

Oxygen-Centered Tetradecaimido Hexatantalum Cluster Complexes

Jamin L. Krinsky, Laura L. Anderson,[†] John Arnold,* and Robert G. Bergman*

Department of Chemistry, University of California, Berkeley, California, 94720

[†]*Department of Chemistry, University of California, Irvine, California, 92697*

Supporting Information

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I. Additional specific experimental procedures.

(PhN)₁₄Ta₆O (2), from compound 1. Compound **1** (100 mg, 0.190 mmol, 1 equiv) was dissolved in 1 mL of benzene. Aniline (89 mg, 0.95 mmol, 5 equiv) was treated with 0.6 μL (0.03 mmol, 0.16 equiv) of degassed water via microsyringe and the resulting mixture was dissolved in 0.5 mL benzene. The two solutions were mixed, and the reaction mixture was transferred to a Kontes reaction vessel. Hexane (4 mL) was then added, causing the formation of a yellow precipitate. The vessel was sealed with a Teflon valve and immersed in a 135 °C oil bath. After a few minutes, most of the yellow solid had dissolved and the solution had developed a red color. After heating for ca. 24 h the reaction vessel was allowed to cool and was transferred to a glove box. The supernatant was removed by pipette and the crystalline product was washed with Et₂O (2 × 2 mL) then pentane (2 × 2 mL). Material collected from the reaction mixture was analytically pure (43 mg, 0.018 mmol, 57%).

(*p*-MeC₆H₄N)₁₄Ta₆O (3), from compound 1. Compound **1** (100 mg, 0.190 mmol, 1 equiv) was dissolved in 1 mL of benzene. *p*-Toluidine (102 mg, 0.950 mmol, 5 equiv) was treated with 0.6 μL (0.03 mmol, 0.16 equiv) of degassed water via microsyringe and the resulting mixture was dissolved in 0.5 mL benzene. The two solutions were mixed, and the reaction mixture was transferred to a Kontes reaction vessel. Hexane (4 mL) was then added, causing the formation of a yellow precipitate. The

vessel was sealed with a Teflon valve and immersed in a 135 °C oil bath. After a few minutes, most of the yellow solid had dissolved and the solution had developed a red color. After heating for ca. 24 h the reaction vessel was allowed to cool and was transferred to a glove box. The supernatant was removed by pipette and the crystalline product was washed with Et₂O (2 × 2 mL) then pentane (2 × 2 mL). Isotopically-enriched samples were prepared in an identical fashion using ¹⁷O/¹⁸O enriched water. Material collected from the reaction mixture was analytically pure (39.2 mg, 0.015 mmol, 48%).

Reaction conditions from which crystals of 7 were obtained. Compound **1** (10.0 mg, 0.019 mmol, 1 equiv) was dissolved in 0.6 mL of C₆D₆, and the solution was added to 13.5 mg (0.106 mmol, 5.56 equiv) of *m*-chloroaniline. The reaction mixture was then transferred to an NMR tube that contained trace tantalum oxide from previous experiments. The NMR tube was flame sealed under reduced pressure and heated at 135 °C in an oil bath for 24 h. The reaction mixture was then allowed to stand at ambient temperature for ca. three weeks during which time red/orange crystals of **7** formed.

Ta(OSiPh₃)₅ (12). Compound **3** (50 mg, 0.019 mmol, 1.0 equiv) was dissolved in 5 mL of benzene and 156 mg (0.564 mmol, 29.0 equiv) of triphenylsilanol were added. The reaction mixture became yellow-orange in color after being stirred for about 1 h. After 2 d, the light yellow solution was cooled to freezing and the solvent was removed under reduced pressure. The resulting amorphous residue was washed with Et₂O (3 × 1 mL), leaving a white powder which was then dissolved with heating in 1 mL of benzene. Pentane vapor (1 mL total) was allowed to diffuse into the benzene solution over 3 d. The supernatant was then decanted and the crystalline **12**·C₆H₆ (103 mg, 0.0629 mmol, 54%) was washed with Et₂O (2 × 1 mL). Some of the crystals were suitable for analysis by X-ray diffraction. ¹H NMR (500 MHz, CD₂Cl₂): δ 7.16 (m, 45H), 6.82 (d, *J* = 7.5 Hz, 30H). ¹³C {¹H} NMR (125.8 MHz, CD₂Cl₂): δ 135.87, 129.77, 128.86, 127.96. Anal. Calcd. for C₉₀H₇₅O₅Si₅Ta·C₆H₆: C, 70.48; H, 4.99. Found: C, 70.38; H, 4.67.

Cp*Cl₂Re=N-*p*-C₆H₄Me (13). Compound **3** (100 mg, 0.0388 mmol, 1.00 equiv) was dissolved in 10 mL of benzene and 223 mg (0.546 mmol, 14.1 equiv) of Cp*Cl₂Re=O was added. The mixture was

transferred to a Pyrex reaction vessel fitted with a vacuum stopcock and heated at 130 °C for 24 h, during which time the solution became deep green in color and a black precipitate formed. NMR tube experiments showed reaction at 75 °C but longer reaction times were necessary at that temperature. Upon cooling, crystalline **13** precipitated. The solvent was removed under vacuum, and the residue was extracted with 15 mL of hot THF. After the extract had cooled to ambient temperature, it was cooled at -30 °C overnight. The supernatant was then removed by pipette and the large green crystals of **13**·0.5THF (176 mg, 0.330 mmol, 61%) were washed with Et₂O (3 × 1 mL). Some of these crystals were suitable for X-ray diffraction analysis. Note: One half of a molecule of THF was located in the asymmetric unit and thus this formulation was used to calculate the yield and elemental analysis. NMR spectra showed that bulk sample only contained 0.43 equivalents of THF per molecule of **13**. ¹H NMR (500 MHz, CD₂Cl₂): δ 7.46 (d, *J* = 8.5 Hz, 2H), 7.12 (d, *J* = 8.5 Hz, 2H), 2.250 (s, 3H), 2.095 (s, 15H). ¹³C {¹H} NMR (125.8 MHz, CD₂Cl₂): δ 155.21, 140.07, 130.75, 123.67, 109.03, 22.30, 12.64. Anal. Calcd. for C₁₇H₂₂Cl₂NRe: C, 41.04; H, 4.46; N, 2.81. Anal. Calcd. for C₁₇H₂₂Cl₂NRe·0.5C₄H₈O: C, 42.77; H, 4.91; N, 2.62. Found: C, 42.19; H, 4.66; N, 2.96.

Cp*Cl₂Re=N-*p*-C₆H₄-*t*-Bu (14). Compound **5** (10 mg, 0.0032 mmol, 1.0 equiv) was dissolved in 0.5 mL of THF-*d*₈, and the solution was added to a vial containing 18 mg (0.044 mmol, 14 equiv) of Cp*Cl₂Re=O. The reaction mixture was then transferred to an NMR tube and flame sealed under reduced pressure. The NMR tube was heated and the reaction was periodically monitored by ¹H NMR. Very little conversion was observed after 7 h at 75 °C; however, signals assigned to **14** were the only observed resonances after the reaction mixture was heated for 14 h at 135 °C. The reaction mixture was filtered and the solvent was removed under reduced pressure (18 mg, 0.033 mmol, 75%). ¹H NMR (500 MHz, CD₂Cl₂): δ 7.50 (d, *J* = 9.0 Hz, 2H), 7.33 (d, *J* = 9.0 Hz, 2H), 2.11 (s, 15H), 1.31 (s, 9H). ¹³C {¹H} NMR (125.8 MHz, CD₂Cl₂): δ 155.08, 152.96, 127.15, 123.44, 109.06, 35.88, 31.04, 12.69. Anal. Calcd. for C₂₀H₂₈Cl₂NRe: C, 44.52; H, 5.23; N, 2.60. Found: C, 44.23; H, 5.12; N, 2.88.

II. Electrospray Mass Spectra for 3 and 4, Including ^{17}O -, ^{18}O -Enriched Samples

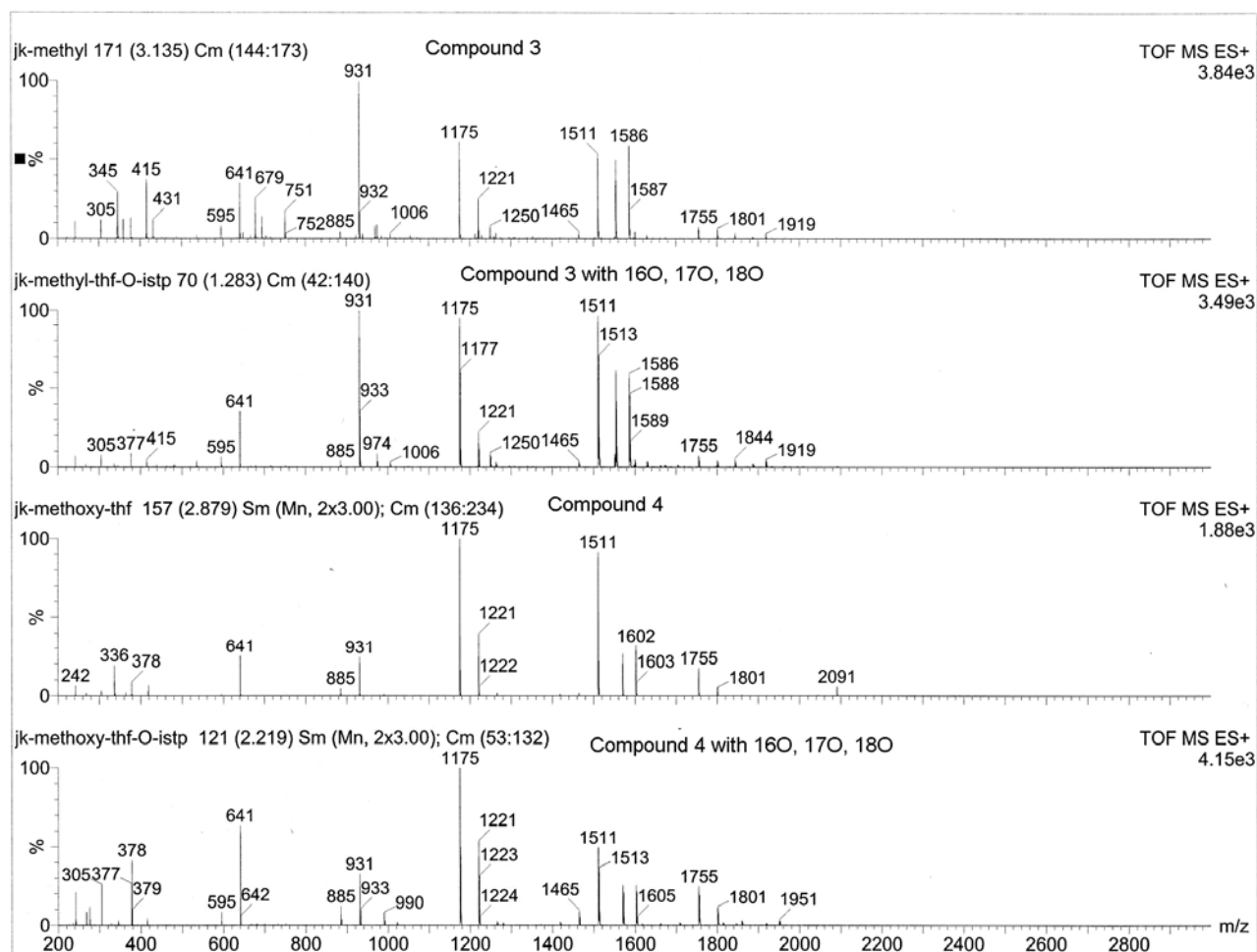


Figure S1. ESI mass spectra of **3**, **3**($^{17,18}\text{O}$), **4**, and **4**($^{17,18}\text{O}$) (from top down, respectively). Full spectral width.

