Electronic Supplementary Material (ESI) for Dalton Transactions.

On the border between localization and delocalization: Tris(iminoxolene)titanium(IV)

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Contents:

I. *In situ* NMR Spectroscopy of Reaction of MeClampH$_6$ with Ti(O^{i}Pr)$_4$

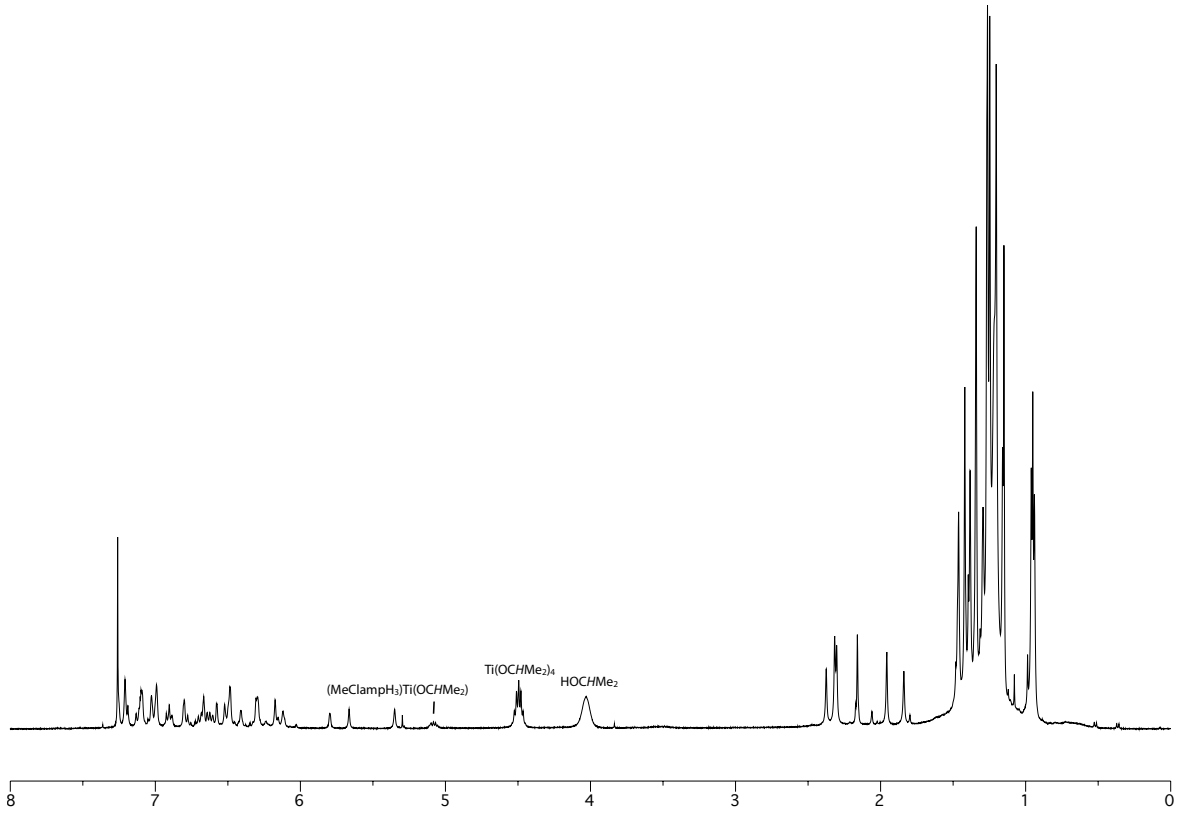

Figure S1. *In situ* ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of the reaction of MeClampH$_6$ with excess Ti(O^{i}Pr)$_4$. The OC*H*(CH$_3$)$_2$ protons from ^{i}PrOH, Ti(O^{i}Pr)$_4$, and (MeClampH$_3$)Ti(O^{i}Pr) are indicated.

II. Calculated Symmetry Breaking in (Clamp)Ti

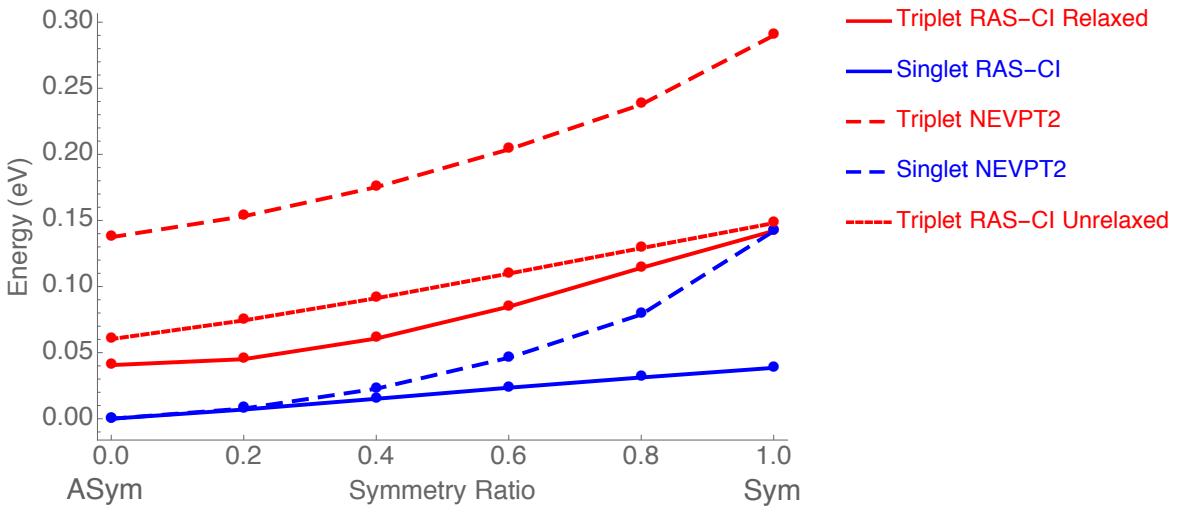

Figure S2. Calculated singlet energies and triplet energies for symmetric, asymmetric and four interpolated (Clamp)Ti geometries, with the symmetry ratio indicating the fractional progress in the bond distances from the asymmetric minimum to the C_3-symmetric optimum.

