54	-4.9574861008	4.4817283816	0.4144100435
H55	-4.4083404788	4.1397795723	-0.4537881612
C56	-4.5152220279	5.5441528253	1.1849498676
H57	-3.6032653924	6.0351305384	0.8694485055
C58	-5.2171599560	5.9372807457	2.3400256508
C59	-6.4429911434	5.2855045325	2.5713144105
H60	-7.0814864820	5.5373499968	3.4083188486
C61	-6.8483453562	4.2345792038	1.7617796166
H62	-7.7705828194	3.6959468935	1.9438679392
C63	-4.6353593423	6.8957701541	3.3326662051
C64	-3.2669569235	7.2262616028	3.3130360911
H65	-2.6030229010	6.8810744296	2.5316569027
C66	-2.7037275472	7.9690378366	4.3383792557
H67	-1.6487234159	8.2132031450	4.3550496389
C68	-4.7759245745	8.1733548263	5.3939843438
H69	-5.3366295480	8.5869762466	6.2238741974
C70	-5.3889440684	7.4394321169	4.3906747625
H71	-6.4616223931	7.3052597047	4.4603303687
O73	-4.6580481740	4.0659882773	7.6242882477
O74	-4.5502278314	2.9075477552	10.2707817934
O75	-2.7741220328	4.2448330571	12.0215763757
H75	-1.2315665965	2.6369040463	0.0678503340
C97	-1.5501243362	2.9144169852	1.0494103672
C98	-1.8739041168	3.2356497908	2.1735322591
C99	-2.0999045975	3.6906660661	3.5152257430
C100	-1.0838252471	4.4215312207	4.1218730089
H101	-0.1714634465	4.6172841026	3.5684776377
C102	-1.2293073067	4.9079768231	5.4325163127
H103	-0.4240201942	5.4811729952	5.8758634618
C104	-2.3823807175	4.6672241365	6.1527136017
H105	-2.4985354765	5.0550514974	7.1543246155
C106	-3.4403467537	3.9164695766	5.8847823131
C107	-3.3123074421	3.4183371943	4.2483043911
C108	-4.3740658219	2.6616336912	3.6949839298
H109	-4.2671802566	2.2581076746	2.6975171046
C110	-5.5197467820	2.4455946676	4.4285404363
H111	-6.333141819	1.8721680167	4.005312923
C112	-5.6735936821	2.9334405135	5.7415800437
H113	-6.5975261373	2.7352802599	6.2683484629

C114	-4.6395819560	3.6314453936	6.3379170192	H33	-1.4720584055	-0.0500859290	3.0328719669
C115	-5.8118404347	3.7388499012	8.4352159614	C34	-3.4245550704	-0.9853190703	5.5220982924
H116	-6.0922267128	2.6936300480	8.2739393478	H35	-4.2664750892	-1.6542014162	5.6576056181
H117	-6.6507036067	4.3844337255	8.1487977613	C36	-2.8788953735	-0.2737634647	6.5820213275
C118	-5.4774577095	3.9173306948	9.8999722969	H37	-3.3190390046	-0.4127507735	7.5629866097
H119	-5.0792966212	4.9236187861	10.0916469759	C38	-3.5936042310	-1.58951511174	3.0915784885
H120	-6.4155554604	3.8174797135	10.4648627123	H39	-2.7878000958	-2.0888468544	2.5493394890
C121	-4.5123873411	2.5995501106	11.6755678773	H40	-4.2314855105	-2.3595901622	3.5268421600
H122	-3.8385489339	1.7431842544	11.7575514883	C41	-4.3777239943	-0.6440006925	2.1934824673
H123	-5.5076755657	2.2870489814	12.0217521555	C42	-5.7320111613	-0.3733097112	2.4370271812
C124	-4.0201495090	3.7465138857	12.5440732946	H43	-6.2669990547	-0.9085767071	3.2167421254
H125	-4.7527218430	4.5618831416	12.5838406324	C44	-6.4128287467	0.5905654489	1.6900647958
H126	-3.8857703797	3.3762356599	13.5660691369	H45	-7.4623091428	0.7779776454	1.9026304294
C127	-1.8639428650	4.7216880623	12.9958196348	C46	-5.7542253587	1.3145919533	0.6849168223
C128	-0.8378676077	3.8527370620	13.4219918061	C47	-4.4434594176	0.9447810357	0.3521885638
C129	0.0660301982	4.3422345852	14.3741217379	H48	-3.9381111631	1.4127164000	-0.4875533075
H130	0.8609491224	3.6985687631	14.7381256805	C49	-3.7649019102	-0.0234337843	1.0953438443
C131	-0.0495878678	5.6330446864	14.8795474676	H50	-2.7518466226	-0.2901949493	0.8077212553
H132	0.6541578973	5.9882712827	15.6255565750	C51	-6.4248314899	2.5031403747	0.0074632006
C133	-1.0726816962	6.4666028907	14.4367797339	H52	-7.5131372652	2.4210996128	0.0091009101
H134	-1.1544487160	7.4677306721	14.8480330414	H53	-6.0974420639	2.6305178785	-1.0260137718
C135	-2.0042989435	6.0346419420	13.4842590375	C54	-4.9574861008	4.4817283816	0.4144100435
C136	-0.7173016206	2.4137905714	12.9260782138	H55	-4.4083404788	4.1397795723	-0.4537881612
H137	-1.4382198858	2.2844781941	12.1099216081	C56	-4.5152220279	5.5441528253	1.1849498676
C138	-3.1349460701	6.9619023994	13.0465403745	H57	-3.6032653924	6.0351305384	0.8694485055
H139	-3.6535588428	6.4806890765	12.2073645842	C58	-5.2171599560	5.9372807457	2.3400256508
C140	0.6829757123	2.1009632844	12.3636942279	C59	-6.4429911434	5.2855045325	2.5713144105
H141	0.9730861429	2.7986044275	11.5675110400	H60	-7.0814864820	5.5373499968	3.4083188486
H142	0.7152319192	1.0845213237	11.9576066071	C61	-6.8483453562	4.2345792038	1.7617796166
H143	1.4546735025	2.1620600054	13.1357761250	H62	-7.7705828194	3.6959468935	1.9438679392
C144	-1.0857877489	1.4080350772	14.0359217221	C63	-4.6353593423	6.8957701541	3.3326662051
H145	-0.3910448490	1.4797923330	14.8778922681	C64	-3.2669569235	7.2262616028	3.3130360911
H146	-1.0449203610	0.3808603317	13.6591876323	H65	-2.6030229010	6.8810744296	2.5316569027
H147	-2.0915258625	1.5885841724	14.4277505253	C66	-2.7037275472	7.9690378366	4.3383792557
C148	-2.6118839931	8.3211829876	12.5444398387	H67	-1.6487234159	8.2132031450	4.3550496389
H149	-2.1245230464	8.8877571949	13.3427056162	C68	-4.7759245745	8.1733548263	5.3939843438
H150	-3.4405380936	8.9358492635	12.1768870489	H69	-5.3366295480	8.5869762466	6.2328741974
H151	-1.8837140250	8.2019429253	11.7348471200	C70	-5.3889440684	7.4394321169	4.6906747625
C152	-4.1603989896	7.1618948291	14.1818541341	H71	-6.4616223931	7.3052597047	4.4603303687
H153	-4.5678169885	6.2100170316	14.5360670198	O73	-4.6580481740	4.0659882773	7.6242882477
H154	-4.9938217239	7.7868689983	13.8457267529	O74	-4.5502278314	2.9075477552	10.270717934
H155	-3.6999908335	7.6584802835	15.0411330475	O75	-2.7741220328	4.2448330571	12.0215763757
H156	1.0129921273	6.7333453125	7.9958889954	H75	-1.2315665965	2.6369040463	0.0678503340
				C97	-1.5501243362	2.9144169852	1.0494103672
				C98	-1.8739041168	3.2356497908	2.1735322591
				C99	-2.0999045975	3.6906660661	3.5152257430
				C100	-1.0838252471	4.4215312207	4.1218730089
				H101	-0.1714634465	4.6172841026	3.5684776377
				C102	-1.2293073067	4.9079768231	5.4325163127
				H103	-0.4240201942	5.4811729952	5.8758634618
				C104	-2.3823807175	4.6672241365	6.1527136017
				H105	-2.4985354765	5.0550514974	7.1543246155
				C106	-3.4403467537	3.9164695766	5.5884782313
				C107	-3.3123074421	3.4183371943	4.2483043911
				C108	-4.3740658219	2.6616336912	3.6949839298
				H109	-4.2671802566	2.2581076746	2.6975171046
				C110	-5.5197467820	2.4455946676	4.4285404363
				H111	-6.3333141819	1.8721680167	4.0005312923
				C112	-5.6735936821	2.9334405135	5.7415800437
				H113	-6.5975261373	2.7352802599	6.2683484629
				C114	-4.6395819560	3.6314453936	6.3379170192
				C115	-5.8118404347	3.7388499012	8.4352159614
				H116	-6.0922267128	2.6936300480	8.2739393478
				H117	-6.6507036067	4.3844337255	8.1487977613
				C118	-5.4774577095	3.9173306948	9.8999722969
				H119	-5.0792966212	4.9236187861	10.0916469759
				H120	-6.4155554604	3.8174797135	10.4648627123
				C121	-4.5123873411	2.5995501106	11.6755678773
				H122	-3.8385489339	1.7431842544	11.7575514883
				H123	-5.5076755657	2.2870489814	12.0217521555
				C124	-4.0201495090	3.7465138857	12.5440732946
				H125	-4.7527218430	4.5618831416	12.5838406324
				H126	-3.8857703797	3.3762356599	13.5660691369
				C127	-1.8639428650	4.7216880623	12.9958196348
				C128	-0.8378676077	3.8527370620	13.4219918061
				C129	0.0660301982	4.3422345852	14.3741217379
				H130	0.8609491224	3.6985687631	14.7381256805
				C131	-0.0495878678	5.6330446864	14.8795474676
				H132	0.6541578973	5.9882712827	15.6255565750
				C133	-1.0726816962	6.4666028907	14.4367797339
				H134	-1.1544487160	7.4677306721	14.8480330414