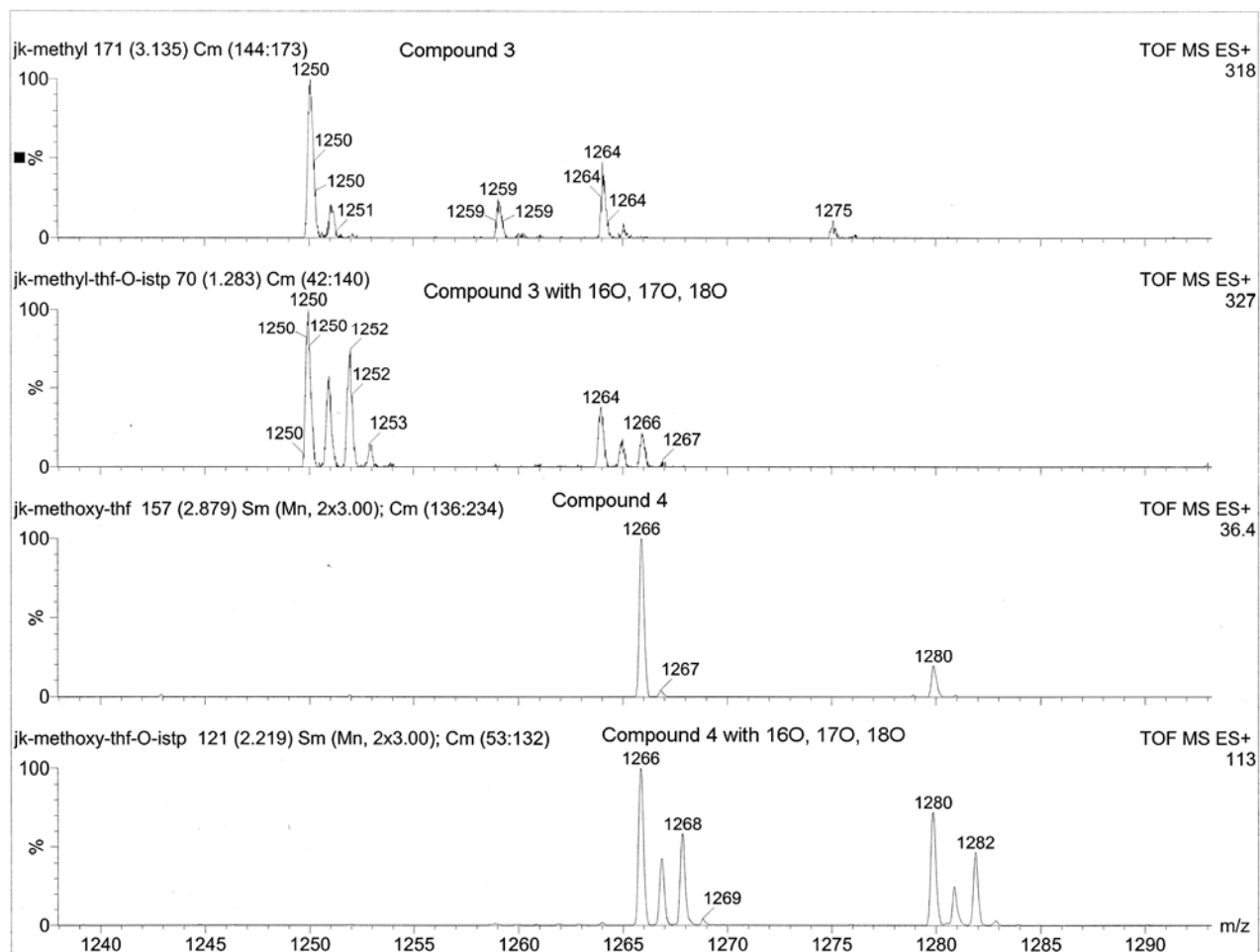


Figure S2. Enlargement #1, showing 16 Da shifts of compound **4** peaks relative to those of **3**.

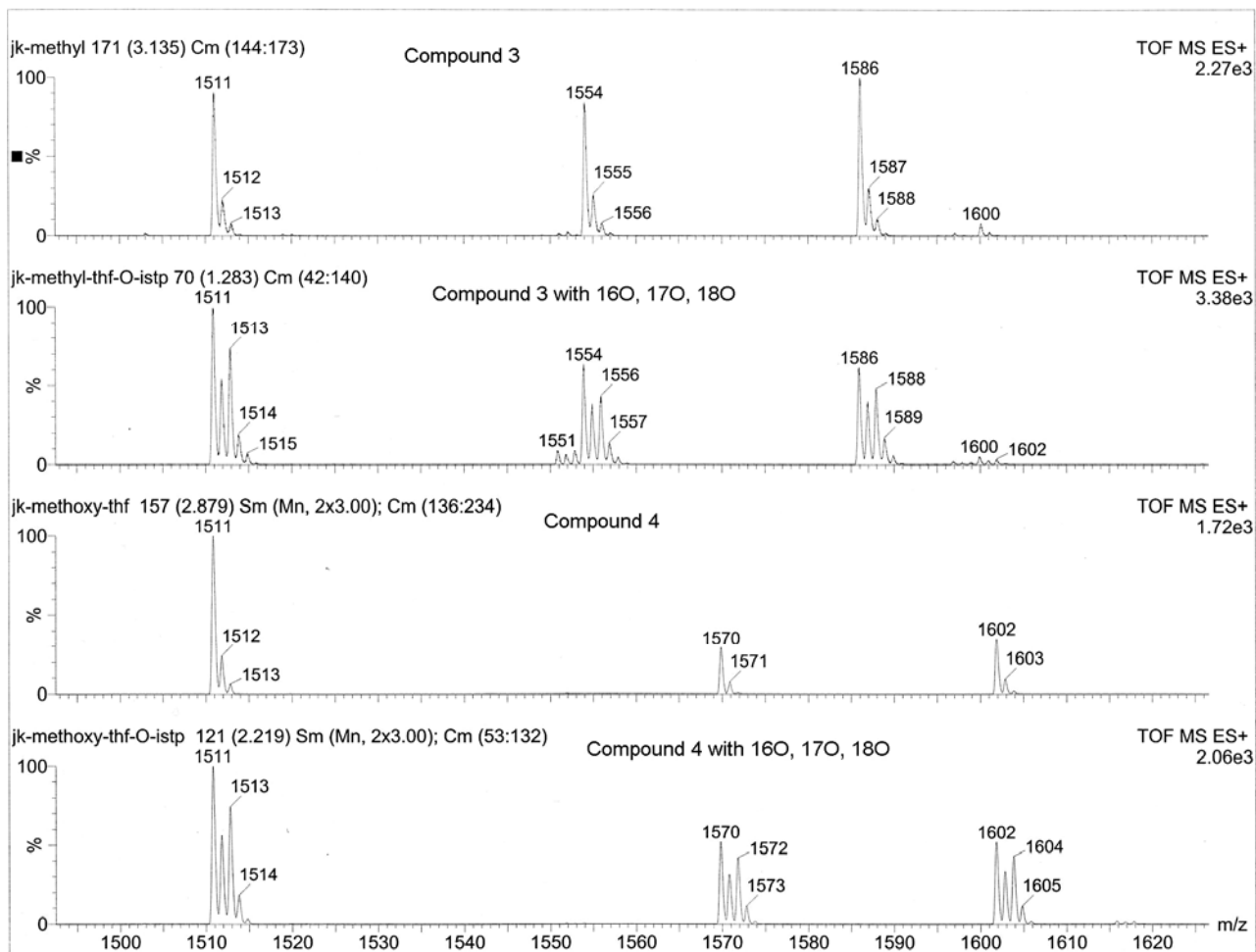


Figure S3. Enlargement #2, showing peak that is common to **3** and **4**, no ligands remaining on cluster core.

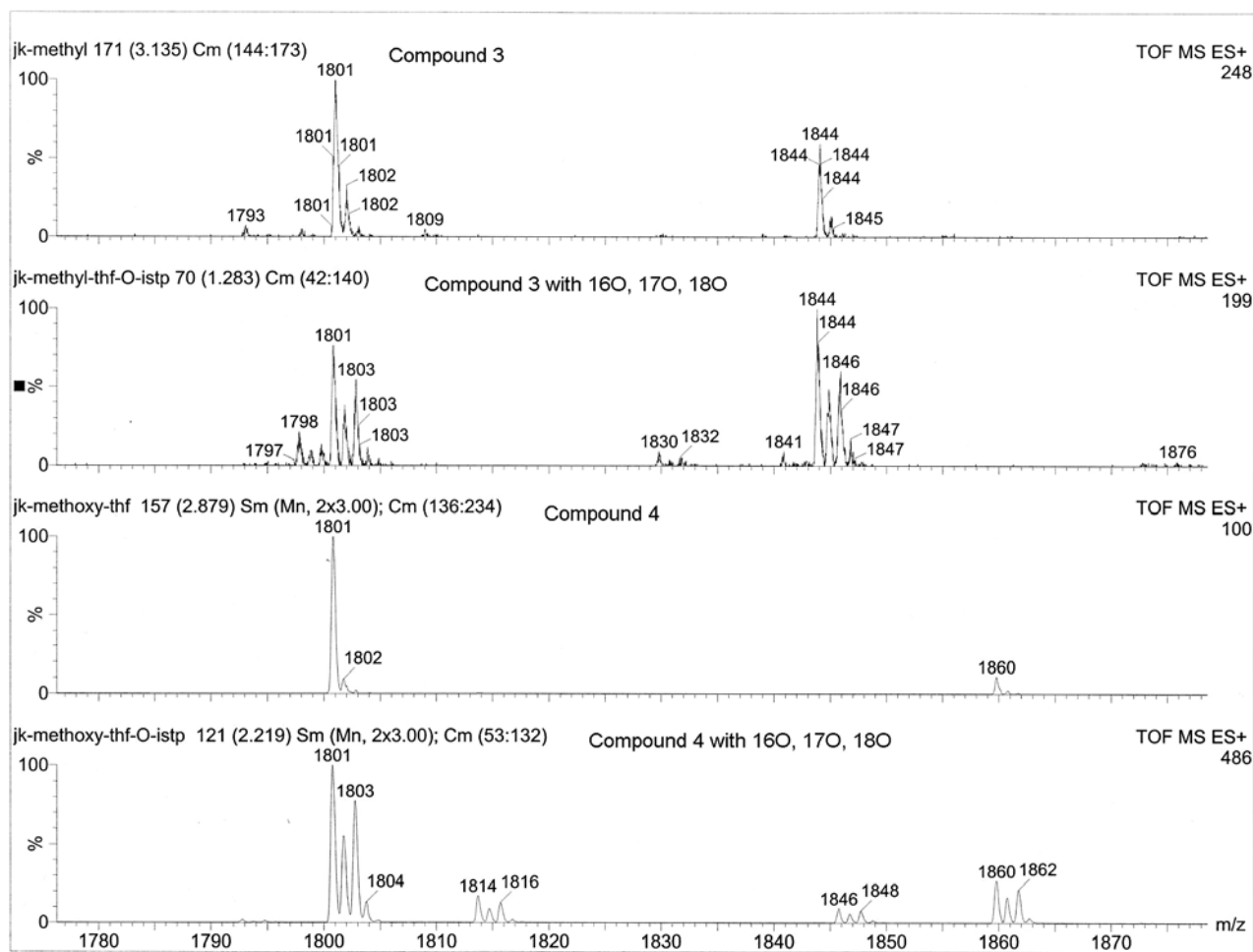


Figure S4. Enlargement #3, showing higher-mass peaks.