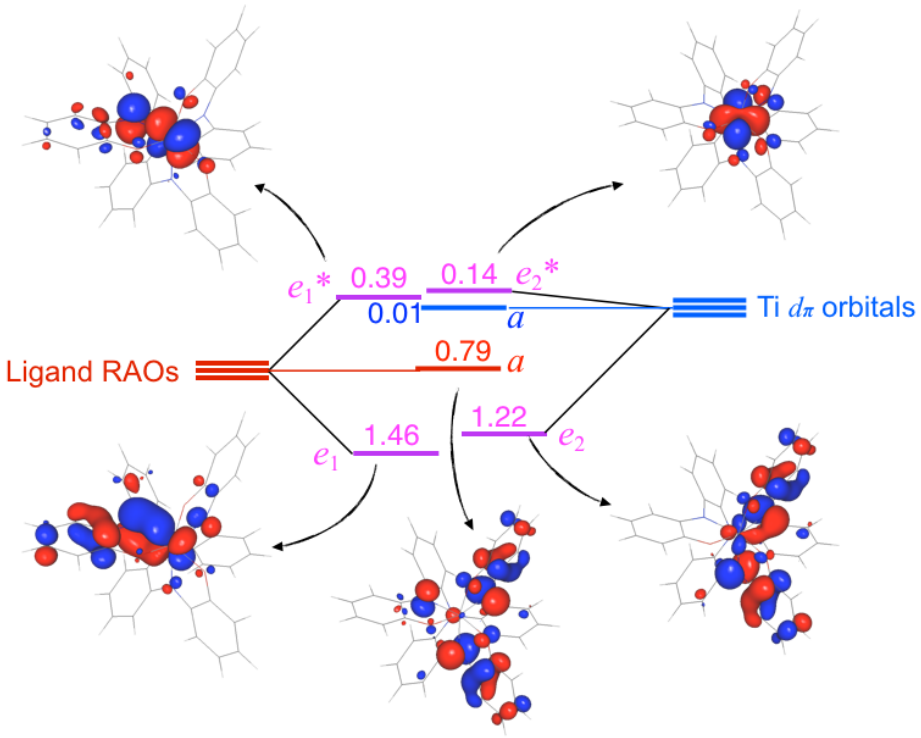

Figure S3. Shape and occupation number of RAS-CI natural orbitals of ground singlet (Clamp)Ti in C_1 geometry.

III. Cartesian Coordinates and Calculated Energies of Optimized Structures

A. C_3-symmetric (Clamp)Ti

1. Singlet State
    a. B3LYP functional, TZVP basis

Energy: -2681.2983571 Hartree

Ti	0.0000000000	0.0000000000	-1.2885056412
O	0.1818683434	-1.6233423767	-2.3014349514
O	-1.4967899090	0.6541685828	-2.3014349514
O	1.3149215655	0.9691737939	-2.3014349514
N	1.4241681824	-1.1766401220	-0.1380250810
N	-1.7310843280	-0.6450457642	-0.1380250810
N	0.3069161456	1.8216858862	-0.1380250810
N	0.0000000000	0.0000000000	1.8337391654
C	0.9877122164	-2.5902910947	-1.9339567219
C	1.7117281605	-2.3757572108	-0.7180897529
C	2.5458549509	-3.4090217924	-0.2377671296
H	3.0595123005	-3.2973862396	0.7061931994
C	2.6746995680	-4.5776429036	-0.9585874349
H	3.3073666737	-5.3701630737	-0.5797589852
C	1.9854330348	-4.7604981051	-2.1699173871
H	2.1077111496	-5.6844063241	-2.7208070481
C	1.1399918824	-3.7795510916	-2.6532263177
H	0.5853344470	-3.9062113892	-3.5735039909
C	-2.7371139995	0.4397616763	-1.9339567219
C	-2.9133301780	-0.2945214659	-0.7180897529
C	-4.2252269498	-0.5002641656	-0.2377671296
H	-4.3853763998	-1.0009222556	0.7061931994
C	-5.3017048280	-0.0275363216	-0.9585874349
H	-6.3043809812	-0.1791820222	-0.5797589852
C	-5.1154288111	0.6608136069	-2.1699173871
H	-5.9766958569	1.0168717626	-2.7208070481
C	-3.8431832014	0.9025136156	-2.6532263177
H	-3.6755455191	1.4461911938	-3.5735039909
C	1.7494017830	2.1505294184	-1.9339567219
C	1.2016020175	2.6702786768	-0.7180897529
C	1.6793719988	3.9092859581	-0.2377671296
H	1.3258640993	4.2983084952	0.7061931994
C	2.6270052600	4.6051792252	-0.9585874349
H	2.9970143075	5.5493450959	-0.5797589852
C	3.1299957763	4.0996844982	-2.1699173871
H	3.8689847073	4.6675345614	-2.7208070481
C	2.7031913191	2.8770374760	-2.6532263177
H	3.0902110721	2.4600201954	-3.5735039909
C	1.4109845706	0.0000671239	1.9446737540
C	2.1370578082	-0.6956295069	0.9548071783
C	3.5358031285	-0.7457274508	1.0704713044
H	4.1122631213	-1.2412716076	0.3022410008
C	4.1804177762	-0.0914755727	2.1069125321
H	5.2614171305	-0.1175501028	2.1614493967
C	3.4529783915	0.6259831417	3.0559217751
H	3.9631074934	1.1388045536	3.8608321536
C	2.0699916166	0.6755234986	2.9686721414
H	1.4885076296	1.2219566793	3.6997871170
C	-0.7054341543	-1.2219820444	1.9446737540

C	-1.6709617287	-1.5029315978	0.9548071783
C	-2.4137204809	-2.6892316067	1.0704713044
H	-3.1311043059	-2.9406885263	0.3022410008
C	-2.1694290579	-3.5746102062	2.1069125321
H	-2.7325099405	-4.4977458435	2.1614493967
C	-1.1843718927	-3.3033585766	3.0559217751
H	-0.9953200733	-4.0015540441	3.8608321536
C	-0.4499752977	-2.1304270749	2.9686721414
H	0.3139917118	-1.9000637606	3.6997871170
C	-0.7055504163	1.2219149205	1.9446737540
C	-0.4660960795	2.1985611047	0.9548071783
C	-1.1220826476	3.4349590575	1.0704713044
H	-0.9811588155	4.1819601339	0.3022410008
C	-2.0109887182	3.6660857790	2.1069125321
H	-2.5289071900	4.6152959463	2.1614493967
C	-2.2686064988	2.6773754349	3.0559217751
H	-2.9677874201	2.8627494904	3.8608321536
C	-1.6200163189	1.4549035763	2.9686721414
H	-1.8024993414	0.6781070814	3.6997871170

