Supporting Information

Highly selective visible light-induced Ti−O bond splitting in an *ansa*-titanocene dihydroxido complex

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1. Experimental details

General information.

All manipulations were carried out in an oxygen- and moisture-free argon atmosphere using standard Schlenk- and glovebox techniques. All solvents were dried over sodium/benzophenone and freshly distilled prior to use. Deionised water was degassed prior to use. Terephthalic acid was obtained from Sigma Aldrich and used as received. The synthesis of compounds **1**[1] and **4**[2] were described elsewhere. The following instruments were used:

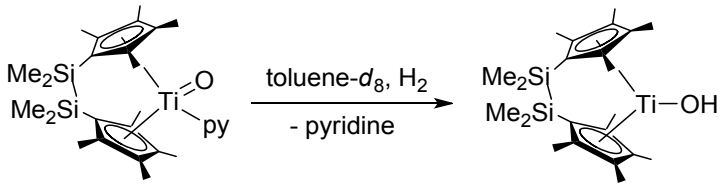
NMR:
Bruker AV 300. ^{1}H and ^{13}C chemical shifts are given in ppm (δ) and were referenced using the chemical shifts of residual protio solvent resonances: benzene-d_6 (δ H 7.16, δ C 128.0).

EPR:
In situ EPR spectra in X-band were recorded by a Bruker EMX CW-micro spectrometer equipped with an ER 4131VT Digital Temperature Control System and an ER 4119HS-WI high-sensitivity optical resonator. A solution of complex **1** in toluene (c = 10.0 mg mL^{-1}, 0.050 mL) was filled into a J. Young EPR tube in a glovebox in the dark and introduced into the EPR spectrometer. The sample was irradiated with a Xe lamp/420 nm cut-off filter (300 W, LOT-Oriel GmbH & Co. KG) to remove radiation below 420 nm and to ensure irradiation by visible light only.[3] Different band pass filter (Lot Oriel 7-Piece visible set, FWHM/ bandwidth 10 nm) were applied for the testing of the wavelength dependence. Spectra were recorded at given reaction/irradiation times. The following parameters were used: microwave frequency: 9.421 GHz, microwave power: 6.92 mW, receiver gain: $1*10^3$, modulation frequency: 100 kHz, modulation amplitude: 0.4 G, Sweep time: 61.44 s. *g* factor have been calculated from the resonance field B_0 and the resonance frequency ν using the resonance condition $h\nu = g\beta B_0$. The calibration of the *g* values was performed using E4100MK Bruker Marker Accessory (g = 1.980±0.0005). Analysis of the experimental spectra was performed using the simulation program EPRSim32 of Sojka and co-workers.[4] The signal at 250 K shows typical hyperfine structure (hfs) splitting which results from the coupling of the single electron of Ti^{III} to the nuclear spin of the isotopes ^{47}Ti (I = 5/2, 7.44 % natural abundance) and ^{49}Ti (I = 7/2, 5.41 % natural abundance). This is characteristic for isolated $Cp^*_2Ti^{III}OR$ complexes.[5]

IR:
The in situ ATR-IR spectroscopic measurements were performed on a Nicolet Avatar 370 (Thermo Electron) FTIR spectrometer equipped with a MCT detector. A Specac Gateway multireflection horizontal accessory, coupled to a custom-made flow-through cell with quartz window containing a ZnSe crystal on the bottom plate, was used for in situ experiments. The 45° internal reflection element of 72x10x6 mm^3 allows six reflections. In each run, 0.3 mL of a solution of **1** (20 mg/mL) was filled into the cell. Then, the cell was irradiated with a Xe lamp/420 nm cut-off filter (300 W, LOT-Oriel GmbH & Co. KG) for 1140 min. All spectra were recorded with 64 scans at 4 cm^{-1} resolution.

X-ray analysis:
Diffraction data were collected on a Bruker Kappa Apex II using graphite-monochromated Mo-Kα radiation. The structures were solved by direct methods (SHELXS-97) and refined by full-matrix least-squares procedures on F^2 (SHELXL-97).[6] Diamond was used for graphical representation.[7]
Crystal data for complex **6**: $C_{70}H_{90}N_2O_8Si_4Ti_2$, M = 1295.60, triclinic, space group P-1, a = 10.0526(16), b = 11.8019(18), c = 14.793(2)Å, α = 74.190(3), β = 89.420(3), γ = 75.231(3)°, V = 1629.6(4) $Å^3$, T = 150(2) K, Z = 1, 31473 reflections measured, 7875 independent reflections (R_{int} = 0.0559), final R values ($I > 2\sigma(I)$): R_1 = 0.0376, wR_2 = 0.0854, final R values (all data): R_1 = 0.0640, wR_2 = 0.0943, 400 parameters.
CCDC 1011531 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/data_request/cif.

Synthesis of compound 2 by hydrogenolysis:



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Scheme S1. Hydrogenation of *ansa*-titanocene oxido complex Cp'$_2$Ti(py)O to give **2**.

In a J. Young NMR tube, titanocene oxido complex (0.025 g, 0.05 mmol) was dissolved in toluene-d_8 (0.5 mL) and the yellow solution was frozen in liquid nitrogen and degassed. Subsequently, 1 atm of hydrogen gas was added at this temperature and the tube was allowed to warm to room temperature. Heating of the solution at 50 °C over night gave a dark green solution. NMR analysis of this mixture shows decreasing signals of the starting complex and increasing signals which are characteristic for complex **1**, further heating at 50 °C resulted in a slow decrease of the NMR signals for both complexes.

2. EPR spectra

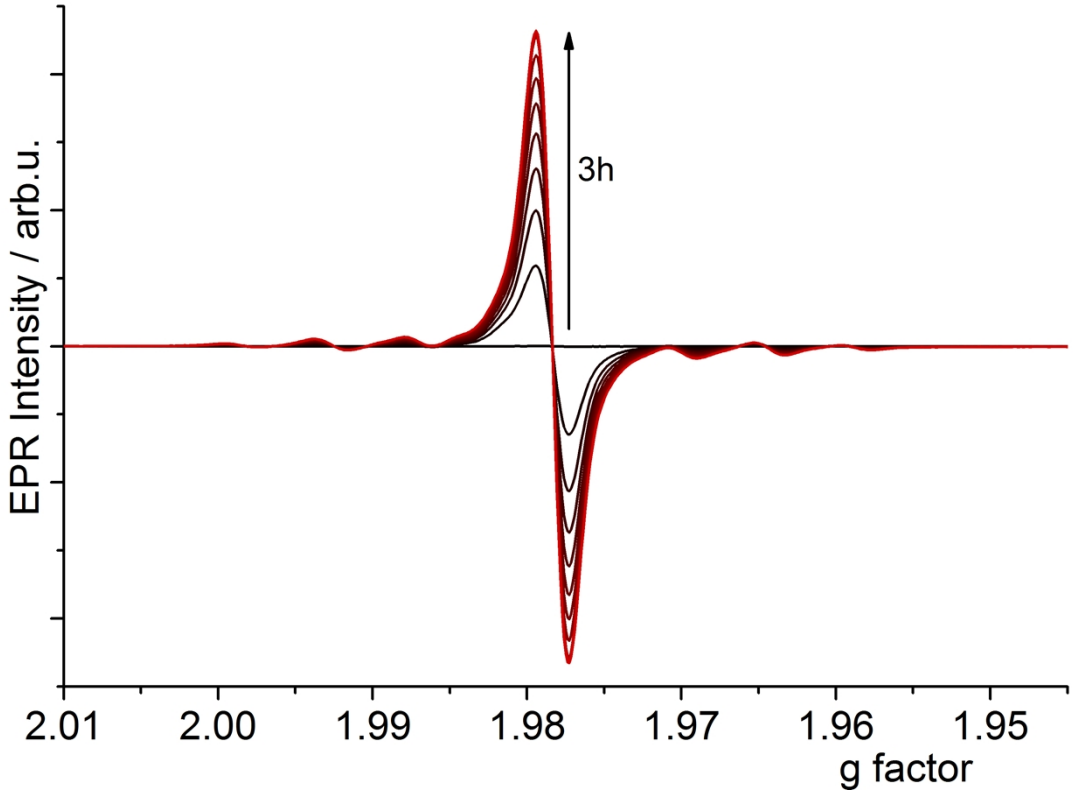


Figure S1. EPR spectra recorded during irradiation with visible light (λ > 420 nm) of complex **1** in toluene at 250 K.

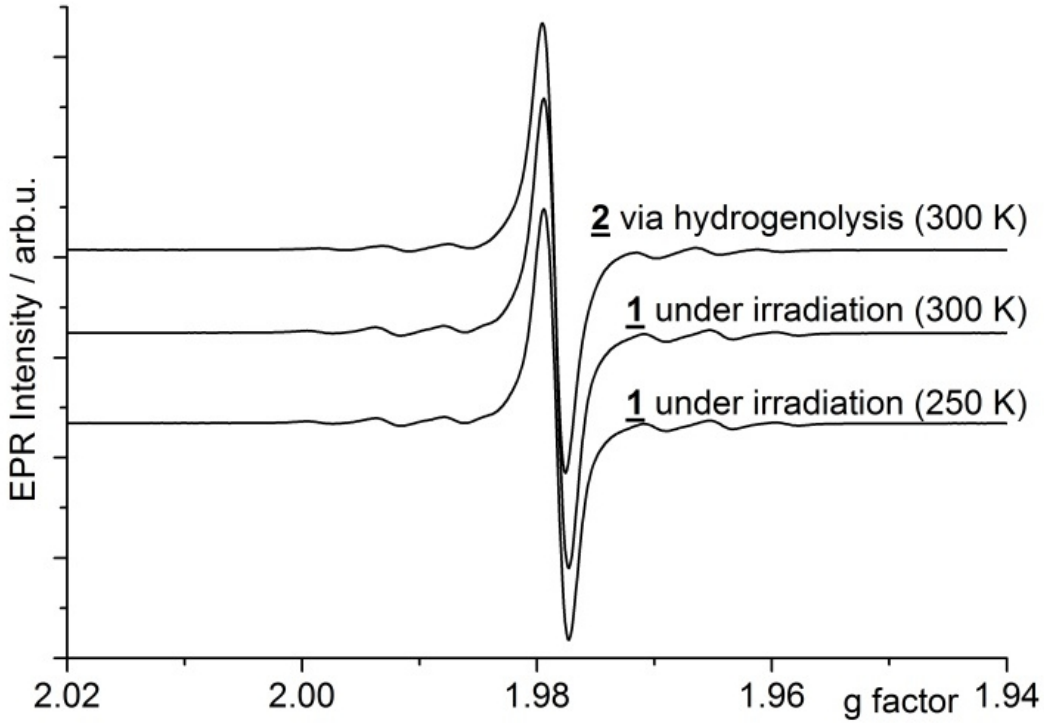


Figure S2. EPR spectra of **2** prepared via hydrogenolysis (toluene) in comparison with complex **1** irradiated in toluene at 250 K and 300 K. EPR parameters of **1** (*T* = 300 K, toluene): g=1.978, A_{Ti}=9.7 G, linewidth ΔB = 3.9 G.