III. Positional coordinates of computed structures.

Table S1. Calculated coordinates for optimized **2**, unconstrained.

Ta1	1.2806743833	-0.8537378180	1.5971574106
Ta2	0.1572970891	2.0112842388	0.9697664333
Ta3	-1.8100981746	-0.4348225289	1.1928484134
N4	-0.2459704993	0.4426922028	2.4684537392
N5	2.1322883908	1.0258682528	0.9017255418
N6	2.2963615069	-1.5854991031	2.8718160051
N7	0.2779376663	3.6086951996	1.7607308190
N8	0.4720756545	2.1820154373	-1.1977352550
N9	-1.8999774085	1.6155086839	0.3754197685
N10	-3.2759591765	-0.7994299133	2.1503842702
O11	0.0047097086	0.0131439042	-0.0039601891
C12	-0.3715422756	0.5462608774	3.8923886073
C13	-0.1036635726	1.7391893568	4.5796361817
H14	0.1958538477	2.6207525502	4.0242482342
C15	-0.2215297416	1.7979643395	5.9687029083

H16	-0.0092860434	2.7349305122	6.4771152386
C17	-0.6026969401	0.6737025869	6.7019867278
H18	-0.6909100408	0.7244392244	7.7837884831
C19	-0.8667262502	-0.5185744253	6.0259882814
H20	-1.1612113902	-1.4082868954	6.5768559207
C21	-0.7537674555	-0.5834512471	4.6392821199
H22	-0.9573369144	-1.5201158017	4.1278861355
C23	3.2953218147	1.6978295268	1.3981479109
C24	3.8275348826	1.4091295638	2.6647411592
H25	3.3566410629	0.6545721500	3.2851788691
C26	4.9600439590	2.0773064419	3.1274416764
H27	5.3530276217	1.8317890590	4.1106900731
C28	5.5855391416	3.0469123757	2.3442285083
H29	6.4699321639	3.5624270710	2.7080288185
C30	5.0583213812	3.3472598441	1.0876952903
H31	5.5282747224	4.1019720542	0.4625765007
C32	3.9255116725	2.6851422753	0.6203330722
H33	3.5253327472	2.9298151442	-0.3586589119
C34	3.0635336594	-2.1902246561	3.8451181281
C35	4.0509835853	-3.1278249887	3.4899718331
H36	4.2095927902	-3.3534383514	2.4396899502
C37	4.8158552086	-3.7416295927	4.4772949127
H38	5.5757743384	-4.4647215089	4.1916118154
C39	4.6140501205	-3.4340901375	5.8242182655
H40	5.2141171556	-3.9167714162	6.5909221821
C41	3.6363444193	-2.5029149198	6.1799438918
H42	3.4719301122	-2.2593809537	7.2265762648
C43	2.8626420560	-1.8817657770	5.2033906085
H44	2.0901390833	-1.1670148122	5.4719095530
C45	0.3628083449	4.8364732702	2.3839802365
C46	1.6119939554	5.3343539625	2.7994707005
H47	2.5032107183	4.7416629677	2.6122847910
C48	1.6908588663	6.5696812311	3.4357003348
H49	2.6597022848	6.9459407991	3.7541524162
C50	0.5381434493	7.3230312643	3.6658239126
H51	0.6061444386	8.2862762339	4.1642693428
C52	-0.7024896965	6.8322211183	3.2531400665
H53	-1.6040007162	7.4134363182	3.4296249416
C54	-0.7979457927	5.5984674946	2.6157389536
H55	-1.7587733726	5.2047443332	2.2963819269
C56	0.6766234825	3.3600946347	-1.9838291286
C57	1.0040544702	3.2497691366	-3.3478545451
H58	1.1110873328	2.2658611328	-3.7958446104
C59	1.1831253971	4.3871698623	-4.1318158827
H60	1.4313650739	4.2727454495	-5.1838264297
C61	1.0427285747	5.6602216496	-3.5757560562
H62	1.1824549739	6.5469554691	-4.1877502392
C63	0.7177796879	5.7775560538	-2.2246017181
H64	0.6023039151	6.7597776783	-1.7734669623
C65	0.5337894373	4.6431367073	-1.4343870201
H66	0.2788424737	4.7504524551	-0.3858201228

C67	-2.9337707458	2.5720098040	0.6240569355
C68	-3.6184841225	2.5984271410	1.8513932926
H69	-3.3684090532	1.8758075539	2.6205240307
C70	-4.6205213021	3.5365331451	2.0884584905
H71	-5.1363797712	3.5305740569	3.0452107282
C72	-4.9597620523	4.4733919312	1.1111934319
H73	-5.7429531504	5.2033643942	1.2959777160
C74	-4.2776754492	4.4600882846	-0.1057686037
H75	-4.5242127023	5.1830469490	-0.8789950213
C76	-3.2744210352	3.5231726866	-0.3491789246
H77	-2.7562341096	3.5243622915	-1.3032267446
C78	-4.3960045950	-1.0864358024	2.9032978559
C79	-4.4849277867	-0.6518645544	4.2396572743
H80	-3.6560114358	-0.0975635074	4.6691504969
C81	-5.6133399760	-0.9499022367	4.9981658665
H82	-5.6689511583	-0.6104992271	6.0295442267
C83	-6.6661393076	-1.6812520855	4.4451418375
H84	-7.5441904735	-1.9128497292	5.0420295344
C85	-6.5827200436	-2.1139024227	3.1205001511
H86	-7.3987254494	-2.6825715838	2.6816114802
C87	-5.4608352121	-1.8220415880	2.3497100265
H88	-5.3965722317	-2.1441045717	1.3147606515
Ta89	-1.2715442143	0.8839694287	-1.6025761335
Ta90	-0.1443228855	-1.9887385192	-0.9685264689
Ta91	1.8123771318	0.4567723414	-1.2045765289
N92	0.2424450042	-0.4284393375	-2.4768448266
N93	-2.1289135483	-0.9944216154	-0.8931372313
N94	-2.3034713854	1.5953122157	-2.8746438851
N95	-0.2794642053	-3.6023866744	-1.7246974866
N96	-0.4584365595	-2.1581735754	1.1831116860
N97	1.9165318915	-1.5846597216	-0.3844573947
N98	3.2713527105	0.7979393182	-2.1782941016
C99	0.3580492545	-0.7776678697	-3.8606834990
C100	-0.7699727477	-0.7906105824	-4.6982341219
H101	-1.7401955903	-0.5177169910	-4.2955928216
C102	-0.6577468568	-1.1417634149	-6.0424528023
H103	-1.5495994324	-1.1383180112	-6.6638602696
C104	0.5780966789	-1.4934859070	-6.5877963982
H105	0.6621045384	-1.7654073375	-7.6359639944
C106	1.7034473283	-1.4880847321	-5.7618893432
H107	2.6770820895	-1.7585454337	-6.1622061792
C108	1.5976756913	-1.1389386950	-4.4160739388
H109	2.4842452257	-1.1402252638	-3.7905097377
C110	-3.3965108196	-1.4632677610	-1.3656139175
C111	-4.5492006092	-0.6827858421	-1.1591789693
H112	-4.4659546867	0.2701838626	-0.6441095867
C113	-5.7945218503	-1.1185061194	-1.6057696324
H114	-6.6689100147	-0.4971078484	-1.4294929442
C115	-5.9201754036	-2.3402933075	-2.2700827153
H116	-6.8918266216	-2.6809659407	-2.6169521212
C117	-4.7811561644	-3.1164636455	-2.4821601287

H118	-4.8589066097	-4.0700813312	-2.9981301695
C119	-3.5311053760	-2.6864684175	-2.0374536850
H120	-2.6561730361	-3.3027864571	-2.2084569176
C121	-3.1127120915	2.1603205171	-3.8383171991
C122	-4.2306867997	1.4626313910	-4.3315071632
H123	-4.4506090807	0.4749658496	-3.9374802636
C124	-5.0459665602	2.0465006499	-5.2968596809
H125	-5.9087501507	1.4994806695	-5.6689113970
C126	-4.7651448832	3.3249054455	-5.7832603070
H127	-5.4066409944	3.7770619217	-6.5349110811
C128	-3.6551839909	4.0187856738	-5.2971334515
H129	-3.4286622783	5.0140666838	-5.6712167376
C130	-2.8305724187	3.4470438253	-4.3324895590
H131	-1.9615936360	3.9774243288	-3.9534318327
C132	-0.4135815931	-4.8484876692	-2.3052684243
C133	-0.7777745486	-5.9663248822	-1.5283699623
H134	-0.9481583469	-5.8333487956	-0.4637750357
C135	-0.9212822379	-7.2138722055	-2.1292654490
H136	-1.2043431570	-8.0706338823	-1.5229750568
C137	-0.7069117347	-7.3677652863	-3.5005180876
H138	-0.8222836833	-8.3431403410	-3.9656960213
C139	-0.3446162506	-6.2618236973	-4.2716221354
H140	-0.1759996981	-6.3751742228	-5.3394781753
C141	-0.1970752290	-5.0075363491	-3.6860015705
H142	0.0829289780	-4.1409238903	-4.2782895006
C143	-0.6985120285	-3.4313582629	1.7913774833
C144	-2.0070773612	-3.9107581865	1.9712840039
H145	-2.8480739731	-3.3043881322	1.6520432691
C146	-2.2376314140	-5.1509594939	2.5634053526
H147	-3.2610549989	-5.4931357048	2.6939475569
C148	-1.1715533937	-5.9462135529	2.9842326695
H149	-1.3534136447	-6.9118509016	3.4478161382
C150	0.1317312570	-5.4835753079	2.8000672323
H151	0.9774162232	-6.0876939291	3.1184081234
C152	0.3686163732	-4.2439408892	2.2083144156
H153	1.3889131146	-3.8999411922	2.0765673958
C154	3.0835101270	-2.4033214644	-0.5199639341
C155	3.0127185060	-3.7181467277	-1.0042551535
H156	2.0526364281	-4.1287022057	-1.2945247340
C157	4.1654271855	-4.4946427967	-1.1170134962
H158	4.0830996764	-5.5098152514	-1.4968337874
C159	5.4097600620	-3.9822360760	-0.7495486743
H160	6.3047438414	-4.5916955116	-0.8389240919
C161	5.4894161829	-2.6747889161	-0.2658353626
H162	6.4486575672	-2.2551792804	0.0263269156
C163	4.3421422205	-1.8926525574	-0.1520379946
H164	4.4197087022	-0.8777944305	0.2280438241
C165	4.3884653931	1.0371412418	-2.9497263911
C166	5.2555743313	-0.0188063774	-3.2882590909
H167	5.0448569777	-1.0153310046	-2.9115438420
C168	6.3719121770	0.2227262614	-4.0837501551

H169	7.0334885579	-0.6011934980	-4.3393034838
C170	6.6450961803	1.5097476016	-4.5505016377
H171	7.5169369639	1.6924980301	-5.1728346597
C172	5.7905842063	2.5608059050	-4.2126341942
H173	5.9958336606	3.5662134397	-4.5715383172
C174	4.6702537627	2.3337093013	-3.4189100750
H175	3.9942482895	3.1441972493	-3.1631001794

Table S2. Calculated coordinates for C_i -optimized **2**.