b. B3LYP functional, SVP basis

Energy: -2679.2173931494 Hartree

Ti	0.0000000000	0.0000000000	-1.2884344778
O	0.1763069441	-1.6149676764	-2.2930159060
O	-1.4867565061	0.6547975457	-2.2930159060
O	1.3104495620	0.9601701307	-2.2930159060
N	1.4198044808	-1.1774184286	-0.1317660300
N	-1.7295765104	-0.6408775345	-0.1317660300
N	0.3097720296	1.8182959631	-0.1317660300
N	0.0000000000	0.0000000000	1.8548085708
C	0.9800627009	-2.5877031663	-1.9400830144
C	1.7062832812	-2.3786665819	-0.7145093325
C	2.5434134739	-3.4189761384	-0.2339913122
H	3.0568293435	-3.3104713014	0.7213772731
C	2.6801967700	-4.5877958181	-0.9684912873
H	3.3190295861	-5.3884105565	-0.5880730706
C	1.9955316621	-4.7637116650	-2.1920647000
H	2.1269869639	-5.6914114524	-2.7549667514
C	1.1438315423	-3.7763092204	-2.6751404929
H	0.5898798912	-3.8957199781	-3.6082575937
C	-2.7310480300	0.4450923869	-1.9400830144
C	-2.9131273277	-0.2883513766	-0.7145093325
C	-4.2326269278	-0.4931726115	-0.2339913122
H	-4.3953669173	-0.9920562158	0.7213772731
C	-5.3132461108	-0.0272205809	-0.9684912873
H	-6.3260152209	-0.1801586592	-0.5880730706
C	-5.1232611492	0.6536747191	-2.1920647000
H	-5.9924003831	1.0036809819	-2.7549667514
C	-3.8422954886	0.8975674369	-2.6751404929
H	-3.6687324126	1.4370090181	-3.6082575937
C	1.7509853290	2.1426107795	-1.9400830144
C	1.2068440465	2.6670179585	-0.7145093325
C	1.6892134539	3.9121487499	-0.2339913122
H	1.3385375738	4.3025275172	0.7213772731
C	2.6330493408	4.6150163990	-0.9684912873

H	3.0069856349	5.5685692157	-0.5880730706
C	3.1277294871	4.1100369459	-2.1920647000
H	3.8654134192	4.6877304705	-2.7549667514
C	2.6984639463	2.8787417835	-2.6751404929
H	3.0788525215	2.4587109600	-3.6082575937
C	1.4135877649	0.0064820444	1.9574352392
C	2.1394865615	-0.6897054965	0.9557742275
C	3.5465741508	-0.7415192344	1.0660434472
H	4.1239859169	-1.2437232450	0.2891893070
C	4.2001409206	-0.0919644026	2.1103822811
H	5.2914804211	-0.1246606749	2.1626709570
C	3.4733775381	0.6258919017	3.0710425428
H	3.9931426306	1.1364962812	3.8854258880
C	2.0819726404	0.6789928618	2.9884258304
H	1.4977191505	1.2240762971	3.7324323935
C	-0.7011802673	-1.2274439371	1.9574352392
C	-1.6670457619	-1.5079969651	0.9557742275
C	-2.4154615698	-2.7006636938	1.0660434472
H	-3.1390888839	-2.9496149464	0.2891893070
C	-2.1797139692	-3.5914465354	2.1103822811
H	-2.7536995218	-4.5202261309	2.1626709570
C	-1.1946504821	-3.3209791358	3.0710425428
H	-1.0123366645	-4.0264110996	3.8854258880
C	-0.4529612529	-2.1425376274	2.9884258304
H	0.3112215942	-1.9091009806	3.7324323935
C	-0.7124074976	1.2209618927	1.9574352392
C	-0.4724407997	2.1977024616	0.9557742275
C	-1.1311125811	3.4421829282	1.0660434472
H	-0.9848970330	4.1933381913	0.2891893070
C	-2.0204269514	3.6834109380	2.1103822811
H	-2.5377808993	4.6448868057	2.1626709570
C	-2.2787270559	2.6950872340	3.0710425428
H	-2.9808059661	2.8899148185	3.8854258880
C	-1.6290113875	1.4635447656	2.9884258304
H	-1.8089407447	0.6850246835	3.7324323935

2. Triplet
   a. B3LYP functional, TZVP basis

      Energy: -2681.29183691 Hartree

Ti	0.0000000000	0.0000000000	-1.3113904118
O	0.1634200189	-1.6341749218	-2.2938954166
O	-1.4969470060	0.6755615731	-2.2938954166
O	1.3335269871	0.9586133487	-2.2938954166
N	1.4059333926	-1.1875713651	-0.1234701604
N	-1.7314336673	-0.6237883515	-0.1234701604
N	0.3255002747	1.8113597166	-0.1234701604
N	0.0000000000	0.0000000000	1.8886446634
C	0.9756569606	-2.6006572793	-1.9222244307
C	1.6916619022	-2.3855449271	-0.7005754235
C	2.5274096716	-3.4166358928	-0.2167097415
H	3.0365207091	-3.3008234398	0.7293527203
C	2.6669764447	-4.5830788600	-0.9395144075
H	3.3020770124	-5.3731163364	-0.5596747139
C	1.9862433463	-4.7649335503	-2.1546867599
H	2.1145711379	-5.6869992134	-2.7072608180

C	1.1393611928	-3.7841154408	-2.6426838244
H	0.5925624453	-3.9120746671	-3.5674465073
C	-2.7400637507	0.4553849264	-1.9222244307
C	-2.9117734598	-0.2722497184	-0.7005754235
C	-4.2225983144	-0.4804830350	-0.2167097415
H	-4.3768573068	-0.9792923533	0.7293527203
C	-5.3025509426	-0.0181299224	-0.9395144075
H	-6.3042937511	-0.1731244098	-0.5596747139
C	-5.1196751751	0.6623295792	-2.1546867599
H	-5.9823713591	1.0122272832	-2.7072608180
C	-3.8468206990	0.9053419833	-2.6426838244
H	-3.6842372659	1.4428632026	-3.5674465073
C	1.7644067901	2.1452723529	-1.9222244307
C	1.2201115576	2.6577946455	-0.7005754235
C	1.6951886429	3.8971189278	-0.2167097415
H	1.3403365977	4.2801157931	0.7293527203
C	2.6355744979	4.6012087824	-0.9395144075
H	3.0022167386	5.5462407462	-0.5596747139
C	3.1334318288	4.1026039712	-2.1546867599
H	3.8678002212	4.6747719303	-2.7072608180
C	2.7074595062	2.8787734574	-2.6426838244
H	3.0916748206	2.4692114645	-3.5674465073
C	1.4138606712	-0.0007200440	1.9624156564
C	2.1280353224	-0.6902679728	0.9592215421
C	3.5279805716	-0.7253222710	1.0418164040
H	4.0894121690	-1.2152499177	0.2586067919
C	4.1931367131	-0.0674120472	2.0646837875
H	5.2752304205	-0.0840502555	2.0937402933
C	3.4799052229	0.6379604693	3.0305658664
H	4.0014962186	1.1566393831	3.8243873984
C	2.0929101008	0.6688624963	2.9757383806
H	1.5230207210	1.2046912140	3.7238265391
C	-0.7075539120	-1.2240792367	1.9624156564
C	-1.6618072610	-1.4977986630	0.9592215421
C	-2.3921377984	-2.6926596636	1.0418164040
H	-3.0971433852	-2.9339098660	0.2586067919
C	-2.1549489020	-3.5976568915	2.0646837875
H	-2.7104048667	-4.5264584272	2.0937402933
C	-1.1874626384	-3.3326665604	3.0305658664
H	-0.9990690206	-4.0437170700	3.8243873984
C	-0.4672031369	-2.1469445633	2.9757383806
H	0.2817828346	-1.9213202419	3.7238265391
C	-0.7063067592	1.2247992807	1.9624156564
C	-0.4662280614	2.1880666357	0.9592215421
C	-1.1358427732	3.4179819346	1.0418164040
H	-0.9922687838	4.1491597838	0.2586067919
C	-2.0381878111	3.6650689387	2.0646837875
H	-2.5648255537	4.6105086827	2.0937402933
C	-2.2924425845	2.6947060911	3.0305658664
H	-3.0024271981	2.8870776869	3.8243873984
C	-1.6257069638	1.4780820670	2.9757383806
H	-1.8048035556	0.7166290279	3.7238265391