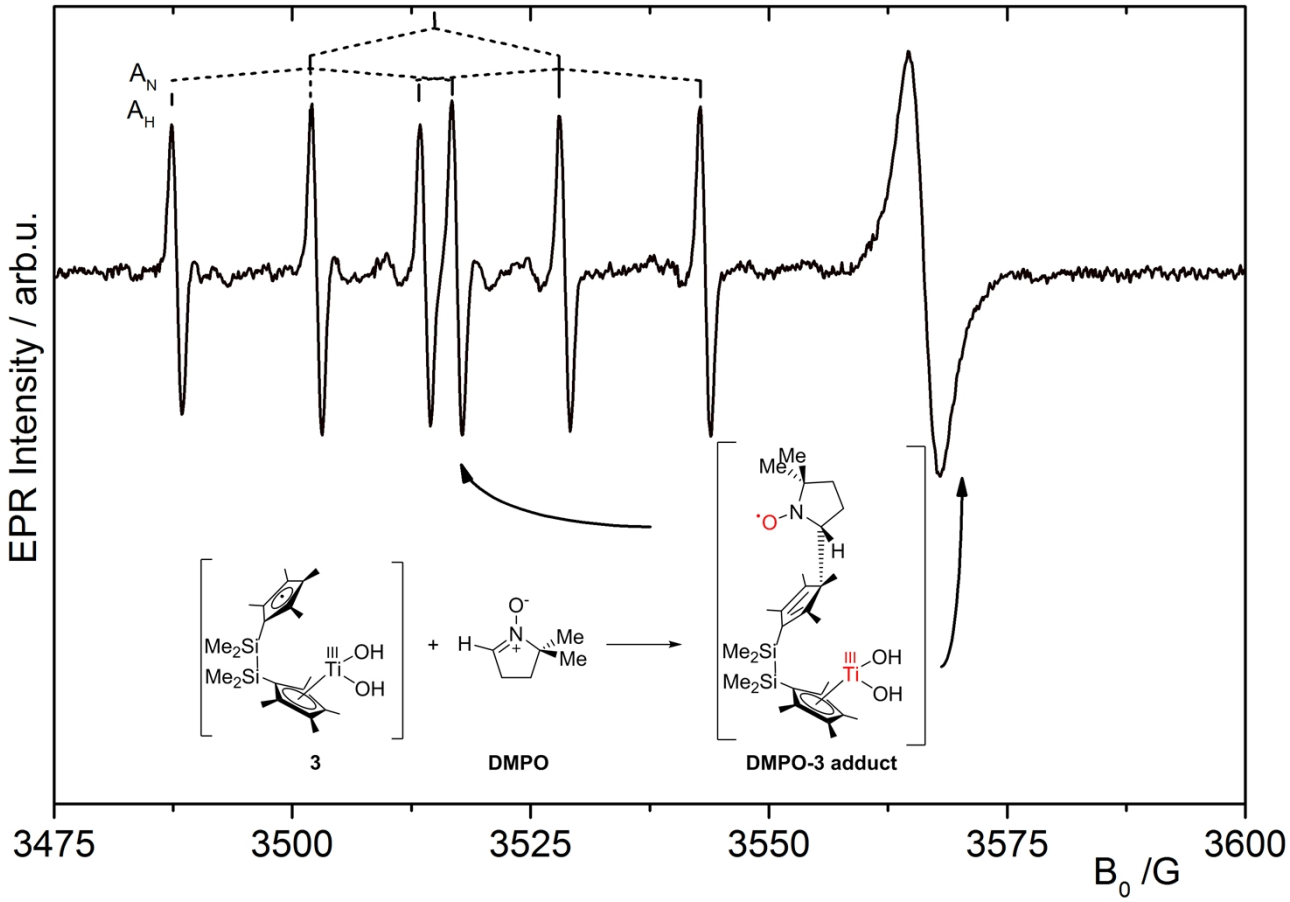


Figure S3. EPR spectrum of complex **1** in the presense of DMPO irradiated in toluene at 300 K. EPR parameters of DMPO adduct **3** (*T* = 300 K, toluene): g_{DMPO}=2.0064, A_N=14.8 G, A_H=26.0 G, linewidth ΔB = 1 G; $g_{Ti(III)}$=1.9779, A_{Ti} not resolved, linewidth ΔB = 3.5 G.

3. UV-Vis spectrum of complex 1

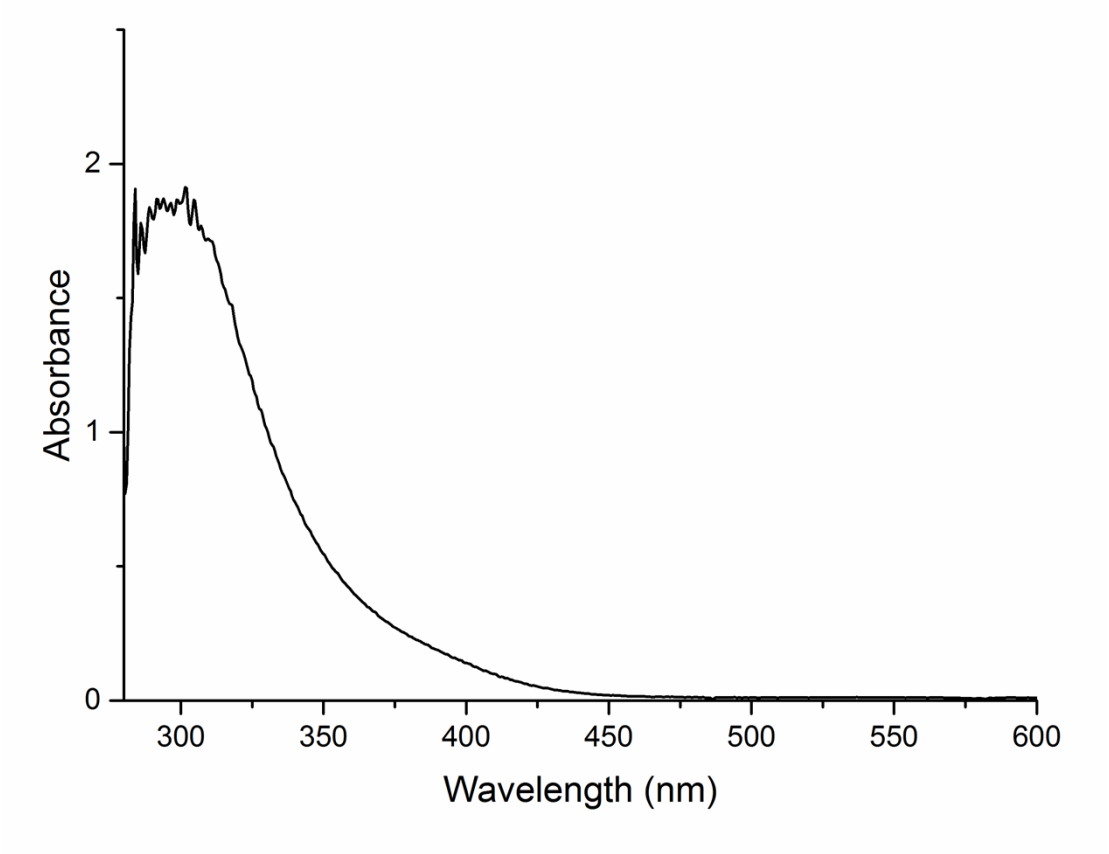
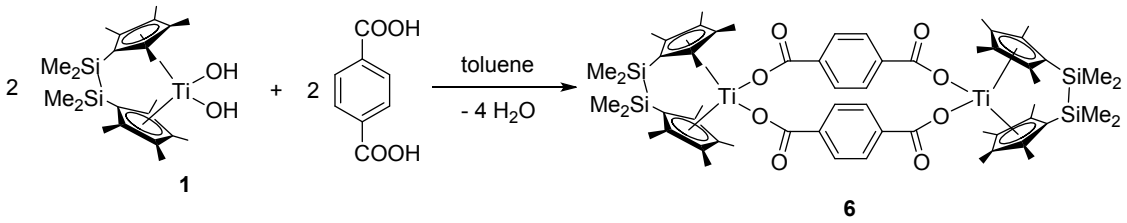


Figure S4. UV-Vis spectrum of complex **1** in toluene (T = 298 K, c = $1.25 \cdot 10^{-7}$ mol·l^{-1}).

4. Molecular structure of complex 6

Upon mixture of a solution of complex **1** with terephthalic acid (TA), formation of a dinuclear adduct **6** was observed (Scheme S2). Its molecular structure is depicted in Figure S4.



Scheme S2. Formation of a dinuclear Ti(IV) complex **6** from **1** and TA.