[1 ⊂ CBPQT]Cl₄

N1	-0.4741605364	3.6574322279	9.0594728056
N2	-2.9313697414	-0.8750594224	4.2651787360
N3	-6.0874734324	3.8041305061	0.7284291009
N4	-3.4422244465	8.4055350730	5.3847790466
C5	-2.7624734098	9.1032534896	6.5586002943
H6	-3.5475154767	9.6622530135	7.0706285615
H7	-2.0685567278	9.8249233508	6.1227338681
C8	-2.0563716940	8.1238757526	7.4824580191
C9	-2.7596381939	7.4444622071	8.4879450031
H10	-3.8053091266	7.6732783341	8.6751014607
C11	-2.1316947322	6.4700812483	9.2655596402
H12	-2.6896958795	5.9581917103	10.0445067479
C13	-0.7848075702	6.1405664711	9.0453406216
C14	-0.0537497132	6.9002269392	8.1222023737
C15	-0.6817699118	7.8832689776	7.3513976587
H16	-0.0863309421	8.4620777204	6.6496866142
C17	-0.1513901661	4.9599692774	9.7726330924
H18	0.9362637306	5.0379472894	9.8040937558
H19	-0.5203748283	4.8596100254	10.7964611409
C20	0.3966483409	3.1210317137	8.1702057048
H21	1.3786038945	3.5758874750	8.1124452411
C22	0.0308639214	2.0606718949	7.3588907349
H23	0.7726063496	1.6737796495	6.6696254911
C24	-1.2719289630	1.5277901112	7.4258809517
C25	-2.0994303299	2.0235873313	8.4440020102
H26	-3.1105021108	1.6724882183	8.6116423982
C27	-1.6833764711	3.0817762140	9.2444352978
H28	-2.3208706927	3.4957892273	10.0223592778
C29	-1.7901604487	0.5926927851	6.3769135203
C30	-1.2611308413	0.6263261297	5.0725270839
H31	-0.4226979351	1.2623627381	4.8183799594
C32	-1.8443099481	-0.0982946841	4.0485675207

C135	-2.0042989435	6.0346419420	13.4842590375
C136	-0.7173016206	2.4137905714	12.9260782138
H137	-1.4382198858	2.2844781941	12.1099216081
C138	-3.1349460701	6.9619023994	13.0465403745
H139	-3.6535588428	6.4806890765	12.2073645842
C140	0.6829757113	2.1009632844	12.3636942279
H141	0.9730861429	2.7986044275	11.5675110400
H142	0.7152319192	1.0845213237	11.9576066071
H143	1.4546735025	2.1620600054	13.1357761250
C144	-1.0857877489	1.4080350772	14.0359217221
H145	-0.3910448490	1.4797923330	14.8778922681
H146	-1.0449203610	0.3808603317	13.6591876323
H147	-2.0915258625	1.5885841724	14.4277505253
C148	-2.6118839931	8.3211829876	12.5444398387
H149	-2.1245230464	8.8877571949	13.3427056162
H150	-3.4405380936	8.9358492635	12.1768870489
H151	-1.8837140250	8.2019429253	11.7348471200
C152	-4.1603989896	7.1618948291	14.1818541341
H153	-4.5678169885	6.2100170316	14.5360670198
H154	-4.9938217239	7.7868689983	13.8457267529
H155	-3.6999908335	7.6584802835	15.0411330475
H156	1.0129921272	6.7333453123	7.9958889952
Cl157	-3.5202517659	3.1740203451	-2.1025503040
Cl158	-5.9334828364	9.0763177182	8.1713062215
Cl159	2.5090370487	5.0120688749	6.9159689731
Cl160	-6.3434070388	-0.6984000358	5.9489087792

b) M06-L optimized geometries
CBPQT⁴⁺

C1	2.5113237414	4.0230881492	-1.9536481764
C2	2.8899125716	4.1405189720	0.8304681489
C3	3.6101175080	3.3954294523	-1.3596012808
C4	1.6200233478	4.7344198869	-1.1438873231
C5	1.8042469381	4.7884020303	0.2340147233
C6	3.7998677986	3.4576590211	0.0173518516
H7	4.3487807521	2.8850585187	-1.9729848098
H8	0.7960378124	5.2877147778	-1.5884405453
H9	1.1150771542	5.3739556845	0.8377986576
H10	4.6887277023	3.0035612405	0.4492946230
C11	2.2896423066	3.9341563941	-3.4449877306
H12	3.2239564899	3.8629206659	-4.0042837358
H13	1.7299328040	4.7871297654	-3.8345411302
C14	3.0783795460	4.1786345949	2.3285191662
H15	4.1243532064	4.0598102818	2.6192798680
H16	2.7106081947	5.1041626931	2.7736252029
N17	2.3171640062	3.0533897452	2.9782872278
C18	0.7581462342	0.8941594807	3.7701512531
C19	2.183439739	1.8013034829	2.9054345266
C20	1.1039378908	3.2698435719	3.5309418494
C21	0.3105041867	2.2123101458	3.9345665155
C22	2.0673518851	0.7148202453	3.2983897146
H23	3.8179397554	1.7057220026	2.4964486922
H24	0.7876834691	4.3037839186	3.6177815087
H25	-0.6545684748	2.4380322623	4.3741983759
H26	2.5006997695	-0.2720290916	3.1804129314
N27	1.4896223534	2.7017760970	-3.7752444405
C28	0.0506116777	0.3309779889	-3.9393515161
C29	2.1053019982	1.5714733626	-4.1845985070
C30	0.1580806152	2.7078787841	-3.5489975642
C31	-0.5790973606	1.5462375306	-3.6311641517
C32	1.4105538140	0.3801730988	-4.2760754075
H33	3.1629285236	1.6502452767	-4.4121237421
H34	-0.2792478368	3.6608541062	-3.2729496185
H35	-1.6369872142	1.5972809184	-3.3987679505
H36	1.9486251872	-0.4995360382	-4.6111860046
C37	-0.6763997717	-0.9481305224	-3.7706301777
N38	-2.0337269077	-3.2422529675	-2.9865149220
C39	-2.0693336277	-1.0451499677	-3.8940317252
C40	0.0124463458	-2.0940840681	-3.3446357949
C41	-0.6836455456	-3.2172644553	-2.9540611249
C42	-2.7216268452	-2.1974691771	-3.4958165539
H43	-2.6659365207	-0.2338346908	-4.2972253228
H44	1.0933166841	-2.1106578980	-3.2598819391
H45	-0.1943211156	-4.1087493115	-2.5778300509
H46	-3.7991057112	-2.3081886461	-3.5527510519
C47	-0.1337216369	-0.2750818920	3.9433370617
N48	-1.7732975431	-2.5121932488	3.7830868488
C49	-1.5088083846	-0.1550870106	3.6918488993
C50	0.3575200505	-1.5572058350	4.2271742678
C51	-0.4778344318	-2.6548487433	4.1380975127
C52	-2.3000024985	-1.2805553292	3.6106380202
H53	-1.9724705951	0.8067168405	3.5031507013
H54	1.3892071962	-1.7232327151	4.5183482591
H55	-0.1349803222	-3.6667954805	4.3248154165
H56	-3.3580792448	-1.2371371893	3.3776542744
C57	-2.7528614115	-4.3965933496	-2.3386547617
H58	-2.2498630665	-5.3070732169	-2.6716174551
H59	-3.7651523171	-4.4052685113	-2.7461561558
C60	-2.6158158484	-3.7160518108	3.4527513839
H61	-2.1723221311	-4.5648993593	3.9757773968
H62	-3.6036087371	-3.5363346658	3.8825894264
C63	-2.6673787389	-3.9185581072	1.9568790734
C64	-2.7339450552	-4.2458393925	-0.8357462935
C65	-3.6854059038	-3.3343378074	1.1958483164
C66	-1.7002401285	-4.6929334859	1.3097434992
C67	-1.7359235904	-4.8585279517	-0.0716426472
C68	-3.7155885620	-3.4917882914	-0.1858911608
H69	-4.4884528393	-2.7852463738	1.6821049224
H70	-0.9327935541	-5.2057488447	1.8845290019
H71	-1.0010912074	-5.5054470572	-0.5453358577
H72	-4.5347191130	-3.0536241443	-0.7511188564