b. B3LYP functional, SVP basis

Energy: -2679.2108735918 Hartree

Ti	0.0000000000	0.0000000000	-1.2941340686
O	0.1418786148	-1.6262127751	-2.2653186234
O	-1.4792808826	0.6902359029	-2.2653186234
O	1.3374022678	0.9359768722	-2.2653186234
N	1.4024978676	-1.1973178001	-0.1052619286
N	-1.7381565651	-0.6159398820	-0.1052619286
N	0.3356586975	1.8132576821	-0.1052619286
N	0.0000000000	0.0000000000	1.9091548048
C	0.9569153825	-2.5983481660	-1.9193513184
C	1.6877606646	-2.3929976876	-0.6946965092
C	2.5371761114	-3.4309091571	-0.2278757643
H	3.0581177705	-3.3235142666	0.7238655610
C	2.6815005018	-4.5920148451	-0.9743511372
H	3.3327677488	-5.3896127780	-0.6083701932
C	1.9896787557	-4.7623046073	-2.1933564325
H	2.1234529499	-5.6832041688	-2.7663278761
C	1.1255158691	-3.7764695081	-2.6634371130
H	0.5669237212	-3.8940708880	-3.5939965316
C	-2.7286932109	0.4704610525	-1.9193513184
C	-2.9162771210	-0.2651447672	-0.6946965092
C	-4.2398425438	-0.4818043878	-0.2278757643
H	-4.4073066700	-0.9866505438	0.7238655610
C	-5.3175517613	-0.0262401322	-0.9743511372
H	-6.3339254567	-0.1914551464	-0.6083701932
C	-5.1191161483	0.6580399559	-2.1933564325
H	-5.9835256600	1.0026378861	-2.7663278761
C	-3.8332764652	0.9135094190	-2.6634371130
H	-3.6558261737	1.4560650995	-3.5939965316
C	1.7717778284	2.1278871135	-1.9193513184
C	1.2285164564	2.6581424549	-0.6946965092
C	1.7026664325	3.9127135449	-0.2278757643
H	1.3491888994	4.3101648103	0.7238655610
C	2.6360512596	4.6182549774	-0.9743511372
H	3.0011577079	5.5810679244	-0.6083701932
C	3.1294373927	4.1042646514	-2.1933564325
H	3.8600727102	4.6805662828	-2.7663278761
C	2.7077605961	2.8629600891	-2.6634371130
H	3.0889024526	2.4380057885	-3.5939965316
C	1.4160186260	0.0022992119	1.9810221522
C	2.1321195555	-0.6913034466	0.9694101801
C	3.5405307102	-0.7248462016	1.0488467076
H	4.1056364160	-1.2200357959	0.2581641735
C	4.2114231430	-0.0655485999	2.0779989322
H	5.3039241264	-0.0824014062	2.1052353073
C	3.4960171715	0.6395400107	3.0536429002
H	4.0240575410	1.1587861402	3.8569354252
C	2.1009233104	0.6720661344	3.0011454157
H	1.5262153426	1.2078762105	3.7597010208
C	-0.7060181371	-1.2274577083	1.9810221522
C	-1.6647461242	-1.5008179756	0.9694101801
C	-2.3980005795	-2.7037664371	1.0488467076
H	-3.1094002008	-2.9455675370	0.2581641735
C	-2.1624783242	-3.6144251279	2.0779989322
H	-2.7233237743	-4.5521323301	2.1052353073
C	-1.1941506897	-3.3474096879	3.0536429002

H	-1.0084905355	-4.0643291269	3.8569354252
C	-0.4684353098	-2.1554860254	3.0011454157
H	0.2829438116	-1.9256793636	3.7597010208
C	-0.7100004889	1.2251584964	1.9810221522
C	-0.4673734313	2.1921214222	0.9694101801
C	-1.1425301307	3.4286126387	1.0488467076
H	-0.9962362152	4.1656033329	0.2581641735
C	-2.0489448188	3.6799737278	2.0779989322
H	-2.5806003521	4.6345337363	2.1052353073
C	-2.3018664818	2.7078696772	3.0536429002
H	-3.0155670054	2.9055429867	3.8569354252
C	-1.6324880006	1.4834198910	3.0011454157
H	-1.8091591543	0.7178031531	3.7597010208