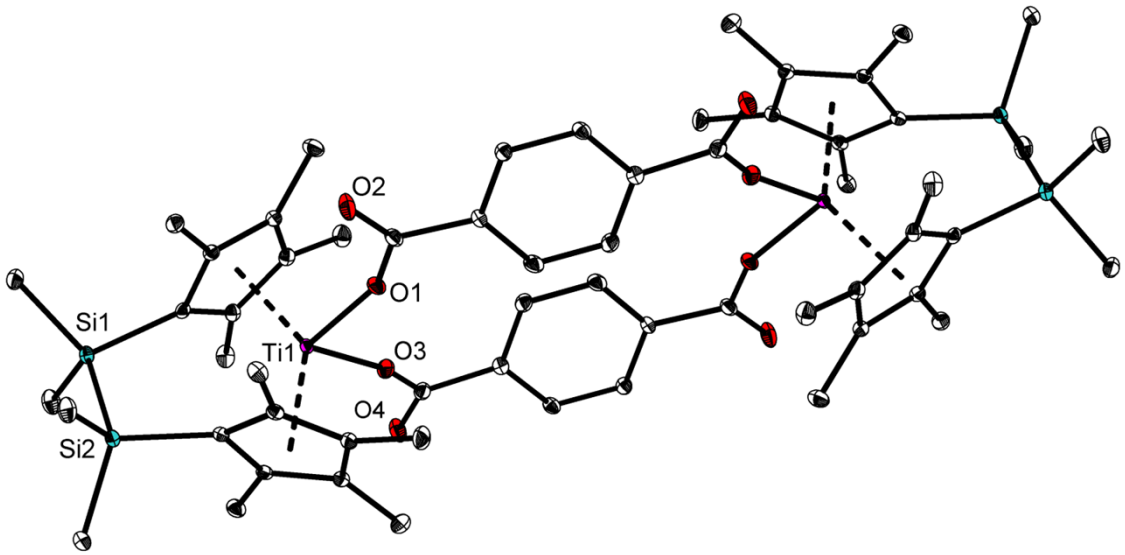


Figure S5. Molecular structure of complex **6**. Thermal ellipsoids correspond to 30 % probability. Hydrogen atoms and co-crystallised pyridine are omitted for clarity.

5. NMR spectra

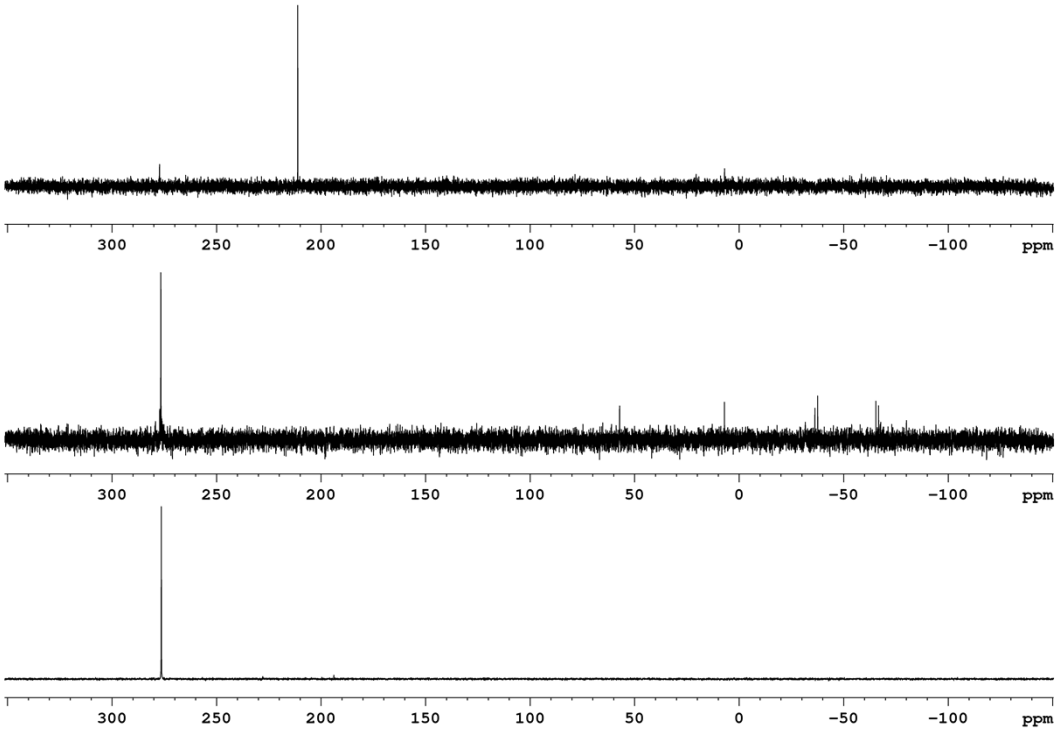
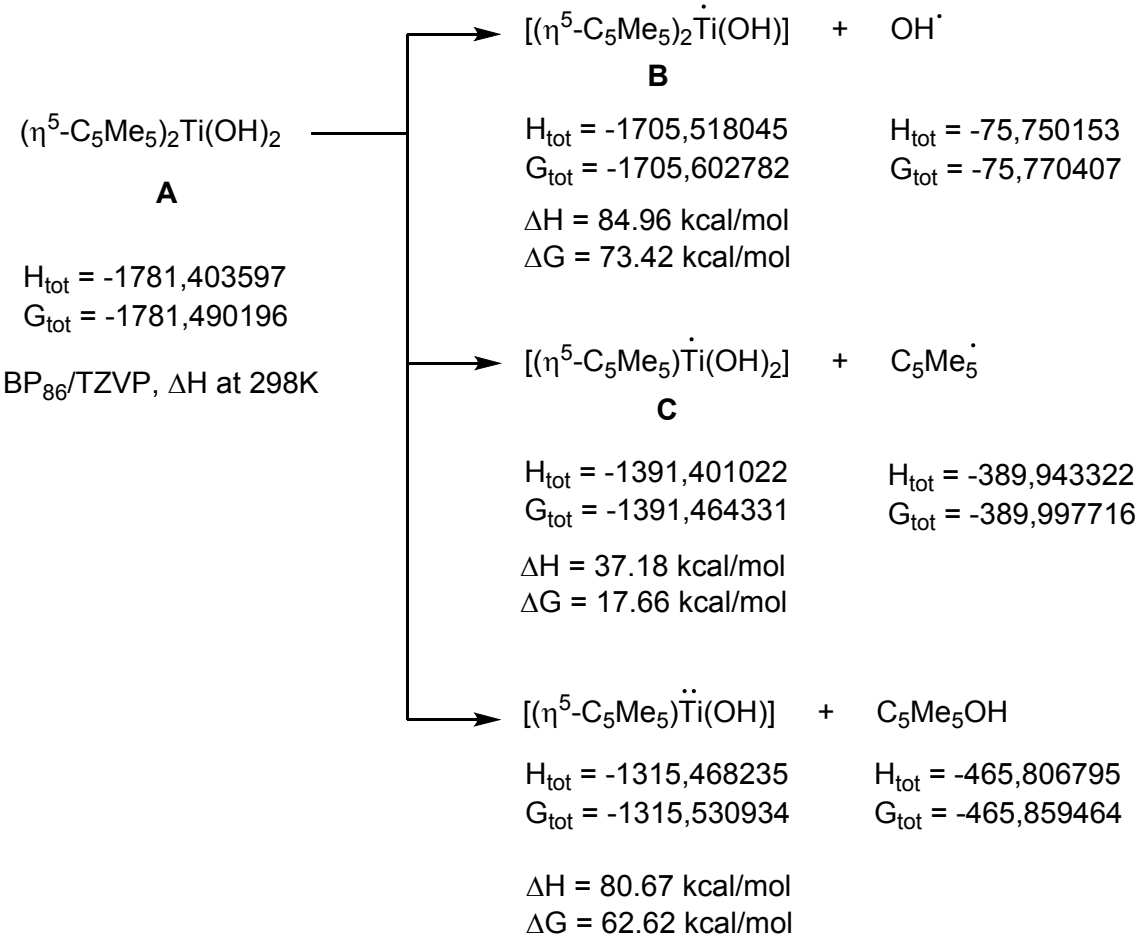


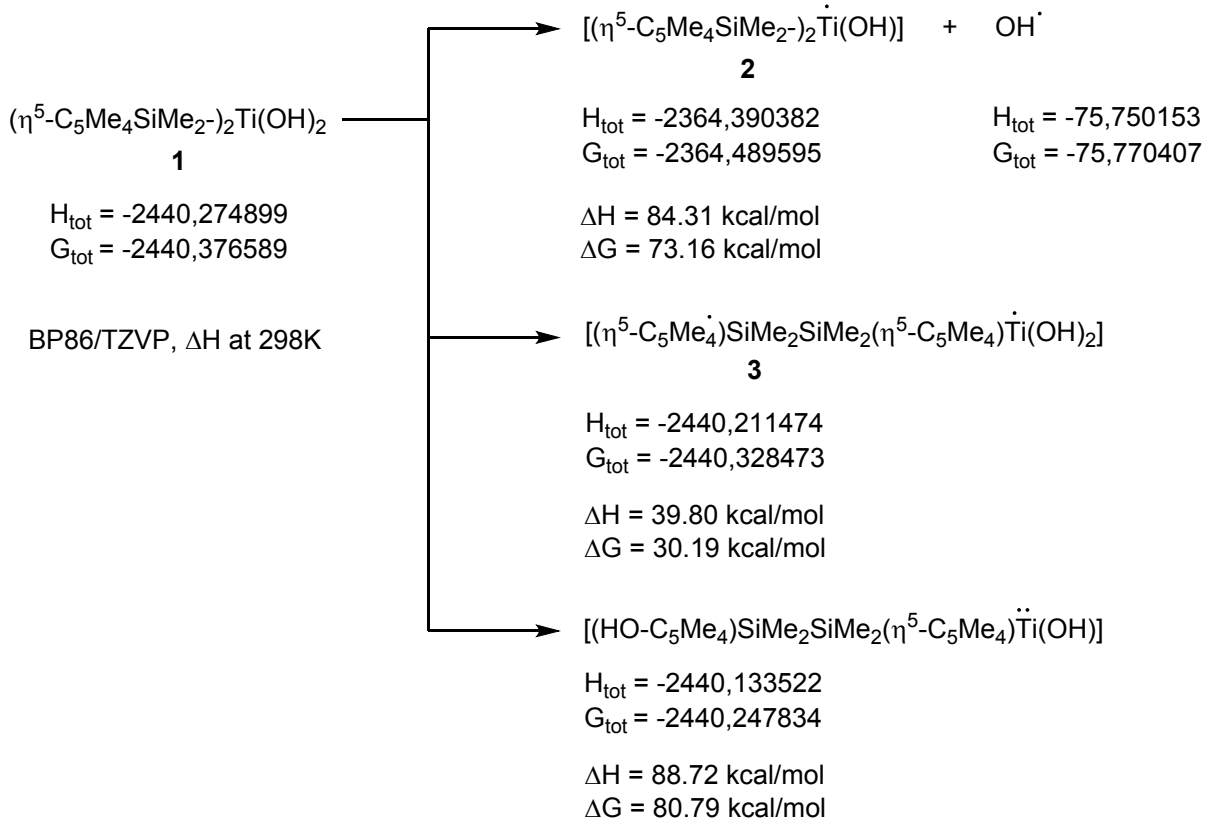
Figure S6. ^{31}P NMR spectra of the biradicaloid $[PN(Ter)]_2$ (**4**) (bottom), the irradiated biradicaloid **4** (middle) and the irradiated mixture of complex **1** and the biradicaloid **4** (top).

