

Supporting information for: Toward the H₂O catalyzed N₂-fixation over TiO₂ doped Ru_n clusters (n=5, 6): a mechanistic and kinetic approach

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S1. Kinetics methodology

The rate constants of elementary reaction steps were computed from conventional transition state theory (TST)^{1,2} using Eq. (1).

$$k^{TST}(T) = \Gamma(T) \times \sigma \times \frac{k_b T}{h} \frac{Q^{TS}(T)}{N_A Q^R(T)} e^{-\frac{E^\ddagger}{k_b T}} \quad (1)$$

In Eq. (1), $\Gamma(T)$, σ , k_b , T , h , Q^{TS} , Q^R and E^\ddagger are denoted as multiplicative transmission coefficient, reaction path degeneracy, Boltzmann's constant, temperature, Planck's constant, total partition functions of transition state, reactants and zero-point excluded energy difference between the transition state (TS) and reactants (R), respectively. Multiplicative factor is determined by using tunneling treatment based on unsymmetrical Eckart potential energy barrier. To calculate TST rate constant, one just needs the thermodynamic information only for transition state (first-order saddle point) and reactants in the PES. Furthermore, $k^{TST}(T)$ can also be computed from the standard Gibbs free energy calculation using Eq. (2).

$$k^{TST}(T) = \Gamma(T) \times \sigma \times \frac{k_b T}{h} \left(\frac{RT}{P^0} \right)^{\Delta n} e^{-\frac{\Delta G^{0,\ddagger}(T)}{k_b T}} \quad (2)$$

In Eq. (2), $\Delta G^{0,\ddagger}(T)$ is denoted as the standard Gibbs free energy of activation. For gas-phase bimolecular or unimolecular reactions Δn belongs to 1 or 0. The reaction path degeneracy σ is calculated from the Eq. (3), in which, n^R and n^\ddagger are the number of chiral isomers of the reactant(s) and transition state, respectively, and σ^R and σ^\ddagger are the rotational symmetry numbers.^{1,2}

$$\sigma = \frac{n^\ddagger \sigma^R}{n^R \sigma^\ddagger} \quad (3)$$

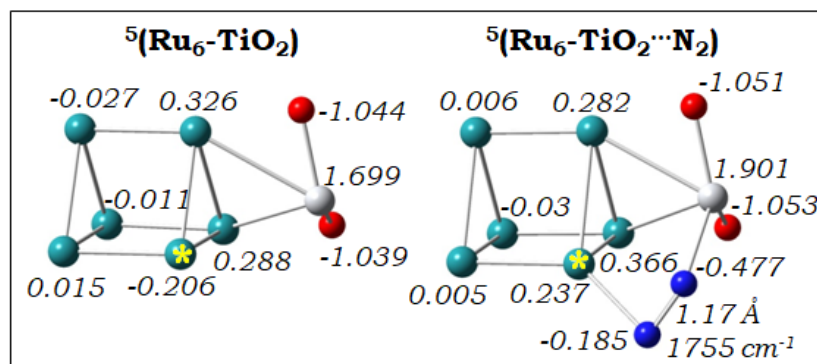


Figure S1: Calculated Bader charges over different elements in N₂ free and adsorbed TiO₂ doped Ru₆ cluster.

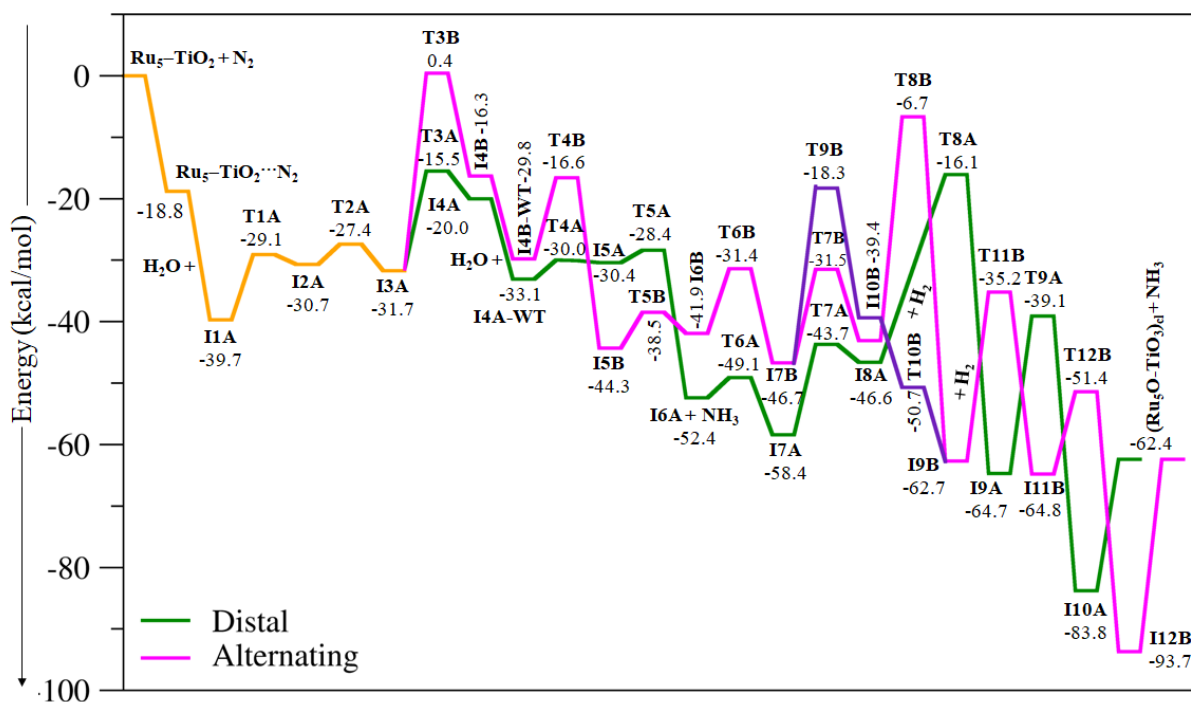


Figure S2: Schematic potential energy diagram for two H₂O and H₂ driven N₂ fixation over TiO₂ doped Ru₅ cluster in accordance with the distal and alternating-type mechanism.

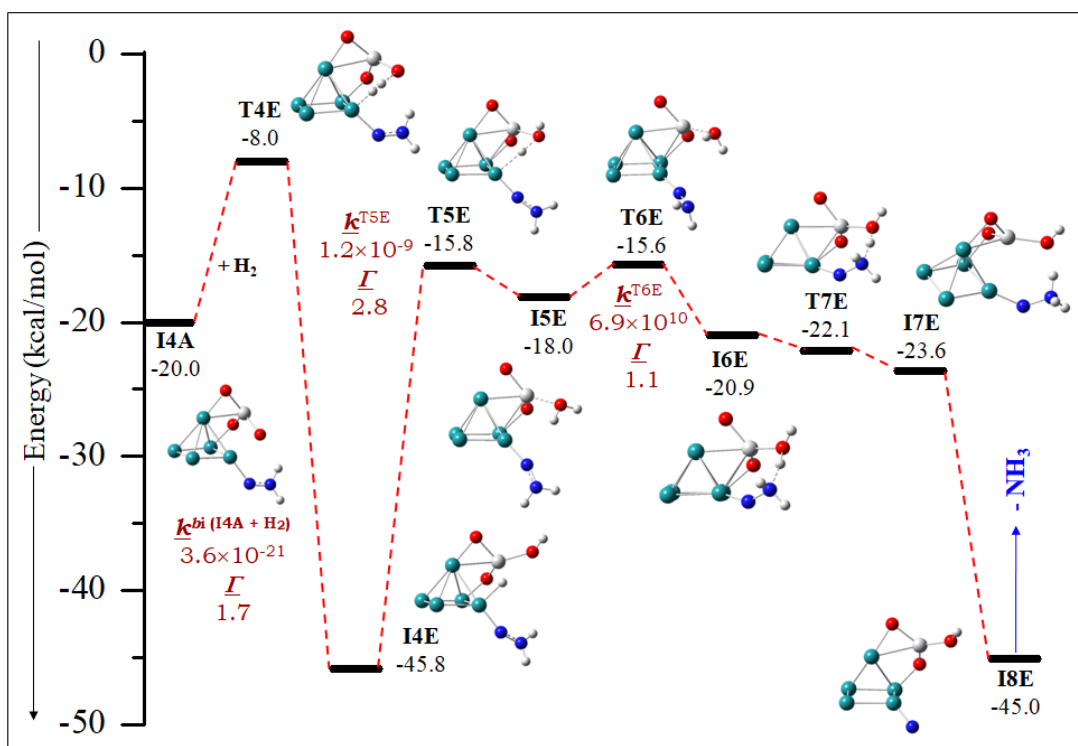


Figure S3: ZPE-corrected B3LYP/def2-TZVP level calculated potential energy diagram for NH₃ formation via hydrogenation of I4A. 1st (k , sec⁻¹) and 2nd (k^{bi} , cm³/molecule/sec) order rate coefficients of various elementary hydrogenation steps along with tunneling correction (Γ) have also been supplied in the figure.

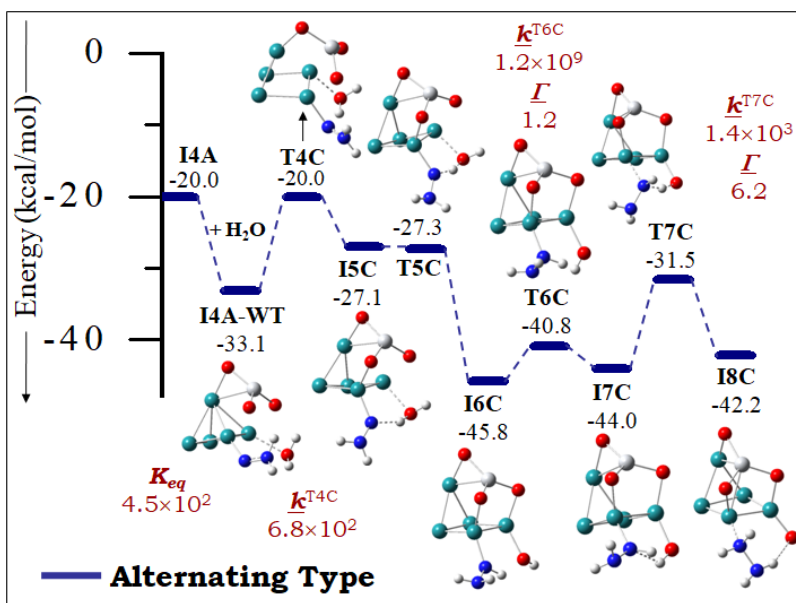


Figure S4: ZPE-corrected B3LYP/def2-TZVP level calculated potential energy diagram for N_2 to N_2H_4 conversion followed by alternating-type mechanism. 1st order rate constant (k , sec^{-1}) of various unimolecular steps along with tunneling correction (Γ) and equilibrium constant of complexes (K_{eq} , atm^{-1}) have also been supplied in the figure.

S2. Alternating-type mechanism over TiO_2 doped Ru_5 cluster

Aside a pure alternating mechanism discussed in the main text, fixation of N_2 into hydrazine could have also been possible via $\text{I4A} + \text{H}_2\text{O}$ capture reaction, which follows somewhat different protocol than the typical hydrogenation sequence of conventional alternating mechanism. In typical alternating mechanism, sequential hydrogenation of two end-on N atoms are occurred alternatively. However, I4A is seen to be formed through consecutive hydrogenation of terminal N atom of the end-on adsorbed $^*\text{N}_2$ molecule. Thus, the present mechanism is denoted by ‘Alternating Type’. Starting from I4A-WT , formation of hydrazine could also be viable via four elementary reaction steps, as shown in Figure S4. In I4A-WT , H of $^*\text{H}_2\text{O}$ is closer to the terminal N of $^*\text{N-NH}_2$. An immediate geometrical reorganization is necessary to make a room for $^*\text{HOH}\cdots^*\text{N-NH}_2$ interaction within I5C intermediate. For this, NH_2 group is rotated around N-N-Ru-Ru dihedral by 110° in anticlockwise direction. Rotational barrier is calculated as 13.1 kcal/mol. In the next steps, I5C passes through a barrierless pathway and accepts a H from adjacent $^*\text{H}_2\text{O}$ to form $^*\text{N}_2\text{H}_3$ moiety

in I6C intermediate, which finally generates $*N_2H_4$ in I8C intermediate via two consecutive unimolecular steps through transition structures T6C and T7C. Barrier heights of the last two steps are calculated as 5 and 12.5 kcal/mol. Analysis of individual unimolecular rate constant suggests that the first step is the RDS for hydrazine formation. Overall 2nd order rate coefficient of water driven $I4A \rightarrow N_2H_4$ conversion is calculated as $\sim 10^{-14}$ cm³/molecule/sec, which is found to be two fold higher than that of pure alternating mechanism, as presented in the Figure 6 of main text.

S3. Enzymatic mechanism over TiO₂ doped Ru₅ cluster

Next, we demonstrate the elementary reactions of enzymatic mechanism, in which two N atoms of side-on N₂ ($*N*N$) are hydrogenated alternately. Basically, alternating and enzymatic mechanisms differ from each other with respect to their different N₂ binding patterns.³ To explore the enzymatic NRR over Ru₅-TiO₂ cluster, here, we assume that two $*H_2O$ molecules attack $*N*N$ simultaneously (see Figure S5). Sequential adsorption of two water on Ti and Ru atoms of Ru₅-TiO₂ yields I1D intermediate in the entrance channel. In the first three elementary steps, $*N*N$ (I1D) is gradually converted into side-on $*NH*NH$ (I4D) through consecutive reduction by two adjacent $*H_2O$ molecules. This conversion goes on through T1D, T2D and T3D transition structures, with calculated energy barriers 9.3, 26.6 and 22.6 kcal/mol, respectively. Second unimolecular step containing T2D is found to be the RDS for diazene formation, with computed 1st order rate coefficient 2×10^{-7} sec⁻¹. In comparison to the alternating mechanism, relative kinetics analysis suggests that formation rate coefficient of I4D is 4 orders of magnitude higher than that of I4B. This indicates that the side-on $*NH*NH$ formation is more favourable than that of end-on $*N_2H_2$. $*NH*NH$ is gradually converted into $*NH_2*NH_2$ in the next five elementary steps. For this, $*NH*NH$ of I4D is reduced by adjacent $*OH$ groups to form I9D and the reaction passes through transition structures T4D, T5D, T6D, T7D and T8D with energy barriers 2.0, 17.1, 4.0, 30.8 and 26.1 kcal/mol, respectively. The first two TS correspond to the geometrical isomerization of $I4D \rightarrow I5D \rightarrow I6D$ conversion via $*OH$ bond rotation; on the other hand, the last three TSs correspond to the reduction of two N