B. Unconstrained (C_1-symmetry) (Clamp)Ti

1. Singlet State

a. B3LYP functional, TZVP basis

Energy: -2681.29904617 Hartree

Ti	0.1401534614	-0.0606342381	0.6830092461
O	-1.1785265066	-1.2075229956	1.5427530353
O	1.5712497456	-0.5553682121	1.8835735308
O	-0.3743555601	1.5064238878	1.6046646855
N	-1.5618716901	-0.0803351742	-0.7075533493
N	1.1763623433	-1.7206523445	-0.3508880291
N	1.1813145701	1.4547807338	-0.3650458728
N	0.4965242037	-0.1425240247	-2.4592471754
C	-2.3542526762	-1.4257722772	1.0182983713
C	-2.6132790134	-0.8002582270	-0.2489485554
C	-3.8503419530	-1.0471041466	-0.8920791068
H	-4.0401723190	-0.6334875616	-1.8717550139
C	-4.7902893706	-1.8447365199	-0.2818451124
H	-5.7306865580	-2.0411559667	-0.7805311590
C	-4.5388014583	-2.4245693027	0.9771231418
H	-5.2983772785	-3.0424633922	1.4391311384
C	-3.3318986679	-2.2286171231	1.6194593612
H	-3.1161264580	-2.6799445329	2.5785950958
C	2.3924516187	-1.5372195651	1.6264271157
C	2.2043891973	-2.2207359055	0.3768305449
C	3.1109571646	-3.2495686194	0.0249861334
H	3.0302179600	-3.7344484656	-0.9370809349
C	4.1189728837	-3.6006712958	0.8929859523
H	4.8187352073	-4.3776783283	0.6129986367
C	4.2672618264	-2.9491693378	2.1335202651
H	5.0647095394	-3.2500719670	2.8011682165
C	3.4202251634	-1.9223235379	2.4968673300
H	3.5285965788	-1.3967936186	3.4362076506
C	0.0781810536	2.7035252903	1.2591097391
C	0.9610482121	2.7142719717	0.1455769484
C	1.4319047131	3.9511694164	-0.3254785043
H	2.0660855890	3.9959582905	-1.1993396438
C	1.0582083445	5.1194383489	0.3190832291
H	1.4208449393	6.0693850942	-0.0530540419
C	0.2151849676	5.0897054447	1.4351965238
H	-0.0588789494	6.0135550202	1.9282685599
C	-0.2830670278	3.8829905575	1.9045536838
H	-0.9494080503	3.8335586766	2.7556928908
C	-0.5538517527	0.7739727851	-2.7028314744
C	-1.6596015471	0.7394327707	-1.8284633270
C	-2.7268881526	1.6200430722	-2.0594099160
H	-3.5584774498	1.6376355963	-1.3690910910
C	-2.6770408746	2.5245854463	-3.1066850490
H	-3.4966428035	3.2164523636	-3.2530083552
C	-1.5653854944	2.5725083913	-3.9461946372
H	-1.5280745189	3.2843368764	-4.7606120083
C	-0.5044141097	1.7030141865	-3.7391341866
H	0.3645501249	1.7287126755	-4.3836427411
C	0.2513095574	-1.5305560374	-2.5519919726
C	0.6920858697	-2.3524612913	-1.4909624856
C	0.4894977755	-3.7389129998	-1.5912399470

H	0.7831732736	-4.3755122071	-0.7686952541
C	-0.1648203647	-4.2800493371	-2.6847306965
H	-0.3381796251	-5.3477237492	-2.7282380387
C	-0.6291869354	-3.4549463640	-3.7080431887
H	-1.1436793602	-3.8799344138	-4.5602257555
C	-0.4247963706	-2.0853370967	-3.6367334517
H	-0.7731061616	-1.4353675726	-4.4290354643
C	1.8304460847	0.3380023189	-2.3913516501
C	2.1458429935	1.2311017450	-1.3476871180
C	3.4491645556	1.7481947919	-1.2942019496
H	3.7193979956	2.4117144619	-0.4846096500
C	4.4053750585	1.3543174044	-2.2170163133
H	5.4119126074	1.7461432552	-2.1399008220
C	4.0905354981	0.4382576440	-3.2185783369
H	4.8421382284	0.1288359309	-3.9332248285
C	2.8028075282	-0.0704699633	-3.3005852300
H	2.5364876240	-0.7755757365	-4.0777565882

b. B3LYP functional, SVP basis

Energy: -2679.21819460 Hartree

Ti	0.1412289580	-0.0576491335	0.6762351463
O	-1.1503910814	-1.2226500085	1.5182201435
O	1.5794677919	-0.5272639453	1.8579817946
O	-0.3902968010	1.4993788101	1.5788154070
N	-1.5603139194	-0.0746302519	-0.7124480038
N	1.1780908338	-1.7184868698	-0.3593492850
N	1.1793160027	1.4609012830	-0.3763543749
N	0.4974462457	-0.1419124539	-2.4705050142
C	-2.3302861936	-1.4510817840	1.0082629487
C	-2.6087925735	-0.8070055641	-0.2549389411
C	-3.8578055061	-1.0525837636	-0.8906105072
H	-4.0650946856	-0.6201159170	-1.8696864859
C	-4.7915662755	-1.8701308728	-0.2763369296
H	-5.7461519521	-2.0650411074	-0.7711106742
C	-4.5202272481	-2.4710810877	0.9763186753
H	-5.2772349640	-3.1071407319	1.4421239213
C	-3.3005708047	-2.2742992379	1.6122597451
H	-3.0660525732	-2.7407777231	2.5708571524
C	2.4035242808	-1.5107643210	1.6187111885
C	2.2104353991	-2.2141048958	0.3710435378
C	3.1173690789	-3.2556522248	0.0279303181
H	3.0318129637	-3.7578785172	-0.9360849011
C	4.1311512276	-3.6019022729	0.9050605112
H	4.8329510762	-4.3936718630	0.6316430493
C	4.2847045653	-2.9320555359	2.1432137616
H	5.0894235472	-3.2304760177	2.8199506198
C	3.4369136174	-1.8913996085	2.4977350155
H	3.5472943655	-1.3486666771	3.4384038691
C	0.0525980454	2.7017141643	1.2471453229
C	0.9517808685	2.7200864225	0.1341836798
C	1.4287090423	3.9671427052	-0.3283108147
H	2.0785448335	4.0176530661	-1.2026720066
C	1.0461815135	5.1370938758	0.3247573859
H	1.4155227525	6.0986141562	-0.0411187143
C	0.1870275259	5.1005720701	1.4386669471

H	-0.0942953777	6.0305696570	1.9388359261
C	-0.3179556851	3.8848363597	1.8997448149
H	-0.9985266389	3.8267711161	2.7515440506
C	-0.5444470912	0.7896879892	-2.7066129326
C	-1.6552441833	0.7601795425	-1.8240674113
C	-2.7224226627	1.6546261475	-2.0515349577
H	-3.5625757379	1.6734981286	-1.3559701469
C	-2.6666054691	2.5670541319	-3.1028862502
H	-3.4899200199	3.2706759397	-3.2485623808
C	-1.5498683417	2.6100663027	-3.9485838409
H	-1.5087198665	3.3309805838	-4.7685499683
C	-0.4888429667	1.7267985861	-3.7456543021
H	0.3864992582	1.7451641272	-4.3980339897
C	0.2334394416	-1.5290962837	-2.5584522976
C	0.6754728449	-2.3553810307	-1.4894542852
C	0.4578270078	-3.7481871651	-1.5821878967
H	0.7559556843	-4.3902897840	-0.7524379104
C	-0.2121895323	-4.2902767702	-2.6760497667
H	-0.3970415764	-5.3666265462	-2.7147520540
C	-0.6787769209	-3.4606490108	-3.7052799286
H	-1.2081620874	-3.8889692516	-4.5597906504
C	-0.4591839931	-2.0847079633	-3.6424393877
H	-0.8080768929	-1.4280061901	-4.4421567461
C	1.8381605507	0.3241088755	-2.3955494526
C	2.1543399970	1.2253746309	-1.3467444845
C	3.4675912029	1.7381531722	-1.2860633181
H	3.7381025684	2.4117076645	-0.4715748510
C	4.4327123926	1.3321371501	-2.2063347142
H	5.4502875532	1.7229033159	-2.1242594451
C	4.1178228873	0.4067435214	-3.2100824413
H	4.8800471415	0.0859249712	-3.9241362588
C	2.8202471413	-0.0978731887	-3.3001383099
H	2.5514644152	-0.8112818962	-4.0824249004