6. Computational details

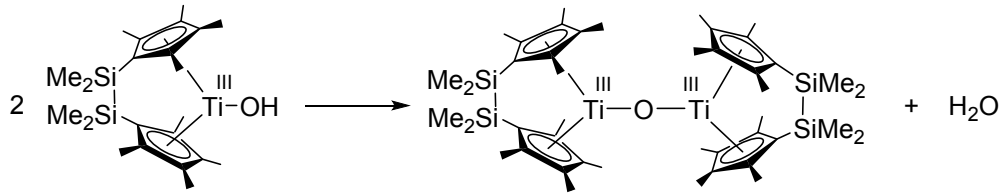
In our calculations we used all real-size model systems without any simplification or constrains. We employed the BP86[8] functional in combination with the TZVP[9] basis set (BP86/TZVP) for the equilibrium geometry optimizations and the subsequent frequency calculations, which characterise the optimised structures as energy minimums without imaginary frequencies; and this is because that BP86/TZVP can give not only reasonable geometries but also the right relative energies for titanocene chemistry.[10] The computed Gibbs free energies (ΔG) at 298 K deduced the frequency calculations were used for discussion and comparison. The Gaussian 09 program was used for all calculations.[11]



Scheme S3. Computed energies for photolytic bond cleavage reactions starting from complex **A**.



Scheme S4. Computed energies for photolytic bond cleavage reactions starting from complex **1**.



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Δ*G*(298 K) = 37.91 kcal/mol (BP86/TZVP)
Δ*G*(298 K) = 17.23 kcal/mol (wB97XD/TZVP//BP86/TZVP)

Scheme S5. ΔG/ΔH of the intermolecular condensation reaction of complex **2**.

The decomposition reaction of complex **2** to give the dinuclear compound and water is strongly endergonic (37.91 kcal/mol at BP86 and 17.23 kcal/mol after dispersion correction at ωB97XD).[12] This is well in line with Mach's experimental observation[13] of a reaction of the dinuclear Ti(III) complex $[Cp^*_2Ti]_2O$ with water to give the monomer $Cp^*_2Ti(OH)$ (**B**) (exergonic by 37.57 kcal/mol at BP86 and 16.13 kcal/mol at ωB97XD).

Table S1. BP86 computed energetic total electronic energies (E_{tot}, au), Zero-point energies (ZPE, kcal/mol, the number of imaginary frequencies (including the value of the imaginary frequencies), as well the thermal enthalpies (H_{tot}, au) and free energies (G_{tot}, au).

Compounds	BP86/TZVP	BP86/TZVP	ωB97XD/TZVP[b]
$(\eta^5\text{-}C_5Me_5)_2Ti(OH)_2$ (**A**)	E_{tot}=-1781.8931024 ZPE= 287.63822 NImag=0	H_{tot}=-1781.403597 G_{tot}= -1781.490196	
$(\eta^5\text{-}C_5Me_5)_2Ti(OH)_1$] – Radical (**B**)	E_{tot} =-1705.9923995 ZPE = 279.19244 NImag= 0	H_{tot}=-1705.518045 G_{tot}= -1705.602782	
OH-Radical	E_{tot} =-75.7615944 ZPE=5.10579 NImag=0	H_{tot}=-75.750153 G_{tot}= -75.770407	
$[(\eta^5\text{-}C_5Me_5)_1Ti(OH)_2]$ Radical (**C**)	E_{tot} =-1391.6591746 ZPE=150.21608 NImag=0	H_{tot}= -1391.401022 G_{tot}= -1391.464331	
$[(\eta^5\text{-}C_5Me_5)$ Radical	E_{tot} =-390.1675952 ZPE=131.77825 NIMag=0	H_{tot}=-389.943322 G_{tot}= -389.997716	
$[(\eta^5\text{-}C_5Me_5)_1Ti(OH)_1]$- triplet state	E_{tot} =-1315.7120889 ZPE=141.87645 NImag=0	H_{tot}=-1315.468235 G_{tot}= -1315.530934	
$(C_5Me_5)(OH)$	E_{tot} =-466.0499609 ZPE=143.46585 NImag=0	H_{tot}=-465.806795 G_{tot}= -465.859464	
$(\eta^5\text{-}C_5Me_4\text{-}ansa)_2Ti(OH)_2$ (**1**)	E_{tot} =-2440.8443064 ZPE=333.09929 NIMag=0	H_{tot}=-2440.274899 G_{tot}= -2440.376589	
$[(\eta^5\text{-}C_5Me_4\text{-}ansa)_2Ti(OH)_1]$ –Radical (**2**)	E_{tot} =-2364.9446559 ZPE=324.67638 NImag=0	H_{tot}=-2364.390382 G_{tot}= -2364.489595	
$[C_5Me_4\text{-}ansa\text{-}(\eta^5\text{-}C_5Me_4)_1Ti(OH)_2]$ (**3**) – triplet state	E_{tot} =-2440.7779413 ZPE=329.36008 NImag=0	H_{tot}=-2440.211474 G_{tot}= -2440.328473	
$[(HO)C_5Me_4\text{-}ansa\text{-}(\eta^5\text{-}C_5Me_4)_1Ti(OH)_1]$ – triplet state	E_{tot} =-2440.7027479 ZPE=331.74114 NIMag=0	H_{tot}=-2440.133522 G_{tot}= -2440.247834	
$[(\eta^5\text{-}C_5Me_4\text{-}ansa)_2Ti(OH)_1]$ –Radical (**2**)[a]	HF=-914.5490458 ZPE= 279.10370 NImag=0	Htot= -914.074803 Gtot= -914.159458	HF=-914.2642478
$[(\eta^5\text{-}C_5Me_4\text{-}ansa)_2]$Ti-O-Ti$[(\eta^5\text{-}C_5Me_4\text{-}ansa)_2]$ Triplet state (**3**)[a]	HF=-3070.4926923 ZPE= 636.29922 NImag=0	Htot= -3069.407559 Gtot= -3069.574696	HF=-3069.8539615
$[(\eta^5\text{-}C_5Me_5)_2]$Ti-O-Ti$[(\eta^5\text{-}C_5Me_5)_2]$ Triplet state[a]	HF=-1752,588828 ZPE= 545,09129 NImag=0	Htot= -1751,664083 Gtot= -1751,801287	HF=-1752,0791566
$[(\eta^5\text{-}C_5Me_5\text{-}ansa)_2Ti(OH)_1]$[a]	HF=-914,5490458 ZPE= 279,10370 NImag=0	Htot= -914,074803 Gtot= -914,159458	HF=-914,2642478
H_2O[a]	HF=-76.4606717 ZPE=12.92167 NImag=0	Htot=-76.436299 Gtot= -76.457754	HF=-76.4349398

[a] Optimisation and frequency calculation at BP86/TZVP. [b] Single-point energy calculations at ωB97XD/TZVP (LAL2DZ basis set for Ti) on the BP86/TZVP optimised geometries for the dispersion correction[11]