C1	2.5113237414	4.0230881492	-1.9536481764	O2	-4.9805162776	3.3189656841	7.9681281523
C2	2.8899125716	4.1405189720	0.8304681489	O3	-4.0317416297	2.0639480511	10.2951223522
C3	3.6101175080	3.3954294523	-1.3596012808	O4	-1.8019566672	3.3892222559	11.7670584730
C4	1.6200233478	4.7344198869	-1.1438873231	H4	-4.4991792321	4.2581700839	-0.2233961440
C5	1.8042469381	4.7884020303	0.2340147233	C26	-4.2991377850	4.2232589146	0.8202805679
C6	3.7998677986	3.4576590211	0.0173518516	C27	-4.0673049975	4.1833604787	2.0084050432
H7	4.3487807521	2.8850585187	-1.9729848098	C28	-3.7702935670	4.1414372731	3.3975182695
H8	0.7960378124	5.2877147778	-1.5884405453	C29	-2.5053843897	4.5019008738	3.8432584207
H9	1.1150771542	5.3739556845	0.8377986576	H30	-1.7633085343	4.8141338919	3.1157824870
H10	4.6887277023	3.0035612405	0.4492946230	C31	-2.1782044696	4.4572871642	5.2060845094
C11	2.2896423066	3.9341563941	-3.4449877306	H32	-1.1772432171	4.7317267372	5.5272661008
H12	3.2239564899	3.8629206659	-4.0042837358	C33	-3.1132644995	4.0600710455	6.1338275263
H13	1.7299328040	4.7871297654	-3.8345411302	H34	-2.8670089882	4.0012710395	7.1888059911
C14	3.0783795460	4.1786345949	2.3285191662	C35	-4.4140081462	3.6980166572	5.7248156762
H15	4.1243532064	4.0598102818	2.6192798680	C36	-4.7635305670	3.7235967867	4.3420049159
H16	2.7106081947	5.1041626931	2.7736252029	C37	-6.0629780448	3.3282932518	3.9480739254
N17	2.3171640062	3.0533897452	2.9782872278	H38	-6.3204201063	3.3473182417	2.8941693103
C18	0.7581462342	0.8941594807	3.7701512531	C39	-6.9728400099	2.9205522942	4.8900994693
C19	2.8183439739	1.8013034829	2.9054345266	H40	-7.9676793732	2.6117078731	4.5824194966
C20	1.1039378908	3.2698435719	3.5309418494	C41	-6.6522423481	2.8928401747	6.2621426424
C21	0.3105041867	2.2123101458	3.9345665155	H42	-7.3980086290	2.5684552702	6.9784633821
C22	2.0673518851	0.7148202453	3.2983897146	C43	-5.3965008662	3.2842953183	6.6739399899
H23	3.8179397554	1.7057220026	2.4964486922	C44	-5.8515538118	2.7706859696	8.9380898132
H24	0.7876834691	4.3037839186	3.6177815087	H45	-6.0742055826	1.7220341080	6.6935982897
H25	-0.6545684748	2.4380322623	4.3741983759	H46	-6.8020723811	3.3257576283	8.9627764891
H26	2.5006997695	-0.2720290916	3.1804129314	C47	-5.1851823382	2.8702845998	10.2819897181
N27	1.4896223534	2.7017760970	-3.7752444407	H48	-4.9438593115	3.9249855139	10.4909512326
C28	0.0506116777	0.3309779889	-3.9393515161	H49	-5.9046713297	2.5386491191	11.0524023381
C29	2.1053019982	1.5714733626	-4.1845985068	C50	-3.5711250719	1.7902113240	11.5993637031
C30	0.1580806152	2.7078787841	-3.5489975642	H51	-2.7792625487	1.0433080832	11.4900980136
C31	-0.5790973606	1.5462375306	-3.6311641517	H52	-4.3812698047	1.3440621013	12.2043620467
C32	1.4105538140	0.3801730988	-4.2760754075	C53	-3.0277422039	2.9818943818	12.3525993220
H33	3.1629285236	1.6502452767	-4.4121237423	H54	-3.7461116719	3.8176636409	12.3493730335
H34	-0.2792478368	3.6608541062	-3.2729496185	H55	-2.8819930283	2.6956762458	13.4075379927
H35	-1.6369872142	1.5972809184	-3.3987679505	C56	-1.3802921152	4.6397219695	12.1921080380
H36	1.9486251872	-0.4995360382	-4.6111860046	C57	-0.7091856728	4.7676569372	13.4172040657
C37	-0.6763997717	-0.9481305224	-3.7706301777	C58	-0.2905767645	6.0417204462	13.8034176695
N38	-2.0337269077	-3.2422529675	-2.9865149220	H59	0.2270483846	6.1637394769	14.7528959141
C39	-2.0693336277	-1.0451499677	-3.8940317252	C60	-0.5211412147	7.1478111494	12.9958301570
C40	0.0124463458	-2.0940840681	-3.3446357949	H61	-0.1874314150	8.1317606177	13.3127978043
C41	-0.6836455456	-3.2172644553	-2.9540611249	C62	-1.1747196277	6.9917455979	11.7809501481
C42	-2.7216268452	-2.1974691771	-3.4958165539	H63	-1.3495419176	7.8576365263	11.1450337057
H43	-2.6659365207	-0.2338346908	-4.2972253228	C64	-1.6189000627	5.7379527126	11.3550699808
H44	1.0933166841	-2.1106578980	-3.2598819391	C65	-0.4492627847	3.5707675914	14.3060305086
H45	-0.1943211156	-4.1087493115	-2.5778300509	H66	-0.7390896522	2.6760101402	13.7428115479
H46	-3.7991057112	-2.3081886461	-3.5527510519	C67	-2.3297766933	5.5824207504	10.0280640016
C47	-0.1337216369	-0.2750818920	3.9433370617	H68	-2.5628808251	4.5178683587	9.8988863957
N48	-1.7732975431	-2.5121932488	3.7830868488	C69	1.0295086249	3.4318890368	14.6575200711
C49	-1.5088083846	-0.1550870106	3.6918488993	H70	1.6520408092	3.3696041559	13.7612314947
C50	0.3575200505	-1.5572058350	4.2271742678	H71	1.2029541587	2.5311850950	15.2548426969
C51	-0.4778344318	-2.6548487433	4.1380975127	H72	1.3826478061	4.2842746799	15.2480036194
C52	-2.3000024985	-1.2805553293	3.6106380201	C73	-1.2936520038	3.6412527266	15.5782425392
H53	-1.9724705951	0.8067168405	3.5031507013	H74	-1.0164363840	4.5154992241	16.1781867375
H54	1.3892071962	-1.7232327151	4.5183482591	H75	-1.1467039890	2.7531048348	16.2011876438
H55	-0.1349803222	-3.6667954805	4.3248154165	H76	-2.3622394126	3.7270240916	15.3562342267
H56	-3.3580792449	-1.2371371892	3.3776542745	C77	-1.4275758103	6.0181472947	8.8750099336
C57	-2.7528614115	-4.3965933496	-2.3386547617	H78	-1.1022988724	7.0572605255	8.9987097445
H58	-2.2498630665	-5.3070732169	-2.6716174551	H79	-1.9541263955	5.9563782593	7.9175012087
H59	-3.7651523171	-4.4052685113	-2.7461561558	H80	-0.5290048970	5.3973544628	8.8126273568
C60	-2.6158158484	-3.7160518108	3.4527513839	C81	-3.6423847378	6.3637917159	10.0020682548
H61	-2.1723221311	-4.5648993593	3.9757773968	H82	-4.2936060611	6.0931904133	10.8409861133
H62	-3.6036087371	-3.5363346658	3.8825894264	H83	-4.1883953876	6.1698336290	9.0721040213
C63	-2.6673787389	-3.9185581072	1.9568790734	H84	-3.4649172346	7.4435981036	10.0660254757
C64	-2.7339450552	-4.2458393925	-0.8357462935				
C65	-3.6854059038	-3.3343378074	1.1958483164				
C66	-1.7002401285	-4.6929334859	1.3097434992				
C67	-1.7359235904	-4.8585279517	-0.0716426472	[1 ⊂ CBPQT] ⁴⁺			
C68	-3.7155885620	-3.4917882914	-0.1858911608	N1	-0.5094367915	3.8100686712	8.7994230042
H69	-4.4884528393	-2.7852463738	1.6821049224	N2	-2.8109398632	-1.0688990560	4.3071517912
H70	-0.9327935541	-5.2057488447	1.8845290019	N3	-6.0169920776	3.6238889331	1.3531505518
H71	-1.0010912074	-5.5054470572	-0.5453358577	N4	-3.4071140034	8.5605675050	5.6647376833
H72	-4.5347191130	-3.0536241443	-0.7511188564	C5	-2.7117116930	9.3188428140	6.7605801254
C173	2.4969040567	2.1724800800	-6.6809654406	H6	-3.4818883859	9.8832758427	7.2980003542
C174	0.0543351515	-6.2376373688	-2.7327914046	H7	-2.0401114496	10.0336109685	6.2815474316
C175	2.0517911860	4.7464891686	5.5535860886	C8	-1.9859853519	8.3383804654	7.6474666450
C176	-5.3481594243	-1.8321881469	3.9312876430	C9	-2.6597514728	7.6677072826	8.6735928248
				H10	-3.6747579799	7.9550481333	8.9458817807
				C11	-2.0431663527	6.6272731701	9.3612505302
				H12	-2.5770437067	6.1008293714	10.1525656334