2. Triplet State

I. B3LYP functional, TZVP basis

Energy: -2681.29490832 Hartree

Ti	0.1641146293	-0.0484004880	0.7117247351
O	-1.1566751911	-1.2431244702	1.5404145465
O	1.6059832881	-0.5690791181	1.8975154638
O	-0.3757619635	1.4951116095	1.6047990431
N	-1.5438170201	-0.0869378749	-0.7120656837
N	1.2226771816	-1.7172036438	-0.3682955806
N	1.1764090265	1.4254840891	-0.3464207653
N	0.5051039520	-0.1436459956	-2.5058600079
C	-2.3334633652	-1.4382693228	1.0130084031
C	-2.5908702112	-0.8017008748	-0.2553074715
C	-3.8339662502	-1.0320479375	-0.8997409790
H	-4.0184536858	-0.6073497861	-1.8757564381
C	-4.7814339189	-1.8204087937	-0.2937533074
H	-5.7252235105	-2.0039367612	-0.7906580913
C	-4.5327392881	-2.4084610768	0.9634976744
H	-5.2983895766	-3.0208948868	1.4229608665
C	-3.3238444862	-2.2293562710	1.6081383668
H	-3.1156380767	-2.6882431584	2.5652976073

C	2.4166890713	-1.5533517581	1.6267930753
C	2.2420404203	-2.2167869266	0.3581683536
C	3.1515184632	-3.2447633057	-0.0012649466
H	3.0807204628	-3.7066708672	-0.9755365562
C	4.1422700028	-3.6188582625	0.8731986571
H	4.8440638751	-4.3924042884	0.5890245281
C	4.2728882438	-2.9929346290	2.1312485760
H	5.0592957634	-3.3114577265	2.8038631002
C	3.4268620978	-1.9695404840	2.5044844575
H	3.5251300203	-1.4654332441	3.4564843396
C	0.0524125052	2.7088802681	1.2368713154
C	0.9315553792	2.7051398002	0.1290399221
C	1.3850371661	3.9322795789	-0.3676867072
H	2.0294374073	3.9663049284	-1.2348940120
C	0.9895631932	5.1135877442	0.2506945872
H	1.3448233017	6.0588809236	-0.1402875699
C	0.1445264022	5.0977462905	1.3590288670
H	-0.1485168156	6.0268788213	1.8305649814
C	-0.3343270337	3.8886507676	1.8552053262
H	-1.0021772771	3.8467538668	2.7057335542
C	-0.5467502213	0.7797447673	-2.7151793516
C	-1.6379347776	0.7526848953	-1.8229004743
C	-2.6917179913	1.6553121291	-2.0130964342
H	-3.5046937323	1.6775377914	-1.3005768771
C	-2.6530016029	2.5745680298	-3.0500535639
H	-3.4634670410	3.2824114043	-3.1668297197
C	-1.5633977928	2.6097026588	-3.9146230536
H	-1.5302580114	3.3310848450	-4.7208547640
C	-0.5140007088	1.7153903281	-3.7443459425
H	0.3384689239	1.7336646420	-4.4108681709
C	0.2520520872	-1.5306577408	-2.5561510718
C	0.7123283582	-2.3478791375	-1.4978303101
C	0.4976036917	-3.7337542772	-1.5754769457
H	0.8067451371	-4.3597936628	-0.7503014503
C	-0.1876540866	-4.2865856699	-2.6441741380
H	-0.3703316064	-5.3531675688	-2.6687410608
C	-0.6688590989	-3.4696023942	-3.6649789625
H	-1.2102042763	-3.8993714990	-4.4980394986
C	-0.4461686290	-2.1010378251	-3.6187088077
H	-0.8030977517	-1.4602093297	-4.4147219295
C	1.8382829930	0.3407467431	-2.4012989175
C	2.1474816250	1.2003337811	-1.3294307191
C	3.4524394956	1.7043757400	-1.2461735723
H	3.7138968245	2.3473118711	-0.4167931029
C	4.4182430548	1.3368424810	-2.1717084621
H	5.4249356803	1.7233948263	-2.0721289966
C	4.1092137302	0.4575113894	-3.2056156078
H	4.8658536735	0.1660116852	-3.9225129511
C	2.8172888697	-0.0369898692	-3.3165339736
H	2.5527040007	-0.7126667703	-4.1202304005

II. B3LYP functional, SVP basis

Energy: -2679.21394547 Hartree

Ti	0.1684833092	-0.0461886375	0.7027983426
O	-1.1270840748	-1.2559163486	1.5145033581