Table S2. BP86 Computed Cartesian Coordinates

$(\eta^5\text{-}C_5Me_5)_2Ti(OH)_2$ (**A**)	$(\eta^5\text{-}C_5Me_5)_2Ti(OH)_1]$ – Radical (**B**)
Ti,0,0.,0.4798906207,0. O,0,-1.4492155591,1.7325452419,0.1243407385 O,0,1.4492155591,1.7325452419,-0.1243407385 H,0,-1.589727152,2.2523135821,-0.6850939753 H,0,1.589727152,2.2523135821,0.6850939753 C,0,0.9216018861,-1.0241447159,1.7473077237 C,0,-0.9216018861,-1.0241447159,-1.7473077237 C,0,-0.4798188794,-1.3384276374,1.6755521121 C,0,0.4798188794,-1.3384276374,-1.6755521121 C,0,-1.2074567105,-0.18547849,2.0865320783 C,0,1.2074567105,-0.18547849,-2.0865320783 C,0,-0.2639353069,0.8322148301,2.4513601804 C,0,0.2639353069,0.8322148301,-2.4513601804 C,0,1.0440328034,0.3048742357,2.2602168316 C,0,-1.0440328034,0.3048742357,-2.2602168316 C,0,0.638247558,2.1770035982,-2.9952737558 C,0,-0.638247558,2.1770035982,2.9952737558 C,0,2.0717924702,-1.9845770576,1.6364994286 C,0,-2.0717924702,-1.9845770576,-1.6364994286 H,0,1.780212784,-2.9275518285,1.1577718855 H,0,-1.780212784,-2.9275518285,-1.1577718855 H,0,2.4575170164,-2.2371468395,2.6405710085 H,0,-2.4575170164,-2.2371468395,-2.6405710085 H,0,2.9163682219,-1.5639489523,1.0686006322 H,0,-2.9163682219,-1.5639489523,-1.0686006322 C,0,2.3449945261,0.9555582528,2.6227507434 C,0,-2.3449945261,0.9555582528,-2.6227507434 H,0,3.0854650768,0.8675948014,1.8129961714 H,0,-3.0854650768,0.8675948014,-1.8129961714 H,0,2.7780558711,0.4838105978,3.5218678416 H,0,-2.7780558711,0.4838105977,-3.5218678416 H,0,2.2221859406,2.0242396851,2.8560903067 H,0,-2.2221859406,2.0242396851,-2.8560903067 H,0,-1.3665396312,2.6658541705,2.3303024956 H,0,1.3665396312,2.6658541705,-2.3303024956 H,0,0.2331853939,2.8405107554,3.0962270532 H,0,-0.2331853939,2.8405107554,-3.0962270532 H,0,-1.0952668086,2.0844878885,3.9955821189 H,0,1.0952668086,2.0844878885,-3.9955821189 C,0,-2.6931039641,-0.0457453335,2.2193768233 C,0,2.6931039641,-0.0457453334,-2.2193768233 H,0,-3.228271955,-0.8963148532,1.7737060146 H,0,3.228271955,-0.8963148532,-1.7737060146 H,0,-3.0340931777,0.8751494269,1.7215665863 H,0,3.0340931777,0.8751494269,-1.7215665863 H,0,-2.9906413284,0.0109988052,3.2808948368 H,0,2.9906413284,0.0109988052,-3.2808948368 C,0,-1.0645463527,-2.7128487271,1.5282839027 C,0,1.0645463527,-2.7128487271,-1.5282839027 H,0,-1.0999747846,-3.2068514832,2.5157937126 H,0,1.0999747846,-3.2068514832,-2.5157937126 H,0,-0.4706482017,-3.3613958045,0.8711263866 H,0,0.4706482017,-3.3613958045,-0.8711263866 H,0,-2.0926446263,-2.6902656377,1.1434833982 H,0,2.0926446263,-2.6902656377,-1.1434833982	C,0,-1.3423129795,1.1590698353,3.9285021775 C,0,-0.9810301357,1.7840313116,5.164474247 C,0,0.4483723356,1.7575285201,5.2601330828 C,0,0.972675203,1.1699812785,4.0630890299 C,0,-0.1395507189,0.7810012177,3.2504986697 C,0,-2.7459699453,0.7816664695,3.5478075234 H,0,-2.8235936384,0.4819435181,2.4946450592 H,0,-3.4625020645,1.599433345,3.7189772179 H,0,-3.0888125232,-0.0751878219,4.1541853784 C,0,-1.9336722856,2.2375443669,6.2355068798 H,0,-2.150471061,1.423924003,6.9517067374 H,0,-2.8950211047,2.5618289685,5.8110797812 H,0,-1.5281146165,3.0812876188,6.8129873363 C,0,1.2511439328,2.1515757056,6.4644118189 H,0,1.3714732395,1.2975953521,7.1533037432 H,0,0.7657887615,2.9541527093,7.0429805303 H,0,2.2674251908,2.4827696311,6.1962672523 C,0,2.4187265505,0.8698310807,3.7817371518 H,0,3.0856252595,1.6314130981,4.2119652276 H,0,2.6206982961,0.8286888239,2.7014555418 H,0,2.7171861702,-0.1057256959,4.207351623 C,0,-0.0317616664,-0.0716953789,2.0180537165 H,0,0.760604597,0.2727036007,1.3361372716 H,0,-0.9718842187,-0.1032343826,1.4521644146 H,0,0.214689253,-1.1121477541,2.2940118119 C,0,0.3968435932,4.9971191441,1.853853874 C,0,-0.8021137956,5.3752481718,2.530804554 C,0,-1.8156009326,4.4131747712,2.2208449476 C,0,-1.2425278007,3.4562772915,1.3169039032 C,0,0.1378066126,3.7971420196,1.1178017217 C,0,1.6878536648,5.7580383505,1.9081837378 H,0,2.5247327854,5.1713091649,1.5025122041 H,0,1.9333885518,6.0262532789,2.9466127152 H,0,1.6217151644,6.6895522682,1.3193159832 C,0,-0.9500009847,6.5899886002,3.3974485803 H,0,-1.8765317443,6.5590222706,3.9888696763 H,0,-0.9787663231,7.5091739834,2.7866061917 H,0,-0.1039751656,6.669636999,4.0963143977 C,0,-3.2693165505,4.5218441167,2.5894133605 H,0,-3.4059380197,4.9577632121,3.5899433197 H,0,-3.7710314355,3.5435606595,2.5819824454 H,0,-3.8125268696,5.1680359305,1.8762969001 C,0,-2.0178485423,2.4667574342,0.4960115296 H,0,-2.3838635895,2.9483898698,-0.4289529299 H,0,-2.9010166206,2.0834542847,1.0247752812 H,0,-1.4068788855,1.6081425149,0.1861235642 C,0,1.0755349717,3.1518566339,0.1353665675 H,0,1.0180615405,3.6457337279,-0.8515335609 H,0,0.8397682326,2.0897872265,-0.0234371268 H,0,2.1221570438,3.2138969131,0.4677643503 O,0,0.8948805104,4.4446175537,4.5544187379 Ti,0,-0.0998692138,3.2387110464,3.4620183934 H,0,1.2777479714,4.1526921412,5.3973024573
$[(\eta^5\text{-}C_5Me_5)_1Ti(OH)_2]$ Radical (**C**)	$[(\eta^5\text{-}C_5Me_5)_1Ti(OH)_1]$- triplet state
Ti,0,0.0150747277,0.6947596905,-0.4093008918 O,0,-1.2268608906,0.3557721529,0.8943633824 O,0,1.3570825225,1.9265608211,0.0115762367 H,0,-2.0157115708,-0.119808215,1.1886939183 H,0,1.4885636818,2.4182584198,0.8372713389	Ti,0,0.6938088352,0.0058463664,1.1045674682 O,0,1.7855909306,0.0125332921,2.5796396216 H,0,2.407765924,0.0178504934,3.315764802 C,0,-1.4752067192,-0.0338557701,0.0418035088 C,0,-0.726913834,-1.169574955,-0.4025207461