C13	-0.7401359587	6.2421683091	9.0346778797	C115	-5.7220316910	5.0043929931	8.2721718304
C14	-0.0331449211	6.9739167656	8.0776592883	H116	-6.5294149971	4.3951122411	7.8648668432
C15	-0.6519406842	8.0110529382	7.3874579219	H117	-6.0584348890	6.0474449978	8.2699551079
H16	-0.0890283028	8.5667462983	6.6406257156	C118	-5.3813634929	4.5939275085	9.6791463035
C17	-0.1494759245	4.9980322258	9.6420914437	H119	-4.6881835221	5.3252114191	10.1294823101
H18	0.9406745064	5.0319786141	9.6945863503	H120	-6.3064345398	4.6112738455	10.2758091589
H19	-0.5379938338	4.7991685952	10.6490768818	C121	-4.7631645204	2.6810074681	10.9339511191
C20	0.3725698998	3.3036936570	7.9098274218	H122	-4.1472857683	1.7848755693	10.7984180799
H21	1.3633719703	3.7454734563	7.9084910924	H123	-5.7705712318	2.3575007603	11.2326744193
C22	0.0163981694	2.2768325780	7.0581503269	C124	-4.1890666589	3.5612690746	12.0199204187
H23	0.7701953095	1.8942949436	6.3789356104	H125	-4.8851662175	4.3669437677	12.2963001794
C24	-1.2773926188	1.7356426044	7.1158116432	H126	-4.0165305981	2.9608941482	12.9221192477
C25	-2.1536913205	2.2696952594	8.0705802776	C127	-2.0943600640	4.5436287033	12.5677119374
H26	-3.1832341190	1.9394993586	8.1661780121	C128	-1.0390200911	3.6863370908	12.9188004862
C27	-1.7602744047	3.3055671765	8.8909017603	C129	-0.1710706726	4.1125708198	13.9339514027
H28	-2.4239378643	3.7297739747	9.6449674448	H130	0.6448315246	3.4644535271	14.2428321339
C29	-1.7424281774	0.6933187831	6.1794750658	C131	-0.3489899206	5.3370341543	14.5607649970
C30	-1.1526139462	0.5184193758	4.9191690960	H132	0.3250712662	5.6453767041	15.3526975222
H31	-0.2904336892	1.0965384147	4.6071661418	C133	-1.3951992056	6.1673588605	14.1776997506
C32	-1.7089467175	-0.3471613835	4.0026100933	H134	-1.5291666346	7.1236669492	14.6763252185
H33	-1.3085143741	-0.4734740711	3.0029679772	C135	-2.2918850460	5.7919554825	13.1680372497
C34	-3.3572239903	-0.9826471584	5.5393541974	C136	-0.8523594002	2.3359652719	12.2654736989
H35	-4.2138668467	-1.6188531122	5.7324271387	H137	-1.5272427071	2.2931345884	11.3979335668
C36	-2.8464609882	-0.1172678820	6.48825243910	C138	-3.4388011602	6.7012249746	12.7899847119
H37	-3.3191264308	-0.0912458394	7.4577023610	H139	-3.9085880609	6.2865260584	11.8830189884
C38	-3.5103142858	-1.8402317152	3.2219918531	C140	0.5770328166	2.1235325800	11.7681872850
H39	-2.7356672542	-2.3251571446	2.6244678070	H141	0.9246056213	2.9376862854	11.1203853750
H40	-4.0953037412	-2.6197832478	3.7132587996	H142	0.6562845991	1.1847518523	11.2112522464
C41	-4.3559371214	-0.8851039888	2.4184948958	H143	1.2890820074	2.0586203683	12.5955208538
C42	-5.6401982594	-0.5375208214	2.8493233610	C144	-1.2545521561	1.2124993491	13.2224232882
H43	-6.0981930337	-1.0637369729	3.6840836249	H145	-0.6257403432	1.2186654679	14.1176255744
C44	-6.3417112678	0.4831449053	2.2185814426	H146	-1.1409770305	0.2333542271	12.7490789627
H45	-7.3388985363	0.7406930719	2.5682781987	H147	-2.2914556221	1.3096230679	13.556759073
C46	-5.7715638740	1.1796845432	1.1480631584	C148	-2.9660133219	8.1172352686	12.672481415
C47	-4.5309945795	0.7666377700	0.6590616515	H149	-2.5658201498	8.6194470720	13.3523497347
H48	-4.1044979339	1.2450197766	-0.2197779831	H150	-3.8005679739	8.7289929610	12.1116654535
C49	-3.8297479406	-0.2573457076	1.2882188331	H151	-2.1801477553	8.1279576483	11.7051703482
H50	-2.8650110175	-0.5675039902	0.8932062701	C152	-4.4926271465	6.7315400386	13.8993174526
C51	-6.4442113927	2.4049933626	0.5840841806	H153	-4.8639284933	5.7331925244	14.1485174872
H52	-7.5327203854	2.3572994284	0.6498885472	H154	-5.3457511857	7.3516651782	13.6116987985
C53	-6.1796711408	2.5840831857	-0.4601762730	H155	-4.0754541324	7.1567909725	14.8169712431
C54	-4.8349892912	4.2169591138	1.0660498879	H156	1.0048587111	6.7318296341	7.8601662697
H55	-4.2899359929	3.8231763737	0.2155878800				
C56	-4.3629343024	5.2649546167	1.8228199135				
H57	-3.4057738362	5.6849384313	1.5380917500				
C58	-5.0833931423	5.7364385534	2.9354865818				
C59	-6.3130359770	5.1062558580	3.1907157384				
H60	-6.9610638572	5.4105181614	4.0029427853				
C61	-6.7516369600	4.0682971408	2.3963571557				
H62	-7.6977292069	3.5669376285	2.5674663205				
C63	-4.5433880433	6.7844705820	3.8248422952				
C64	-3.3226370406	7.4349454287	3.5693070734				
H65	-2.7638532597	7.2763206580	2.6551507153				
C66	-2.7788272089	8.3003916299	4.4963685152				
H67	-1.8280330344	8.7983042712	4.3400049318				
C68	-4.6148724750	8.0049282232	5.9128642561				
H69	-5.0843741855	8.2813149105	6.8500104099				
C70	-5.1944183050	7.1350095221	5.0212918607				
H71	-6.1551963755	6.7162053427	5.2946606153				
O73	-4.5496000634	4.9454525278	7.4400325752				
O74	-4.7969555019	3.3082460612	9.6491852779				
O75	-2.9622483345	4.1278681493	11.5487105450				
H75	-1.3733138631	1.7363022936	0.4579341297				
C97	-1.6067972039	2.2110458877	1.3853786295				
C98	-1.8121122540	2.7905210129	2.4305490817				
C99	-1.9831616404	3.5262914338	3.6339306656				
C100	-0.9964515725	4.4277320656	4.0123595692				
H101	-0.1117377609	4.5333411280	3.3932923250				
C102	-1.1362392594	5.1958076408	5.1786222254				
H103	-0.3433061420	5.8830647002	5.4634887205				
C104	-2.2718752661	5.0968266633	5.9536532279				
H105	-2.3867181231	5.7026805606	6.8467991001				
C106	-3.3007567357	4.1924060950	5.6085478645				
C107	-3.1532865927	3.3644410619	4.4521054967				
C108	-4.1476102566	2.4050590410	4.1576078505				
H109	-4.0312602539	1.7754066733	3.2792183613				
C110	-5.2222279455	2.2545736211	5.0043381396				
H111	-5.9642977536	1.4862091874	4.8016477996				
C112	-5.4007590202	3.0695046885	6.1374614985				
H113	-6.2566102680	2.8939214627	6.7766638494				
C114	-4.4771286965	4.0575317076	6.4223315250				