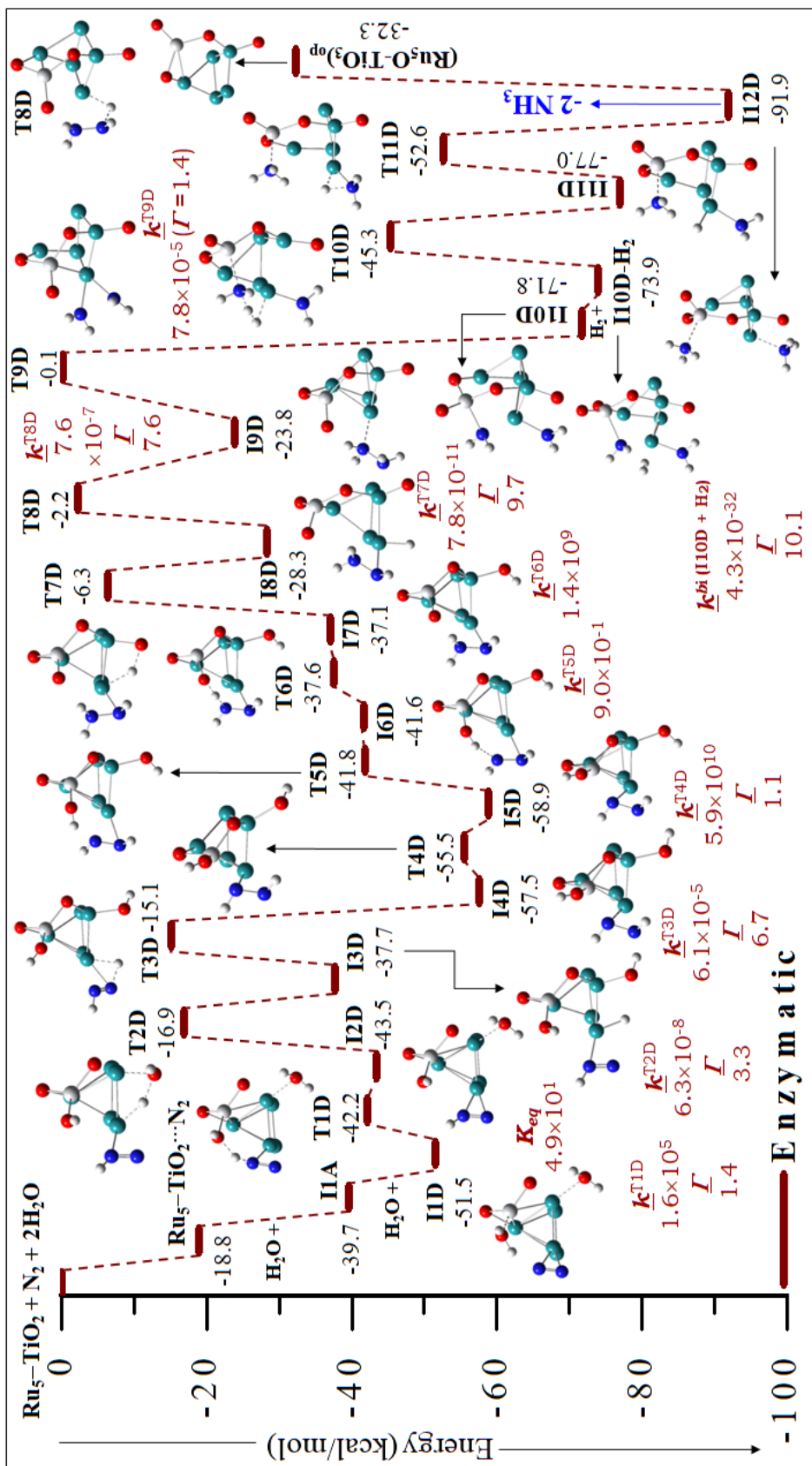


Figure S5: Relative electronic energies of various intermediates and transition states with respect to the isolated reactants ($\text{Ru}_5\text{-TiO}_2$, N_2 , two H_2O and H_2) in associated with the NH_3 formation via enzymatic mechanism over TiO_2 doped Ru_5 cluster based on zpe-corrected B3LYP/def2-TZVP level of calculation. 1st (k , sec^{-1}) and 2nd (k^{bi} , $\text{cm}^3/\text{molecule}/\text{sec}$) order rate coefficients of various elementary reactions along with tunneling correction (Γ) have also been supplied in the figure.

atoms of side-on *NH*NH group. In I4D, N of *NH*NH and H of *OH are far apart from each other and thus, rotation of Ti adsorbed *OH group is essential to make a room for N...H interaction between hydroxyl and diazene groups of I6D intermediate. Thereafter, feasible H-migration from *OH to N of *NH*NH results in *NH*NH₂ containing I7D intermediate, which eventually forms *NH₂*NH₂ containing I9D intermediate with appreciable energy barrier. Like alternating, here also, N-N bond within *NH₂*NH₂ needs to be ruptured to eliminate two *NH₂ groups in terms of ammonia. To cleave N-N bond, side-on *NH₂*NH₂ requires 12.7 kcal/mol less activation energy than that of end-on *N₂H₄. Ultimately, sequential hydrogenation of two *NH₂ within I10D liberates two molecules of NH₃, leaving Ru₅O-TiO₃ oxide cluster at an end. Notably, that Ru₅O-TiO₃ oxide cluster generated from the enzymatic mechanism has a different geometrical configuration than those were generated via other two mechanisms which were closed in nature ((Ru₅O-TiO₃)_{cl}) and the former is energetically ~ 30.1 kcal/mol less stable than the closed structure. Elimination of two NH₃ from I10D occurs through two elementary reaction steps, covering transition structures T10D and T11D with calculated hydrogenation barriers 28.6 and 24.4 kcal/mol, respectively. Summarizing, like alternating, the mechanism of enzymatic is also less effective to convert N₂ into NH₃.

References

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- (2) Canneaux, S.; Bohr, F.; Henon, E. KiSThElP: a program to predict thermodynamic properties and rate constants from quantum chemistry results. *Journal of computational chemistry* **2014**, *35*, 82–93.
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Table S1: Optimized geometries and zpe-corrected electronic energies from the B3LYP/def2-TZVP level of calculation.

Species	Cartesian coordinates	(E) _{zpe}
Ru₅ (sqp)	Ru,0,0.,1.60662587,0.38048842 Ru,0,-1.60662587,0.,0.38048842 Ru,0,0.,-1.60662587,0.38048842 Ru,0,1.60662587,0.,0.38048842	-474.569151
Ru₅ (tbp)	Ru,0,-0.0196827706,0.0133092279,-0.0780779431 Ru,0,-0.0041653261,-0.0004178788,2.4583202988 Ru,0,2.1313710493,-0.0117753344,1.1773848163 Ru,0,0.8395672495,1.9066819984,1.1954883941 Ru,0,0.806883798,-1.9077980131,1.1749314338	-474.518782
N₂	N,0,0.,0.,0.5454531693 N,0,0.,0.,-0.5454531693	-109.567674
Ru₅···N₂ (End-On)	Ru,0,1.4322594285,0.6786091587,0.4767393739 Ru,0,-0.7240364159,1.0294120151,1.0880689202 Ru,0,-1.4063399757,0.1647574302,-0.8952879487 Ru,0,0.7609327216,-0.1968310099,-1.5249390096 N,0,1.6430447381,-1.3701421596,-2.9001728666 N,0,2.1193468422,-2.067074461,-3.61904397 Ru,0,-0.0600849289,-1.3065452836,0.5893185609	-584.163636
Ru₅···N₂ (Side-On)	Ru,0,1.4267289406,0.6248285441,0.5133694063 Ru,0,-0.7089781648,1.2024477765,0.9906901307 Ru,0,-1.4148213101,0.1101388725,-0.861161222 Ru,0,0.7359838804,-0.4623220585,-1.3721204186 N,0,1.7070867355,-1.385139492,-3.0271005833 N,0,1.5062751664,-2.2409479337,-2.2924403163 Ru,0,-0.2057402481,-1.2201847088,0.8578600032	-584.159520
H₂O	O,0,0.,0.,-0.1309831008 H,0,0.,-0.7649494602,0.4533331204 H,0,0.,0.7649494602,0.4533331204	-76.441815
I1	Ru,0,1.4397055276,0.6134999388,0.4937050021 Ru,0,-0.6972885711,1.2047657506,0.9888055393 Ru,0,-1.4333780955,0.1099584287,-0.8473983886 Ru,0,0.7116645942,-0.4795147987,-1.376874559 N,0,1.7341915427,-1.3709660865,-3.0186309777 N,0,1.5149357422,-2.2385797661,-2.3001288112 Ru,0,-0.2232971615,-1.2103415772,0.8696191432 O,0,3.6610337379,0.6508674105,1.0795762571 H,0,4.2757307737,0.8158817805,0.3536716605 H,0,3.8966809099,-0.2049870806,1.4568561344	-660.621081
T1	Ru,0,1.093316634,0.1159966035,0.6666466558 Ru,0,-0.9754711955,0.9205703419,1.0281686449 Ru,0,-1.6694162661,0.2332237844,-1.0200653274 Ru,0,0.5154987835,-0.537728439,-1.4280698247 N,0,2.4486759339,-0.9769024516,-1.8705820248 N,0,1.9087559774,-2.0318679896,-1.6436844395 Ru,0,-0.8339958742,-1.4827319334,0.5438379023 O,0,3.1065524066,0.1638383793,0.2467417425 H,0,3.2027265858,-0.5465344215,-1.1645091872 H,0,3.7950290145,-0.025776874,0.8946088581	-660.557535
I2	Ru,0,1.483112493,0.5703045554,0.7458701853 Ru,0,-0.6484388777,1.264511272,0.9761823563	-660.594824

	Ru,0,-1.219018882,0.2395198259,-0.9643905722 Ru,0,0.9844581066,-0.3893318689,-1.2820317138 N,0,2.2289888692,-1.2474994006,-2.6858338616 N,0,1.6884577712,-2.1084229098,-2.0084269848 Ru,0,-0.3078754614,-1.1674166952,0.8134472887 O,0,3.1207238115,1.2292008478,1.4736969755 H,0,2.9703529618,-1.5048291741,-3.3541845323 H,0,3.2676862078,1.2577545475,2.4253668588	
T2	Ru,0,1.4039502461,0.8996130076,0.4698593528 Ru,0,-0.7023745468,0.9664869981,1.2236919419 Ru,0,-1.4755920927,-0.2502122381,-0.518636395 Ru,0,0.6987267939,-0.3587265459,-1.3919157381 N,0,2.0175333338,-2.0754161318,-2.3340753035 N,0,1.4006223032,-2.1278625115,-1.2706514882 Ru,0,0.3008779158,-1.2980236145,0.846799205 O,0,2.9785136825,1.8474266611,0.9638497495 H,0,2.6549161082,-2.8704163585,-2.5023617829 H,0,3.4784952559,1.6712387336,1.7670684584	-660.586270
I3	Ru,0,1.6095074678,0.7985290298,0.5553112149 Ru,0,-0.4306276579,0.6087102818,1.426146868 Ru,0,-1.2891611951,-0.1826170762,-0.5203662541 Ru,0,0.8042838495,0.0627514336,-1.5433081779 N,0,1.8838849081,-2.4222561205,-2.4617052302 N,0,1.3286656746,-1.8350710021,-1.5304583387 Ru,0,0.6495202809,-1.5176790007,0.2792060051 O,0,3.0073992461,1.9102271321,1.1846986563 H,0,2.1731742174,-3.3706821068,-2.1753107654 H,0,3.0190212087,2.3521924291,2.0394130221	-660.598721
T3	Ru,0,1.2398386898,1.0867606128,0.5137094665 Ru,0,-0.808617596,0.896062019,1.3539824513 Ru,0,-1.6680999269,-0.0218766892,-0.6324229542 Ru,0,0.4610954542,0.2990023635,-1.6323026189 N,0,2.8533150874,-0.9135427827,-1.2483142077 N,0,1.5834666936,-1.2275434411,-1.1731582295 Ru,0,0.2674362508,-1.2007622942,0.281714489 O,0,3.0377858364,0.9440345777,0.4071329336 H,0,3.4508173898,-1.7412076775,-1.2597018632 H,0,3.151407121,0.0228633116,-0.4709444668	-660.547714
I4	Ru,0,1.1761611859,1.0634696885,0.781905799 Ru,0,-0.8797034621,0.5851146677,1.5020864502 Ru,0,-1.5709470992,-0.1193045493,-0.646899307 Ru,0,0.589563271,0.3408364894,-1.388214677 N,0,2.6873704046,-1.7312255544,-1.5496781929 N,0,1.4040786882,-1.423399703,-1.2364717085 Ru,0,0.2585066193,-1.3985435125,0.2936486334 O,0,2.2371984828,2.2651302608,1.3303266856 H,0,2.9837258599,-2.6280842458,-1.184099875 H,0,3.3720280496,-0.9962535415,-1.3996378077	-660.576411
T3'	Ru,0,1.2722202101,1.3483761221,0.0768717573 Ru,0,-0.9516522959,1.5398410789,0.5718628643 Ru,0,-1.4954513159,0.0389755424,-1.0671937263 Ru,0,0.8132860405,-0.1184750286,-1.5921673117 N,0,2.6581141983,-0.6443515273,-2.3628101629 N,0,2.3685286011,-1.2411786962,-1.2211015475 Ru,0,-0.0017011079,-0.7139505494,0.7332450154 O,0,2.6785204337,0.3525638681,0.6697455008 H,0,3.3996922871,0.0626922437,-2.2793875674	-660.521787

	H,0,2.7658239489,-0.5979840537,-0.2025488218	
I4'	Ru,0,1.1083322415,0.7848400232,0.84104309 Ru,0,-1.0958624027,1.1299950784,0.9617358908 Ru,0,-1.4865746685,-0.233779275,-0.8523873973 Ru,0,0.8016154327,-0.5267452833,-1.0299164387 N,0,2.5235813258,-0.7853135162,-2.0896580922 N,0,2.1456086131,-1.9558538605,-1.554808758 Ru,0,-0.4483399683,-1.2979083576,1.05196436 O,0,2.483460055,1.6728108394,1.2814051895 H,0,3.3909511716,-0.4110664344,-1.6942605309 H,0,2.7753291996,-2.293669214,-0.8188463132	-660.567849
I4WT	O,0,2.0862473035,2.1829713,1.2647541784 Ru,0,1.0541482785,0.9331049515,0.7564817023 Ru,0,0.1847208913,-1.563332696,0.1608981618 N,0,1.2728170095,-1.411815908,-1.4098139598 N,0,2.6650855169,-1.4082230147,-1.6801107692 Ru,0,-0.9264042375,0.2914808789,1.5637902093 Ru,0,-1.7286694581,-0.2961037728,-0.5723151198 Ru,0,0.3740338524,0.3160068571,-1.3975506294 O,0,1.9731780005,1.0388167955,-2.8391287879 H,0,2.9325981038,-2.3175045947,-2.0472422394 H,0,3.2008010286,-1.2188549165,-0.8347559374 H,0,2.5561865898,0.2528556316,-2.7057618488 H,0,2.4558871207,1.806257488,-2.50783896	-737.043947
T4	O,0,2.2327221959,1.8373752291,1.4046244729 Ru,0,0.8761754927,0.9603585274,0.8878172972 Ru,0,0.3620185693,-1.4115969469,0.2856503646 N,0,1.1232494205,-1.4721272362,-1.5074783314 N,0,2.8191614645,-1.3398616759,-1.7902349991 Ru,0,-1.255627873,0.5821565721,1.4926703255 Ru,0,-1.6846930461,-0.3191334752,-0.538262792 Ru,0,0.4623382251,0.3160603845,-1.4273496657 O,0,1.7123992769,0.9978960277,-2.8256192738 H,0,3.1150023805,-2.1865858074,-2.262591757 H,0,3.3502996974,-1.1746126737,-0.9405981209 H,0,2.8281519377,-0.5046235523,-2.4010227306 H,0,2.0696882588,1.8765756268,-2.6530677896	-737.023751
I5	O,0,2.6570399547,2.1778438273,0.4483368039 Ru,0,1.4015789241,1.0652721455,0.3215868388 Ru,0,1.6016357216,-1.1896697292,-0.6332263086 N,0,1.1233627221,-0.2906484853,-2.0791299594 Ru,0,-0.2795576678,0.4050492999,1.6639839013 Ru,0,-0.7745954983,-0.8687967784,-0.1604973819 Ru,0,-0.0560124328,0.919074838,-1.6861242653 O,0,-0.9001305299,2.2454144543,-2.764214893 H,0,-0.6658961936,2.3958774277,-3.6860887358	-680.534232
H₂	H,0,-0.4462930319,0.50802138,0. H,0,0.2976299119,0.50802138,0.	-1.169574
I5H₂	O,0,2.7631535461,1.8791862396,0.4529844034 Ru,0,1.3919328103,0.9151096985,0.3457919322 Ru,0,1.2760570001,-1.4093635164,-0.5171827562 N,0,0.9174534626,-0.5090183992,-2.0185992608 Ru,0,-0.395598826,0.5896199804,1.6673994258 Ru,0,-1.0896598727,-0.686014509,-0.0617809063 Ru,0,-0.0582364995,0.8680082373,-1.6711642967 O,0,-0.7399177919,2.2761242244,-2.7606764409 H,0,-0.5115819024,2.3713347112,-3.6912713762	-681.717046