C,0,-0.9496486587,-0.8564819856,-1.9333130105 C,0,0.43087313,-1.2061920657,-1.7509259305 C,0,1.2259199017,-0.1369350155,-2.2908999945 C,0,0.3431494304,0.8774328615,-2.7686771975 C,0,-1.007085492,0.4429638673,-2.5363871995 C,0,0.7684288557,2.1712562945,-3.4021752653 C,0,-2.1304667059,-1.7127738764,-1.5736998245 H,0,-1.905737766,-2.3853071285,-0.7322019858 H,0,-2.4378596789,-2.348166558,-2.422659525 H,0,-3.0051212449,-1.1065969872,-1.292423581 C,0,-2.2561716522,1.1640531921,-2.9609050427 H,0,-3.1005237458,0.9521643385,-2.2885776749 H,0,-2.5635746685,0.8587432541,-3.9770305815 H,0,-2.1129091517,2.2542515052,-2.9778287267 H,0,1.6590330491,2.5859746035,-2.9075204039 H,0,-0.0245139396,2.9309531171,-3.3478369876 H,0,1.0141553792,2.0283432582,-4.4690471864 C,0,2.7257709471,-0.0774190692,-2.3434146696 H,0,3.1849115993,-0.8101476711,-1.6647127172 H,0,3.0983416969,0.9176140069,-2.0580341855 H,0,3.0939969327,-0.2953490703,-3.3609240761 C,0,0.9464861365,-2.5154856266,-1.2213470986 H,0,1.0446322881,-3.2609617937,-2.0307754135 H,0,0.2727334447,-2.9439541601,-0.4649194614 H,0,1.9368094423,-2.4063131607,-0.7561002451	C,0,0.4357520679,-0.6925012844,-1.1002436273 C,0,0.4000497154,0.7480581789,-1.0815352347 C,0,-0.7842119297,1.1486739316,-0.3721620215 C,0,1.354579801,1.662592943,-1.7998630709 C,0,-2.7752353185,-0.0758438606,0.7954481438 H,0,-2.8535840823,-0.9737034593,1.4265229334 H,0,-3.6356668809,-0.0878863405,0.1030781553 H,0,-2.8972220266,0.8000867537,1.4499804304 C,0,-1.2490610823,2.5643238802,-0.1687697585 H,0,-1.8728004432,2.6655694612,0.7316608691 H,0,-1.8539062095,2.9115399629,-1.0256865152 H,0,-0.4046052959,3.262400841,-0.0655314712 H,0,2.3757441795,1.2535165806,-1.8248268779 H,0,1.4086830907,2.6529272718,-1.3239849774 H,0,1.042735348,1.8212261602,-2.8482417987 C,0,1.4342899762,-1.5395326775,-1.8411145299 H,0,1.5397848744,-2.5371844916,-1.3897144165 H,0,2.4331003202,-1.0781717147,-1.8562738052 H,0,1.1292788882,-1.688135089,-2.8929603855 C,0,-1.1211627602,-2.611296063,-0.2367821531 H,0,-1.7077380334,-2.9654564196,-1.1034920719 H,0,-1.7394697726,-2.7666386043,0.6596702396 H,0,-0.2432455632,-3.2691853874,-0.1504017105
[(η^5-C_5Me_5) Radical C,0,-1.3516673565,1.239481904,3.9769456997 C,0,-1.0043180735,1.9714961415,5.0925182921 C,0,0.4071270651,1.7117041358,5.3561046081 C,0,0.9145792151,0.7992173186,4.3696123314 C,0,-0.1417766466,0.4965384197,3.5160426538 C,0,-2.6795902181,1.1553814792,3.2953754473 H,0,-2.6213049543,1.4842346048,2.2424378963 H,0,-3.4342899264,1.7791436843,3.7945234179 H,0,-3.0651645011,0.1204258805,3.2755170327 C,0,-1.8601047703,2.879816317,5.9237409878 H,0,-1.9168438602,2.5471244361,6.9752149138 H,0,-2.8903220605,2.9274232127,5.5427320817 H,0,-1.4712234423,3.9132296433,5.9410619213 C,0,1.1790862766,2.3127871806,6.4816014891 H,0,0.7313300539,2.0561926513,7.4588071449 H,0,1.1741774234,3.416647239,6.4286194834 H,0,2.2259410014,1.9796706067,6.491628819 C,0,2.328018424,0.2933066171,4.3093491726 H,0,3.0583057197,1.1117522471,4.1866438144 H,0,2.4722884777,-0.3942512951,3.4635889364 H,0,2.6127193867,-0.2565210182,5.2230590486 C,0,-0.1392036967,-0.4055166624,2.3266495926 H,0,-0.4256279118,0.1351519452,1.4067386194 H,0,-0.8691576896,-1.2271982585,2.4391514401 H,0,0.8470970643,-0.8578164303,2.1535021555	(C_5Me_5)(OH) C,0,0.1789031186,-0.4765276495,1.0133233291 C,0,-0.0353535172,-0.1095990938,-0.2745387692 C,0,-0.0250405859,-1.3238920643,-1.1494816573 C,0,0.1954682214,-2.4269806601,-0.3920500294 C,0,0.3753927357,-1.9953436723,1.0672779181 C,0,0.2683985831,-3.8650910993,-0.7889284126 H,0,1.291561826,-4.2691304707,-0.6848581029 H,0,-0.0433886905,-4.0231465207,-1.8311618149 H,0,-0.3761143579,-4.4811355986,-0.1389624853 C,0,-0.2275470077,-1.2502262989,-2.6336616329 H,0,0.5611765294,-0.648860993,-3.1171548651 H,0,-1.1882067569,-0.771760439,-2.8891959945 H,0,-0.2154685878,-2.2463463268,-3.0970021167 C,0,0.2325505488,0.355824843,2.2523972596 H,0,1.251937666,0.3964042489,2.6768318032 H,0,-0.4135527743,-0.0729605916,3.0372902522 H,0,-0.0893704379,1.3909604085,2.0699019877 C,0,-0.2489735741,1.2726382729,-0.8158446248 H,0,0.5425036271,1.5497742237,-1.5329570702 H,0,-0.2517660556,2.0274880264,-0.017546777 H,0,-1.2062511955,1.3528765245,-1.3583166713 C,0,1.7576587555,-2.3741081342,1.6092404216 H,0,2.5480086499,-1.9229440005,0.9924063182 H,0,1.8804494841,-3.4671324707,1.6040048532 H,0,1.8681751041,-2.0218893194,2.6453558676 O,0,-0.5823733682,-2.6406687418,1.9516057184 H,0,-1.4666759951,-2.4048131171,1.6138492963
OH H,0,-1.0339405473,3.0879880422,0.9987029483 O,0,-0.6785374527,2.2980889578,1.4712330517	
(η^5-C_5Me_4-*ansa*)$_2$Ti(OH)$_2$ (**1**) Ti,0,-0.9748426275,0.6463692796,0.5489030944 C,0,-2.0433325658,0.8502611021,-1.7712869073 C,0,-0.9672329618,-0.0715196481,-1.838757204 C,0,0.2700646423,0.6390687593,-1.5730258338 C,0,-0.0890506146,2.0062494789,-1.3137858732 C,0,-1.5117774652,2.1224744325,-1.402215133 C,0,-1.1484542462,-0.9601359861,2.5116039523	[(η^5-C_5Me_4-*ansa*)$_2$Ti(OH)$_1$] –Radical (**2**) Ti,0,-0.9174265402,0.5020807328,0.4709791892 C,0,-1.9637726218,0.9741680837,-1.6787348117 C,0,-0.9255065502,0.0158550653,-1.8802325622 C,0,0.3423014581,0.6431775916,-1.5751373848 C,0,0.0530748149,1.9898844824,-1.1390572393 C,0,-1.361930714,2.1886725319,-1.2267290611 C,0,-1.1062011479,-0.8917313559,2.4785788304

C,0,-0.2237666771,0.0437553712,2.9034340245 C,0,0.8896933328,-0.0139177806,2.0068721413 C,0,0.6876065885,-1.102859618,1.0855803931 C,0,-0.608026831,-1.6590291853,1.3866460299 Si,0,1.990807128,-0.1439128869,-1.8339463687 Si,0,2.0563082625,-1.7511303055,-0.0826174674 C,0,-2.4333135806,-1.3114239012,3.1990276904 H,0,-3.2223894793,-1.5800007645,2.4780729398 H,0,-2.8054252099,-0.4880391083,3.8278269627 H,0,-2.301097852,-2.1842472203,3.8616523868 C,0,-0.3459706975,0.9936524665,4.0526154641 H,0,-1.2806031032,0.8430372871,4.6112912842 H,0,-0.3280826101,2.0319775442,3.6832503042 H,0,0.4899479141,0.8637173678,4.7599620376 C,0,2.0744538018,0.9022002902,2.1229749165 H,0,1.7379556066,1.9306612063,2.3223505643 H,0,2.6757002563,0.9185192943,1.2039937264 H,0,2.7415147333,0.5963813766,2.9478680816 C,0,-1.2691003581,-2.8745785394,0.7997350575 H,0,-2.342116615,-2.701583633,0.6206720907 H,0,-1.1915057445,-3.7328226297,1.4905291411 H,0,-0.8175939893,-3.1783824202,-0.1495795163 C,0,-1.1072821394,-1.4786881727,-2.3486729535 H,0,-2.003406472,-1.9755535349,-1.9507919011 H,0,-0.2400447792,-2.0989821986,-2.0896324455 H,0,-1.1899824533,-1.4841257903,-3.4497563275 C,0,-3.4880441598,0.5697098737,-2.0311450424 H,0,-4.0368442686,0.5544189964,-1.0729314752 H,0,-3.6321389294,-0.3996291717,-2.5285379962 H,0,-3.9315605599,1.3480739775,-2.6723050627 C,0,-2.3414170871,3.3613781977,-1.2251320374 H,0,-3.2597053707,3.1454342357,-0.6583859687 H,0,-2.643298188,3.7808112974,-2.2007199405 H,0,-1.796656476,4.1627232213,-0.7014255647 C,0,0.8484318844,3.1545306558,-1.0663905279 H,0,0.320616225,4.0249422229,-0.65165206 H,0,1.3172843684,3.4866403312,-2.0080105819 H,0,1.6499584086,2.8969159889,-0.3625967286 C,0,3.4309252394,1.1076184039,-1.699832835 H,0,3.3291975936,1.9092471305,-2.4472959299 H,0,4.3732393048,0.5761721243,-1.9077294004 H,0,3.5253984069,1.5761276589,-0.710833673 C,0,2.1273150311,-0.8504368066,-3.607819068 H,0,1.401394944,-1.6492050649,-3.8112100321 H,0,3.136265401,-1.2619971245,-3.7694914575 H,0,1.9671134335,-0.050789694,-4.3485818281 C,0,3.7238935271,-1.8370923145,0.8542056898 H,0,4.1049816968,-0.8557935827,1.1648249973 H,0,4.4825283373,-2.3049340608,0.2067909204 H,0,3.6204081368,-2.4615485359,1.7559120028 C,0,1.7833504971,-3.5568327806,-0.662743358 H,0,0.9394036991,-3.7026387914,-1.3502216345 H,0,1.6395974409,-4.2268901096,0.1992991763 H,0,2.6943480482,-3.883390626,-1.189545399 O,0,-2.8692224777,0.5232386219,0.7715261519 H,0,-3.1654480497,0.3904140988,1.688128251 O,0,-0.6811027179,2.3037909261,1.4678222667 H,0,-1.0313749457,3.082286137,1.0021136654	C,0,-0.209134673,0.1764498363,2.7813699396 C,0,0.9301724724,0.0577128525,1.9295652845 C,0,0.756048887,-1.1152878953,1.0983183434 C,0,-0.5352758671,-1.6772478177,1.427239801 Si,0,2.033821188,-0.2018436889,-1.8579091274 Si,0,2.1014269625,-1.7822659385,-0.0784049167 C,0,-2.4156938864,-1.1158154321,3.1731652067 H,0,-2.9944507268,-1.9263588741,2.7087857062 H,0,-3.0271512472,-0.2006168331,3.1410788434 H,0,-2.2570280143,-1.386904201,4.2309306122 C,0,-0.4476254583,1.2210943664,3.8314256543 H,0,-0.2666636988,0.8146039538,4.841965407 H,0,-1.4863888082,1.580809196,3.7935657406 H,0,0.2157382464,2.088650149,3.7036712103 C,0,2.1598893933,0.9182931262,2.0348207563 H,0,1.9095497335,1.9568158929,2.2977161643 H,0,2.7266215809,0.9442203508,1.0939784843 H,0,2.8435686854,0.5399023239,2.8150036175 C,0,-1.1310960324,-2.9616413554,0.9155394032 H,0,-2.2263840183,-2.9591406753,1.0126538096 H,0,-0.7565176831,-3.8298948053,1.4861918898 H,0,-0.8955364533,-3.1413824851,-0.1403171426 C,0,-1.1420732312,-1.3481065346,-2.4761502191 H,0,-2.0996929707,-1.7857085579,-2.1576348127 H,0,-0.3478823281,-2.0517892731,-2.1926236056 H,0,-1.1555505679,-1.3008068446,-3.5793139853 C,0,-3.4252274432,0.7558603323,-1.9495572828 H,0,-4.0654127998,1.3836460833,-1.3119085861 H,0,-3.7211898864,-0.2893810825,-1.7787567091 H,0,-3.6743884282,1.0009953803,-2.9969580429 C,0,-2.0791666309,3.4799234537,-0.9536823524 H,0,-3.1555585132,3.3271596737,-0.7760816426 H,0,-2.0021868931,4.1627717949,-1.8173792865 H,0,-1.6681365493,4.0087766938,-0.0807746182 C,0,1.0311227671,3.0895190097,-0.8227739797 H,0,0.5758375463,3.8529125989,-0.174808821 H,0,1.3641022357,3.6029409428,-1.7425437075 H,0,1.9292323117,2.7195201517,-0.3141271071 C,0,3.5084987053,1.0186618115,-1.8139563907 H,0,3.3698856554,1.8371377423,-2.5372870269 H,0,4.4174110675,0.4674848928,-2.1038602692 H,0,3.6961788704,1.4648774692,-0.8278820485 C,0,2.1085510192,-0.9565241501,-3.6166201767 H,0,1.3872056167,-1.7693381733,-3.7738456773 H,0,3.116515626,-1.3613381758,-3.8001845762 H,0,1.9148320198,-0.1795774182,-4.3734369051 C,0,3.7858297405,-1.8979210168,0.8249648089 H,0,4.1791438673,-0.9225754008,1.1406347326 H,0,4.5308836604,-2.3630995509,0.1600925413 H,0,3.6918255532,-2.5314322488,1.7214864625 C,0,1.7755075599,-3.5693493848,-0.6840278392 H,0,0.8999452222,-3.6726529525,-1.3393505628 H,0,1.6466062342,-4.2579892362,0.1653554457 H,0,2.6561438826,-3.9044176054,-1.2551286021 O,0,-2.4456807776,1.2705791281,1.3114933473 H,0,-3.0083814225,1.8940082693,0.8238308467
[C_5Me_4-*ansa*-(η^5-C_5Me_4)$_1$Ti(OH)$_2$] (**3**) –triplet state Ti,0,0.00149623,-0.5336326538,0.9106904681 O,0,-1.4599854474,-1.4721526945,1.5347283037 H,0,-2.2773232699,-1.8897507413,1.2271428804 O,0,1.2022039337,-0.0409873527,2.2246119152 H,0,2.0435763804,0.4253749254,2.3324356912 C,0,1.4347709361,-0.5896290988,-1.0164662074 C,0,1.07491741,0.76559446,-0.7518942893 C,0,-0.364049948,0.9083676082,-0.878084396	[(HO)C_5Me_4-*ansa*-(η^5-C_5Me_4)$_1$Ti(OH)$_1$] –triplet state Ti,0,-4.0227782797,-0.2632280756,-1.2728919768 O,0,-4.6196356938,-0.61905983,-2.9710828635 H,0,-4.8458945502,-0.8101034659,-3.8886512992 C,0,-4.1626446379,0.9371000597,0.8215430819 C,0,-2.9280859364,1.2280148771,0.1610896543 C,0,-2.1623140852,-0.0040131502,0.0425400091 C,0,-2.9677058645,-1.0421775317,0.6679553681 C,0,-4.1868159285,-0.4579831735,1.1332087128