Ta1	1.2792696352	-0.9206652122	1.5736753355
Ta2	0.2060455097	1.9833567331	0.9806115666
Ta3	-1.8088255836	-0.4273567693	1.2170053725
N4	-0.2040941221	0.3947175746	2.4764755010
N5	2.1754757491	0.9094017597	0.9059241824
N6	2.2907007824	-1.7218594681	2.8117794926
N7	0.4349557612	3.5725637237	1.7644629300
N8	0.5451980369	2.1728011567	-1.1670576029
N9	-1.8508676926	1.6652733032	0.4382430588
N10	-3.2941999681	-0.7575413702	2.1549412685
O11	0.0000000000	0.0000000000	0.0000000000
C12	-0.3062871444	0.7738951731	3.8509594451
C13	0.7982117100	0.6975878133	4.7146509825
H14	1.7487380385	0.3329557894	4.3380206048
C15	0.6861467758	1.0856675521	6.0489282211
H16	1.5565348238	1.0105929950	6.6964596374
C17	-0.5230054332	1.5674451770	6.5513229655
H18	-0.6061463528	1.8692141749	7.5919932134
C19	-1.6216129163	1.6626984342	5.6962225772
H20	-2.5705871049	2.0455939134	6.0638198440
C21	-1.5163698765	1.2737750666	4.3625989213
H22	-2.3787306584	1.3578790516	3.7077467258
C23	3.3839518773	1.5489229644	1.3310008455
C24	4.3019630879	0.9132659800	2.1815829369
H25	4.0988800787	-0.0929828892	2.5309936314
C26	5.4657948124	1.5674003389	2.5856698607
H27	6.1593325682	1.0528327128	3.2466535929
C28	5.7402394683	2.8654008537	2.1567583228
H29	6.6460959722	3.3727311947	2.4778794453
C30	4.8338990441	3.5045216495	1.3094739761
H31	5.0262588954	4.5170890200	0.9635752055
C32	3.6726100149	2.8559801355	0.8989428824
H33	2.9783068384	3.3690053734	0.2399955124
C34	3.0569554648	-2.3803015742	3.7516277150
C35	4.2951920193	-2.9444952228	3.3910477652
H36	4.6282923767	-2.8686315786	2.3596113537
C37	5.0700778343	-3.5951596980	4.3472031878
H38	6.0246605740	-4.0275181075	4.0564825047
C39	4.6311908977	-3.6947605645	5.6685268003
H40	5.2411757176	-4.2031751518	6.4107669471
C41	3.4021638230	-3.1391745765	6.0298891889

H42	3.0510158658	-3.2145534868	7.0562429247
C43	2.6168210874	-2.4863278021	5.0845978931
H44	1.6605423803	-2.0499206476	5.3578098065
C45	0.6491723913	4.7863049571	2.3834555104
C46	0.7431947644	5.9651546566	1.6200170167
H47	0.6490699902	5.9004242857	0.5391929943
C48	0.9506041688	7.1895060768	2.2496777296
H49	1.0231660679	8.0935833490	1.6494258518
C50	1.0663872218	7.2599938203	3.6386096808
H51	1.2261181260	8.2185013233	4.1258951549
C52	0.9751014252	6.0918252296	4.3989783779
H53	1.0652012493	6.1393660934	5.4815205488
C54	0.7690390183	4.8609336310	3.7837549305
H55	0.6948227073	3.9473484965	4.3672507794
C56	0.7186345497	3.4399131000	-1.8123031319
C57	1.9254936414	3.7924316562	-2.4346555162
H58	2.7548577550	3.0947597270	-2.4250511781
C59	2.0609881124	5.0244860718	-3.0733444452
H60	3.0063202604	5.2710094035	-3.5507718031
C61	1.0008456398	5.9289233304	-3.1103043883
H62	1.1087808696	6.8852122459	-3.6151072141
C63	-0.2034768238	5.5872032378	-2.4929222996
H64	-1.0449730680	6.2754811199	-2.5129490319
C65	-0.3439107105	4.3607841811	-1.8482428344
H66	-1.2889628253	4.1095520007	-1.3749971050
C67	-2.9902567402	2.5058245121	0.6455141426
C68	-2.8627514971	3.8296224671	1.0935170180
H69	-1.8764007026	4.2320602240	1.2961121547
C70	-3.9926545593	4.6198649153	1.3019284241
H71	-3.8652547684	5.6405359319	1.6546581610
C72	-5.2709152896	4.1135557050	1.0709336278
H73	-6.1481109650	4.7317385106	1.2421074862
C74	-5.4077939045	2.8006042713	0.6171758900
H75	-6.3950464000	2.3835907340	0.4330563041
C76	-4.2835951241	2.0079780460	0.4003004788
H77	-4.4067179747	0.9891556884	0.0444977211
C78	-4.4656403691	-0.9997955765	2.8411297247
C79	-4.4849715649	-0.9895904744	4.2481797070
H80	-3.5649857758	-0.7767431022	4.7847517288
C81	-5.6709280059	-1.2402526938	4.9317452725
H82	-5.6741011075	-1.2262212582	6.0191425861
C83	-6.8490916988	-1.5086640692	4.2326342127
H84	-7.7721834314	-1.7052520677	4.7719189874
C85	-6.8335154522	-1.5250623723	2.8365242301
H86	-7.7454604736	-1.7386119635	2.2841042195
C87	-5.6550323808	-1.2744380750	2.1399791165
H88	-5.6325031731	-1.2960176711	1.0540967970
Ta89	-1.2792696352	0.9206652122	-1.5736753355
Ta90	-0.2060455097	-1.9833567331	-0.9806115666
Ta91	1.8088255836	0.4273567693	-1.2170053725
N92	0.2040941221	-0.3947175746	-2.4764755010

N93	-2.1754757491	-0.9094017597	-0.9059241824
N94	-2.2907007824	1.7218594681	-2.8117794926
N95	-0.4349557612	-3.5725637237	-1.7644629300
N96	-0.5451980369	-2.1728011567	1.1670576029
N97	1.8508676926	-1.6652733032	-0.4382430588
N98	3.2941999681	0.7575413702	-2.1549412685
C99	0.3062871444	-0.7738951731	-3.8509594451
C100	-0.7982117100	-0.6975878133	-4.7146509825
H101	-1.7487380385	-0.3329557894	-4.3380206048
C102	-0.6861467758	-1.0856675521	-6.0489282211
H103	-1.5565348238	-1.0105929950	-6.6964596374
C104	0.5230054332	-1.5674451770	-6.5513229655
H105	0.6061463528	-1.8692141749	-7.5919932134
C106	1.6216129163	-1.6626984342	-5.6962225772
H107	2.5705871049	-2.0455939134	-6.0638198440
C108	1.5163698765	-1.2737750666	-4.3625989213
H109	2.3787306584	-1.3578790516	-3.7077467258
C110	-3.3839518773	-1.5489229644	-1.3310008455
C111	-4.3019630879	-0.9132659800	-2.1815829369
H112	-4.0988800787	0.0929828892	-2.5309936314
C113	-5.4657948124	-1.5674003389	-2.5856698607
H114	-6.1593325682	-1.0528327128	-3.2466535929
C115	-5.7402394683	-2.8654008537	-2.1567583228
H116	-6.6460959722	-3.3727311947	-2.4778794453
C117	-4.8338990441	-3.5045216495	-1.3094739761
H118	-5.0262588954	-4.5170890200	-0.9635752055
C119	-3.6726100149	-2.8559801355	-0.8989428824
H120	-2.9783068384	-3.3690053734	-0.2399955124
C121	-3.0569554648	2.3803015742	-3.7516277150
C122	-4.2951920193	2.9444952228	-3.3910477652
H123	-4.6282923767	2.8686315786	-2.3596113537
C124	-5.0700778343	3.5951596980	-4.3472031878
H125	-6.0246605740	4.0275181075	-4.0564825047
C126	-4.6311908977	3.6947605645	-5.6685268003
H127	-5.2411757176	4.2031751518	-6.4107669471
C128	-3.4021638230	3.1391745765	-6.0298891889
H129	-3.0510158658	3.2145534868	-7.0562429247
C130	-2.6168210874	2.4863278021	-5.0845978931
H131	-1.6605423803	2.0499206476	-5.3578098065
C132	-0.6491723913	-4.7863049571	-2.3834555104
C133	-0.7431947644	-5.9651546566	-1.6200170167
H134	-0.6490699902	-5.9004242857	-0.5391929943
C135	-0.9506041688	-7.1895060768	-2.2496777296
H136	-1.0231660679	-8.0935833490	-1.6494258518
C137	-1.0663872218	-7.2599938203	-3.6386096808
H138	-1.2261181260	-8.2185013233	-4.1258951549
C139	-0.9751014252	-6.0918252296	-4.3989783779
H140	-1.0652012493	-6.1393660934	-5.4815205488
C141	-0.7690390183	-4.8609336310	-3.7837549305
H142	-0.6948227073	-3.9473484965	-4.3672507794
C143	-0.7186345497	-3.4399131000	1.8123031319

C144	-1.9254936414	-3.7924316562	2.4346555162
H145	-2.7548577550	-3.0947597270	2.4250511781
C146	-2.0609881124	-5.0244860718	3.0733444452
H147	-3.0063202604	-5.2710094035	3.5507718031
C148	-1.0008456398	-5.9289233304	3.1103043883
H149	-1.1087808696	-6.8852122459	3.6151072141
C150	0.2034768238	-5.5872032378	2.4929222996
H151	1.0449730680	-6.2754811199	2.5129490319
C152	0.3439107105	-4.3607841811	1.8482428344
H153	1.2889628253	-4.1095520007	1.3749971050
C154	2.9902567402	-2.5058245121	-0.6455141426
C155	2.8627514971	-3.8296224671	-1.0935170180
H156	1.8764007026	-4.2320602240	-1.2961121547
C157	3.9926545593	-4.6198649153	-1.3019284241
H158	3.8652547684	-5.6405359319	-1.6546581610
C159	5.2709152896	-4.1135557050	-1.0709336278
H160	6.1481109650	-4.7317385106	-1.2421074862
C161	5.4077939045	-2.8006042713	-0.6171758900
H162	6.3950464000	-2.3835907340	-0.4330563041
C163	4.2835951241	-2.0079780460	-0.4003004788
H164	4.4067179747	-0.9891556884	-0.0444977211
C165	4.4656403691	0.9997955765	-2.8411297247
C166	4.4849715649	0.9895904744	-4.2481797070
H167	3.5649857758	0.7767431022	-4.7847517288
C168	5.6709280059	1.2402526938	-4.9317452725
H169	5.6741011075	1.2262212582	-6.0191425861
C170	6.8490916988	1.5086640692	-4.2326342127
H171	7.7721834314	1.7052520677	-4.7719189874
C172	6.8335154522	1.5250623723	-2.8365242301
H173	7.7454604736	1.7386119635	-2.2841042195
C174	5.6550323808	1.2744380750	-2.1399791165
H175	5.6325031731	1.2960176711	-1.0540967970

Table S3. Calculated coordinates for C_i -optimized **3**.