	H,0,3.0785234152,-1.5723636253,-0.5130807215 H,0,2.8464346582,-2.3345510415,-0.7354740029	
T5	O,0,2.8326705291,1.8658953558,0.5411491101 Ru,0,1.4500359751,0.9286325246,0.3559938979 Ru,0,1.4057264694,-1.4289314593,-0.2740598671 N,0,1.1636359638,-0.7602547435,-2.0030642793 Ru,0,-0.5074292009,0.8506631719,1.4826646194 Ru,0,-1.0741654401,-0.6890972654,-0.0472566192 Ru,0,0.1665230225,0.6703024718,-1.7123451162 O,0,-0.4432339383,2.1468342057,-2.7225032115 H,0,-0.6644637442,2.0226353059,-3.6540160203 H,0,2.7706731179,-2.2118964386,0.126338608 H,0,2.3785872458,-1.0067121288,-1.5959551219	-681.671889
I6	O,0,2.4788232234,1.8424516995,0.7847500843 Ru,0,1.2169788193,0.7740577877,0.4734803213 Ru,0,0.9492725145,-1.5127816328,-0.0630112923 N,0,0.8779869102,-1.1547049476,-1.8921079404 Ru,0,-0.6174656275,0.2478452364,1.7686649401 Ru,0,-1.7727645648,-0.3349507276,-0.008682512 Ru,0,-0.1009221661,0.3878129672,-1.5238539241 O,0,-0.7810020654,1.8353982283,-2.53289577 H,0,-1.5880462222,1.6955513145,-3.0452590225 H,0,2.4707755863,-1.8985869991,-0.298268705 H,0,1.5837755926,-1.2822559264,-2.6178101794	-681.711101
T6	O,0,2.6663603222,2.4226539748,0.5415051047 Ru,0,1.5042140221,1.2367644321,0.2341630074 Ru,0,1.0700420668,-1.2467265974,-0.2890785319 N,0,1.3449266997,-0.7905075344,-2.2377473561 Ru,0,-0.0288742644,0.2874339092,1.5416373826 Ru,0,-1.2161039353,-0.4330896766,-0.3420271198 Ru,0,0.2814662286,0.7229438575,-1.7425652268 O,0,-0.3793251633,2.2357505948,-2.6865899321 H,0,-1.0675056483,2.0728430051,-3.3447814597 H,0,1.6970206725,-2.0169659115,-1.6450911737 H,0,2.2431479994,-0.6465150536,-2.6986766947	-681.683453
I7	O,0,2.4993294195,1.8157890655,0.871377342 Ru,0,1.1061799336,0.8983851149,0.6125474185 Ru,0,0.7397925706,-1.4473024288,-0.0478414217 N,0,1.0810359064,-1.1775859749,-2.0582976738 Ru,0,-0.6265093972,0.1226995146,1.8280907904 Ru,0,-1.5613224498,-0.6413694046,-0.0825843712 Ru,0,0.029635512,0.4703064432,-1.5333679447 O,0,-0.5008257536,2.0402625251,-2.4661584584 H,0,-1.2854105541,1.9921864521,-3.0287043676 H,0,2.0357264752,-1.0024580336,-2.3635164562 H,0,0.6397493372,-1.7964022734,-2.7318958574	-681.732099
I7'	O,0,2.5452158826,1.8956287194,0.4029222807 Ru,0,1.1355515788,0.9732930334,0.2538798259 Ru,0,0.6868229982,-1.3748304369,-0.3754749399 N,0,1.0098152711,-1.0765214888,-2.3832284138 Ru,0,-0.5482589949,0.2483628882,1.5576300113 Ru,0,-1.594193997,-0.5068914797,-0.3032461652 Ru,0,-0.0539543162,0.5522951614,-1.8265778062 O,0,-0.6760922863,2.0450374941,-2.8348759537 H,0,-0.1833691628,2.8644075326,-2.6909964975 H,0,1.9648382669,-0.8974617502,-2.6839579416 H,0,0.5628217597,-1.6728496734,-3.0737344	-681.734109

T7	O,0,2.4264628242,1.950602009,0.7793424496 Ru,0,1.222668115,0.7858749107,0.5997953954 Ru,0,0.5764826773,-1.3627400204,-0.2874372837 N,0,0.7818607331,-0.2886611606,-3.0908870162 Ru,0,-0.4977261054,-0.1011499799,1.7663448837 Ru,0,-1.6299835492,-0.4979058775,-0.1991185649 Ru,0,-0.1174614898,0.7634025579,-1.510756502 O,0,-0.2800587638,1.7716402972,-3.0009613161 H,0,0.3230983655,0.834595389,-3.5321277921 H,0,1.7861132237,-0.4055801151,-3.041500921 H,0,0.3281939696,-1.1359940103,-3.4061433327	-681.657516
Ru₅O₂	O,0,2.5750770366,1.8163036972,0.7058160611 Ru,0,1.2110525453,0.8578860498,0.5574104371 Ru,0,0.5114784491,-1.3029994285,-0.3968649405 Ru,0,-0.3461445734,-0.1749651597,1.7504241904 Ru,0,-1.8614141425,-0.3263132918,-0.1779745385 Ru,0,-0.4079591497,0.6905601259,-1.5088834999 O,0,-0.2937311653,1.5352720071,-2.9490007097	-625.121302
NH₃	N,0,0,0,-0.12910107 H,0,-0.0000000025,-0.9429656822,0.2429972659 H,0,-0.8166322344,0.4714828433,0.2429972659 H,0,0.8166322369,0.4714828389,0.2429972659	-56.551514
Ru₅-TiO₂	O,0,2.1985184991,-0.2105892619,2.1282281337 Ru,0,0.9622254282,0.8031454627,0.8154847807 Ru,0,-1.2279721705,1.6132144357,0.5125190599 Ru,0,-1.3729658062,0.5694057479,-1.4388298124 Ru,0,0.7250236016,-0.2950813331,-1.2174577581 Ru,0,-0.8751092892,-0.8640867454,0.6520623297 O,0,-0.1491977822,-2.1696849362,1.9915791523 Ti,0,1.3921765191,-1.5656283697,1.3523061143	-1474.737824
Ru₅-TiO₂••N₂ (End-On)	O,0,2.225970656,-0.2306069872,1.9349763492 Ru,0,0.9468697088,0.8663488323,0.7673859093 Ru,0,-1.2530193848,1.6399087778,0.6019787213 Ru,0,-1.5150234336,0.6787694688,-1.3625740317 Ru,0,0.641843137,-0.2057219674,-1.320626189 N,0,2.1341561123,-1.1495734192,-2.2695796356 N,0,2.8951083517,-1.6326587264,-2.9190257388 Ru,0,-0.8587420504,-0.8429949637,0.6205297648 O,0,0.0008142325,-2.2645677935,1.7308243688 Ti,0,1.4725769805,-1.5464362315,1.0460941417	-1584.333762
Ru₅-TiO₂••N₂ (Side-On)	O,0,2.300485444,-0.3554137185,1.7207738882 Ru,0,0.9263423306,0.8713037164,0.7411528565 Ru,0,-1.2561138618,1.6902800789,0.5848642579 Ru,0,-1.5939719308,0.6959855267,-1.3386138757 Ru,0,0.5685878092,-0.2126318203,-1.3102053484 N,0,2.250848136,-1.2351580947,-2.1812992625 N,0,2.008276053,-1.832529245,-1.2224364186 Ru,0,-0.8993962213,-0.8087833341,0.6623829053 O,0,-0.0369950767,-2.2823079896,1.6737882578 Ti,0,1.4407803178,-1.6350001198,0.8982457395	-1584.335532
IIA	O,0,2.1993314781,-0.2284707496,2.1208747965 Ru,0,0.950940649,0.814051939,0.8057259068 Ru,0,-1.2403457836,1.5973217333,0.5069174479 Ru,0,-1.3829754103,0.5759908794,-1.4360445287 Ru,0,0.7500966023,-0.265447973,-1.2536676979 N,0,2.1393556622,-1.0394675396,-2.6235114904 N,0,1.9167884365,-1.9454816657,-1.9437282022	-1660.810540

	Ru,0,-0.8726366004,-0.8672924521,0.6716085916 O,0,-0.1679625718,-2.1482464136,2.0037252526 O,0,2.6868551693,-3.0463007519,0.4254463509 H,0,3.6139575814,-3.2101964786,0.6321152456 H,0,2.5834363467,-3.0052205882,-0.5522252504 Ti,0,1.4162514407,-1.5972129393,1.3767525779	
T1A	O,0,2.0998751988,-0.2687408999,2.0796968131 Ru,0,0.875217668,0.6923692106,0.7472464548 Ru,0,-1.3166419285,1.4796922845,0.5157524776 Ru,0,-1.5398732742,0.5042628074,-1.4361795912 Ru,0,0.6188364901,-0.336243053,-1.3336950178 N,0,2.1663304873,-1.1556864142,-2.4581571576 N,0,1.7437777557,-1.9554269385,-1.6832205565 Ru,0,-0.9416195676,-0.9823111017,0.6336070952 O,0,-0.2651164321,-2.2347256773,1.9709300142 O,0,2.4769844074,-3.0193984031,0.4131768159 H,0,3.4015902413,-3.2386547731,0.5625031552 H,0,2.1983618644,-2.7154551397,-0.9824663279 Ti,0,1.3774980895,-1.733798902,1.426800825	-1660.793747
I2A	O,0,2.1706341979,-0.0497302244,2.1614596369 Ru,0,1.034335657,0.70845535,0.6907784478 Ru,0,-1.1322102241,1.5290916522,0.5660301248 Ru,0,-1.4206151699,0.5498160391,-1.3834144116 Ru,0,0.7031483482,-0.3046134339,-1.3521997099 N,0,1.9593260966,-0.7387548981,-2.8537176128 N,0,1.7627001744,-1.7987572747,-2.2907029417 Ru,0,-0.829816423,-0.9200632488,0.7172186844 O,0,-0.2622053936,-2.0254698991,2.2000516277 O,0,2.5739166217,-3.0294354091,1.3246847926 H,0,3.5302056236,-3.0629113532,1.2379279326 H,0,2.2879458108,-2.65167601,-2.5282339446 Ti,0,1.4659236804,-1.6448042903,1.827294374	-1660.796204
T2A	O,0,1.9400095363,0.0530379772,2.4009409146 Ru,0,1.1034787738,0.7003851154,0.7581121578 Ru,0,-1.0004097189,1.5609522278,0.3749239568 Ru,0,-1.2056080079,0.3992760574,-1.4940727744 Ru,0,0.8842248962,-0.537897442,-1.1865527128 N,0,1.9300962704,-0.7750129283,-2.7740391245 N,0,1.9150339668,-1.968392643,-3.0291651685 Ru,0,-0.8301622952,-0.8996367297,0.7238181701 O,0,-0.4807388571,-1.9090049026,2.3574870206 O,0,2.3724313642,-3.039062185,1.9227260421 H,0,3.3181769509,-3.1858878771,1.8503611196 H,0,2.6298557277,-2.2408446351,-3.7312861159 Ti,0,1.2668983927,-1.596767035,2.1439245146	-1660.791011
I3A	O,0,1.7116661873,-0.3433262966,2.3061475528 Ru,0,1.0756172067,0.6827551501,0.7927754644 Ru,0,-0.8303884286,1.9479450649,0.610241675 Ru,0,-1.2043702318,1.1770835649,-1.4560733524 Ru,0,0.6534937667,-0.1322362945,-1.3603347797 N,0,1.914036174,-0.9282712407,-2.4182846879 N,0,2.6484898018,-1.2890356092,-3.3016193762 Ru,0,-1.1217257037,-0.4937835909,0.5416917784 O,0,-0.979316186,-1.8425403907,1.9443278767 O,0,1.6479280244,-3.3809042996,1.4074671323 H,0,2.5463117523,-3.6894334064,1.2702084025 H,0,2.6178980365,-0.6898856085,-4.1489739612	-1660.797888