C,0,-0.8573953478,-0.3966350535,-1.2789252652
C,0,0.2385064762,-1.310910136,-1.3409822165
C,0,2.8226377908,-1.1672782246,-1.0134112606
H,0,3.2903780665,-1.0795260569,-2.0096655986
H,0,2.8160234482,-2.2348322209,-0.7491522804
H,0,3.4827788452,-0.6576498094,-0.2972968238
C,0,0.1771461612,-2.7575676693,-1.7451356997
H,0,0.980684207,-3.34414384,-1.2767058126
H,0,0.286548109,-2.8680093114,-2.8384205739
H,0,-0.7765981193,-3.2262616473,-1.4636629779
C,0,-2.2804031845,-0.7628992519,-1.6037515075
H,0,-2.4008574073,-1.8527751807,-1.6846834872
H,0,-2.5881375047,-0.3339000516,-2.5723632033
H,0,-2.9902308673,-0.4018468981,-0.8468753562
C,0,2.0572318527,1.854452167,-0.4134645945
H,0,3.0586108433,1.4423049923,-0.2234904483
H,0,1.7576578185,2.4279454815,0.4747824249
H,0,2.157167315,2.5703328376,-1.246669583
Si,0,-1.3584082648,2.537789593,-0.7714237571
Si,0,-1.3420585328,3.6397923483,-2.8989575066
C,0,-0.6749904486,3.6776823917,0.6081167825
H,0,0.3101693214,4.1067802641,0.3781392273
H,0,-0.5947882807,3.1295159771,1.5604504594
H,0,-1.3768859887,4.5128954487,0.7587086654
C,0,-3.1847957267,2.2310329922,-0.290938796
H,0,-3.2574536028,1.6459238535,0.6395182548
H,0,-3.7615968588,1.7163200893,-1.0714910742
H,0,-3.6614649973,3.2086425104,-0.1184949107
C,0,0.4329656425,4.1554177635,-3.4089746033
H,0,1.0526203968,3.2560868114,-3.5516142402
H,0,0.9344176599,4.7961789066,-2.6712158399
H,0,0.4069618957,4.7008305063,-4.3660874203
C,0,-1.8508111656,2.351637677,-4.2256112892
H,0,-1.0354923181,1.6177648659,-4.3245189687
H,0,-1.9987821614,2.8278134253,-5.207487712
H,0,-2.7634304229,1.7925572119,-3.9743699666
C,0,-2.4846652003,5.1583934916,-2.8807175232
C,0,-3.8014938916,5.3013798279,-3.3747181964
C,0,-2.1458416359,6.4378221685,-2.3253961367
C,0,-3.2575146481,7.3744923976,-2.5141455071
C,0,-4.2677021992,6.6894744486,-3.1503526611
C,0,-0.8697226353,6.8305818857,-1.6566303576
H,0,-0.1619160772,7.2782222751,-2.3797593165
H,0,-0.3619812748,5.9733974034,-1.1947742764
H,0,-1.0419338286,7.58990873,-0.8780494315
C,0,-3.2374795087,8.8062526695,-2.071571284
H,0,-2.412727934,9.3708086038,-2.5399655741
H,0,-3.1035134659,8.8999923378,-0.9795111778
H,0,-4.1738581011,9.3212342502,-2.3290202018
C,0,-5.6141573881,7.1910138471,-3.5686046593
H,0,-5.7513170354,8.2506291975,-3.3111737137
H,0,-6.4312035563,6.6261002018,-3.0863241586
H,0,-5.7680616241,7.0929369863,-4.6576012516
C,0,-4.6844646859,4.2845174895,-4.019793326
H,0,-4.225946741,3.2916891951,-4.0610001187
H,0,-4.9462883107,4.5807494999,-5.0520831346
H,0,-5.6437384122,4.1963449958,-3.4792701185
C,0,-5.2382127692,1.9294450301,1.1678680322
H,0,-5.0340446155,2.4142439054,2.138953326
H,0,-6.2239835699,1.4483078907,1.2457362411
H,0,-5.3216392703,2.7286340942,0.4165054848
C,0,-5.2912381289,-1.173662309,1.8612766376
H,0,-6.2611963107,-0.6747741738,1.7199580023
H,0,-5.0957165793,-1.2048004834,2.9477617479
H,0,-5.4041219233,-2.2137585548,1.521406008
C,0,-2.577858676,-2.4814256342,0.8854720713
H,0,-3.433229741,-3.0736066527,1.240407074
H,0,-1.7850508627,-2.5665226234,1.6491323105
H,0,-2.2016976636,-2.9612868053,-0.0285407868
C,0,-2.492799986,2.6109546141,-0.2503884837
H,0,-3.3239940382,3.3256937598,-0.1700195373
H,0,-2.1226486387,2.6514808992,-1.2842263755
H,0,-1.6831042655,2.981688544,0.4022580591
Si,0,-0.3824755737,-0.1910458682,-0.6195828272
Si,0,1.1863616158,0.10507,1.1621962126
C,0,0.0088301612,1.0852655591,-1.9904182471
H,0,0.0460461755,2.121587418,-1.627792677
H,0,-0.7348542025,1.0305100293,-2.8016976999
H,0,0.9947793155,0.84372992,-2.4173306055
C,0,-0.1099854311,-1.8967644701,-1.4434460809
H,0,-0.8863280445,-2.0913341772,-2.2009877776
H,0,-0.1099051353,-2.7327376807,-0.7308418784
H,0,0.8654149989,-1.8917046156,-1.9539504811
C,0,0.7842429497,1.7293713553,2.0944031722
H,0,-0.1936764559,1.6141298262,2.5877431872
H,0,0.7270961853,2.6077355085,1.4378336895
H,0,1.5321064456,1.9346536042,2.8766151046
C,0,0.9984001963,-1.2573425563,2.4965772258
H,0,0.0383085167,-1.1208964743,3.0186221563
H,0,1.8034342547,-1.1711105503,3.2437554174
H,0,1.0215895281,-2.2794572567,2.095829081
C,0,2.9673172837,0.1041355096,0.4532162819
C,0,3.7075922908,-1.0104541598,0.1871813792
C,0,3.7800880897,1.3068790166,0.0476146048
C,0,4.9919035382,0.9141007723,-0.4185142471
C,0,5.0927252627,-0.6035846226,-0.3171055547
C,0,3.2855240204,2.7202312752,0.1359387709
H,0,3.1322363728,3.0357063517,1.1804205612
H,0,2.3173555646,2.8374120608,-0.3779612886
H,0,3.9927487112,3.4249113905,-0.3233753359
C,0,6.120239638,1.7318801419,-0.958211312
H,0,7.0262078425,1.6571226652,-0.3296369803
H,0,5.8622484086,2.797392837,-1.0316022636
H,0,6.4073693507,1.3969010929,-1.9720854713
C,0,3.375063041,-2.4639716263,0.2902909491
H,0,2.2967000795,-2.6409291422,0.3796345016
H,0,3.8665828624,-2.9416094197,1.1573564126
H,0,3.7384360456,-2.9884236951,-0.6084939463
C,0,6.1851319901,-1.0227056916,0.6865186203
O,0,5.3135840939,-1.2507284776,-1.5966925907
H,0,7.1775786487,-0.6903706353,0.3374977091
H,0,6.00345327,-0.5700646656,1.672668718
H,0,6.2074943338,-2.1175085526,0.7926878239
H,0,6.2285167752,-1.0507122075,-1.866925812