[1 ⊂ CBPQT]Cl₄

N1	-0.5094383033	3.8100727399	8.7994275358
N2	-2.8109428753	-1.0689000972	4.3071511892
N3	-6.0169918016	3.6238891058	1.3531503736
N4	-3.4071137906	8.5605671013	5.6647379583
C5	-2.7117119968	9.3188427704	6.7605803484
H6	-3.4818883859	9.8832758427	7.2908003542
H7	-2.0401114496	10.0336109685	6.2815474316
C8	-1.9859851340	8.3383804877	7.6474664913
C9	-2.6597514728	7.6677072826	8.6735928248
H10	-3.6747579799	7.9550481333	8.9458817807
C11	-2.0431663527	6.6272731701	9.3612505302
H12	-2.5770437067	6.1008293714	10.1525656334
C13	-0.7401359587	6.2421683091	9.0346778796
C14	-0.0331449211	6.9739167656	8.0776592883
C15	-0.6519406842	8.0110529382	7.3874579219
H16	-0.0890283028	8.5667462983	6.6406257156
C17	-0.1494759245	4.9980322258	9.6420914437
H18	0.9406745064	5.0319786141	9.6945863503
H19	-0.5379938338	4.7991685952	10.6490768818
C20	0.3725698998	3.3036936570	7.9098274218
H21	1.3633719703	3.7454734563	7.9084910924
C22	0.0163981694	2.2768325780	7.0581503269
H23	0.7701953095	1.8942949436	6.3789356104
C24	-1.2773926188	1.7356426044	7.1158116432
C25	-2.1536913205	2.2696952594	8.0705802776
H26	-3.1832341190	1.9394993586	8.1661780121
C27	-1.7602744047	3.3055671765	8.8909017603
H28	-2.4239378643	3.7297739747	9.6449674448
C29	-1.7424281774	0.6933187831	6.1794750658
C30	-1.1526139462	0.5184193758	4.9191690960
H31	-0.2904336892	1.0965384147	4.6071661418
C32	-1.7089467175	-0.3471613835	4.0026100933
H33	-1.3085143741	-0.4734740711	3.0029679772
C34	-3.3572239903	-0.9826471584	5.5393541974
H35	-4.2138668467	-1.6188531122	5.7324271387
C36	-2.8464609882	-0.1172678820	6.48825243910
H37	-3.3191264308	-0.0912458394	7.4577023610
C38	-3.5103142858	-1.8402317152	3.2219918531
H39	-2.7356672542	-2.3251571446	2.6244678070
H40	-4.0953037412	-2.6197832478	3.7132587996
C41	-4.3559371214	-0.8851039888	2.4184948958
C42	-5.6401982594	-0.5375208214	2.8493233610
H43	-6.0981930337	-1.0637369729	3.6840836249
C44	-6.3417112678	0.4831449053	2.2185814426
H45	-7.3388985363	0.7406930719	2.5682781987
C46	-5.7715638740	1.1796845432	1.1480631584
C47	-4.5309945795	0.7666377700	0.6590616515
H48	-4.1044979339	1.2450197766	-0.2197779831
C49	-3.8297479406	-0.2573457076	1.2882188331
H50	-2.8650110175	-0.5675039902	0.8932062701
C51	-6.4442113927	2.4049933626	0.5840841806
H52	-7.5327203854	2.3572994284	0.6498885472
C53	-6.1796711408	2.5840831857	-0.4601762730
C54	-4.8349892912	4.2169591138	1.0660498879
H55	-4.2899359929	3.8231763737	0.2155878800
C56	-4.3629343024	5.2649546167	1.8228199135
H57	-3.4057738362	5.6849384313	1.5380917500
C58	-5.0833931423	5.7364385534	2.9354865818
C59	-6.3130359770	5.1062558580	3.1907157384
H60	-6.9610638572	5.4105181614	4.0029427853
C61	-6.7516369600	4.0682971408	2.3963571557
H62	-7.6977292069	3.5669376285	2.5674663205
C63	-4.5433880433	6.7844705820	3.8248422952
C64	-3.322637040		