Ta1	1.2911648475	-0.9060375040	1.5776917436
Ta2	0.1946624062	1.9867967395	0.9777478551
Ta3	-1.8006018899	-0.4403472166	1.2264390966
N4	-0.2011589879	0.3989993187	2.4775766130
N5	2.1778538078	0.9198198000	0.8981969288
N6	2.3002499997	-1.6769515646	2.8395050872
N7	0.4289794848	3.5628436745	1.7898415324
N8	0.5332727277	2.1749552646	-1.1753355401
N9	-1.8530160603	1.6610950601	0.4433484561
N10	-3.2770435890	-0.7727683729	2.1804835401
O11	0.0000000000	0.0000000000	0.0000000000
C12	-0.3424310167	0.7855539058	3.8465433840
C13	0.7251525235	0.6850344440	4.7531456263
H14	1.6774952876	0.2919746478	4.4132386797
C15	0.5788387179	1.0871111795	6.0786034531
H16	1.4287769112	0.9919975737	6.7519114027

C17	-0.6275812443	1.6130121014	6.5591595101
C19	-1.6841085361	1.7235334522	5.6499248330
H20	-2.6350340514	2.1366905029	5.9796717799
C21	-1.5498306060	1.3223269160	4.3217914564
H22	-2.3916169735	1.4330902904	3.6446786583
C23	3.3886462686	1.5664674697	1.3051399205
C24	4.3268774827	0.9421077476	2.1430934624
H25	4.1329924629	-0.0599224912	2.5090142334
C26	5.4986886401	1.5979774183	2.5150054243
H27	6.2024931623	1.0829474631	3.1663462895
C28	5.7887414854	2.8957077482	2.0763129425
C30	4.8505731755	3.5138286056	1.2432723310
H31	5.0365167068	4.5224348311	0.8806015959
C32	3.6772660501	2.8677379041	0.8613451359
H33	2.9761878901	3.3808942896	0.2099760758
C34	3.0631748424	-2.3096681518	3.8006435829
C35	4.3251305462	-2.8469398738	3.4796256770
H36	4.6823034693	-2.7764538159	2.4558381350
C37	5.0949324438	-3.4651050016	4.4586755088
H38	6.0669180484	-3.8734704296	4.1876985146
C39	4.6485127429	-3.5748610291	5.7834319084
C41	3.3909165262	-3.0450529941	6.0915039851
H42	3.0152246385	-3.1198216538	7.1099338566
C43	2.6049133392	-2.4237708887	5.1246461592
H44	1.6303959039	-2.0201672554	5.3813229840
C45	0.6803204986	4.7463281449	2.4533142545
C46	0.7851879233	5.9606798097	1.7480731721
H47	0.6653354339	5.9538072128	0.6678601288
C48	1.0447687800	7.1463170957	2.4271574545
H49	1.1248537440	8.0732049429	1.8617478102
C50	1.2085279609	7.1728528364	3.8192369329
C52	1.1000130034	5.9611094505	4.5110397892
H53	1.2239026956	5.9517820150	5.5920631659
C54	0.8409315469	4.7636676538	3.8497377141
H55	0.7636834421	3.8304595620	4.4004203294
C56	0.6849611069	3.4468885786	-1.8175585912
C57	1.8744999116	3.8281968863	-2.4585646823
H58	2.7149549406	3.1432402812	-2.4763790989
C59	1.9786946615	5.0671377700	-3.0867943554
H60	2.9143781077	5.3271516470	-3.5782416184
C61	0.9136881963	5.9763289754	-3.1081210125
C63	-0.2670831836	5.5943932632	-2.4633341299
H64	-1.1195797530	6.2702761865	-2.4583662510
C65	-0.3824716970	4.3600259482	-1.8274836328
H66	-1.3169087536	4.0996254539	-1.3388287338
C67	-2.9960720242	2.4961712174	0.6538720663
C68	-2.8834638256	3.8181021374	1.1156470526
H69	-1.9015159795	4.2283637661	1.3249526822
C70	-4.0180044314	4.5979718975	1.3274792986
H71	-3.8923770438	5.6163175990	1.6906191243
C72	-5.3077168825	4.1041890963	1.0946677588

C74	-5.4153249558	2.7896281328	0.6302729628
H75	-6.3992085839	2.3654508190	0.4409053604
C76	-4.2880096393	2.0014172238	0.4079279315
H77	-4.4123257825	0.9843536128	0.0481292008
C78	-4.4590461642	-0.9963312059	2.8565684671
C79	-4.5142339215	-0.9385086131	4.2624224027
H80	-3.6078986945	-0.7083885318	4.8147810296
C81	-5.7134569697	-1.1654852465	4.9276512883
H82	-5.7332314981	-1.1145304369	6.0147919703
C83	-6.8949467777	-1.4581229395	4.2313949793
C85	-6.8300570157	-1.5173902556	2.8352998084
H86	-7.7305330659	-1.7453046585	2.2685139578
C87	-5.6384260721	-1.2928999391	2.1507471922
H88	-5.6029597484	-1.3516237355	1.0667500094
Ta89	-1.2911648475	0.9060375040	-1.5776917436
Ta90	-0.1946624062	-1.9867967395	-0.9777478551
Ta91	1.8006018899	0.4403472166	-1.2264390966
N92	0.2011589879	-0.3989993187	-2.4775766130
N93	-2.1778538078	-0.9198198000	-0.8981969288
N94	-2.3002499997	1.6769515646	-2.8395050872
N95	-0.4289794848	-3.5628436745	-1.7898415324
N96	-0.5332727277	-2.1749552646	1.1753355401
N97	1.8530160603	-1.6610950601	-0.4433484561
N98	3.2770435890	0.7727683729	-2.1804835401
C99	0.3424310167	-0.7855539058	-3.8465433840
C100	-0.7251525235	-0.6850344440	-4.7531456263
H101	-1.6774952876	-0.2919746478	-4.4132386797
C102	-0.5788387179	-1.0871111795	-6.0786034531
H103	-1.4287769112	-0.9919975737	-6.7519114027
C104	0.6275812443	-1.6130121014	-6.5591595101
C106	1.6841085361	-1.7235334522	-5.6499248330
H107	2.6350340514	-2.1366905029	-5.9796717799
C108	1.5498306060	-1.3223269160	-4.3217914564
H109	2.3916169735	-1.4330902904	-3.6446786583
C110	-3.3886462686	-1.5664674697	-1.3051399205
C111	-4.3268774827	-0.9421077476	-2.1430934624
H112	-4.1329924629	0.0599224912	-2.5090142334
C113	-5.4986886401	-1.5979774183	-2.5150054243
H114	-6.2024931623	-1.0829474631	-3.1663462895
C115	-5.7887414854	-2.8957077482	-2.0763129425
C117	-4.8505731755	-3.5138286056	-1.2432723310
H118	-5.0365167068	-4.5224348311	-0.8806015959
C119	-3.6772660501	-2.8677379041	-0.8613451359
H120	-2.9761878901	-3.3808942896	-0.2099760758
C121	-3.0631748424	2.3096681518	-3.8006435829
C122	-4.3251305462	2.8469398738	-3.4796256770
H123	-4.6823034693	2.7764538159	-2.4558381350
C124	-5.0949324438	3.4651050016	-4.4586755088
H125	-6.0669180484	3.8734704296	-4.1876985146
C126	-4.6485127429	3.5748610291	-5.7834319084
C128	-3.3909165262	3.0450529941	-6.0915039851

H129	-3.0152246385	3.1198216538	-7.1099338566
C130	-2.6049133392	2.4237708887	-5.1246461592
H131	-1.6303959039	2.0201672554	-5.3813229840
C132	-0.6803204986	-4.7463281449	-2.4533142545
C133	-0.7851879233	-5.9606798097	-1.7480731721
H134	-0.6653354339	-5.9538072128	-0.6678601288
C135	-1.0447687800	-7.1463170957	-2.4271574545
H136	-1.1248537440	-8.0732049429	-1.8617478102
C137	-1.2085279609	-7.1728528364	-3.8192369329
C139	-1.1000130034	-5.9611094505	-4.5110397892
H140	-1.2239026956	-5.9517820150	-5.5920631659
C141	-0.8409315469	-4.7636676538	-3.8497377141
H142	-0.7636834421	-3.8304595620	-4.4004203294
C143	-0.6849611069	-3.4468885786	1.8175585912
C144	-1.8744999116	-3.8281968863	2.4585646823
H145	-2.7149549406	-3.1432402812	2.4763790989
C146	-1.9786946615	-5.0671377700	3.0867943554
H147	-2.9143781077	-5.3271516470	3.5782416184
C148	-0.9136881963	-5.9763289754	3.1081210125
C150	0.2670831836	-5.5943932632	2.4633341299
H151	1.1195797530	-6.2702761865	2.4583662510
C152	0.3824716970	-4.3600259482	1.8274836328
H153	1.3169087536	-4.0996254539	1.3388287338
C154	2.9960720242	-2.4961712174	-0.6538720663
C155	2.8834638256	-3.8181021374	-1.1156470526
H156	1.9015159795	-4.2283637661	-1.3249526822
C157	4.0180044314	-4.5979718975	-1.3274792986
H158	3.8923770438	-5.6163175990	-1.6906191243
C159	5.3077168825	-4.1041890963	-1.0946677588
C161	5.4153249558	-2.7896281328	-0.6302729628
H162	6.3992085839	-2.3654508190	-0.4409053604
C163	4.2880096393	-2.0014172238	-0.4079279315
H164	4.4123257825	-0.9843536128	-0.0481292008
C165	4.4590461642	0.9963312059	-2.8565684671
C166	4.5142339215	0.9385086131	-4.2624224027
H167	3.6078986945	0.7083885318	-4.8147810296
C168	5.7134569697	1.1654852465	-4.9276512883
H169	5.7332314981	1.1145304369	-6.0147919703
C170	6.8949467777	1.4581229395	-4.2313949793
C172	6.8300570157	1.5173902556	-2.8352998084
H173	7.7305330659	1.7453046585	-2.2685139578
C174	5.6384260721	1.2928999391	-2.1507471922
H175	5.6029597484	1.3516237355	-1.0667500094
C176	-5.5015980045	4.2453292131	-6.8357063568
H177	-5.0045661941	4.2474486727	-7.8112742511
H178	-6.4666545816	3.7362231811	-6.9555025118
H179	-5.7207763898	5.2879753600	-6.5719373836
C179	5.5015980045	-4.2453292131	6.8357063568
H180	5.0045661941	-4.2474486727	7.8112742511
H181	5.7207763898	-5.2879753600	6.5719373836
H182	6.4666545816	-3.7362231811	6.9555025118