[(η^5-C_5Me_5)$_2$]Ti-O-Ti[(η^5-C_5Me_5)$_2$] Triplet state

C,0,-2.5099680156,-2.1822151075,0.8331061954
C,0,-2.5099680156,2.1822151075,-0.8331061954
C,0,2.5099680156,-0.8331061954,-2.1822151075
C,0,2.5099680156,0.8331061954,2.1822151075
C,0,-3.7562262851,-1.4793492122,0.9049849646
C,0,-3.7562262851,1.4793492122,-0.9049849646
C,0,3.7562262851,-0.9049849646,-1.4793492122
C,0,3.7562262851,0.9049849646,1.4793492122
C,0,-3.6225894337,-0.4322158626,1.8609695991
C,0,-3.6225894337,0.4322158626,-1.8609695991
C,0,3.6225894337,-1.8609695991,-0.4322158626

[(η^5-C_5Me_5-*ansa*)$_2$Ti(OH)$_1$]

C,0,-1.3439764877,1.1678987183,3.9210874614
C,0,-0.9830799975,1.7941669902,5.1555093609
C,0,0.4464432401,1.7762104433,5.2461433718
C,0,0.9706798116,1.1797960147,4.0538608109
C,0,-0.1412892788,0.7896722784,3.2429677077
C,0,-2.7473180328,0.7863116789,3.5444191704
H,0,-2.8241198347,0.4712841031,2.4957862378
H,0,-3.4637105642,1.606621566,3.7032247614
H,0,-3.0906113528,-0.0617030209,4.1627172595
C,0,-1.9349496652,2.2461996496,6.2272147315
H,0,-2.1531821103,1.4304372853,6.940452536

C,0,3.6225894337,1.8609695991,0.4322158626
C,0,-2.3058950337,-0.4967740543,2.4098599195
C,0,-2.3058950337,0.4967740543,-2.4098599195
C,0,2.3058950337,-2.4098599195,-0.4967740543
C,0,2.3058950337,2.4098599195,0.4967740543
C,0,-1.6293938035,-1.6010370711,1.8071350688
C,0,-1.6293938035,1.6010370711,-1.8071350688
C,0,1.6293938035,-1.8071350688,-1.6010370711
C,0,1.6293938035,1.8071350688,1.6010370711
Ti,0,-1.9050331522,0.,0.
Ti,0,1.9050331522,0.,0.
O,0,0.,0.,0.
C,0,4.7262429,2.4733962573,-0.3810982403
C,0,4.7262429,-2.4733962573,0.3810982403
C,0,-4.7262429,0.3810982403,2.4733962573
C,0,-4.7262429,-0.3810982403,-2.4733962573
H,0,5.6429073414,1.8714266518,-0.3705941752
H,0,5.6429073414,-1.8714266518,0.3705941752
H,0,-5.6429073414,0.3705941752,1.8714266518
H,0,-5.6429073414,-0.3705941752,-1.8714266518
H,0,4.9848278231,3.466053362,0.030548236
H,0,4.9848278231,-3.466053362,-0.030548236
H,0,-4.9848278231,-0.030548236,3.466053362
H,0,-4.9848278231,0.030548236,-3.466053362
H,0,4.440368661,2.6341950982,-1.4319439471
H,0,4.440368661,-2.6341950982,1.4319439471
H,0,-4.440368661,1.4319439471,2.6341950982
H,0,-4.440368661,-1.4319439471,-2.6341950982
C,0,2.3058913129,0.1073532855,3.48267926
C,0,2.3058913129,-0.1073532855,-3.48267926
C,0,-2.3058913129,-3.48267926,0.1073532855
C,0,-2.3058913129,3.48267926,-0.1073532855
H,0,2.8079930313,-0.8715206412,3.4924844032
H,0,2.8079930313,0.8715206412,-3.4924844032
H,0,-2.8079930313,-3.4924844032,-0.8715206412
H,0,-2.8079930313,3.4924844032,0.8715206412
H,0,1.2432545783,-0.0722254374,3.6895534304
H,0,1.2432545783,0.0722254374,-3.6895534304
H,0,-1.2432545783,-3.6895534304,-0.0722254374
H,0,-1.2432545783,3.6895534304,0.0722254374
H,0,2.7132206394,0.6906354095,4.3291335516
H,0,2.7132206394,-0.6906354095,-4.3291335516
H,0,-2.7132206394,-4.3291335516,0.6906354095
H,0,-2.7132206394,4.3291335516,-0.6906354095
C,0,0.3161735778,2.2526777336,2.1563101983
C,0,0.3161735778,-2.2526777336,-2.1563101983
C,0,-0.3161735778,-2.1563101983,2.2526777336
C,0,-0.3161735778,2.1563101983,-2.2526777336
H,0,0.2786153138,2.1022794756,3.2442053028
H,0,0.2786153138,-2.1022794756,-3.2442053028
H,0,-0.2786153138,-3.2442053028,2.1022794756
H,0,-0.2786153138,3.2442053028,-2.1022794756
H,0,-0.5332467529,1.7040365089,1.7083036835
H,0,-0.5332467529,-1.7040365089,-1.7083036835
H,0,0.5332467529,-1.7083036835,1.7040365089
H,0,0.5332467529,1.7083036835,-1.7040365089
H,0,0.1574192823,3.325704433,1.9721429418
H,0,0.1574192823,-3.325704433,-1.9721429418
H,0,-0.1574192823,-1.9721429418,3.325704433
H,0,-0.1574192823,1.9721429418,-3.325704433
C,0,1.8963008206,3.6532270211,-0.2389531219
C,0,1.8963008206,-3.6532270211,0.2389531219
C,0,-1.8963008206,0.2389531219,3.6532270211
C,0,-1.8963008206,-0.2389531219,-3.6532270211
H,0,2.1640100595,3.6199762807,-1.3051478276
H,0,2.1640100595,-3.6199762807,1.3051478276
H,0,-2.1640100595,1.3051478276,3.6199762807
H,0,-2.1640100595,-1.3051478276,-3.6199762807
H,0,2.4042045168,4.534584967,0.1946320751
H,0,2.4042045168,-4.534584967,-0.1946320751
H,0,-2.8957922612,2.5734763597,5.8039533587
H,0,-1.5276525626,3.0871797251,6.8073420468
C,0,1.2481949938,2.1609367325,6.4534451291
H,0,1.3648963507,1.3035603613,7.1385615321
H,0,0.7648979112,2.9622027538,7.0356255396
H,0,2.2661951566,2.4900667091,6.1890780677
C,0,2.4161610575,0.8780614513,3.7737262111
H,0,3.0835456269,1.6372710388,4.2071816294
H,0,2.6199790616,0.8391453289,2.6937156223
H,0,2.7116628101,-0.0992212905,4.1972807151
C,0,-0.0328046397,-0.0673986935,2.0139343835
H,0,0.7520241468,0.2810828181,1.3255013825
H,0,-0.9759575583,-0.1109138493,1.4541412964
H,0,0.2250561052,-1.1039566257,2.2937997106
C,0,0.3989643166,4.9877587521,1.8636986492
C,0,-0.7996840703,5.3654948298,2.540380976
C,0,-1.8125608908,4.4036276964,2.230770661
C,0,-1.2394196345,3.4474689706,1.3267501824
C,0,0.1405976704,3.7881478513,1.1280897993
C,0,1.6887549549,5.7498274584,1.9145792402
H,0,2.5269560086,5.1603402548,1.5156278947
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H,0,-0.9872877846,7.4987673512,2.7912161949
H,0,-0.1012577237,6.6674072486,4.0990376018
C,0,-3.2661378402,4.5145940211,2.5979504022
H,0,-3.403098365,4.9415783167,3.6022957263
H,0,-3.7719448335,3.5386534473,2.5799042618
H,0,-3.8048735348,5.1699033669,1.8899342068
C,0,-2.0153416365,2.4617334982,0.5023607532
H,0,-2.3804060579,2.9482438293,-0.4203889605
H,0,-2.8990883422,2.0770041067,1.0288901696
H,0,-1.4055123222,1.6038722602,0.1885695241
C,0,1.0787278314,3.1454852457,0.1447705016
H,0,1.0281704187,3.6482023067,-0.8379160809
H,0,0.8372355897,2.086352226,-0.0241513519
H,0,2.1243599227,3.1985004407,0.4818814759
O,0,0.8917994238,4.4440206639,4.5476181385
Ti,0,-0.1008070926,3.2378597796,3.4606203675
H,0,1.2757072877,4.1534659024,5.3904915527

H,0,-2.4042045168,-0.1946320751,4.534584967 H,0,-2.4042045168,0.1946320751,-4.534584967 H,0,0.8171587959,3.8360745435,-0.1766486419 H,0,0.8171587959,-3.8360745435,0.1766486419 H,0,-0.8171587959,0.1766486419,3.8360745435 H,0,-0.8171587959,-0.1766486419,-3.8360745435 C,0,5.0477754323,-0.3264471718,-1.9760194572 C,0,5.0477754323,0.3264471718,1.9760194572 C,0,-5.0477754323,1.9760194572,-0.3264471718 C,0,-5.0477754323,-1.9760194572,0.3264471718 H,0,5.4936499608,-1.0052270722,-2.7259376942 H,0,5.4936499608,1.0052270722,2.7259376942 H,0,-5.4936499608,2.7259376942,-1.0052270722 H,0,-5.4936499608,-2.7259376942,1.0052270722 H,0,4.9147590299,-0.6464521588,2.4673058379 H,0,4.9147590299,0.6464521588,-2.4673058379 H,0,-4.9147590299,-2.4673058379,-0.6464521588 H,0,-4.9147590299,2.4673058379,0.6464521588 H,0,5.7907164841,0.2013248705,1.1767113409 H,0,5.7907164841,-0.2013248705,-1.1767113409 H,0,-5.7907164841,-1.1767113409,0.2013248705 H,0,-5.7907164841,1.1767113409,-0.2013248705	

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