C36	-2.8464609880	-0.1172678824	6.4825243910	C138	-3.4388011602	6.7012249746	12.7899847119
H37	-3.3191264308	-0.0912458394	7.4577023610	H139	-3.9085880609	6.2865260584	11.8830189884
C38	-3.5103130708	-1.8402307406	3.2219913029	C140	0.5770324613	2.1235324701	11.7681869560
H39	-2.7356672541	-2.3251571446	2.6244678070	H141	0.9246069987	2.9376860782	11.1203825571
H40	-4.0953026842	-2.6197797901	3.7132613893	H142	0.6562845991	1.1847518523	11.2112522464
C41	-4.3559372810	-0.8851049079	2.4184939712	H143	1.2890820074	2.0586203683	12.5955208538
C42	-5.6401982817	-0.5375208665	2.8493233309	C144	-1.254521561	1.2124993491	13.2224232882
H43	-6.0981930337	-1.0637369728	3.6840836250	H145	-0.6257403432	1.2186654679	14.1176255744
C44	-6.3417112677	0.4831449053	2.2185814427	H146	-1.1409770305	0.2333542271	12.7490789627
H45	-7.3388985363	0.7406930719	2.5682781987	H147	-2.2914556221	1.3096230679	13.5567759073
C46	-5.7715638742	1.1796845430	1.1480631584	C148	-2.9660133219	8.1172352686	12.4672481415
C47	-4.5309945795	0.7666377701	0.6590616516	H149	-2.5658201498	8.6194470720	13.3523497347
H48	-4.1044979339	1.2450197766	-0.2197779831	H150	-3.8005679739	8.7289929610	12.1116654535
C49	-3.8297479407	-0.2573457078	1.2882188329	H151	-2.1801477553	8.1279576483	11.7051703482
H50	-2.8650110175	-0.5675039901	0.8932062701	C152	-4.4926271465	6.7315400386	13.8993174526
C51	-6.4442134738	2.4049920284	0.5840848526	H153	-4.8639284933	5.7331925244	14.1485174872
H52	-7.5327203856	2.3572994284	0.6498885473	H154	-5.3457511857	7.3516651782	13.6116987985
H53	-6.1796692867	2.5840845371	-0.4601760570	H155	-4.0754541324	7.1567909725	14.8169712431
C54	-4.8349894573	4.2169590376	1.0660490467	H156	1.0048587111	6.7318296341	7.8601662697
H55	-4.2899359929	3.8231763737	0.2155878799	C157	-6.0116363963	8.4283274404	8.7606711107
C56	-4.3629343514	5.2649546840	1.8228198508	C158	3.0612886907	4.4686195190	9.0272968135
H57	-3.4057738362	5.6849384313	1.5380917500	C159	-5.6921823974	-3.1379713963	5.4364724356
C58	-5.0833931423	5.7364385534	2.9354865818	C160	-3.5973849137	3.1401100334	-1.6188297270
C59	-6.3130359770	5.1062558580	3.1907157384				
H60	-6.9610638572	5.4105181614	4.0029427853				
C61	-6.7516367937	4.0682969601	2.3963573498				
H62	-7.6977292069	3.5669376285	2.5674663205				
C63	-4.5433880433	6.7844705820	3.8248422952				
C64	-3.3226370406	7.4349454288	3.5693070734				
H65	-2.7638532597	7.2763206580	2.6551507153				
C66	-2.7788269360	8.3003917450	4.4963681925				
H67	-1.8280330344	8.7983042712	4.3400049318				
C68	-4.6148729025	8.0049284866	5.9128642053				
H69	-5.0843741855	8.2813149105	6.8500104099				
C70	-5.1944183051	7.1350095222	5.0212918606				
H71	-6.1551963755	6.7162053427	5.2946606153				
O73	-4.5496000545	4.9454525303	7.4400325798				
O74	-4.7969555019	3.3082460612	9.6491852779				
O75	-2.9622483157	4.1278681931	11.5487105696				
H75	-1.3733138631	1.7363022936	0.4579341297				
C97	-1.6067972039	2.2110458877	1.3853786295				
C98	-1.8121122540	2.7905210129	2.4305490817				
C99	-1.9836164040	3.5262914338	3.6339306656				
C100	-0.9964515725	4.4277320656	4.0123595692				
H101	-0.1117377609	4.5333411280	3.3932923250				
C102	-1.1362392594	5.1958076408	5.1786222254				
H103	-0.3433061420	5.8830647002	5.4634887205				
C104	-2.2718752661	5.0968266633	5.9536532279				
H105	-2.3867181231	5.7026805606	6.8467991001				
C106	-3.3007567357	4.1924060950	5.6085478645				
C107	-3.1532865927	3.3644410619	4.4521054967				
C108	-4.1476102566	2.4050590410	4.1576078505				
H109	-4.0312602539	1.7754066733	3.2792183613				
C110	-5.2222794555	2.2545736211	5.0043381396				
H111	-5.9642977536	1.4862091874	4.8016477996				
C112	-5.4007590202	3.0695046885	6.1374614985				
H113	-6.2566102680	2.8939214627	6.7766638494				
C114	-4.4771286965	4.0575317076	6.4223315250				
C115	-5.7220316910	5.0043929931	8.2721718304				
H116	-6.5294149971	4.3951122411	7.8648668432				
H117	-6.0584348890	6.0474449978	8.2699551079				
C118	-5.3813634929	4.5939275085	9.6791463035				
H119	-4.6881835221	5.3252114191	10.1294823101				
H120	-6.3064345398	4.6112738455	10.2758091589				
C121	-4.7631645204	2.6810074681	10.9339511191				
H122	-4.1472857683	1.7848755693	10.7984180799				
H123	-5.7705712318	2.3575007603	11.2326744193				
C124	-4.1890666589	3.5612690746	12.0199204187				
H125	-4.8851662175	4.3669437677	12.2963001794				
H126	-4.0165305981	2.9608941482	12.9221192477				
C127	-2.0943600640	4.5436287033	12.5677119374				
C128	-1.0390200911	3.6863370908	12.9188004862				
C129	-0.1710706726	4.1125708198	13.9339514027				
H130	0.6448315246	3.4644535271	14.2428321339				
C131	-0.3489899206	5.3370341543	14.5607649970				
H132	0.3250712662	5.6453767041	15.3526975222				
C133	-1.3951992056	6.1673588605	14.1776997506				
H134	-1.5291666346	7.1236669492	14.6763252185				
C135	-2.2918850460	5.7919554825	13.1680372497				
C136	-0.8523592615	2.3359654645	12.2654740154				
H137	-1.5272427071	2.2931345884	11.3979335668				

c) PBE optimizations

CBPQT⁴⁺

C1	2.5572087855	4.0836418268	-1.9693927614
C2	2.9336762399	4.2093533381	0.8331392266
C3	3.6634625537	3.4529389546	-1.3688059861
C4	1.6705691162	4.8210680100	-1.1607178578
C5	1.8534586740	4.8787015876	0.2272022005
C6	3.8528491347	3.5202140961	0.0178820517
H7	4.4086144348	2.9347950547	-1.9816783783
H8	0.8508384280	5.3914563476	-1.6106870474
H9	1.1657113847	5.4825168455	0.8285425885
H10	4.7485198259	3.0631574118	0.4523977724
C11	2.3232878584	3.9721796907	-3.4692823777
H12	3.2632101631	3.8904086388	-4.0345558336
H13	1.7606111135	4.8303682475	-3.8676555501
C14	3.1071045237	4.2318531606	2.3450659505
H15	4.1595795904	4.1117196994	2.6448484767
H16	2.7295861020	5.1613558150	2.7956793920
N17	2.3365020195	3.0903699614	2.9815626980
C18	0.7555113608	0.9025107541	3.7548439852
C19	2.8322949853	1.8269939490	2.8894750335
C20	1.1179774324	3.2999797225	3.5485355798
C21	0.3152785833	2.2312652718	3.9444049289
C22	2.0715015348	0.7284556358	3.2692163351
H23	3.8379336504	1.7256762373	2.4766820325
H24	0.8001249068	4.3393294709	3.6609658323
H25	-0.6505175732	2.4613908201	4.4020923520
H26	2.5071349596	-0.2639711022	3.1328801206
N27	1.5117641703	2.7297597054	-3.7842740741
C28	0.0554625106	0.3338126129	-3.9253069879
C29	2.1200604200	1.5898470652	-4.2094958792
C30	0.1745377207	2.7315178181	-3.5350679985
C31	-0.5694363051	1.5597998974	-3.6026098993
C32	1.4186566551	0.3884198401	-4.2917754264
H33	3.1800442915	1.6639213250	-4.4643289622
H34	-0.2684548638	3.6885524207	-3.2523571264
H35	-1.6309400587	1.6149666910	-3.3505042847
H36	1.9573620911	-0.4936773145	-4.6479614844
C37	-0.6787636130	-0.9538689521	-3.7560986469
N38	-2.0577701770	-3.2764878018	-2.9903875171
C39	-2.0803399178	-1.0571910249	-3.8981032403
C40	0.0071727979	-2.1118410553	-3.3241140722
C41	-0.6985329357	-3.2473678319	-2.9462839228
C42	-2.7415402985	-2.2205883842	-3.5077639241
H43	-2.6808714511	-0.2440113717	-4.3142991019
H44	1.0951328818	-2.1327638331	-3.2278482941
H45	-0.2026761849	-4.1452934064	-2.5721162502
H46	-3.8262759476	-2.3275616785	-3.5847266906
C47	-0.1410046858	-0.2770373512	3.9297325561
N48	-1.7920081402	-2.5438256534	3.7929036447
C49	-1.5263057234	-0.1669817341	3.6721362985
C50	0.3512299882	-1.5653065730	4.2362171144
C51	-0.4878762041	-2.6749634988	4.1567526627
C52	-2.3214720223	-1.3048379377	3.6058334221
H53	-1.9990011324	0.7970623331	3.4705905042
H54	1.3875762019	-1.7304375424	4.5424403089
H55	-0.1348637674	-3.6879018083	4.3647417652
H56	-3.3872324170	-1.2588731796	3.3731787104
C57	-2.7902859409	-4.4429330510	-2.3544459156
H58	-2.2861420727	-5.3601599153	-2.6956893879
H59	-3.8096986022	-4.4419717755	-2.7673897721
C60	-2.6362602926	-3.7640439989	3.4771371474
H61	-2.1782782299	-4.6137104014	4.0043514040
H62	-3.6297242252	-3.5867626578	3.9169441429
C63	-2.7041907570	-3.9846213981	1.9725170147
C64	-2.7795415122	-4.3107430801	-0.8382512986
C65	-3.7421274851	-3.4101479174	1.2128638780
C66	-1.7335875636	-4.7669541372	1.3184492382
C67	-1.7743206954	-4.9328770095	-0.0725799599
C68	-3.7764824689	-3.5665811284	-0.1787955338
H69	-4.5573985327	-2.8685645494	1.7046434807
H70	-0.9581846681	-5.2855234515	1.8921274249
H71	-1.0360662911	-5.5866154224	-0.5495476318
H72	-4.6103185959	-3.1332806524	-0.7411551015