C182	1.4959294264	8.4696285393	4.5409598215
H183	1.5970775267	8.3123358769	5.6198007434
H184	2.4257038817	8.9311842890	4.1839530500
H185	0.6947402753	9.2037488369	4.3857320531
C185	-1.4959294264	-8.4696285393	-4.5409598215
H186	-1.5970775267	-8.3123358769	-5.6198007434
H187	-0.6947402753	-9.2037488369	-4.3857320531
H188	-2.4257038817	-8.9311842890	-4.1839530500
C188	8.1899046111	1.6999672803	-4.9724162812
H189	9.0108258552	1.9195816647	-4.2820859703
H190	8.4815741546	0.8251809860	-5.5678680478
H191	8.1044327181	2.5451648523	-5.6674411227
C191	-8.1899046111	-1.6999672803	4.9724162812
H192	-9.0108258552	-1.9195816647	4.2820859703
H193	-8.1044327181	-2.5451648523	5.6674411227
H194	-8.4815741546	-0.8251809860	5.5678680478
C194	-0.7713025129	2.0475853472	7.9996106520
H195	-1.7727699537	2.4423636307	8.1991838199
H196	-0.5990796501	1.2127456598	8.6910300504
H197	-0.0473606009	2.8309905165	8.2577835273
C197	0.7713025129	-2.0475853472	-7.9996106520
H198	1.7727699537	-2.4423636307	-8.1991838199
H199	0.0473606009	-2.8309905165	-8.2577835273
H200	0.5990796501	-1.2127456598	-8.6910300504
C200	-6.5285956453	4.9604191240	1.3401703038
H201	-7.4503585970	4.4152369478	1.1124187752
H202	-6.5856382713	5.2874731518	2.3861349206
H203	-6.5159235589	5.8668083283	0.7214065633
C203	6.5285956453	-4.9604191240	-1.3401703038
H204	7.4503585970	-4.4152369478	-1.1124187752
H205	6.5159235589	-5.8668083283	-0.7214065633
H206	6.5856382713	-5.2874731518	-2.3861349206
C206	7.0631985444	3.5959764205	2.4882629828
H207	7.1295861584	4.5944841329	2.0440892703
H208	7.1237929614	3.7125709534	3.5777655581
H209	7.9520741669	3.0327914833	2.1762325576
C209	-1.0379754058	-7.3108888447	3.8061984799
H210	-0.1156260964	-7.8941201379	3.7181354771
H211	-1.2504362603	-7.1858040795	4.8756001541
H212	-1.8543698952	-7.9118204756	3.3856529233
C212	-7.0631985444	-3.5959764205	-2.4882629828
H213	-7.1295861584	-4.5944841329	-2.0440892703
H214	-7.9520741669	-3.0327914833	-2.1762325576
H215	-7.1237929614	-3.7125709534	-3.5777655581
C215	1.0379754058	7.3108888447	-3.8061984799
H216	0.1156260964	7.8941201379	-3.7181354771
H217	1.8543698952	7.9118204756	-3.3856529233
H218	1.2504362603	7.1858040795	-4.8756001541

Table S4. Calculated coordinates for C_i -optimized **4**.

Ta1	-0.0310201169	-2.2135575039	-0.2663058695
Ta2	0.9670547207	0.2294047805	-1.9873534119
Ta3	1.9949174152	-0.1471941447	0.9666879508
N4	1.9185981053	-1.4027886316	-0.8248383617
N5	-0.7066669223	-1.2703159575	-2.0656468044
N6	-0.0690089018	-3.9994856974	-0.4142555644
N7	1.6899554931	0.3188865310	-3.6227105600
N8	-0.6878318399	1.6416965318	-1.7927498521
N9	1.9633520882	1.4857006301	-0.5639314384
N10	3.6085774166	-0.2210067354	1.7425857746
O11	0.0000000000	0.0000000000	0.0000000000
C12	3.0652157415	-2.0376422353	-1.3975894774
C13	2.9663823852	-3.2755263779	-2.0576381299
H14	2.0019546233	-3.7691190704	-2.1176360329
C15	4.0783226181	-3.8738221160	-2.6377776170
H16	3.9935120642	-4.8308856820	-3.1441614856
C17	5.3310039985	-3.2491209091	-2.5868536006
C19	5.4474216802	-2.0129529215	-1.9454338233
H20	6.3974131545	-1.4928073596	-1.8941234254
C21	4.3248295006	-1.4222362944	-1.3629367151
H22	4.4371310306	-0.4564309451	-0.8799274226
C23	-1.1527839344	-1.8219545575	-3.3070730385
C24	-1.3888915105	-3.1972474051	-3.4830803929
H25	-1.2098643322	-3.8798933579	-2.6589439670
C26	-1.8453528328	-3.6956942748	-4.6985304174
H27	-2.0264353074	-4.7585824790	-4.8291267969
C28	-2.0768924847	-2.8386978554	-5.7811928733
C30	-1.8403520267	-1.4696198979	-5.6274402823
H31	-2.0031463146	-0.7741806152	-6.4430914272
C32	-1.3868733135	-0.9785972977	-4.4043456312
H33	-1.2157105344	0.0888456170	-4.3046177030
C34	-0.0925319726	-5.3803404174	-0.4586471368
C35	-1.3137741183	-6.0860871096	-0.4856273041
H36	-2.2456968854	-5.5283170321	-0.4538065978
C37	-1.3279496862	-7.4718571005	-0.5397114962
H38	-2.2642514165	-8.0216894752	-0.5587161165
C39	-0.1282612159	-8.1960541987	-0.5695657998
C40	1.0906260589	-7.5111145191	-0.5373765006
H41	2.0338582862	-8.0456147012	-0.5540535087
C42	1.1021753228	-6.1183550650	-0.4803442151
H43	2.0479080080	-5.5863949959	-0.4498896829
C44	2.1939407148	0.2340820742	-4.9041651202
C45	1.9336751207	1.2329558022	-5.8646562135
H46	1.3304259202	2.0917411496	-5.5825032642
C47	2.4250159456	1.1145163159	-7.1569352520
H48	2.2246508651	1.8764687577	-7.9044024196
C49	3.1857433730	-0.0022118766	-7.5293791412
C51	3.4597923581	-0.9969144480	-6.5849782433
H52	4.0454279693	-1.8716372708	-6.8454439408

C53	2.9671397581	-0.8744278643	-5.2878303745
H54	3.1661854478	-1.6523814924	-4.5564832938
C55	-0.9304083343	2.6638163728	-2.7652349283
C56	-2.1222969601	2.7351672851	-3.5082116044
H57	-2.8957495376	1.9910783264	-3.3499367613
C58	-2.3331507894	3.7579327956	-4.4254293449
H59	-3.2586876712	3.8135897554	-4.9908548760
C60	-1.3630998834	4.7462378683	-4.6312852902
C62	-0.1677506729	4.6867961313	-3.9086177280
H63	0.6075684415	5.4335210588	-4.0380673530
C64	0.0369936661	3.6541530788	-2.9942467825
H65	0.9711297497	3.6284033399	-2.4411898493
C66	3.0964961566	2.3411112805	-0.7220735905
C67	3.6515489269	2.6218369203	-1.9842779016
H68	3.2106150183	2.1785093696	-2.8713470771
C69	4.7715331518	3.4341368323	-2.1112068460
H70	5.1991214520	3.6409418914	-3.0878976494
C71	5.3803289597	3.9941920822	-0.9818056794
C73	4.8390543708	3.7344973594	0.2808753589
H74	5.2838174348	4.1462062999	1.1800387322
C75	3.7099294810	2.9232238474	0.3978131600
H76	3.3071513267	2.7314176963	1.3875990420
C77	4.8568155589	-0.1774425727	2.3302298425
C78	5.8806253717	-1.0698954393	1.9488755388
H79	5.6769225749	-1.8051572661	1.1762056649
C80	7.1334393615	-1.0021800512	2.5390606575
H81	7.9271290569	-1.6841872659	2.2486388268
C82	7.4042470958	-0.0453340210	3.5269781637
C84	6.3971699098	0.8400814187	3.9234935121
H85	6.5775391954	1.5860837664	4.6896770590
C86	5.1383962081	0.7699371548	3.3284898346
H87	4.3545395745	1.4549003403	3.6377165308
Ta88	0.0310201169	2.2135575039	0.2663058695
Ta89	-0.9670547207	-0.2294047805	1.9873534119
Ta90	-1.9949174152	0.1471941447	-0.9666879508
N91	-1.9185981053	1.4027886316	0.8248383617
N92	0.7066669223	1.2703159575	2.0656468044
N93	0.0690089018	3.9994856974	0.4142555644
N94	-1.6899554931	-0.3188865310	3.6227105600
N95	0.6878318399	-1.6416965318	1.7927498521
N96	-1.9633520882	-1.4857006301	0.5639314384
N97	-3.6085774166	0.2210067354	-1.7425857746
C98	-3.0652157415	2.0376422353	1.3975894774
C99	-2.9663823852	3.2755263779	2.0576381299
H100	-2.0019546233	3.7691190704	2.1176360329
C101	-4.0783226181	3.8738221160	2.6377776170
H102	-3.9935120642	4.8308856820	3.1441614856
C103	-5.3310039985	3.2491209091	2.5868536006
C105	-5.4474216802	2.0129529215	1.9454338233
H106	-6.3974131545	1.4928073596	1.8941234254
C107	-4.3248295006	1.4222362944	1.3629367151

H108	-4.4371310306	0.4564309451	0.8799274226
C109	1.1527839344	1.8219545575	3.3070730385
C110	1.3888915105	3.1972474051	3.4830803929
H111	1.2098643322	3.8798933579	2.6589439670
C112	1.8453528328	3.6956942748	4.6985304174
H113	2.0264353074	4.7585824790	4.8291267969
C114	2.0768924847	2.8386978554	5.7811928733
C116	1.8403520267	1.4696198979	5.6274402823
H117	2.0031463146	0.7741806152	6.4430914272
C118	1.3868733135	0.9785972977	4.4043456312
H119	1.2157105344	-0.0888456170	4.3046177030
C120	0.0925319726	5.3803404174	0.4586471368
C121	1.3137741183	6.0860871096	0.4856273041
H122	2.2456968854	5.5283170321	0.4538065978
C123	1.3279496862	7.4718571005	0.5397114962
H124	2.2642514165	8.0216894752	0.5587161165
C125	0.1282612159	8.1960541987	0.5695657998
C126	-1.0906260589	7.5111145191	0.5373765006
H127	-2.0338582862	8.0456147012	0.5540535087
C128	-1.1021753228	6.1183550650	0.4803442151
H129	-2.0479080080	5.5863949959	0.4498896829
C130	-2.1939407148	-0.2340820742	4.9041651202
C131	-1.9336751207	-1.2329558022	5.8646562135
H132	-1.3304259202	-2.0917411496	5.5825032642
C133	-2.4250159456	-1.1145163159	7.1569352520
H134	-2.2246508651	-1.8764687577	7.9044024196
C135	-3.1857433730	0.0022118766	7.5293791412
C137	-3.4597923581	0.9969144480	6.5849782433
H138	-4.0454279693	1.8716372708	6.8454439408
C139	-2.9671397581	0.8744278643	5.2878303745
H140	-3.1661854478	1.6523814924	4.5564832938
C141	0.9304083343	-2.6638163728	2.7652349283
C142	2.1222969601	-2.7351672851	3.5082116044
H143	2.8957495376	-1.9910783264	3.3499367613
C144	2.3331507894	-3.7579327956	4.4254293449
H145	3.2586876712	-3.8135897554	4.9908548760
C146	1.3630998834	-4.7462378683	4.6312852902
C148	0.1677506729	-4.6867961313	3.9086177280
H149	-0.6075684415	-5.4335210588	4.0380673530
C150	-0.0369936661	-3.6541530788	2.9942467825
H151	-0.9711297497	-3.6284033399	2.4411898493
C152	-3.0964961566	-2.3411112805	0.7220735905
C153	-3.6515489269	-2.6218369203	1.9842779016
H154	-3.2106150183	-2.1785093696	2.8713470771
C155	-4.7715331518	-3.4341368323	2.1112068460
H156	-5.1991214520	-3.6409418914	3.0878976494
C157	-5.3803289597	-3.9941920822	0.9818056794
C159	-4.8390543708	-3.7344973594	-0.2808753589
H160	-5.2838174348	-4.1462062999	-1.1800387322
C161	-3.7099294810	-2.9232238474	-0.3978131600
H162	-3.3071513267	-2.7314176963	-1.3875990420