	Ti,0,0.7982176004,-1.8045220428,1.7580662754	
T3A	O,0,2.0337072186,-0.193906947,2.0767817729 Ru,0,1.1331610404,0.8474484019,0.68805585 Ru,0,-0.7072114198,1.9768103356,0.1611184022 Ru,0,-1.3968837947,0.3371320303,-1.3176993531 Ru,0,0.4702645674,-0.8968762484,-0.9392836284 N,0,1.9214579194,-1.227398886,-2.0610996918 N,0,2.8330392387,-2.0160564863,-1.7182063904 Ru,0,-0.9887767068,-0.4095543222,1.1199906546 O,0,-0.5716002157,-1.7953828393,2.4507431812 O,0,1.393681368,-2.5752108468,0.0981151868 H,0,2.4096827053,-2.5357126191,-0.6860124056 H,0,3.516566503,-2.2730365467,-2.4314912605 Ti,0,1.0577015764,-1.6851710259,1.696491682	-1660.772024
I4A	O,0,1.9894148916,-0.2099732022,1.9636543237 Ru,0,1.1608758228,0.8148398674,0.5627491284 Ru,0,-0.6467823376,1.9902368416,0.0184973439 Ru,0,-1.3757972201,0.2843400391,-1.4001073965 Ru,0,0.4712293776,-0.9541273038,-1.0024679677 N,0,1.818626847,-1.2304463258,-2.2087606329 N,0,2.9180833672,-1.8506703486,-2.0251540428 Ru,0,-1.0209917051,-0.3454781604,1.0465350007 O,0,-0.7082825567,-1.7362546544,2.3817947338 O,0,1.1673972316,-2.5780248307,0.0944865608 H,0,3.0654004211,-2.3447942675,-1.1417766148 H,0,3.5232326947,-2.0350823325,-2.8163653113 Ti,0,0.9488791658,-1.7275203222,1.6611078749	-1660.779252
T3B	O,0,1.9405726328,-0.2326060593,2.0840856065 Ru,0,1.1515346557,0.7899999133,0.6292485352 Ru,0,-0.5899117704,1.9946983589,-0.007067843 Ru,0,-1.2554787044,0.313608383,-1.5051500877 Ru,0,0.4912309289,-0.9613011914,-0.9830521971 N,0,2.2398335705,-1.6023488887,-1.6762188923 N,0,2.9939080284,-1.490351614,-2.6392222598 Ru,0,-1.044927794,-0.3650952206,0.9760820398 O,0,-0.7372113635,-1.7228231366,2.3446708629 O,0,1.3637535042,-2.7008600768,0.2228295577 H,0,2.1725457169,-2.4201587527,-0.67060443 H,0,2.6640104472,-0.7415324499,-3.2805926334 Ti,0,0.9560751477,-1.7227352654,1.7182587412	-1660.746672
I4B	O,0,1.7513388341,-0.202634223,2.3088234623 Ru,0,1.1762458267,0.7938237534,0.7556169491 Ru,0,-0.4810763316,1.984456928,-0.1149508936 Ru,0,-1.0106245446,0.1892979139,-1.559853196 Ru,0,0.6960655387,-1.0338336469,-0.7973726806 N,0,2.3068230418,-1.5387993356,-1.8630213956 N,0,2.7653496803,-1.2566575949,-2.994252591 Ru,0,-1.0949543325,-0.2804656556,0.9360281138 O,0,-0.9959199213,-1.6092655476,2.3634769106 O,0,1.1161353644,-2.6148996329,0.3968652121 H,0,2.8681513026,-2.2686905739,-1.4075294778 H,0,2.1737166546,-0.5168941713,-3.3958115861 Ti,0,0.7460728868,-1.7063162137,1.9080211727	-1660.773231
I4A-WT	O,0,0.2532003602,0.0866915139,0.05525586 O,0,1.7596547199,-0.057943435,2.7521842195 Ru,0,2.4823688207,-1.7933255918,1.8729734161 Ru,0,0.0087794399,-2.63803817,1.7689032636	-1737.241943

	O,0,-1.1041225024,-1.2628603041,2.5599293632 Ru,0,1.2441993664,-1.64539556,-0.2434817755 Ru,0,1.0325597164,-3.8486118705,-0.2580197265 Ru,0,2.1555659935,-4.0270400109,1.7795220088 N,0,4.1008635929,-0.9616824492,1.6934116804 N,0,4.3125099383,0.3091261805,1.7032171485 H,0,3.5369133839,0.9079057848,2.0071032424 H,0,5.2657217891,0.6346752481,1.8154478576 O,0,2.2698747452,-0.1761878408,-1.6146772122 H,0,3.1600243876,0.0382506225,-1.3104289201 H,0,1.669217659,0.5225412746,-1.2808450329 Ti,0,0.1863715896,-0.1798833921,1.8729796071	
T4A	O,0,-0.0042177115,0.0503717012,0.2657675279 O,0,1.2241666722,-0.244280138,3.1308727927 Ru,0,2.3762078348,-1.4372708809,2.0999067618 Ru,0,-0.1065271558,-2.8468910342,1.6538818541 O,0,-1.4407775506,-1.6911369131,2.4140342351 Ru,0,1.2849762758,-1.4610681317,-0.072004597 Ru,0,1.4840966318,-3.6450136267,-0.2539513664 Ru,0,2.089904069,-3.7786927642,2.002933785 N,0,4.0191997239,-0.8703514283,1.8196886221 N,0,4.3885485325,0.1270378542,0.8761793564 H,0,4.3555291678,1.0362486795,1.3373265882 H,0,5.3566717825,-0.0394341823,0.6065397855 O,0,2.4403720089,0.0644103512,-1.1331358036 H,0,3.2115493582,0.1993801301,-0.51267953 H,0,1.8683143701,0.8443661051,-1.0712281345 Ti,0,-0.2143150096,-0.399450722,2.0093411226	-1737.237004
I5A	O,0,-1.3273557945,2.2922422978,-0.8181944323 O,0,-0.0126702832,1.8772457834,1.9980673528 Ru,0,1.1002552867,0.7053426318,0.8903296975 Ru,0,-1.5288122808,-0.7385559406,0.4873437371 O,0,-2.7254640799,0.5029151809,1.3023401762 Ru,0,-0.1433475943,0.726104863,-1.2410382417 Ru,0,0.0051308321,-1.437971558,-1.4761596008 Ru,0,0.6116217948,-1.6412840849,0.8122422196 N,0,2.7724943936,1.1452295595,0.5879753814 N,0,3.1927142038,1.9789865557,-0.5083106608 H,0,3.6009765388,2.8247401443,-0.111699537 H,0,3.9473296852,1.488530826,-0.9881364062 O,0,1.1141003395,2.1661610837,-2.2506291583 H,0,1.9261535462,2.2346704584,-1.6491608918 H,0,0.6224246943,2.9988311624,-2.1936552768 Ti,0,-1.4584042823,1.7738240365,0.9065436412	-1737.237507
T5A	O,0,-1.4498052644,2.3312023154,-0.6575017125 O,0,-0.0548048691,1.7726385934,2.0818471308 Ru,0,1.0921715343,0.7003963512,0.9448359562 Ru,0,-1.569206899,-0.7479503806,0.4965445236 O,0,-2.7973440337,0.4378271552,1.3523284884 Ru,0,-0.1294606641,0.9179342851,-1.1752636968 Ru,0,-0.0835721916,-1.2317123963,-1.5442657451 Ru,0,0.6039080748,-1.6227872608,0.701058871 N,0,2.7618569325,1.0864996975,0.6797057015 N,0,3.2049178037,2.039608007,-0.6120088918 H,0,3.5445297011,2.9078084844,-0.2102495985 H,0,3.974159956,1.5487840369,-1.0573377565 O,0,1.0994483161,2.0880317956,-2.2123471148	-1737.234416

	H,0,2.4123507068,2.2013818143,-1.3001605644 H,0,0.6422737431,2.7290807973,-2.769044444 Ti,0,-1.5542748465,1.7382707044,1.0297178529	
I6A	O,0,-1.6161473257,2.082640532,-0.6086096402 O,0,-0.147920409,1.5764828624,2.0657436758 Ru,0,1.1594646882,0.8271538468,0.8564292229 Ru,0,-1.7007622219,-1.0129476718,0.6780571069 O,0,-2.9066592457,0.1075384211,1.6157822378 Ru,0,-0.0318940683,1.2414937892,-1.2329104383 Ru,0,-0.4207894511,-0.9096336488,-1.4627078771 Ru,0,0.6460538146,-1.4829946261,0.556543512 N,0,2.7389750017,1.063623935,0.6654566639 O,0,1.5226981422,1.8834935808,-2.1168530918 H,0,1.372274256,1.9724332722,-3.0701508115 Ti,0,-1.686565181,1.3681387073,1.0898984397	-1680.721100
T6A	O,0,-1.6791636861,2.1518570313,-0.5176511719 O,0,-0.089687137,1.5248219697,2.1054717864 Ru,0,1.1491094567,0.805316929,0.823782509 Ru,0,-1.7271181664,-1.0101242245,0.6584138614 O,0,-2.8768627033,0.0992170497,1.6571454936 Ru,0,-0.0939723025,1.3244619413,-1.2013181143 Ru,0,-0.506726023,-0.7943653973,-1.515164187 Ru,0,0.6067922018,-1.4970672535,0.4205731926 N,0,2.7166081711,1.038422841,0.5293421832 O,0,1.3937346366,2.0566675179,-2.1543525164 H,0,1.9090352205,1.4986402104,-2.7469156217 Ti,0,-1.6521966684,1.3704253851,1.140688585	-1680.715842
I7A	O,0,-1.4091897376,2.0865279377,-0.5268333221 O,0,0.2721772506,1.5303538426,2.0361498705 Ru,0,1.4354683784,0.7481491415,0.7228525811 Ru,0,-1.4800770303,-1.0113304322,0.7926731054 O,0,-2.5753582935,0.1630100237,1.7969387715 Ru,0,0.1006727355,1.1819694149,-1.2580768976 Ru,0,-0.3734319893,-0.9557078081,-1.4390373363 Ru,0,0.8459511825,-1.5434784366,0.4907791508 N,0,2.9799765995,0.9996716632,0.3099820719 O,0,1.5504594914,1.6929294692,-2.3340407052 H,0,2.4131701474,1.7120523604,-1.8832479837 Ti,0,-1.3463147346,1.3659778237,1.1665256937	-1680.730687
T7A	O,0,-1.6461624789,2.0776608579,-0.6427113459 O,0,0.0308459129,1.5439792935,1.9947046449 Ru,0,1.1195384272,0.7205316534,0.6303794695 Ru,0,-1.7370346629,-0.9936986548,0.7098993492 O,0,-2.8076510523,0.1997794825,1.7124858585 Ru,0,-0.1309180163,1.1750223145,-1.3111971811 Ru,0,-0.6316237052,-0.994608084,-1.5282798681 Ru,0,0.6206973504,-1.5495291825,0.3831773127 N,0,2.5681626724,1.1536183334,-0.1307704664 O,0,1.3342572843,1.6430826117,-2.1706753792 H,0,2.3438193197,1.4945959012,-1.2457388291 Ti,0,-1.5584260513,1.3795624733,1.089134435	-1680.707277
I8A	O,0,-1.3880999632,2.0322634755,-0.5536090043 O,0,0.2917535676,1.5134400285,2.0827639339 Ru,0,1.3689233638,0.7227991085,0.6766473582 Ru,0,-1.4934664709,-0.9975781675,0.7737786871 O,0,-2.5483074016,0.1830164635,1.8070635065 Ru,0,0.1321403041,1.185344427,-1.2557546478	-1680.711840

	Ru,0,-0.4393237924,-0.9982498831,-1.4334833957 Ru,0,0.8655956744,-1.5047355148,0.4857309952 N,0,2.9759017478,1.1095477047,0.1362549556 O,0,1.2769422638,1.6867720799,-2.4014394156 H,0,3.1991967247,1.5454990477,-0.7739103906 Ti,0,-1.2946470182,1.3754472301,1.1985734175	
T8A	O,0,-1.3623395773,2.0598215368,-0.5405181803 O,0,0.2747409248,1.5731265073,2.0327816209 Ru,0,1.455570599,0.7337542567,0.6625348137 Ru,0,-1.4768992875,-1.0022506018,0.7799135263 O,0,-2.524480986,0.1474173797,1.8394242847 Ru,0,0.098836806,1.2310587139,-1.320395754 Ru,0,-0.4312933186,-0.9787950222,-1.4343507405 Ru,0,0.9065926086,-1.4545393515,0.4527077424 N,0,3.0905806316,1.0618763819,-0.0933901887 O,0,1.2249260553,1.6963452858,-2.4835131419 H,0,3.1284653477,1.5442714526,-0.9957198028 Ti,0,-1.2864267836,1.36258657,1.2092649873 H,0,3.2082306863,0.9332269372,1.2496598515 H,0,2.6908592936,0.5992159537,2.0359889813	-1681.832891
I9A	O,0,-1.3532863985,2.0483880472,-0.5056416676 O,0,0.1972925082,1.4936103212,2.1074398981 Ru,0,1.4738516769,0.7011196037,0.7827447821 Ru,0,-1.5037346434,-1.0544413328,0.7857690888 O,0,-2.5716679833,0.0846000807,1.841533314 Ru,0,0.0691516228,1.262253796,-1.3558657415 Ru,0,-0.4617693499,-0.9799413497,-1.3775536924 Ru,0,0.9232065201,-1.4022025901,0.5282330073 N,0,3.0851714542,1.0672486502,-0.1238705077 O,0,1.25065332,1.6701429463,-2.4738936288 H,0,3.1024598831,1.3925244663,-1.0850484163 Ti,0,-1.3254745092,1.3087050314,1.2394534329 H,0,3.9941903745,1.0658970547,0.3153010508 H,0,2.3866695245,0.4821112751,2.0930330804	-1681.910339
T9A	O,0,-1.2681860358,2.0252792391,-0.3963952338 O,0,0.1948235772,1.2577356999,2.1796541216 Ru,0,1.3698645599,0.5699125049,0.7133655902 Ru,0,-1.6886477848,-1.1025406878,0.698337146 O,0,-2.6862748712,0.0802295407,1.7835061278 Ru,0,0.1486608209,1.1595433094,-1.3058743311 Ru,0,-0.6766950504,-0.9862072334,-1.4087790557 Ru,0,0.6406515342,-1.5300865869,0.6405242275 N,0,3.223944161,0.9392916738,0.0194943478 O,0,1.2220930722,1.6557670632,-2.5038936139 H,0,3.283206289,1.6722123403,-0.6810042984 Ti,0,-1.3315843758,1.2532691495,1.2809937916 H,0,4.1323695984,0.7624917644,0.4263419005 H,0,2.7024865052,1.3831162228,1.3253642798	-1681.869520
I10A	O,0,-1.0356593612,2.0068428819,-0.4281391662 O,0,0.7695755532,1.1950447354,1.9396094948 Ru,0,1.2554149348,0.1685102069,0.3266344371 Ru,0,-1.8826813139,-1.0048802434,0.7338310144 O,0,-2.396922333,0.3314797518,1.9552360865 Ru,0,0.0542970757,0.8921480525,-1.5394110622 Ru,0,-1.1150759507,-1.0818961059,-1.5055762838 Ru,0,0.3069075321,-1.8362359429,0.3368827006 N,0,3.1751922119,1.2876056006,0.5059674623	-1681.940722