CBPQT Cl₄

C1	2.5572087855	4.0836418268	-1.9693927614
C2	2.9336762399	4.2093533381	0.8331392266
C3	3.6634625537	3.4529389546	-1.3688059861
C4	1.6705691162	4.8210680100	-1.1607178578
C5	1.8534586740	4.8787015876	0.2272022005
C6	3.8528491347	3.5202140961	0.0178820517
H7	4.4086144348	2.9347950547	-1.9816783783
H8	0.8508384280	5.3914563476	-1.6106870474
H9	1.1657113847	5.4825168455	0.8285425885
H10	4.7485198259	3.0631574118	0.4523977724
C11	2.3232878584	3.9721796907	-3.4692823777
H12	3.2632101631	3.8904086388	-4.0345558336
H13	1.7606111135	4.8303682475	-3.8676555501
C14	3.1071045237	4.2318531606	2.3450659505
H15	4.1595795904	4.1117196994	2.6448484767
H16	2.7295861020	5.1613558150	2.7956793920
N17	2.3365020195	3.0903699614	2.9815626980
C18	0.7555113608	0.9025107541	3.7548439852
C19	2.8322949853	1.8269939490	2.8894750335
C20	1.1179774324	3.2999797225	3.5485355799
C21	0.3152785833	2.2312652718	3.9444049289
C22	2.0715015348	0.7284556358	3.2692163351
H23	3.8379336504	1.7256762373	2.4766820325
H24	0.8001249068	4.3393294709	3.6609658323
H25	-0.6505175732	2.4613908201	4.4020923520
H26	2.5071349596	-0.2639711022	3.1328801206
N27	1.5117641703	2.7297597054	-3.7842740741
C30	0.1745377207	2.7315178181	-3.5350679985
C31	-0.5694363051	1.5597998974	-3.6026098993
C32	1.4186566551	0.3884198401	-4.2917754264
H33	3.1800442915	1.6639213250	-4.4643289622
H34	-0.2684548638	3.6885524207	-3.2523571264
H35	-1.6309400587	1.6149666910	-3.3505042847
H36	1.9573620911	-0.4936773145	-4.6479614844
C37	-0.6787636130	-0.9538689521	-3.7560986469
N38	-2.0577701770	-3.2764878018	-2.9903875171
C39	-2.0803399178	-1.0571910249	-3.8981032403
C40	0.0071727979	-2.1118410553	-3.3241140722
C41	-0.6985329357	-3.2473678319	-2.9462839228
C42	-2.7415402985	-2.2205883842	-3.5077639241
H43	-2.6808714511	-0.2440113717	-4.3142991019
H44	1.0951328818	-2.1327638331	-3.2278482941
H45	-0.2026761849	-4.1452934064	-2.5721162502
H46	-3.8262759476	-2.3275616785	-3.5847266906
C47	-0.1410046858	-0.2770373512	3.9297325561
N48	-1.7920081402	-2.5438256534	3.7929036447
C49	-1.5263057234	-0.1669817341	3.6721362985
C50	0.3512299882	-1.5653065730	4.2362171144
C51	-0.4878762041	-2.6749634988	4.1567526627
C52	-2.3214720223	-1.3048379377	3.6058334221
H53	-1.9990011324	0.7970623331	3.4705905042
H54	1.3875762019	-1.7304375424	4.5424403089
H55	-0.1348637674	-3.6879018083	4.3647417652
H56	-3.3872324170	-1.2588731796	3.3731787103
C57	-2.7902859409	-4.4429330510	-2.3544459156
H58	-2.2861420727	-5.3601599153	-2.6956893879
H59	-3.8096986022	-4.4419717755	-2.7673897721
C60	-2.6362602926	-3.7640439989	3.4771371474
H61	-2.1782782299	-4.6137104014	4.0043514040
H62	-3.6297242252	-3.5867626578	3.9169441429
C63	-2.7041907570	-3.9846213981	1.9725170147
C64	-2.7795415122	-4.3107430801	-0.8382512986
C65	-3.7421274851	-3.4101479174	1.2128638780
C66	-1.7335875636	-4.7669541372	1.3184492382
C67	-1.7743206954	-4.9328770095	-0.0725799599
C68	-3.7764824689	-3.5665811284	-0.1787955338
H69	-4.5573985327	-2.8685645494	1.7046434807
H70	-0.9581846681	-5.2855234515	1.8921274249
H71	-1.0360662911	-5.5866154224	-0.5495476318
H72	-4.6103185959	-3.1332806524	-0.7411551015

O2	-5.0777059346	3.2280909492	7.8705761429
O3	-4.2420171537	2.1574178122	10.3873924394
O4	-2.0700507871	3.5861961750	11.8436898149
H4	-3.9362601023	3.9257591221	-0.3426584973
C26	-3.8356583257	3.9661420506	0.7240201164
C27	-3.7160580178	4.0138647947	1.9400357875
C28	-3.5564068692	4.0787372047	3.3574495277
C29	-2.4153267267	4.6830596195	3.8977801656
H30	-1.6660845343	5.0971052501	3.2180817288
C31	-2.2242778835	4.7537653487	5.2939674259
H32	-1.3189340287	5.2218121976	5.6917313829
C33	-3.1712066329	4.2298189395	6.1605435969
H34	-3.0231815360	4.2673677758	7.2420067398
C35	-4.3489022643	3.6178371961	5.6544403617
C36	-4.5583383395	3.5241954812	4.2358772465
C37	-5.7303871280	2.8879049381	3.7408969289
H38	-5.8763907014	2.8206340155	2.6601420796
C39	-6.6577957767	2.3627007007	4.6212233670
H40	-7.556131293	1.8692069465	4.2367685483
C41	-6.4773893933	2.4485725723	6.0248070764
H42	-7.2339979879	2.0250529594	6.6877564408
C43	-5.3454872254	3.0723947290	6.5366570467
C44	-5.9714088863	2.6129096818	8.8000485847
H45	-6.0263480993	1.5232978912	8.6127581426
H46	-6.9893238062	3.0410443262	8.7003862836
C47	-5.4585807102	2.8686646228	10.2051439860
H48	-5.3293913660	3.9602331763	10.3566636812
H49	-6.2345663926	2.5185933846	10.9217510670
C50	-3.8675582483	1.9950544613	11.7502930051
H51	-3.0747127862	1.2281455581	11.7511120795
H52	-4.7227070014	1.6104318399	12.3496779100
C53	-3.3331625936	3.2490371810	12.4332162708
H54	-4.0431626962	4.0951424193	12.3392493583
H55	-3.2149654223	3.0416329011	13.5179032994
C56	-1.5400682851	4.7885592430	12.3163154514
C57	-0.6840432660	4.7639159357	13.4417958920
C58	-0.1453475420	5.9853966570	13.8820651354
H59	0.5219363774	5.9949163888	14.7509982665
C60	-0.4423437603	7.1845287982	13.2260328360
H61	-0.0163178136	8.1259342778	13.5867703376
C62	-1.2719164767	7.1777132530	12.0997877880
H63	-1.4834535374	8.1177202116	11.5783393275
C64	-1.8328212755	5.9824039806	11.6170340362
C65	-0.3285575293	3.4546684160	14.1392486963
H66	-0.8449632766	2.6477216427	13.5920882971
C67	-2.7021239429	5.9722400878	10.3636206092
H68	-2.9620103984	4.9191230135	10.1586330832
C69	1.1842614757	3.1695665211	14.0550753182
H70	1.5273755112	3.1475819181	13.0086267261
H71	1.4225414556	2.1957915436	14.5158885481
H72	1.7687588669	3.9411052686	14.5848334687
C73	-0.8106616665	3.4366707310	15.6033730066
H74	-0.3078975504	4.2179000562	16.1993855276
H75	-0.5895221221	2.4642209962	16.0752342896
H76	-1.8966075273	3.6140330266	15.6757554987
C77	-1.9257721526	6.5050217161	9.1424673829
H78	-1.6286992250	7.5588574739	9.2809084796
H79	-2.5479212792	6.4518364603	8.2329110304
H80	-1.0090269982	5.9186363160	8.9687476051
C81	-4.0071403305	6.7674396763	10.5680066848
H82	-4.5824044318	6.3927426553	11.4317593999
H83	-4.6471998070	6.6994297402	9.6719382431
H84	-3.8003847550	7.8361491856	10.7511365769