O	1.6179257909	-0.5405862947	1.8696595779
O	-0.3872341983	1.4832275027	1.5801822990
N	-1.5424909970	-0.0822671810	-0.7208301019
N	1.2315176053	-1.7163840695	-0.3793704954
N	1.1716591370	1.4331037156	-0.3603407554
N	0.5070313875	-0.1447262624	-2.5150791390
C	-2.3097084340	-1.4587306857	1.0043281979
C	-2.5882397360	-0.8050851686	-0.2600213419
C	-3.8448308628	-1.0329350407	-0.8939831337
H	-4.0473717705	-0.5914768192	-1.8700690911
C	-4.7870735352	-1.8380764472	-0.2805951510
H	-5.7463129183	-2.0190750381	-0.7713099463
C	-4.5172085388	-2.4453991412	0.9707591785
H	-5.2808474693	-3.0732663648	1.4370812266
C	-3.2935251225	-2.2672959386	1.6057347384
H	-3.0653794107	-2.7405821751	2.5624549110
C	2.4310262383	-1.5280949955	1.6192853556
C	2.2535209774	-2.2120935030	0.3527478751
C	3.1626175815	-3.2539499681	0.0043137593
H	3.0884830663	-3.7336602061	-0.9722348047
C	4.1570053425	-3.6241637152	0.8904115957
H	4.8602258566	-4.4137048633	0.6145421788
C	4.2908665771	-2.9790464384	2.1461097951
H	5.0824599209	-3.2956225751	2.8301223968
C	3.4445124679	-1.9402725881	2.5081103375
H	3.5433304017	-1.4185178582	3.4617381850
C	0.0270573476	2.7040815805	1.2271117171
C	0.9189309967	2.7111890830	0.1171280960
C	1.3738876111	3.9504220679	-0.3713054322
H	2.0307729976	3.9925159230	-1.2411787038
C	0.9687910301	5.1316282352	0.2582064539
H	1.3269408055	6.0900559680	-0.1268233860
C	0.1111598867	5.1055881274	1.3671567308
H	-0.1897407709	6.0397031562	1.8476745641
C	-0.3698946416	3.8855552462	1.8553180003
H	-1.0491279581	3.8321546106	2.7086566399
C	-0.5363436376	0.7920689861	-2.7220609920
C	-1.6340031565	0.7700800482	-1.8234149952
C	-2.6885979593	1.6844800864	-2.0142896813
H	-3.5115102993	1.7087378339	-1.2981463354
C	-2.6429085489	2.6093915331	-3.0572460031
H	-3.4576751374	3.3276187669	-3.1762926133
C	-1.5465795009	2.6396268534	-3.9260616918
H	-1.5092476956	3.3682195592	-4.7394615200
C	-0.4963719745	1.7337763615	-3.7558009671
H	0.3635520093	1.7441387818	-4.4286045362
C	0.2371220844	-1.5309552844	-2.5620084197
C	0.7026246731	-2.3527375284	-1.4975929146
C	0.4753883215	-3.7452049147	-1.5682714217
H	0.7919061685	-4.3770811835	-0.7372939025
C	-0.2275589136	-4.2987601921	-2.6356721024
H	-0.4202502897	-5.3741143307	-2.6556178260
C	-0.7149205088	-3.4769909305	-3.6604846356
H	-1.2727596354	-3.9100271162	-4.4943785560
C	-0.4792390999	-2.1020740896	-3.6224414896

H	-0.8398991221	-1.4544799991	-4.4244556198
C	1.8461440341	0.3278033676	-2.4065034109
C	2.1536636854	1.1982837675	-1.3310079823
C	3.4667926462	1.7022723918	-1.2421943160
H	3.7269397113	2.3567557643	-0.4085391684
C	4.4421425834	1.3238709895	-2.1653936186
H	5.4586235884	1.7126629540	-2.0620312198
C	4.1355350653	0.4322980591	-3.1999353199
H	4.9034060426	0.1303050619	-3.9161872425
C	2.8354560791	-0.0623091919	-3.3172229008
H	2.5702548896	-0.7484152975	-4.1250186259

C. (*o*-$C_6H_4[NH]_2)_3Ti$, $(bd)_3Ti$

Symmetry unconstrained, optimizes to C_3 symmetry

B3LYP functional, 6-31G+ basis set, singlet state

Energy: -1874.84556153 Hartree

Ti	0.087523	-0.103504	0.781309
N	-1.434236	-1.015504	1.822228
N	1.413530	-0.811242	2.185525
N	-0.178673	1.571806	1.948490
N	-1.360587	-0.485873	-0.632622
N	1.359260	-1.333428	-0.270957
N	0.736154	1.460841	-0.388200
C	-2.544772	-1.400292	1.158901
C	-2.510543	-1.077625	-0.248286
C	-3.627454	-1.393094	-1.059704
H	-3.604069	-1.141784	-2.117861
C	-4.724804	-2.024831	-0.505290
H	-5.577997	-2.272377	-1.130721
C	-4.750643	-2.358091	0.871366
H	-5.625281	-2.852793	1.284317
C	-3.680221	-2.056687	1.692547
H	-3.701417	-2.306418	2.751075
C	2.396990	-1.648790	1.795350
C	2.352857	-1.965320	0.387215
C	3.306729	-2.862456	-0.151965
H	3.266806	-3.107909	-1.211004
C	4.282362	-3.402905	0.664421
H	5.016990	-4.086238	0.247694
C	4.338919	-3.075398	2.041647
H	5.114720	-3.513506	2.663445
C	3.415781	-2.212097	2.601517
H	3.454516	-1.963637	3.659981
C	0.153770	2.779586	1.446757
C	0.701754	2.713100	0.112332
C	1.132093	3.904920	-0.520672
H	1.556945	3.852985	-1.520848
C	0.997407	5.117591	0.128841
H	1.320248	6.031487	-0.362098
C	0.437202	5.185592	1.428351
H	0.340383	6.150457	1.918280
C	0.019122	4.039765	2.078977
H	-0.405420	4.089633	3.079334
H	-1.337300	-0.220054	-1.614574
H	1.294269	-1.574277	-1.257405
H	1.153367	1.393021	-1.313804
H	1.453067	-0.552950	3.168924
H	-1.429077	-1.268776	2.807705
H	-0.598823	1.608132	2.874553

D. *fac*-(*o*-C_6H_4[NH]O)$_3$Ti, fac-(ap)$_3$Ti

1. Unconstrained (C_1-symmetric)

B3LYP functional, 6-31G+ basis set, singlet

Energy: -1934.48481841 Hartree

Ti	0.089278	-0.071230	0.864138
O	-1.319997	-1.132917	1.775661
O	1.463346	-0.674614	2.124576
O	-0.306202	1.530308	1.835049
N	-1.380433	-0.354880	-0.613569
N	1.289357	-1.357715	-0.279019
N	0.847522	1.388023	-0.343786
C	-2.429166	-1.420983	1.152398
C	-2.503462	-0.975454	-0.225274
C	-3.677054	-1.232793	-0.984485
H	-3.736526	-0.891105	-2.015088
C	-4.720961	-1.916727	-0.397933
H	-5.621271	-2.123040	-0.969794
C	-4.637825	-2.359883	0.949287
H	-5.479920	-2.893480	1.381487
C	-3.510488	-2.122765	1.719157
H	-3.439268	-2.453896	2.750170
C	2.354625	-1.561849	1.763417
C	2.285002	-1.975858	0.380149
C	3.216088	-2.927057	-0.111668
H	3.168351	-3.240114	-1.152031
C	4.170433	-3.439725	0.744762
H	4.887833	-4.168542	0.377987
C	4.230989	-3.029947	2.101498
H	4.992337	-3.456127	2.748888
C	3.338145	-2.100484	2.612294
H	3.373466	-1.777444	3.647810
C	0.099190	2.712617	1.390589
C	0.774293	2.661707	0.129144
C	1.252326	3.854736	-0.451719
H	1.770148	3.825144	-1.407904
C	1.052433	5.057028	0.214376
H	1.419038	5.980699	-0.225360
C	0.381223	5.097415	1.453025
H	0.241733	6.051555	1.953689
C	-0.101487	3.931950	2.044849
H	-0.619833	3.945420	2.998467
H	-1.383899	-0.017270	-1.573375
H	1.207775	-1.608344	-1.262058
H	1.301122	1.291851	-1.248766