	O,0,0.8658334492,1.312810973,-2.9614490127 H,0,3.3758672292,1.8431814773,-0.319086644 Ti,0,-0.9190879017,1.2105043204,1.2277126344 H,0,3.9864391404,0.7107169451,0.7027816526 H,0,3.012651124,1.9073252971,1.2969481063	
(Ru₅O-TiO₃)_{cl}	O,0,0.0243669428,1.702862258,-1.5750425196 Ru,0,-0.827306925,1.8131937254,0.1347347357 Ru,0,0.9370434462,1.5320684019,1.5667783102 Ru,0,0.4058207462,-0.8319261459,1.7052547778 Ru,0,-1.1566908123,-0.4971817017,0.1716682362 Ru,0,2.1466034555,-0.0659468745,0.261100364 O,0,2.4141109114,-0.4380034663,-1.5636722418 O,0,-0.786408934,-1.2686120974,-1.5242557044 O,0,-2.0511417511,2.8689761198,0.6042940079 Ti,0,0.6028059203,-0.0342412193,-1.6448789659	-1625.355137
I4B-WT	O,0,1.9717874548,0.1506554318,2.1163655489 Ru,0,1.097124475,1.016853475,0.5012515914 Ru,0,-0.7485644223,1.9898737966,-0.230381472 Ru,0,-1.3225922164,0.0374379801,-1.4285137133 Ru,0,0.5500473107,-0.9943249912,-0.7671029938 N,0,2.0407864665,-1.5494199138,-1.9653683334 N,0,2.3569980256,-1.3452052915,-3.1648074573 Ru,0,-1.0948225742,-0.1757421159,1.0946177524 O,0,-0.7479986581,-1.2895168972,2.6359691064 O,0,1.2353769118,-2.3990316408,0.5232589169 H,0,2.6659838015,-2.2370603613,-1.527765099 H,0,1.7000763658,-0.6488459364,-3.541537081 Ti,0,0.9410832535,-1.3527439101,1.9677583499 O,0,3.2903082435,1.4654880995,0.2722530585 H,0,3.4624429427,0.9521437657,1.0899563465 H,0,3.7103986194,0.9973975094,-0.4592315211	-1737.236607
T4B	O,0,2.0320936689,-0.2306681669,1.8480958073 Ru,0,1.1888418049,0.6161848887,0.226081965 Ru,0,-0.541394529,1.7503392123,-0.5240242173 Ru,0,-1.4821611387,-0.172543705,-1.5381553797 Ru,0,0.3906133182,-1.4283287275,-0.8025406761 N,0,2.061928304,-1.5388106121,-1.6973460592 N,0,2.6959987664,-0.5904448281,-2.364044369 Ru,0,-1.3066516311,-0.2170279494,0.8251353937 O,0,-0.8096803113,-1.3206557069,2.2742976823 O,0,1.2597421499,-2.7958072572,0.5927318687 H,0,2.7311599361,-2.1207816098,-1.1842629905 H,0,2.0059510743,-0.0789949312,-2.9132893008 Ti,0,0.9605041981,-1.6636717692,1.8853163216 O,0,3.0764567973,1.0330516664,-0.5600417037 H,0,3.752136674,0.9271436118,0.1225529722 H,0,3.1465509182,0.2078658842,-1.5192923143	-1737.215588
I5B	O,0,1.4053138776,0.3199518438,2.4899054409 Ru,0,1.434299799,0.8510197454,0.6619350718 Ru,0,-0.6092989775,1.5025694581,0.143040085 Ru,0,-1.1178248676,-0.5347087975,-0.9785078097 Ru,0,0.9933463586,-1.3189158752,-0.5536912505 N,0,1.9984661125,-1.2465806778,-2.1285463981 N,0,3.0511048521,-0.4801617261,-2.6006370588 Ru,0,-1.7334701683,-0.3469473868,1.3398414371 O,0,-1.3661982884,-1.2522219901,2.9534323261 O,0,0.9519153872,-2.37971802,1.0547761417	-1737.259754

	H,0,1.8575648301,-2.0292404593,-2.7675175017 H,0,3.1798025273,0.3197545723,-1.9732686619 Ti,0,0.3496035761,-1.1614163578,2.2642044899 O,0,2.8808482635,1.3371140051,-0.529258589 H,0,3.1012602604,2.274337262,-0.4422077246 H,0,3.9056504576,-1.0264695961,-2.6763959984	
T5B	O,0,1.2706650241,0.5584158862,2.42779949 Ru,0,1.316787674,0.9105031055,0.5655503266 Ru,0,-0.7592223124,1.3661457086,-0.0240695752 Ru,0,-1.0900997694,-0.7977244734,-0.9814740061 Ru,0,1.071131928,-1.364336457,-0.4911992047 N,0,2.0437636058,-1.2507835996,-2.0916745771 N,0,2.9372155692,-0.3540423081,-2.647281926 Ru,0,-1.8050428274,-0.4396914275,1.2728167932 O,0,-1.3983274523,-1.1740379998,2.9590307311 O,0,1.0677302347,-2.2760931738,1.2179590402 H,0,2.0035104146,-2.0765154979,-2.6893247241 H,0,3.0101840034,0.4672223568,-2.0345621007 Ti,0,0.3233516815,-1.0120437223,2.2853048645 O,0,2.8018831531,1.5156135617,-0.585214066 H,0,3.6431055333,1.5345945799,-0.1116418338 H,0,3.8457475398,-0.7788595393,-2.8149162319	-1737.250555
I6B	O,0,1.2924243801,0.491384785,2.44872913 Ru,0,1.4031925417,0.8152790186,0.5802591363 Ru,0,-0.6660369023,1.3720118153,-0.0047396616 Ru,0,-1.077868618,-0.7862966643,-0.9906862213 Ru,0,1.0362100468,-1.4302512646,-0.5094204042 N,0,1.9835893833,-1.267624017,-2.1338477312 N,0,2.6859530887,-0.2834579335,-2.8339016447 Ru,0,-1.8092584677,-0.3653616661,1.2498287434 O,0,-1.4573050514,-1.1311096995,2.9372359936 O,0,0.9870988181,-2.3186661524,1.2193822892 H,0,2.0054869093,-2.1142784651,-2.701472935 H,0,2.6376155687,0.5942756532,-2.3281311766 Ti,0,0.2774396904,-1.032411838,2.2800783847 O,0,2.9973530913,1.3152320494,-0.3454499901 H,0,3.6263083204,0.5975891826,-0.5024969508 H,0,3.6577752005,-0.5450678037,-2.9829219618	-1737.255958
T6B	O,0,1.4696115314,0.5270238946,2.1990970603 Ru,0,1.3068206951,0.8090256286,0.3273084229 Ru,0,-0.8390743791,1.3131004922,-0.0184015456 Ru,0,-1.2897205279,-0.8750528467,-0.9123948281 Ru,0,0.7995436966,-1.4951269052,-0.5726035601 N,0,1.9097298488,-1.5776294393,-2.200739155 N,0,1.835736455,-0.7318883704,-3.3196857736 Ru,0,-1.7692257562,-0.3913859117,1.4422888492 O,0,-1.1757592608,-1.1168636015,3.0631542912 O,0,1.0256756194,-2.3914375309,1.1300855873 H,0,2.8958867531,-1.7171015718,-1.9894185171 H,0,0.9033762075,-0.782300719,-3.7076772441 Ti,0,0.4608187507,-1.0122407725,2.1727753197 O,0,2.7084745507,1.2588807196,-0.8676520194 H,0,3.2896966738,0.5412197748,-1.1506666548 H,0,2.0478391421,0.238051159,-3.0899182328	-1737.239131
I7B	O,0,1.4585218641,-0.6547243494,1.9843284554 Ru,0,1.6133176994,0.7768671112,0.695267379 Ru,0,-0.3163851076,1.840630579,0.6184201117	-1737.263523

	Ru,0,-1.0086721704,0.5237230788,-1.2940483032 Ru,0,0.8777891187,-0.65693476,-1.2861099967 N,0,2.4367301525,-0.2819983653,-2.4456611828 N,0,1.943527767,-1.5045958068,-2.9678347249 Ru,0,-1.7916098183,-0.0514258635,0.9128833573 O,0,-1.6233866566,-1.6414177199,1.8968621554 O,0,0.4698939849,-2.3523269981,-0.427696049 H,0,3.350266573,-0.435921379,-2.0218659203 H,0,1.6365542392,-1.4325795984,-3.9288175383 Ti,0,0.0999452895,-1.5521808899,1.1686900416 O,0,2.9636923183,1.7090044953,-0.2500877318 H,0,2.9828055089,1.5927378759,-1.2095208898 H,0,2.4854662375,-2.3439614101,-2.7926341636	
T7B	O,0,1.415048267,-0.2541049489,2.4884866529 Ru,0,1.7164179809,0.7704438706,0.8512271362 Ru,0,-0.1990815731,1.867208647,0.5444866259 Ru,0,-0.9817667349,0.0160889423,-0.8857346466 Ru,0,0.9548208365,-1.064659375,-0.5394875578 N,0,2.700294729,-0.7969060327,-1.6098373839 N,0,2.702947887,-0.6947156442,-3.0436377072 Ru,0,-1.6907007917,0.1677859002,1.368698184 O,0,-1.6180148979,-1.0800301417,2.7798585802 O,0,0.3699376976,-2.4842564246,0.6001720485 H,0,3.4023260654,-1.4894998952,-1.3550560719 H,0,1.9869063503,-1.2985067763,-3.4360592172 Ti,0,0.0675806128,-1.3681715775,2.0413885722 O,0,3.1739305341,1.1136199842,-0.1344398202 H,0,3.1193904507,0.2455797724,-1.0092140028 H,0,2.4599385864,0.2613696995,-3.2784083923	-1737.239365
I8B	O,0,1.5741692291,0.2462839632,1.5607096965 Ru,0,1.1717067909,1.2401536188,-0.0240337716 Ru,0,-1.0162785908,1.830006502,0.324689975 Ru,0,-1.7018879523,-0.1455270067,-0.950922542 Ru,0,0.4436871185,-0.7004033809,-1.0816520898 N,0,2.1317629994,-1.3867554791,-2.3457050134 N,0,2.7728828984,-0.3917341495,-3.1623721388 Ru,0,-1.740913533,-0.1414135008,1.4242787339 O,0,-0.9853236591,-1.4134276431,2.585444037 O,0,0.835820301,-2.3048542972,-0.0007474961 H,0,1.7999876294,-2.1279143995,-2.9558811918 H,0,2.7214625223,0.4925032466,-2.6649453991 Ti,0,0.4731333697,-1.2260255251,1.4344966104 O,0,2.1825192795,2.2989939059,-0.8789744278 H,0,2.7525682729,-1.8159507006,-1.660335647 H,0,3.7508463243,-0.629029154,-3.2974403353	-1737.257752
T8B	O,0,0.0158632862,-0.3704573822,-0.1302870734 Ru,0,-0.0208179164,-0.2965489072,1.7505697575 Ru,0,2.1515664324,0.2268403203,2.2064423844 Ru,0,2.6111046478,-2.0113965578,2.6880946291 Ru,0,3.2131887869,-1.1755670496,0.5107442479 O,0,2.7747138977,-1.7122602873,-1.2640246196 Ti,0,1.129399687,-1.8333078241,-0.4751874738 Ru,0,0.402692329,-2.5474646505,2.2415942129 N,0,-0.5565482185,-2.6456897834,3.8934979929 O,0,0.5954170046,-3.2920768074,0.4355540264 N,0,-1.8045136419,-3.8568439095,2.8199535104 O,0,-1.1349398044,0.4428968714,2.7952829947	-1737.199762

	H,0,-1.2542002595,-4.5745369135,2.3394050993 H,0,-2.1837808384,-3.2512211273,2.0891106709 H,0,-1.2530370107,-1.9494935518,4.1524580574 H,0,-0.5506244934,-3.3882672642,4.581023956	
I9B	O,0,-0.2206247392,1.9088698258,-1.5601458729 Ti,0,-0.3404359311,2.2464893741,0.2862317825 O,0,1.1889494754,1.8544067652,0.9971595359 Ru,0,1.737799983,-0.0581083431,0.3306268546 N,0,3.148961757,0.278463451,1.6275998993 Ru,0,0.4127631899,0.1812034933,-1.7847563933 O,0,1.178748069,-0.7329863153,-2.971923715 Ru,0,-1.3061573862,-0.9726972084,-0.7714629863 Ru,0,-1.7093919304,0.3741167384,1.0694157902 O,0,-1.8405922333,2.2415317744,1.369994506 Ru,0,0.116376066,-1.2106278237,1.2290272351 N,0,2.8748967718,-1.3696854449,-0.4566730763 H,0,4.0984727552,-0.0376495442,1.4797873378 H,0,3.1127917012,1.1748556965,2.0955097435 H,0,2.7960003795,-1.66746181,-1.4208491554 H,0,3.6944340723,-1.7433786291,0.0032945145	-1737.288973
T11B	O,0,0.0015254851,1.8444249771,-1.8285388035 Ru,0,-1.2371066024,1.5275650449,-0.4853939192 Ru,0,0.2946735985,1.0851554406,1.1834582073 Ru,0,-0.1508094357,-1.3115816252,0.9315865057 Ru,0,-1.4893557943,-1.0273395253,-0.806706172 N,0,-2.5626816056,-1.4723065836,1.0324950575 N,0,-1.8741530329,-2.7780132927,-1.6034006579 Ru,0,1.8944460078,-0.1886671399,0.1702850863 O,0,2.728186811,-0.1535467239,-1.5469417445 O,0,-0.1563249109,-0.9745091562,-2.3462190269 H,0,-2.8244112482,-3.1009463327,-1.7360495502 H,0,-1.3090028612,-2.9758962848,-2.4211320689 O,0,-2.6368816251,2.2212821192,0.1364437505 H,0,-2.957307321,-0.7794528505,1.6574289078 H,0,-3.025768627,-2.3679755534,1.1445258253 Ti,0,1.0213224042,0.2877034587,-2.0702619781 H,0,-3.1770133201,-0.9931497885,-0.1894107037 H,0,-3.1960659221,-0.6519261836,-1.1074547155	-1738.414812
I11B	O,0,0.0011072621,1.8200086734,-1.661210434 Ru,0,-1.1327149465,1.5310223739,-0.1986750055 Ru,0,0.4313158348,0.9475413633,1.4324143276 Ru,0,0.3110942792,-1.3508843149,1.0282007153 Ru,0,-1.3566549807,-1.1673059175,-0.6155895908 N,0,-2.9341624067,-1.4720710285,0.8507176591 N,0,-1.8197107036,-2.8202976463,-1.4373343089 Ru,0,2.1390917008,-0.1203467749,0.1391026027 O,0,2.7970502452,0.0465528144,-1.6179931815 O,0,-0.0410460224,-1.0808636254,-2.2368755254 H,0,-2.4220505986,-3.5478336173,-1.0738962627 H,0,-1.282304391,-3.1221174616,-2.240433752 O,0,-2.3030995133,2.4671091119,0.5880126982 H,0,-2.910511243,-0.7543714854,1.5684423905 H,0,-2.9034981772,-2.3753885152,1.3137563108 Ti,0,0.9970240965,0.2825010489,-1.9958855951 H,0,-3.8315564386,-1.4001510151,0.3788086811 H,0,-2.114682997,0.3233600162,-0.9837447291	-1738.461986
T12B	O,0,-0.0659136959,1.6465262171,-1.8083310105	-1738.440643