[1 ⊂ CBPQT]⁴⁺

N1	-0.4193485555	3.7407313494	8.7440545466
N2	-2.7783696667	-1.2537197562	4.3295340738
N3	-6.0333715616	3.7040294979	1.3780470919
N4	-3.4810831110	8.7368129789	5.6814102637
C5	-2.7150611409	9.4289951426	6.7912266654
H6	-3.4539769960	9.9807229018	7.3919267190
H7	-2.0513935024	10.1634144044	6.3115885473
C8	-1.9488320109	8.4037982885	7.6147385177
C9	-2.5767850805	7.7284632784	8.6789260966
H10	-3.5699629397	8.0380487340	9.0205155723
C11	-1.9433380359	6.6550082332	9.3191150571
H12	-2.4529329470	6.1343013709	10.1361575908
C13	-0.6621409617	6.2360812719	8.9121274586

C14	0.0169780013	6.9899314512	7.9348482047
C15	-0.6208052921	8.0608841198	7.2910007018
H16	-0.0728289896	8.6286183308	6.5310985931
C17	-0.0417354603	4.9865932394	9.5165727538
H18	1.0570851263	5.0337838476	9.5157587638
H19	-0.3803810009	4.8249776393	10.5554366893
C20	0.4945127118	3.1090437392	7.9561741099
H21	1.5097688598	3.5119543211	7.9627468783
C22	0.1430846311	2.0060037721	7.1847076373
H23	0.9268612261	1.5319052642	6.5901756067
C24	-1.1839554296	1.5178118259	7.1953485939
C25	-2.0868282522	2.1615740927	8.0698219016
H26	-3.1375708230	1.8717053131	8.1417209782
C27	-1.6899072092	3.2590771336	8.8277600834
H28	-2.3761470008	3.7573735731	9.5223965009
C29	-1.6519766714	0.4517213595	6.2657923952
C30	-1.0726042215	0.2975030885	4.9855369397
H31	-0.2047929283	0.8831877304	4.6737708109
C32	-1.6538319869	-0.5415914655	4.0416588374
H33	-1.2612775849	-0.6326740567	3.0273902669
C34	-3.2961976255	-1.2120709914	5.5887383113
H35	-4.1599987578	-1.8521847650	5.7811666047
C36	-2.7568356994	-0.3803145771	6.5646852941
H37	-3.2143422692	-0.3905614642	7.5563066262
C38	-3.5255574792	-1.9576339757	3.2122370241
H39	-2.7705830024	-2.4485116229	2.5793639778
H40	-4.1375727754	-2.7417069697	3.6823659641
C41	-4.3610759947	-0.9477941195	2.4384064517
C42	-5.6335958784	-0.5575314772	2.9030995369
H43	-6.0999240163	-1.0850423292	3.7419447240
C44	-6.3186291203	0.5046007516	2.2993919707
H45	-7.3048263066	0.7883447953	2.6805917039
C46	-5.7508163987	1.2013844334	1.2136484057
C47	-4.5423529323	0.7264017380	0.6708601093
H48	-4.1306673131	1.1771540084	-0.2382584560
C49	-3.8532162610	-0.3348785402	1.2777958849
H50	-2.9167621440	-0.6877956097	0.8333256493
C51	-6.4255018933	2.4384111827	0.6385719262
H52	-7.5218545775	2.3725445251	0.6942391442
H53	-6.1523447609	2.5973096609	-0.4163467563
C54	-4.7858804287	4.2268227438	1.2080415226
H55	-4.1317487433	3.7155899687	0.4993292072
C56	-4.3611300762	5.3328726236	1.9310968454
H57	-3.3398888577	5.6658217887	1.7705783512
C58	-5.2033201302	5.9499587879	2.8894704160
C59	-6.5119865052	5.4172239344	2.9939930722
H60	-7.2654241119	5.8606239450	3.6490054464
C61	-6.8947529334	4.3103298206	2.2431391743
H62	-7.8990678775	3.8861629199	2.3094180101
C63	-4.6894173875	7.0214121755	3.7847464461
C64	-3.5095798165	7.7514966069	3.4931828982
H65	-3.0171375881	7.6851880730	2.5205087323
C66	-2.9288862206	8.5819063892	4.4449071260
H67	-2.0049467297	9.1310181060	4.2503274482
C68	-4.6775481709	8.1426074067	5.9515035420
H69	-5.1062546741	8.3447326696	6.9338128087
C70	-5.2943704788	7.3037356413	5.0334747841
H71	-6.2304035315	6.8312421438	5.3359052857
O73	-4.6097285610	5.0761496485	7.3828944989
O74	-4.8934145413	3.3253796762	9.5998910344
O75	-2.9966607107	4.0859483062	11.5469421632
H75	-1.1603319996	1.5824250876	0.5642308883
C97	-1.4497935336	2.0911504040	1.4676034276
C98	-1.7232236653	2.7128966760	2.4865719308
C99	-1.9482641632	3.5271590370	3.6351033080
C100	-1.0164097741	4.5352133996	3.9122377506
H101	-0.1437811254	4.6484305324	3.2642176280
C102	-1.2009668454	5.3877629886	5.0196242533
H103	-0.4526911150	6.1552045006	5.2340964714
C104	-2.3179405889	5.2616590299	5.8359372448
H105	-2.4545494805	5.9248379681	6.6900700678
C106	-3.2922501794	4.2584465268	5.5887798761
C107	-3.1020938687	3.3504851416	4.4880241111
C108	-4.0452501229	2.3103748117	4.2754058919
H109	-3.9107836939	1.6375454689	3.4261285437
C110	-5.1039493471	2.1470965861	5.1550289852
H111	-5.8080314285	1.3238872088	5.0083030655
C112	-5.3129917130	3.0230897966	6.2451440551
H113	-6.1403184162	2.8278394469	6.9274357346
C114	-4.4546139726	4.1028518443	6.4353760395
C115	-5.7942234107	5.0813830405	8.2220874001

C140	0.5638199803	1.9965581198	11.8062859970
H141	0.9173782743	2.7576228543	11.0885685026
H142	0.6047583279	1.0103298606	11.3144830693
H143	1.2955247404	1.9696750325	12.6301611893
C144	-1.2708029542	1.2092437967	13.3590451489
H145	-0.6080252742	1.2465333600	14.2389618733
H146	-1.1955253165	0.1980156448	12.9268030500
H147	-2.3020177747	1.3544195944	13.7182342944
C148	-3.1059997076	8.1315940837	12.5542119472
H149	-2.6785524193	8.6328921403	13.4365558640
H150	-3.9924168478	8.7171256284	12.2591513075
H151	-2.3581507391	8.1923112168	11.7463509378
C152	-4.5315512001	6.6456861441	14.0303517906
H153	-4.8631185640	5.6224437155	14.2694959505
H154	-5.4194758194	7.2501469046	13.7830743714
H155	-4.0868121423	7.0677056851	14.9459922280
H156	1.0495006727	6.7064659836	7.6640900662
Cl157	-4.1301200370	3.3829124004	-1.6734798104
Cl158	-5.7093154209	8.4822617411	9.2375881507
Cl159	2.1706952082	4.8376380720	6.2660796326
Cl160	-6.2212808995	-1.0723334661	6.2764171314