C163	-4.8568155589	0.1774425727	-2.3302298425
C164	-5.8806253717	1.0698954393	-1.9488755388
H165	-5.6769225749	1.8051572661	-1.1762056649
C166	-7.1334393615	1.0021800512	-2.5390606575
H167	-7.9271290569	1.6841872659	-2.2486388268
C168	-7.4042470958	0.0453340210	-3.5269781637
C170	-6.3971699098	-0.8400814187	-3.9234935121
H171	-6.5775391954	-1.5860837664	-4.6896770590
C172	-5.1383962081	-0.7699371548	-3.3284898346
H173	-4.3545395745	-1.4549003403	-3.6377165308
O175	0.2584517277	9.5551139724	0.6269031380
O176	-0.2584517277	-9.5551139724	-0.6269031380
C177	-0.9206702479	10.3373855206	0.6675557193
H178	-0.5909840292	11.3774219831	0.7124993446
H179	-1.5360859034	10.1915875459	-0.2306352662
H180	-1.5268867064	10.1112724633	1.5552731570
C181	0.9206702479	-10.3373855206	-0.6675557193
H182	0.5909840292	-11.3774219831	-0.7124993446
H183	1.5268867064	-10.1112724633	-1.5552731570
H184	1.5360859034	-10.1915875459	0.2306352662
O186	3.6056493882	-0.0274028284	-8.8304342520
O187	-3.6056493882	0.0274028284	8.8304342520
O188	8.6737188417	-0.0618995516	4.0337351866
O189	-8.6737188417	0.0618995516	-4.0337351866
O190	6.4827161258	4.7655623602	-1.2171288806
O191	2.5318481469	3.4269548795	6.9274112472
O192	-6.3578767948	3.9173705031	3.1918777893
O193	-1.6751329272	5.7121917346	-5.5451655131
O194	1.6751329272	-5.7121917346	5.5451655131
O195	-2.5318481469	-3.4269548795	-6.9274112472
O196	-6.4827161258	-4.7655623602	1.2171288806
O197	6.3578767948	-3.9173705031	-3.1918777893
C198	9.0095663792	0.8890334827	5.0261248140
H199	10.0549012337	0.7025057275	5.2812532131
H200	8.9059434377	1.9175859272	4.6538666754
H201	8.3916250761	0.7725269695	5.9268367979
C201	-9.0095663792	-0.8890334827	-5.0261248140
H202	-10.0549012337	-0.7025057275	-5.2812532131
H203	-8.3916250761	-0.7725269695	-5.9268367979
H204	-8.9059434377	-1.9175859272	-4.6538666754
C204	-7.6389432867	3.3144798071	3.1854851332
H205	-8.2995259288	4.0046573842	3.7145533086
H206	-8.0136254937	3.1673792256	2.1634602496
H207	-7.6338815022	2.3468989308	3.7056983515
C207	2.7879965910	2.5949753825	8.0442472370
H208	3.1371015400	3.2569565636	8.8395969908
H209	1.8813947380	2.0734579282	8.3793068036
H210	3.5659772193	1.8504512811	7.8251072310
C210	7.1453297022	5.3379593197	-0.1051763550
H211	7.9867671579	5.9018064177	-0.5134291485
H212	6.4890277889	6.0209551304	0.4514246422

H213	7.5236488836	4.5682336830	0.5812711651
C213	-0.7301818674	6.7414168337	-5.7741278107
H214	-1.1753663485	7.3976642117	-6.5249184018
H215	-0.5297169544	7.3183191421	-4.8611314016
H216	0.2184966733	6.3432560717	-6.1594080436
C216	-4.3517264012	1.1474604757	9.2682852164
H217	-4.5752196043	0.9680589638	10.3221408289
H218	-3.7774427460	2.0793631894	9.1733837498
H219	-5.2934383706	1.2522735528	8.7125304848
C219	4.3517264012	-1.1474604757	-9.2682852164
H220	4.5752196043	-0.9680589638	-10.3221408289
H221	5.2934383706	-1.2522735528	-8.7125304848
H222	3.7774427460	-2.0793631894	-9.1733837498
C222	-2.7879965910	-2.5949753825	-8.0442472370
H223	-3.1371015400	-3.2569565636	-8.8395969908
H224	-3.5659772193	-1.8504512811	-7.8251072310
H225	-1.8813947380	-2.0734579282	-8.3793068036
C225	0.7301818674	-6.7414168337	5.7741278107
H226	1.1753663485	-7.3976642117	6.5249184018
H227	-0.2184966733	-6.3432560717	6.1594080436
H228	0.5297169544	-7.3183191421	4.8611314016
C228	-7.1453297022	-5.3379593197	0.1051763550
H229	-7.9867671579	-5.9018064177	0.5134291485
H230	-7.5236488836	-4.5682336830	-0.5812711651
H231	-6.4890277889	-6.0209551304	-0.4514246422
C231	7.6389432867	-3.3144798071	-3.1854851332
H232	8.2995259288	-4.0046573842	-3.7145533086
H233	7.6338815022	-2.3468989308	-3.7056983515
H234	8.0136254937	-3.1673792256	-2.1634602496

Table S5. Calculated coordinates for C_i -optimized **9**.

Ta1	1.2882211810	-0.9075001947	1.5763630727
Ta2	0.1984084797	1.9882340609	0.9814400156
Ta3	-1.8073976992	-0.4306944224	1.2281612329
N4	-0.1939555675	0.4078395027	2.4824362570
N5	2.1654450741	0.9554526937	0.8829072430
N6	2.2914322480	-1.6918403091	2.8305734755
N7	0.4219645645	3.5664660176	1.7868233748
N8	0.4903632910	2.1739408468	-1.1838290102
N9	-1.8777272505	1.6308505219	0.4445395926
N10	-3.2928120949	-0.7443951709	2.1711652948
O11	0.0000000000	0.0000000000	0.0000000000
C12	-0.3015870995	0.7854559896	3.8546849818
C13	0.7854378329	0.7060555517	4.7361004917
H14	1.7476588765	0.3361185875	4.3999906969
C15	0.6177129084	1.1124503698	6.0590523965
H16	1.4570912321	1.0499508453	6.7496950498
N17	-0.5257187806	1.5898132451	6.5635420370
C18	-1.5576154842	1.6709007668	5.7151119222
H19	-2.4859188956	2.0655566822	6.1247869876

C20	-1.5030583206	1.2909804832	4.3757034217
H21	-2.3822965176	1.3918086412	3.7473981059
C22	3.3784557938	1.5868353923	1.2980240258
C23	4.2957566268	0.9612348343	2.1534589413
H24	4.1013202165	-0.0286133245	2.5490831499
C25	5.4689563045	1.6326627165	2.4969657226
H26	6.1871768388	1.1519188683	3.1594080522
N27	5.7947682408	2.8548911463	2.0649802577
C28	4.9102281170	3.4512851780	1.2559660030
H29	5.1734835885	4.4493216137	0.9103468465
C30	3.7107059294	2.8745518361	0.8461208088
H31	3.0468479967	3.4215786927	0.1839814035
C32	3.0392159625	-2.3534409133	3.7828318416
C33	4.3169132837	-2.8537744465	3.4809867556
H34	4.7300950402	-2.7377916797	2.4839937170
C35	5.0274250250	-3.5105116407	4.4823510033
H36	6.0183768499	-3.9079890915	4.2693210135
N37	4.5734384820	-3.7001588734	5.7269846464
C38	3.3527624358	-3.2234162410	6.0015912374
H39	2.9925698976	-3.3887849622	7.0155599466
C40	2.5493671003	-2.5514230680	5.0846093593
H41	1.5659153621	-2.1863443472	5.3619036608
C42	0.6439260462	4.7724714963	2.4196200238
C43	0.7250716728	5.9690531404	1.6883177850
H44	0.6159094194	5.9612369821	0.6082717555
C45	0.9501728906	7.1556096522	2.3813886034
H46	1.0190026118	8.0950897981	1.8354171055
N47	1.0939371508	7.2360410767	3.7095728406
C48	1.0137625676	6.0883862129	4.3951326705
H49	1.1328218994	6.1673642693	5.4743648541
C50	0.7931249231	4.8427181479	3.8146516492
H51	0.7370514736	3.9431305991	4.4191999024
C52	0.6567981332	3.4405083560	-1.8258116035
C53	1.8456186689	3.8081784781	-2.4702076842
H54	2.6867451846	3.1264700046	-2.5158260793
C55	1.9312999658	5.0651854868	-3.0687174768
H56	2.8523595212	5.3572714956	-3.5705969890
N57	0.9449668698	5.9674114794	-3.0777164955
C58	-0.1889005110	5.6093830292	-2.4626984148
H59	-0.9935517130	6.3426071384	-2.4750891003
C60	-0.3832175306	4.3844796306	-1.8291704693
H61	-1.3330034006	4.1691601920	-1.3493584265
C62	-3.0155165956	2.4711414699	0.6449911988
C63	-2.9027931726	3.7892719950	1.1078208315
H64	-1.9335654254	4.2156940227	1.3392815471
C65	-4.0599344048	4.5485795678	1.2826281878
H66	-3.9784085233	5.5726340271	1.6432446735
N67	-5.2983086906	4.1077940678	1.0395024853
C68	-5.4001063888	2.8481028395	0.5986472161
H69	-6.4093827158	2.4874166903	0.4068090172
C70	-4.3143092234	2.0033127711	0.3821987165