	Ru,0,-1.1996867339,1.2325671976,-0.387407748 Ru,0,0.2659073373,1.2544012239,1.3463928697 Ru,0,0.4391086194,-1.0928940143,1.3815801776 Ru,0,-1.1029758938,-1.1788950735,-0.4931869913 N,0,-2.6385910081,-1.3630236534,1.086263687 N,0,-2.0222049127,-2.5678616439,-1.6388772014 Ru,0,2.1634245547,0.1835655238,0.3294617305 O,0,2.9205748771,0.2020116447,-1.4142390649 O,0,0.2717630325,-1.3496821329,-1.9697305178 H,0,-2.9862948955,-2.873423739,-1.6762262971 H,0,-1.5797331591,-2.654816807,-2.5480535407 O,0,-2.725644281,1.7796595942,0.1371014368 H,0,-2.2818301882,-1.3938341338,2.0363742933 H,0,-3.2229650923,-2.1824350845,0.9469966094 Ti,0,1.1298111666,0.1834177026,-1.8381229768 H,0,-3.2200801176,-0.5282903091,1.0192069192 H,0,-2.5199786095,-1.0905295126,-1.2713833747	
I12B	O,0,-0.1051432911,1.830765244,-1.644815645 Ru,0,-1.1779278019,1.2778070531,-0.2091967023 Ru,0,0.3679129855,0.9607189065,1.4450335992 Ru,0,0.3496613016,-1.3418205472,1.0371947667 Ru,0,-1.2838754257,-1.0250205847,-0.6202498556 N,0,-2.9201205699,-1.1205993097,0.836565156 N,0,-2.0291309093,-2.8583064751,-1.7420726929 Ru,0,2.1298438151,-0.0840731571,0.0903736954 O,0,2.7542964041,0.1750668451,-1.6961210301 O,0,-0.0773331371,-1.1363476396,-2.2468934224 H,0,-2.0422647888,-3.7480225914,-1.2565825853 H,0,-1.2666578876,-2.8492038164,-2.4207034145 O,0,-2.6609304581,1.7834409207,0.5112778976 H,0,-2.6575547834,-1.3888413921,1.7793507722 H,0,-3.6914795008,-1.7148029148,0.5490648897 Ti,0,0.9406972462,0.2972301633,-1.9510715705 H,0,-3.2532281735,-0.1487294337,0.8867278668 H,0,-2.9062840256,-2.7498002706,-2.240836725	-1738.507969
T9B	O,0,1.3343229441,-0.4792705908,2.2171456443 Ru,0,1.5562771185,0.8387510311,0.8276776425 Ru,0,-0.3950000332,1.8122561749,0.5089110806 Ru,0,-0.839172171,0.436345492,-1.425502515 Ru,0,1.1659229795,-0.5599011398,-1.26279693 N,0,2.409444361,-0.0162595808,-2.4410792542 N,0,1.5185585635,-1.8009357976,-3.0245602765 Ru,0,-1.7571993816,-0.1851737139,0.711872631 O,0,-1.6209485093,-1.7198200774,1.7828462581 O,0,0.7852774943,-2.1704996537,-0.2933209959 H,0,3.3634056312,-0.3743111028,-2.4847703095 H,0,1.5671673759,-1.4240943351,-3.9613140395 Ti,0,0.1714374397,-1.5212421798,1.29463531 O,0,2.9711148525,1.7589709196,0.0087805772 H,0,3.1689301494,1.5014343769,-0.9073444033 H,0,2.1789181855,-2.5613538228,-2.89900742	-1737.218313
I10B	O,0,1.1363598024,-0.4960514834,2.2966759804 Ru,0,1.320239099,0.7735162552,0.871722767 Ru,0,-0.6364031355,1.6068426133,0.3297591264 Ru,0,-0.8973389478,0.2796001688,-1.5825038244 Ru,0,1.2049535439,-0.7247623161,-1.3405826829 N,0,2.5083386703,0.170961949,-2.0628584526	-1737.251973

	N,0,0.6639990309,-2.0700140309,-2.6491563007 Ru,0,-1.8204912188,-0.5901072067,0.4906283199 O,0,-1.5980835651,-2.0748628438,1.5806809159 O,0,1.100666743,-2.2866673684,-0.1592601448 H,0,3.389226849,-0.2653835302,-2.3510072592 H,0,0.0983745257,-1.9150268743,-3.4718259557 Ti,0,0.2148751547,-1.6906059026,1.2905003163 O,0,2.7272039924,1.7560844694,0.1551989949 H,0,2.9901861916,1.4859928916,-0.7512126944 H,0,0.5664062645,-3.0073837909,-2.2810451063	
T10B	O,0,1.1978237607,-0.288230309,2.1888159198 Ru,0,1.5750957332,0.8855162765,0.7395626924 Ru,0,-0.4090394304,1.6375449869,0.0575901516 Ru,0,-0.3029255166,-0.0726341769,-1.8561935453 Ru,0,1.7204320444,-0.6476630757,-1.095358754 N,0,3.1150330994,0.2507964946,-1.7997589443 N,0,0.7324505055,-1.6624338479,-2.8011728209 Ru,0,-1.5084609862,-0.465791281,0.0955779838 O,0,-1.521786944,-1.8579010626,1.3806699362 O,0,1.2221539646,-2.3319815869,-0.0633022205 H,0,3.4119382725,0.4581314455,-2.7519768106 H,0,1.0810334175,-1.6127190237,-3.7520111409 Ti,0,0.3222526506,-1.6405191958,1.288806404 O,0,2.9546868092,1.823012611,0.0648270425 H,0,3.2792944564,1.2357975398,-0.8943068281 H,0,0.5156920333,-2.6248506443,-2.5710326158	-1737.269895
T4C	O,0,-0.4730382519,1.6028663194,-2.2498281078 Ru,0,-0.4088011167,1.4636656085,-0.2077497713 Ru,0,0.817130351,1.4687880274,1.6074563922 Ru,0,0.6164830354,-0.882830825,1.7939573078 Ru,0,-0.9457357836,-0.8640388731,-0.0461144814 N,0,-2.803407895,-0.7964640135,0.1689137363 N,0,-3.5771163662,-1.6768353324,-0.3851683974 Ru,0,1.7011370785,-0.1091930857,-0.1703886977 O,0,1.898565359,-0.3684337567,-2.0580903818 O,0,-1.0194054823,-1.3454496558,-2.0356951455 H,0,-3.2094786523,-2.3795520194,-1.0239740053 H,0,-4.5810294931,-1.5816165433,-0.296783281 O,0,-2.5270073401,2.0846796645,-0.2981966218 H,0,-2.6546403589,2.1720485616,-1.2558375251 H,0,-2.9457650538,1.2346207121,-0.0349469459 Ti,0,0.1423899701,-0.0644757886,-2.4669280743	-1737.221056
I5C	O,0,-0.1743367093,1.8761514824,-2.1007868148 Ru,0,-0.520018754,1.3657901988,-0.150938895 Ru,0,0.3860171194,0.8918799591,1.7946351839 Ru,0,0.2823829671,-1.4258284152,1.2946807005 Ru,0,-1.0620721299,-0.9194230257,-0.6042725816 N,0,-2.8601653885,-0.7140239219,-0.3719640511 N,0,-3.7466177067,-1.6478490878,-0.0414328576 Ru,0,1.6648575176,-0.1433640488,-0.1479326452 O,0,2.2720905719,0.0186849655,-1.9438319063 O,0,-0.5229631819,-1.1625491908,-2.5025646644 H,0,-3.4261364855,-2.5503636319,0.2941652068 H,0,-4.6216048309,-1.3176568866,0.3425217008 O,0,-2.5823580251,1.9879932429,-0.4665709765 H,0,-2.6200846096,2.3391378232,-1.368369935 H,0,-2.9867682621,1.0684828215,-0.4808634295	-1737.232257

	Ti,0,0.5480579076,0.2907127152,-2.505846035	
T5C	O,0,-0.1810032116,-0.0817389289,-0.0577395062 O,0,0.9050844056,0.1323407053,2.865674919 Ru,0,2.208583177,-1.0409461694,2.0088245138 Ru,0,-0.0260094734,-2.9047499145,1.7600448971 O,0,-1.4709131521,-1.7456184297,2.1887648665 Ru,0,1.2763011708,-1.5029518446,-0.1566534481 Ru,0,1.6637969224,-3.6469612465,-0.0009196084 Ru,0,2.2299255834,-3.4085504491,2.2940809306 N,0,3.6824934623,-0.2936237934,1.2322413869 N,0,4.9544467381,-0.1814461737,1.6878273563 H,0,5.0713203717,-0.2712767156,2.6912673321 H,0,5.4529668039,0.6103920237,1.2993223471 O,0,2.7061074656,-0.2554244028,-1.0354150013 H,0,3.338747808,-0.1051579956,-0.0536461043 H,0,2.3347246705,0.566467701,-1.3816148397 Ti,0,-0.4221167422,-0.3259063662,1.6943619586	-1737.232582
I6C	O,0,0.2450109712,1.8798872718,-2.1072018661 Ru,0,-0.7773062608,1.6345484501,-0.5308707435 Ru,0,0.6140264597,1.1894212454,1.129636494 Ru,0,0.126990608,-1.1319401726,1.1233203239 Ru,0,-1.2970801052,-0.8548914223,-0.6382325593 N,0,-3.0343489186,-0.6192804448,-0.0138142784 N,0,-4.0024125816,-1.6305356752,0.0004035571 Ru,0,2.0330417754,-0.3474035198,-0.192588486 O,0,2.5665429892,-0.3691991162,-1.999272345 O,0,-0.475804726,-1.1881826227,-2.3369659844 H,0,-3.5859871508,-2.5219568695,0.2409073374 H,0,-4.4986019201,-1.7050766562,-0.8845232533 O,0,-2.6182230755,2.0665046055,-0.1484185369 H,0,-2.7093287536,2.9648792883,0.1964213755 H,0,-3.4450047685,0.3087829097,0.0743503384 Ti,0,0.7990744573,0.1216407286,-2.2085123732	-1737.262153
T6C	O,0,0.4469273417,2.1292145342,-1.4358599967 Ru,0,-0.7126154308,1.5132086736,-0.0258777038 Ru,0,0.5141771108,0.7865548546,1.633367013 Ru,0,0.1643586569,-1.500604454,1.1110159724 Ru,0,-1.0740128174,-0.893204957,-0.720425034 N,0,-2.9110834869,-0.855546158,-0.4298867086 N,0,-3.7658127477,-1.9325368112,-0.7190222742 Ru,0,2.146080412,-0.3953548024,0.2090629037 O,0,2.8656126874,0.0174989138,-1.4708687254 O,0,-0.0763842487,-0.8552401088,-2.3345311261 H,0,-3.3791012987,-2.7979148288,-0.3625096939 H,0,-3.9524722369,-2.0207376554,-1.7146885306 Ti,0,1.0959165401,0.4689157215,-1.8056591744 O,0,-2.5850376657,1.8288752659,0.408061343 H,0,-2.8993553379,1.499420989,1.2571315166 H,0,-3.4115004781,0.0258368229,-0.3420507806	-1737.254159
I7C	O,0,0.2960711124,2.0660575328,-1.5767208183 Ru,0,-0.8336096411,1.5369884667,-0.0954167856 Ru,0,0.4079493227,0.8401183951,1.5807850483 Ru,0,0.0522529908,-1.4531697853,1.0592935723 Ru,0,-1.1777689164,-0.8790162057,-0.7686187242 N,0,-3.0601102926,-0.8803210636,-0.6469712677 N,0,-3.7669558528,-2.0707061648,-0.9338585401	-1737.259309

	Ru,0,2.0494294004,-0.3300770597,0.1718370112 O,0,2.775842968,0.0414714173,-1.5212328538 O,0,-0.1528991193,-0.9641764936,-2.3455991083 H,0,-3.5307610403,-2.7904910057,-0.2630032665 H,0,-3.601606157,-2.4064023816,-1.8788833675 Ti,0,0.9955700607,0.4171912234,-1.8681273382 O,0,-2.599419794,1.7709607819,0.5564663318 H,0,-3.1143009572,0.9657104002,0.7037072669 H,0,-3.6359230844,-0.0790290573,-0.8816361603	
T7C	O,0,0.2188691359,2.0635463196,-1.143650853 Ru,0,-0.989585579,1.2621353142,0.1657371625 Ru,0,0.3772142313,0.3738551427,1.6845989644 Ru,0,0.2922900354,-1.7598786531,0.4488629096 Ru,0,-1.0715819717,-0.8225065987,-1.0673640737 N,0,-3.1262331768,-0.664982786,-0.9271576096 N,0,-3.9462835044,-1.7630217913,-0.4931349978 Ru,0,2.1376277367,-0.2995746583,0.1878185797 O,0,2.9216199381,0.4462427949,-1.356268071 O,0,0.1079157183,-0.6908701115,-2.5667386779 H,0,-3.9256565257,-1.7746126592,0.5206259232 H,0,-3.5525571903,-2.6406539687,-0.8186280979 Ti,0,1.1254022738,0.6503602568,-1.8058430672 O,0,-2.7605493276,1.3571254124,0.4262550459 H,0,-3.1742372208,0.3587907498,-0.1707713226 H,0,-3.5304955732,-0.3108457636,-1.7923218147	-1737.239370
I8C	O,0,-0.362720638,2.1313495242,-0.5949361784 Ru,0,-1.0674061848,1.0346667721,0.8061078666 Ru,0,0.8428599188,0.3457276724,1.8745446594 Ru,0,0.8175307166,-1.6903364416,0.5054812682 Ru,0,-0.9348092591,-0.8377995345,-0.5655512963 N,0,-2.9695949844,-1.1404327724,-1.3329158753 N,0,-4.1289578996,-1.0243413487,-0.4541908829 Ru,0,2.2421508876,0.1327708133,-0.024744902 O,0,2.4349132484,0.9910971317,-1.6883746698 O,0,-0.4811338311,-0.3444053276,-2.4233283245 H,0,-3.9611169987,-0.1900811033,0.1078673067 H,0,-4.0527439993,-1.7930428387,0.2066554714 Ti,0,0.5692033433,0.9412449174,-1.6476263546 O,0,-2.4822097734,1.2725981631,1.7105871545 H,0,-3.0807397301,-0.4375433847,-2.0617308921 H,0,-3.0632478163,-2.0273802427,-1.8229753512	-1737.256312
I1D	O,0,2.2483046114,-0.0933728461,2.0276277505 Ru,0,0.9116262412,0.8437352911,0.7126754014 Ru,0,-1.3206685357,1.5518373634,0.4363534258 Ru,0,-1.5022772436,0.4147746479,-1.4318376484 Ru,0,0.6515352612,-0.3776730936,-1.2743976102 N,0,1.9751235589,-1.2217900161,-2.654172931 N,0,1.7759230659,-2.0840874568,-1.9063254609 Ru,0,-0.908045719,-0.8965129152,0.7317482419 O,0,-0.1307423924,-2.044902505,2.1603302276 O,0,2.5531399089,-3.066899704,0.4817611209 H,0,3.4403650319,-3.3785034384,0.6879422294 H,0,2.4283086752,-3.0572258108,-0.4963100512 Ti,0,1.3951228238,-1.5146140136,1.4114067753 O,0,2.5891062751,2.4069082872,0.7708015711 H,0,3.0180149458,2.5461044987,-0.0811152504 H,0,3.1798594915,1.8554947112,1.3097662081	-1737.271191