2. Constrained to C_3-symmetry

B3LYP functional, 6-31G+ basis set, singlet

Energy: -1934.48449486 Hartree

Ti	0.000000	0.000000	-0.137392
O	1.613046	0.216362	-1.219134
O	-0.619148	-1.505120	-1.219134
O	-0.993898	1.288758	-1.219134
N	1.364173	0.849715	1.175004
N	0.053788	-1.606266	1.175004

N	-1.417962	0.756551	1.175004
C	2.679395	0.795017	-0.720566
C	2.568010	1.178605	0.664008
C	3.661248	1.811659	1.305413
H	3.579687	2.105185	2.349552
C	4.819706	2.042960	0.586754
H	5.664874	2.526783	1.068317
C	4.923665	1.657887	-0.772460
H	5.847162	1.855224	-1.309527
C	3.869224	1.037498	-1.427415
H	3.934448	0.741837	-2.469679
C	-0.651193	-2.717933	-0.720566
C	-0.263303	-2.813264	0.664008
C	-0.261682	-4.076564	1.305413
H	0.033300	-4.152692	2.349552
C	-0.640598	-5.195468	0.586754
H	-0.644179	-6.169317	1.068317
C	-1.026061	-5.092962	-0.772460
H	-1.316910	-5.991403	-1.309527
C	-1.036113	-3.869595	-1.427415
H	-1.324774	-3.778251	-2.469679
C	-2.028203	1.922916	-0.720566
C	-2.304707	1.634659	0.664008
C	-3.399567	2.264905	1.305413
H	-3.612987	2.047507	2.349552
C	-4.179108	3.152508	0.586754
H	-5.020695	3.642533	1.068317
C	-3.897604	3.435076	-0.772460
H	-4.530252	4.136179	-1.309527
C	-2.833112	2.832097	-1.427415
H	-2.609674	3.036413	-2.469679
H	1.233681	1.093251	2.154012
H	0.329943	-1.615025	2.154012
H	-1.563624	0.521773	2.154012

E. (o-$C_6H_4O_2$)$_3$Ti, (Cat)$_3$Ti

1. Unconstrained (optimizes to C2 symmetry)

B3LYP functional, 6-31G+ basis set, singlet

Energy: -1994.11553388 Hartree

Ti	0.105954	0.004212	0.798584
O	-1.238152	-1.184488	1.811455
O	1.526563	-0.529462	2.128391
O	-0.428177	1.499071	1.801173
O	-1.396772	-0.195192	-0.534776
O	1.137178	-1.464588	-0.212228
O	0.971440	1.341698	-0.196464
C	-2.330696	-1.454560	1.182323
C	-2.420283	-0.892380	-0.166604
C	-3.571454	-1.128996	-0.956807
H	-3.623572	-0.705742	-1.954547
C	-4.590583	-1.888785	-0.423998
H	-5.483550	-2.079631	-1.012617
C	-4.506304	-2.436562	0.893738
H	-5.339750	-3.024215	1.268095
C	-3.400829	-2.233560	1.690753
H	-3.325137	-2.643336	2.692577
C	2.360768	-1.445260	1.761042
C	2.138717	-1.979264	0.415919
C	2.995173	-2.990854	-0.088136
H	2.821418	-3.378944	-1.086443
C	4.023323	-3.442697	0.710194
H	4.692227	-4.214855	0.340753
C	4.239103	-2.918952	2.022626
H	5.064153	-3.309896	2.611164
C	3.428667	-1.936943	2.550279
H	3.582533	-1.528840	3.543667
C	0.015929	2.700302	1.389225
C	0.816518	2.610614	0.223223
C	1.355341	3.751998	-0.363042
H	1.965263	3.668927	-1.257158
C	1.084447	4.988849	0.234341
H	1.493188	5.894088	-0.205890
C	0.296062	5.077018	1.388596
H	0.101623	6.049164	1.832912
C	-0.247975	3.931515	1.981626
H	-0.859645	3.984717	2.876916

2. Constrained to C_3 symmetry

B3LYP functional, 6-31G+ basis set, singlet

Energy: -1994.11194399 Hartree

Ti	0.0000000000	0.0000000000	-0.0697141912
O	1.6219991446	0.0331667326	-1.2015012769
O	-0.7822763393	-1.4212758304	-1.2015012769
O	-0.8397228053	1.3881090978	-1.2015012769
O	1.2491736854	1.0318656808	1.0636500724
O	0.2690350501	-1.5977489857	1.0636500724
O	-1.5182087356	0.5658833049	1.0636500724
C	2.6646273557	0.6575615495	-0.7215740733
C	2.4489822360	1.2345096985	0.5878489603

C	3.4841782574	1.9390726019	1.2317121305
H	3.3087739599	2.3651131314	2.2141713501
C	4.7023277798	2.0547444281	0.5828309142
H	5.5158396679	2.5911544833	1.0628048260
C	4.9162571203	1.4838889015	-0.7002350303
H	5.8891750204	1.5968470136	-1.1705170100
C	3.9141717117	0.7894801354	-1.3579011219
H	4.0629457531	0.3509588058	-2.3393817385
C	-0.7628486714	-2.6364157564	-0.7215740733
C	-0.1553743579	-2.7381356791	0.5878489603
C	-0.0628029956	-3.9869231832	1.2317121305
H	0.3938610747	-4.0480388703	2.2141713501
C	-0.5717030168	-5.0997075283	0.5828309142
H	-0.5139142262	-6.0724345172	1.0628048260
C	-1.1730430750	-4.9995480085	-0.7002350303
H	-1.5616774305	-5.8985986818	-1.1705170100
C	-1.2733760028	-3.7845122048	-1.3579011219
H	-1.7275336350	-3.6940936393	-2.3393817385
C	-1.9017786843	1.9788542069	-0.7215740733
C	-2.2936078782	1.5036259806	0.5878489603
C	-3.4213752617	2.0478505812	1.2317121305
H	-3.7026350346	1.6829257389	2.2141713501
C	-4.1306247629	3.0449631002	0.5828309142
H	-5.0019254416	3.4812800339	1.0628048260
C	-3.7432140453	3.5156591070	-0.7002350303
H	-4.3274975899	4.3017516682	-1.1705170100
C	-2.6407957089	2.9950320694	-1.3579011219
H	-2.3354121181	3.3431348334	-2.3393817385