H71	-4.4791632858	0.9934140521	0.0204741125
C72	-4.4690204915	-0.9683479347	2.8567054920
C73	-4.5030799149	-0.9717767014	4.2610826112
H74	-3.5976859943	-0.7923042403	4.8317023260
C75	-5.7203268288	-1.2042167297	4.8958177009
H76	-5.7698797448	-1.2091679813	5.9834385808
N77	-6.8731950237	-1.4305146523	4.2545166764
C78	-6.8278336067	-1.4298208632	2.9164975884
H79	-7.7708222058	-1.6189066470	2.4063252191
C80	-5.6725202591	-1.2085440991	2.1720324171
H81	-5.6936168109	-1.2296742195	1.0872442333
Ta82	-1.2882211810	0.9075001947	-1.5763630727
Ta83	-0.1984084797	-1.9882340609	-0.9814400156
Ta84	1.8073976992	0.4306944224	-1.2281612329
N85	0.1939555675	-0.4078395027	-2.4824362570
N86	-2.1654450741	-0.9554526937	-0.8829072430
N87	-2.2914322480	1.6918403091	-2.8305734755
N88	-0.4219645645	-3.5664660176	-1.7868233748
N89	-0.4903632910	-2.1739408468	1.1838290102
N90	1.8777272505	-1.6308505219	-0.4445395926
N91	3.2928120949	0.7443951709	-2.1711652948
C92	0.3015870995	-0.7854559896	-3.8546849818
C93	-0.7854378329	-0.7060555517	-4.7361004917
H94	-1.7476588765	-0.3361185875	-4.3999906969
C95	-0.6177129084	-1.1124503698	-6.0590523965
H96	-1.4570912321	-1.0499508453	-6.7496950498
N97	0.5257187806	-1.5898132451	-6.5635420370
C98	1.5576154842	-1.6709007668	-5.7151119222
H99	2.4859188956	-2.0655566822	-6.1247869876
C100	1.5030583206	-1.2909804832	-4.3757034217
H101	2.3822965176	-1.3918086412	-3.7473981059
C102	-3.3784557938	-1.5868353923	-1.2980240258
C103	-4.2957566268	-0.9612348343	-2.1534589413
H104	-4.1013202165	0.0286133245	-2.5490831499
C105	-5.4689563045	-1.6326627165	-2.4969657226
H106	-6.1871768388	-1.1519188683	-3.1594080522
N107	-5.7947682408	-2.8548911463	-2.0649802577
C108	-4.9102281170	-3.4512851780	-1.2559660030
H109	-5.1734835885	-4.4493216137	-0.9103468465
C110	-3.7107059294	-2.8745518361	-0.8461208088
H111	-3.0468479967	-3.4215786927	-0.1839814035
C112	-3.0392159625	2.3534409133	-3.7828318416
C113	-4.3169132837	2.8537744465	-3.4809867556
H114	-4.7300950402	2.7377916797	-2.4839937170
C115	-5.0274250250	3.5105116407	-4.4823510033
H116	-6.0183768499	3.9079890915	-4.2693210135
N117	-4.5734384820	3.7001588734	-5.7269846464
C118	-3.3527624358	3.2234162410	-6.0015912374
H119	-2.9925698976	3.3887849622	-7.0155599466
C120	-2.5493671003	2.5514230680	-5.0846093593
H121	-1.5659153621	2.1863443472	-5.3619036608

C122	-0.6439260462	-4.7724714963	-2.4196200238
C123	-0.7250716728	-5.9690531404	-1.6883177850
H124	-0.6159094194	-5.9612369821	-0.6082717555
C125	-0.9501728906	-7.1556096522	-2.3813886034
H126	-1.0190026118	-8.0950897981	-1.8354171055
N127	-1.0939371508	-7.2360410767	-3.7095728406
C128	-1.0137625676	-6.0883862129	-4.3951326705
H129	-1.1328218994	-6.1673642693	-5.4743648541
C130	-0.7931249231	-4.8427181479	-3.8146516492
H131	-0.7370514736	-3.9431305991	-4.4191999024
C132	-0.6567981332	-3.4405083560	1.8258116035
C133	-1.8456186689	-3.8081784781	2.4702076842
H134	-2.6867451846	-3.1264700046	2.5158260793
C135	-1.9312999658	-5.0651854868	3.0687174768
H136	-2.8523595212	-5.3572714956	3.5705969890
N137	-0.9449668698	-5.9674114794	3.0777164955
C138	0.1889005110	-5.6093830292	2.4626984148
H139	0.9935517130	-6.3426071384	2.4750891003
C140	0.3832175306	-4.3844796306	1.8291704693
H141	1.3330034006	-4.1691601920	1.3493584265
C142	3.0155165956	-2.4711414699	-0.6449911988
C143	2.9027931726	-3.7892719950	-1.1078208315
H144	1.9335654254	-4.2156940227	-1.3392815471
C145	4.0599344048	-4.5485795678	-1.2826281878
H146	3.9784085233	-5.5726340271	-1.6432446735
N147	5.2983086906	-4.1077940678	-1.0395024853
C148	5.4001063888	-2.8481028395	-0.5986472161
H149	6.4093827158	-2.4874166903	-0.4068090172
C150	4.3143092234	-2.0033127711	-0.3821987165
H151	4.4791632858	-0.9934140521	-0.0204741125
C152	4.4690204915	0.9683479347	-2.8567054920
C153	4.5030799149	0.9717767014	-4.2610826112
H154	3.5976859943	0.7923042403	-4.8317023260
C155	5.7203268288	1.2042167297	-4.8958177009
H156	5.7698797448	1.2091679813	-5.9834385808
N157	6.8731950237	1.4305146523	-4.2545166764
C158	6.8278336067	1.4298208632	-2.9164975884
H159	7.7708222058	1.6189066470	-2.4063252191
C160	5.6725202591	1.2085440991	-2.1720324171
H161	5.6936168109	1.2296742195	-1.0872442333

Table S6. Calculated coordinates for neutral decamethylcobaltocene.

Co1	0.0004455893	-1.5503681848	-0.2915052919
C2	2.5265748421	-2.4800261974	-2.2281060131
C3	1.0993428086	-2.0229141990	-2.1311961387
C4	0.6506560917	-0.6576885216	-2.1093677931
C5	-0.0840509228	-4.3448190778	-1.9995188407
C6	1.5292912836	0.5529445722	-2.2523203866
C7	-0.7934275759	-0.6453617211	-2.1298017053
C8	-1.6575101107	0.5791204287	-2.2266868944

C9	-1.2270976343	-1.9871483693	-2.0249470239
C10	-2.6459686340	-2.4783118617	-2.0141318910
C11	-0.0519617745	-2.8430763222	-2.0094220631
C12	2.6427667030	-0.6127356446	1.4387989402
C13	1.2253013975	-1.1094131625	1.4451387259
C14	0.7978040881	-2.4535724270	1.5468210869
C15	0.0686241862	1.2425724731	1.4192808077
C16	1.6688279676	-3.6735450994	1.6402269578
C17	-0.6462267189	-2.4486276238	1.5244755610
C18	-1.5185859669	-3.6639322319	1.6651384020
C19	-1.1014967415	-1.0855725917	1.5467272154
C20	-2.5309713794	-0.6345146086	1.6376329433
C21	0.0460183479	-0.2593562354	1.4282832253
H22	0.8472062031	-4.7670737358	-1.6083496672
H23	-0.2249154640	-4.7482851102	-3.0121120204
H24	-0.9052449384	-4.7286432166	-1.3847378633
H25	-2.7703225488	-3.3383467263	-1.3473338635
H26	-2.9677722570	-2.7984642137	-3.0149749450
H27	-3.3406573931	-1.7002872733	-1.6821810659
H28	-1.2101298309	1.4338333489	-1.7073139004
H29	-2.6471204270	0.4121057611	-1.7888108935
H30	-1.8126515867	0.8841332199	-3.2715276328
H31	2.5160759309	0.3931351814	-1.8052514049
H32	1.0871187025	1.4336128012	-1.7744777728
H33	1.6901974259	0.8060311587	-3.3100498688
H34	3.2078094510	-1.7894715260	-1.7190686536
H35	2.8610685796	-2.5493840778	-3.2733269635
H36	2.6673321776	-3.4685272990	-1.7784074102
H37	-1.0651765674	-4.5443300333	1.1976049505
H38	-2.5015901317	-3.5138657610	1.2063999924
H39	-1.6894775693	-3.9114095763	2.7225752440
H40	2.6603154040	-3.4961781835	1.2107071632
H41	1.2309212853	-4.5270683541	1.1108279855
H42	1.8189237571	-3.9862498136	2.6835844239
H43	3.3357857974	-1.3752086644	1.0693143388
H44	2.9750796575	-0.3317972979	2.4483035695
H45	2.7587908158	0.2735735400	0.8055715407
H46	0.8795951016	1.6329388525	0.7949661581
H47	0.2188305612	1.6460851491	2.4304403027
H48	-0.8702429040	1.6583958173	1.0397369739
H49	-2.6791772907	0.3380827330	1.1569051564
H50	-2.8600115320	-0.5331185586	2.6819610940
H51	-3.2117403149	-1.3444557847	1.1552166779

Table S7. Calculated coordinates for the decamethylcobaltocenium cation.

Co1	0.0014421351	-1.5509343939	-0.2918159244
C2	2.5353852039	-2.4477958098	-2.1062280597
C3	1.1103524089	-1.9934118220	-2.0087476733
C4	0.6562120778	-0.6306170157	-2.0533595829
C5	-0.0339023382	-4.3436646988	-1.9354417440

C6	1.5263758862	0.5809253131	-2.2031713838
C7	-0.7795833560	-0.6399670829	-2.0053144468
C8	-1.6734047654	0.5599689633	-2.0979172015
C9	-1.2124914011	-2.0082310270	-1.9295748830
C10	-2.6344695673	-2.4812231207	-1.9286259144
C11	-0.0444061870	-2.8446994730	-1.9326386249
C12	2.6464311422	-0.6578650826	1.3564561003
C13	1.2175729851	-1.1104118472	1.3506478180
C14	0.7648646589	-2.4721074491	1.4242345574
C15	0.0722083474	1.2410823279	1.3492764469
C16	1.6380598192	-3.6869092395	1.5189145163
C17	-0.6709045101	-2.4607287528	1.4689004151
C18	-1.5569359928	-3.6606765247	1.6181249610
C19	-1.1054496129	-1.0923598433	1.4214886301
C20	-2.5235914187	-0.6165637457	1.5120365175
C21	0.0615743853	-0.2577218791	1.3483770978
H22	0.8622889543	-4.7479192423	-1.4568810410
H23	-0.0471976850	-4.7169939041	-2.9675255398
H24	-0.9091497872	-4.7599708688	-1.4294437697
H25	-2.7480492407	-3.4317834753	-1.4008666850
H26	-2.9787753117	-2.6382030513	-2.9589314965
H27	-3.3081890058	-1.7524046340	-1.4698056252
H28	-1.1908247982	1.4588179895	-1.7052168300
H29	-2.6139005440	0.4136478406	-1.5597101077
H30	-1.9271882369	0.7601533062	-3.1472611901
H31	2.5071478358	0.4398472934	-1.7406578368
H32	1.0671053690	1.4711272477	-1.7650906262
H33	1.6965706329	0.7927270948	-3.2669024478
H34	3.2259420074	-1.7200544269	-1.6717752188
H35	2.8183154109	-2.5757588296	-3.1593356530
H36	2.6935118656	-3.4088621227	-1.6094385414
H37	-1.1147482411	-4.5544431534	1.1695528079
H38	-2.5400231268	-3.5022332003	1.1666049623
H39	-1.7196414928	-3.8780279535	2.6818523341
H40	2.5963261391	-3.5427429268	1.0125433968
H41	1.1563026396	-4.5712175071	1.0929135237
H42	1.8570889028	-3.9119077770	2.5708695073
H43	3.3082407010	-1.3909232059	0.8876969869
H44	2.9934942470	-0.5198082610	2.3887739186
H45	2.7754345498	0.2979349892	0.8413051569
H46	0.9527917464	1.6440995989	0.8419190150
H47	0.0912866292	1.6156581956	2.3807499702
H48	-0.8184561934	1.6571519369	0.8704863540
H49	-2.6670609047	0.3423829933	1.0069252152
H50	-2.8060229704	-0.4754140137	2.5631675187
H51	-3.2242975795	-1.3377359117	1.0829272824