T1D	O,0,2.2837580199,-0.2036870934,1.9354853009 Ru,0,0.9905219388,0.708453739,0.6048686058 Ru,0,-1.2282869359,1.4387289638,0.3847298277 Ru,0,-1.4882249532,0.3554189184,-1.5007421722 Ru,0,0.6858638232,-0.4502788357,-1.412277236 N,0,2.1711598154,-1.3287533483,-2.5650096506 N,0,1.7763131692,-2.0905330306,-1.7348446263 Ru,0,-0.8293697772,-1.0191010138,0.6171006181 O,0,-0.095081444,-2.1764068298,2.0182933393 O,0,2.5417576907,-3.0587582166,0.379474081 H,0,3.4306092133,-3.3811418571,0.5509981988 H,0,2.2505148766,-2.8172015099,-0.9999053372 Ti,0,1.4982196956,-1.6878432052,1.3555410094 O,0,2.6889467172,2.2341840057,0.6651945617 H,0,3.1339034438,2.3690113095,-0.179369537 H,0,3.2686097066,1.6843930041,1.2186710167	-1737.256397
I2D	O,0,2.179666796,-0.0418291894,2.0416414467 Ru,0,0.9132922069,0.8274661585,0.6725403825 Ru,0,-1.2821920909,1.5539347693,0.4510876753 Ru,0,-1.5411077048,0.4283049102,-1.4115460219 Ru,0,0.6338267463,-0.3663915694,-1.3081450162 N,0,1.9503944336,-1.1396718907,-2.654987374 N,0,1.5738923103,-2.0175267826,-1.9032804161 Ru,0,-0.896010662,-0.9092786507,0.7292611425 O,0,-0.1966684728,-2.0441926503,2.140610128 O,0,2.5464416362,-2.9371725353,0.8610972925 H,0,3.5060284475,-2.9850233606,0.8603457867 H,0,2.0094038323,-2.9420151106,-1.7877961602 Ti,0,1.4518428927,-1.5898544923,1.5526902652 O,0,2.6163173265,2.3454173407,0.7602557194 H,0,3.0831572913,2.478075756,-0.0726900948 H,0,3.175524011,1.7892252973,1.3296842445	-1737.258394
T2D	O,0,1.9611237185,-0.1459549958,2.267481179 Ru,0,0.8215085366,1.0347175747,0.9944022833 Ru,0,-1.239243085,1.7241565423,0.6821338761 Ru,0,-1.3395357475,0.5384561211,-1.3310135521 Ru,0,0.7968962861,-0.1769361952,-1.1420399342 N,0,2.3336261393,-0.6513380497,-2.4571505592 N,0,1.994624076,-1.6312284844,-1.8410571986 Ru,0,-0.9368014079,-0.8084274613,0.783031354 O,0,-0.3093249841,-2.1565623666,1.996584039 O,0,2.5877456225,-2.9046638973,0.9291357639 H,0,3.5412461546,-2.9481646509,1.0391503082 H,0,2.4242013425,-2.5639706885,-1.90512516 Ti,0,1.3805617772,-1.6317007706,1.5600494699 O,0,2.5137077769,2.0158261992,0.387009288 H,0,1.9266264718,1.0708426406,-0.5996945164 H,0,3.2668463225,1.6844184824,0.8978753592	-1737.215994
I3D	O,0,1.7393460968,-0.2906732698,2.3368935766 Ru,0,1.2493852102,0.7585235165,0.8491589463 Ru,0,-0.985739894,1.4141189971,0.6390899175 Ru,0,-1.1434447766,0.602519419,-1.3877033564 Ru,0,0.9862788017,-0.3329393306,-1.2916060297 N,0,2.1413986524,-0.8601909239,-2.917275303 N,0,1.8016796891,-1.8672739997,-2.3260632137 Ru,0,-0.7390370706,-1.0756030911,0.5494840909 O,0,-0.4542273523,-2.435143584,1.904063704	-1737.249270

	O,0,2.435520452,-3.1968131552,1.0672994851 H,0,3.3936637093,-3.2220733353,1.009237894 H,0,2.0759936305,-2.8112624286,-2.6369749224 Ti,0,1.2431368074,-1.9286906734,1.6890183673 O,0,2.4824575244,2.2035857108,0.6907695806 H,0,1.2676040756,1.2233912888,-1.5800704186 H,0,2.2631864443,2.9776688594,1.2276036817	
T3D	O,0,1.833461881,-0.3231638059,2.4335012735 Ru,0,1.222070105,0.7763018832,1.0413450861 Ru,0,-1.0215041546,1.4860476917,0.7127867599 Ru,0,-1.1326367672,0.5444395059,-1.2332257033 Ru,0,0.9964822898,-0.4472204266,-1.0393616759 N,0,1.8537803966,-0.3980726167,-2.8603810309 N,0,2.2204411108,-1.4928829088,-2.3788063359 Ru,0,-0.7313889025,-1.0181147589,0.7951809319 O,0,-0.3480166426,-2.4148737794,2.0934959685 O,0,2.5294298059,-3.2799353257,1.3094323962 H,0,2.514337698,-4.193023373,1.0172710206 H,0,2.4909135726,-2.216123914,-3.0526295079 Ti,0,1.3337365179,-1.9464507057,1.7168928368 O,0,2.1685592265,2.3080093152,0.4079711884 H,0,1.9435431537,0.6281615333,-1.9384900708 H,0,1.8839927092,3.1460456855,0.797942863	-1737.213148
I4D	O,0,2.0678291863,-0.4143368476,1.5448320033 Ru,0,1.093989695,0.9688639709,0.7308423303 Ru,0,-1.1692964205,1.5473621374,0.9085857683 Ru,0,-1.5598163122,0.9793403001,-1.1811562614 Ru,0,0.5822379375,0.1460401183,-1.4141348936 N,0,2.1619879162,-0.7107132791,-2.419995311 N,0,1.6166311076,-1.6257973772,-1.5386858121 Ru,0,-0.7837620922,-0.8930131461,0.4243156897 O,0,0.0704507466,-2.5377346774,1.0596746751 O,0,2.919818613,-3.2475746827,0.8875704846 H,0,3.014517927,-4.1630863119,1.1554639863 H,0,1.0601301526,-2.2934817781,-2.0681496604 Ti,0,1.6788411618,-1.9495352661,0.5996575635 O,0,2.0233431143,2.6172137722,0.4367002252 H,0,3.0174290236,-0.3292870224,-2.0143918533 H,0,1.9209642434,3.2617610898,1.1512980656	-1737.280734
T4D	O,0,2.1285812265,-0.2552013605,1.211227757 Ru,0,0.9415196539,1.0622075797,0.4066334542 Ru,0,-1.2285552674,1.6086913296,0.6886237906 Ru,0,-1.8166744117,0.6920684397,-1.2667704708 Ru,0,0.3534845433,-0.0151170012,-1.543949039 N,0,2.074581321,-0.7370105127,-2.4509441999 N,0,1.5994055279,-1.6709538347,-1.5557689645 Ru,0,-0.8602088653,-0.8795237773,0.4874133104 O,0,0.1043632126,-2.4540000102,1.0988438022 O,0,3.0009324772,-3.1223009151,0.9713805806 H,0,3.0457553118,-4.0323667025,1.2715921637 H,0,1.1351446213,-2.4169652816,-2.0707556682 Ti,0,1.719910694,-1.8879842275,0.581811202 O,0,2.27901005,2.4468037647,0.5312869792 H,0,2.8656321161,-0.2544198322,-2.0237739212 H,0,1.9395723987,3.3127923318,0.7860681235	-1737.277641
I5D	O,0,2.172161554,-0.4797096848,1.5066560666 Ru,0,1.2016664044,0.9420489719,0.7340164172	-1737.282919

	Ru,0,-1.0622163952,1.6456478174,0.8683472367 Ru,0,-1.4372139741,1.0420158383,-1.2008763644 Ru,0,0.6698472254,0.1183687466,-1.4231120642 N,0,2.1862538179,-0.8228249925,-2.4521194565 N,0,1.6043820026,-1.7016363353,-1.5546070473 Ru,0,-0.719171485,-0.8160888804,0.4495635894 O,0,0.0787550576,-2.4797257549,1.1132085429 O,0,2.8916073612,-3.3472279283,0.8497500809 H,0,2.9659235348,-4.2595173485,1.1336430706 H,0,1.0060237407,-2.3439211641,-2.0694208124 Ti,0,1.7036015337,-1.9956141012,0.5861270745 O,0,1.8204567236,2.7453292976,0.5652174025 H,0,3.0703707719,-0.4962427239,-2.0611676897 H,0,2.2315411665,2.9605487821,-0.2821658867	
T5D	O,0,1.869493085,-0.3340694642,2.3054342765 Ru,0,1.0693196739,0.8786259974,1.118755878 Ru,0,-1.1939554055,1.344953761,0.9932533636 Ru,0,-1.2621062499,0.6742577121,-1.1375412075 Ru,0,0.8694565257,-0.0212640813,-1.0931292356 N,0,2.0588212283,-0.5790103344,-2.6526164948 N,0,1.726572468,-1.7041221257,-1.9577465709 Ru,0,-0.7214924126,-1.1106372567,0.651962436 O,0,-0.1554554164,-2.5895840664,1.7500928176 O,0,2.7796024465,-2.9488284426,0.705035181 H,0,2.902024609,-3.1842972993,-0.2220140329 H,0,0.9252040995,-2.1267579452,-2.4334706618 Ti,0,1.4742378163,-1.9027970386,1.4282787171 O,0,1.8578338492,2.598919522,0.950638305 H,0,3.0143163914,-0.3280395338,-2.3803357837 H,0,2.5014212917,2.6886705958,0.2358270123	-1737.255744
I6D	O,0,1.7222043259,-0.2480221613,2.0463420738 Ru,0,0.9207316865,0.8797688413,0.7852820838 Ru,0,-1.3354933667,1.3639740847,0.7284276396 Ru,0,-1.495428622,0.5734453441,-1.3609968756 Ru,0,0.6265035681,-0.1289978814,-1.3640500724 N,0,1.7671694217,-0.7084725585,-2.9458871909 N,0,1.4649056918,-1.8266025727,-2.2264826329 Ru,0,-0.9234705777,-1.1132191758,0.5114468645 O,0,-0.4062849932,-2.5348442251,1.7017419348 O,0,2.3679586488,-2.8516685052,0.3044142843 H,0,2.3284715673,-2.8104283997,-0.6713439908 H,0,0.6608202105,-2.2733049844,-2.6732898538 Ti,0,1.2404356476,-1.8925357217,1.3493165948 O,0,1.7396784462,2.5654431216,0.4826404253 H,0,2.7301978788,-0.4477702834,-2.7130320835 H,0,2.3687714664,2.5887330774,-0.2501942009	-1737.255452
T6D	O,0,1.9530564189,-0.1641858347,2.0569009687 Ru,0,1.1314954945,0.9348437524,0.8080755521 Ru,0,-1.1353399055,1.4560424835,0.7923469954 Ru,0,-1.3425522184,0.7183323594,-1.2916472208 Ru,0,0.7833776914,-0.0330560011,-1.3466671164 N,0,2.1707198195,-0.6787203318,-2.6889595401 N,0,1.7136474728,-1.7614277462,-1.974838493 Ru,0,-0.7112788806,-1.0088637838,0.5519042425 O,0,-0.2320599074,-2.4743317696,1.6701990422 O,0,2.423701308,-2.6289801137,0.2165554858 H,0,2.2111507967,-2.2858351701,-0.9542220885	-1737.248979

	H,0,1.0771016823,-2.3281935578,-2.529350739 Ti,0,1.4801699251,-1.8819477743,1.4589573528 O,0,1.8834991271,2.6494603487,0.4630823751 H,0,3.0934349876,-0.42672562,-2.328750177 H,0,2.507394188,2.669560759,-0.2749176396	
I7D	O,0,1.8063943985,-0.2362189859,2.0014485894 Ru,0,0.9646368396,0.8248636205,0.7584568435 Ru,0,-1.3035823407,1.3482999953,0.7701214256 Ru,0,-1.5307784371,0.6638182977,-1.3283373519 Ru,0,0.5834994047,-0.1140455448,-1.408506858 N,0,2.0297536296,-0.6994547507,-2.7113372374 N,0,1.5759483359,-1.8198279508,-2.0302131705 Ru,0,-0.8822976202,-1.1065926256,0.4993186543 O,0,-0.4192839701,-2.5735120324,1.5883583742 O,0,2.3181528278,-2.7801984787,0.3615142265 H,0,2.1035158948,-2.2751807446,-1.2450110336 H,0,1.0453545903,-2.4613487066,-2.6078438449 Ti,0,1.335664766,-2.0042399228,1.4766041398 O,0,1.6853130231,2.5501192936,0.3897710147 H,0,2.9553359553,-0.4549480431,-2.3603961409 H,0,2.3024887024,2.5667635789,-0.3540766308	-1737.248246
T7D	O,0,1.8402459036,-0.1528319837,2.2914339855 Ru,0,1.1837457755,0.9808134272,0.9865947186 Ru,0,-1.0494549577,1.5676128505,1.0094947915 Ru,0,-1.2518912727,0.6439287255,-1.1464637069 Ru,0,0.8343894155,-0.1226147379,-1.1253363709 N,0,2.2975639332,-0.3079886307,-2.4877882196 N,0,1.9636260562,-1.6030601418,-2.0890452703 Ru,0,-1.0988428904,-0.8599912349,0.8106561675 O,0,-0.4399096332,-2.4029037198,1.5888823627 O,0,2.4139902611,-2.5810488895,0.4570812109 H,0,2.5061115604,-2.1165676661,-1.3767728936 H,0,1.5548517284,-2.1701692526,-2.8204347262 Ti,0,1.3321422584,-1.7767873073,1.4340271259 O,0,2.0645845286,2.2822549625,0.167539705 H,0,3.2183404531,-0.0550290199,-2.1347971583 H,0,1.6380248801,1.4303536185,-0.9364047217	-1737.199246
I8D	O,0,1.8195351497,-0.5588156911,1.5572052538 Ru,0,1.3396458793,0.9630662859,0.6203570039 Ru,0,-0.9292097377,1.0944548892,1.001000106 Ru,0,-1.263843414,0.1471791502,-1.2518699429 Ru,0,0.9067575638,0.187579998,-1.573442035 N,0,2.0600827249,-0.620680198,-3.0150522192 N,0,2.142397965,-1.4706342496,-1.9073067759 Ru,0,-1.4769794059,-1.0995256093,0.7997872896 O,0,-0.9712163985,-2.6294224738,1.6915211375 O,0,1.5244944788,-3.1431547527,0.2015740038 H,0,2.998193999,-1.538962894,-1.3655306677 H,0,1.682885955,-2.3714641333,-1.9871050872 Ti,0,0.8312421379,-2.1779548652,1.3377276893 O,0,1.9944503936,2.51427416,0.7052438386 H,0,2.9550699566,-0.1746401612,-3.1971708254 H,0,1.0971087524,1.6394165448,-2.2224377692	-1737.234273
T8D	O,0,1.7108619938,-0.2899650112,1.902092032 Ru,0,1.1131152214,0.9792188365,0.6651583351 Ru,0,-1.0804891766,1.4006884159,0.9803128059 Ru,0,-1.5913611502,0.4872422307,-1.1321423953	-1737.192707

	<p>Ru,0,0.5899616599,-0.2063031132,-1.297159464 N,0,2.2888779586,-0.3552306714,-2.6173602403 N,0,1.8550833423,-1.6172709418,-2.2109809784 Ru,0,-1.310624913,-1.0403609602,0.720272131 O,0,-0.584918013,-2.6114312771,1.3950282206 O,0,2.2002718848,-2.7056219705,0.181621791 H,0,2.3053812226,-2.1247019158,-1.4058701582 H,0,1.547211178,-2.1943089541,-2.9839473089 Ti,0,1.1547925338,-1.9609788503,1.2618213136 O,0,2.0343218774,2.3717652406,0.410632451 H,0,3.0767940108,-0.0702880772,-2.0362313714 H,0,1.4013383695,0.698263019,-2.4387471636</p>	
I9D	<p>O,0,1.7534233735,-0.1806363056,1.9030420954 Ru,0,1.0660896715,1.1507501779,0.8015704322 Ru,0,-1.2563008789,1.1820509457,1.1668299327 Ru,0,-1.6638798515,0.404046984,-1.2716069661 Ru,0,0.5389876534,-0.0142936208,-1.1059127836 N,0,2.8123325507,-0.7996303686,-3.1024622516 N,0,1.7293664171,-1.3426106079,-2.298224542 Ru,0,-1.2025181806,-1.0705809582,0.5356987279 O,0,-0.3832167285,-2.6348615601,1.1981568183 O,0,2.4259681356,-2.5397026716,0.0607572873 H,0,2.1313545422,-1.975487192,-1.5732505436 H,0,1.1685059128,-1.9265943613,-2.9137249994 Ti,0,1.3116156191,-1.8504829401,1.0952096249 O,0,1.7402096037,2.6695889444,0.5337575959 H,0,3.6403502063,-0.7955451442,-2.5150441997 H,0,2.5938329536,0.1691826784,-3.3127272286</p>	-1737.224379
T9D	<p>O,0,1.7990209092,-0.1254762002,1.8023841155 Ru,0,1.2301889695,1.1419406167,0.5512612043 Ru,0,-0.9866730922,1.4964600847,0.7817730506 Ru,0,-1.5107696188,0.4163600753,-1.2118720813 Ru,0,0.7775603665,-0.3601102117,-1.2393239249 N,0,2.5805983308,-0.3064460691,-2.2731870722 N,0,1.5466751264,-1.9260932015,-2.2922545989 Ru,0,-1.3653782931,-1.1631333135,0.3009034728 O,0,-0.4114877927,-2.4352260317,1.1684640088 O,0,2.5849656048,-2.713063204,0.335462601 H,0,2.0428888272,-2.6321112159,-1.7385119132 H,0,1.6894790284,-2.0480176448,-3.2851857333 Ti,0,1.381340312,-1.7384588271,0.9158174832 O,0,2.1491855912,2.460078145,0.0421163386 H,0,2.7065601476,-0.0599181218,-3.2470711251 H,0,3.4411966331,-0.6265070605,-1.846525716</p>	-1737.189247
I10D	<p>O,0,1.9330896018,-0.6934979829,1.5553100178 Ru,0,1.5394551647,0.798985443,0.4787790897 Ru,0,-0.5950744866,1.2593363414,1.0172127007 Ru,0,-1.4171918175,0.8591902237,-1.2061183731 Ru,0,0.7624255759,-0.3050288233,-1.578683381 N,0,1.7118977174,0.8229506395,-2.7058953767 N,0,1.4710303774,-2.1790657232,-1.0792782561 Ru,0,-1.4688522421,-0.962050466,-0.0575988968 O,0,-0.8366670947,-2.2661979528,1.0134009801 O,0,1.8004979951,-3.628055788,1.6649790012 H,0,1.0779111303,-2.9333375639,-1.6378684391 H,0,2.4750972638,-2.1798726076,-1.2528189454 Ti,0,1.1167965596,-2.295782752,1.022424325</p>	-1737.303483

	O,0,2.7143555693,1.9216773022,0.0141975281 H,0,1.6253017123,0.8520113028,-3.717774208 H,0,2.3317899733,1.547022407,-2.3471487666	
I10D-H₂	O,0,1.7867111903,-0.93884935,1.63809056 Ru,0,1.5315871889,0.6544887475,0.7143296076 Ru,0,-0.6027676827,1.0808266335,1.3040035254 Ru,0,-1.5096695015,1.1581942359,-0.940975463 Ru,0,0.5628505828,-0.2030148865,-1.5251612864 N,0,1.4710849113,1.1244682831,-2.4856422702 N,0,1.2404838523,-2.1429023279,-1.0383683791 Ru,0,-1.6802694965,-0.8081786019,-0.1019925284 O,0,-1.1859454753,-2.2376580216,0.8903637476 O,0,1.272661214,-3.843078706,1.5472670946 H,0,0.9170964279,-2.8704581905,-1.6678458848 H,0,2.2555419845,-2.1216662607,-1.1229188805 Ti,0,0.7531322877,-2.3981667725,1.006176745 O,0,2.6176621424,1.8305222616,0.189438985 H,0,1.3907211281,1.3105146125,-3.4785611188 H,0,2.0213348718,1.8308607293,-2.0032350165 H,0,0.1747455104,-0.9652040821,-3.1097197444 H,0,-0.5392461361,-0.6150883035,-2.890927693	-1738.476539
T10D	O,0,1.9922435567,-0.7593712304,1.5450724745 Ru,0,1.7368153305,0.8801184077,0.6908920034 Ru,0,-0.4393032377,1.3030032057,1.1509601272 Ru,0,-1.2459046415,1.2720843218,-1.1469697701 Ru,0,0.8124006351,-0.0943700657,-1.6078981409 N,0,1.596535111,1.3038149434,-2.5715315287 N,0,1.3057104308,-2.3040974663,-1.3185653835 Ru,0,-1.4429686001,-0.6500967198,-0.2383928376 O,0,-0.9139261219,-2.101934252,0.7222090627 O,0,1.562878405,-3.640930511,1.4090163232 H,0,0.7429805706,-3.1263411538,-1.5300275003 H,0,2.2699963937,-2.5241113032,-1.55426427 Ti,0,1.0145440805,-2.2059135404,0.8680373419 O,0,2.7862681545,2.0635834972,0.1251630683 H,0,1.4296901099,1.5243000472,-3.5462178057 H,0,2.0875104685,2.0511274585,-2.0851365708 H,0,0.8177763663,-1.636217655,-2.3550875969 H,0,0.2099479881,-0.7665699839,-3.0110159964	-1738.430866
I11D	O,0,1.8938062473,-1.0655400488,1.0964463865 Ru,0,1.3986651499,0.6206917261,0.4582357766 Ru,0,-0.5113803869,1.3190095512,1.5285115804 Ru,0,-1.7292969499,1.3592251141,-0.5105494577 Ru,0,0.2737874571,0.4278503823,-1.488556109 N,0,1.1182643803,1.6208713302,-2.7198865459 N,0,1.322816614,-3.205515882,-1.1252400435 Ru,0,-1.7027624995,-0.6635272496,0.2352663251 O,0,-1.1146753439,-2.2977368153,0.7740121763 O,0,1.2268726713,-3.8038662329,1.8427533776 H,0,0.7807631522,-4.0020784264,-1.4477502342 H,0,2.3051164694,-3.4603264387,-1.1796667332 Ti,0,0.7853617726,-2.5582302731,0.8962317898 O,0,2.4830229803,1.9052858183,0.2232663952 H,0,1.8250120825,1.3040250364,-3.3710522276 H,0,1.2981037185,2.577911431,-2.4371231502 H,0,1.1534644009,-2.4182992517,-1.7593790983 H,0,0.667730084,-0.7211757713,-2.5780032079	-1738.481338

T11D	O,0,1.8685732568,-0.9331861122,0.9687968804 Ru,0,1.3268142034,0.8532649313,0.6317557144 Ru,0,-0.5671479099,1.0815288977,1.8633681299 Ru,0,-1.9174108011,1.5331811837,-0.02877305 Ru,0,-0.0249539468,0.8226659974,-1.3097438449 N,0,1.3079705048,1.241333021,-2.7225229039 N,0,1.2213407352,-3.0201527948,-1.3169142335 Ru,0,-1.8152628299,-0.6048275796,0.2369348211 O,0,-1.0958529587,-2.2200646624,0.6896527474 O,0,1.3558028645,-3.7316337959,1.5837620824 H,0,0.7446217711,-3.8845090858,-1.5565589102 H,0,2.2172198538,-3.1658967658,-1.4543193155 Ti,0,0.812404905,-2.4285734261,0.7640198421 O,0,2.5599860428,2.0039907355,0.5588118661 H,0,2.2928822867,1.2625159731,-2.4824602121 H,0,1.1728353922,1.325476939,-3.7220476953 H,0,0.9069095488,-2.2857710147,-1.9481881985 H,0,0.6870300812,-0.0566354415,-2.5692027197	-1738.442585
I12D	O,0,1.9645642179,-1.2043704357,0.3799935037 Ru,0,1.4099375541,0.5146770236,-0.0101980086 Ru,0,-0.1759926842,1.1795714053,1.4561524131 Ru,0,-1.632402783,1.6592585211,-0.2802312971 Ru,0,-0.0750400067,0.8223867482,-1.7103620067 N,0,1.1952105204,2.2370536123,-2.699633435 N,0,1.2228886288,-4.0667911137,-0.7519231217 Ru,0,-1.3994093453,-0.6509215307,0.2913361127 O,0,-1.1960832295,-2.4282816846,-0.0132401711 O,0,0.7406746571,-3.3147273572,2.1053878587 H,0,1.0758130347,-4.9635625533,-0.2988801447 H,0,2.2053205541,-3.9939919573,-0.9975162975 Ti,0,0.5934449515,-2.4930371871,0.6980762062 O,0,2.6482940935,1.6795308452,-0.3213800036 H,0,1.9822244451,2.2847066585,-2.024692239 H,0,0.7762646692,3.1600373968,-2.7519775449 H,0,0.6704919994,-4.0433993328,-1.6029842097 H,0,1.5624939929,2.0048340114,-3.619728915	-1738.505162
(Ru₅O-TiO₃)_{op}	O,0,1.9845605949,-1.2170974231,0.2254987954 Ru,0,1.4826573617,0.5325809797,-0.0501387147 Ru,0,-0.0773127908,1.1025854715,1.4827373707 Ru,0,-1.6360262488,1.5964941216,-0.1588899819 Ru,0,-0.1387891221,0.6447799288,-1.6465087399 Ru,0,-1.4579087765,-0.6808343196,0.2441278426 O,0,-1.1076169291,-2.4393517337,-0.1919329977 O,0,0.6244670796,-3.1535791561,2.1744653843 Ti,0,0.5313343955,-2.335234386,0.7694136301 O,0,2.6726224355,1.713743517,-0.2532375889	-1625.307222
I13	O,0,-0.5143543569,2.3447889673,-0.1400007602 O,0,1.4992809898,1.3814555613,1.9933059052 Ru,0,1.779988143,0.3663700021,0.3052679119 Ru,0,-1.3577210406,-0.597053252,1.1675432543 O,0,-1.6295932551,0.7530801207,2.4472920451 Ru,0,0.343021883,1.1884114202,-1.3726951122 Ru,0,-0.9334039611,-0.7019416219,-1.1532453341 Ru,0,0.698951778,-1.5562233523,0.4638166089 O,0,0.9358959254,1.5367818149,-2.9072610323 Ti,0,-0.2311304803,1.5637433439,1.5148538952 H,0,3.4953475796,0.9259849002,-0.2742844923	-1626.527505

	H,0,3.539355795,1.0939980957,0.5071381105	
T13	O,0,-0.9444788789,2.0134614969,-0.4599915111 O,0,1.2627435802,1.104154676,1.5292029332 Ru,0,1.2280857317,-0.0948708686,-0.1347159043 Ru,0,-1.8587378433,-0.9130559303,0.8431197417 O,0,-1.9719734229,0.4746260525,2.1196138042 Ru,0,-0.1956453581,0.8082617436,-1.7462694079 Ru,0,-1.5547293442,-1.02694621,-1.5066104043 Ru,0,0.0892837826,-1.9952578415,0.0071367048 O,0,0.3400317071,1.106335148,-3.3131223877 Ti,0,-0.588721411,1.1896727872,1.1291381413 H,0,2.8531523121,0.6781825904,0.0036083831 H,0,2.3289471448,1.0472433559,0.8253439068	-1626.501044
I14	O,0,-0.5112252101,2.3587092579,-0.1078344632 O,0,1.7942564639,1.3459508071,1.9403621139 Ru,0,1.6657274443,0.2180333207,0.1813933611 Ru,0,-1.4027343749,-0.5702076584,1.1696685152 O,0,-1.5288785114,0.8550699082,2.414940322 Ru,0,0.2610283116,1.1407981532,-1.4071699021 Ru,0,-1.1280475403,-0.6840641026,-1.1549916601 Ru,0,0.540595989,-1.7010428132,0.3468392057 O,0,0.7928282452,1.3926099602,-2.984135981 Ti,0,-0.1255795232,1.5283429769,1.4474326692 H,0,3.1773492301,0.6829978798,-0.2201313441 H,0,2.5803324759,1.8742763101,2.1018691634	-1626.533726
T14	O,0,-1.2181364031,2.205433118,-0.5167155036 O,0,1.1179778351,1.3728658761,1.6636981754 Ru,0,1.3103076486,-0.04011953,0.0914529373 Ru,0,-1.8069888159,-1.0264206574,0.8030595497 O,0,-2.0995596344,0.4695379677,1.9067065617 Ru,0,-0.2920487094,0.8657042279,-1.5966011101 Ru,0,-1.3761627896,-1.1048074111,-1.5746635464 Ru,0,0.2484601334,-1.9701970296,0.022839518 O,0,1.1439415581,0.9338656331,-2.6355669296 Ti,0,-0.7415328519,1.2285035426,0.9247135564 H,0,1.7898779788,0.1946416408,-1.514370954 H,0,1.4986010503,1.3098946219,2.5441087451	-1626.502175
I15	O,0,-0.7240709672,2.4477123131,-0.1087928164 O,0,1.5072186542,1.5590992766,2.1224009141 Ru,0,1.6526765908,0.217610688,0.5054957314 Ru,0,-1.5095750732,-0.7188254353,1.0232717564 O,0,-1.7730873141,0.6886818032,2.2568795057 Ru,0,0.236709638,1.2291564185,-1.2784895349 Ru,0,-0.9293579889,-0.6614160352,-1.3305528503 Ru,0,0.5511678871,-1.6916754944,0.3139590841 O,0,1.6498487617,1.3801113898,-2.5219737849 Ti,0,-0.3578212902,1.4291720508,1.3390640146 H,0,2.5206369304,1.0702262542,-2.2371292382 H,0,2.0788171714,2.3325167709,2.1861642185	-1626.539545
I16	O,0,0.0918658379,2.3183161375,0.1829325973 O,0,1.3887021676,2.0687446871,2.9559921268 Ru,0,1.7558090576,-0.3010425662,0.1220883459 Ru,0,-1.470565645,-0.5681551223,1.1406849909 O,0,-1.2843630737,0.7609288121,2.4261321608 Ru,0,0.4674813241,1.1076774282,-1.2710053858 Ru,0,-1.2183158805,-0.3871023165,-1.1817807256	-1627.733921

	Ru,0,0.2018604293,-1.8699694387,0.2170170026 O,0,1.2581606342,1.3237743219,-2.9741822586 Ti,0,0.3144364976,1.3440017465,1.6695440831 H,0,2.161455987,1.0071463233,-3.0890130076 H,0,1.9927461582,2.8115377862,3.0186608578 H,0,3.2992384952,-0.6938011612,0.7673359389 H,0,2.7652580105,-0.3135656381,1.4721252736	
T15	O,0,-0.5515022877,1.9172712291,-0.3869452469 O,0,1.1569035689,1.2182965955,2.2699749705 Ru,0,1.2210466758,-0.6056643327,-0.2413596611 Ru,0,-2.0900943308,-0.9527369504,0.6871097149 O,0,-1.9919236297,0.46373845,1.9331366477 Ru,0,0.0383937921,0.6407042521,-1.7141674112 Ru,0,-1.6707627991,-0.9404850312,-1.6302617262 Ru,0,-0.3165496683,-2.2558848735,-0.1309740045 O,0,0.4389305363,0.7738919376,-3.5627662 Ti,0,-0.4340165214,0.9182584838,1.0955650025 H,0,1.3859792395,0.8542767173,-3.7398593358 H,0,1.621955927,2.0338979414,2.4844465928 H,0,2.4361865541,-0.2458598005,1.0154207166 H,0,1.8650879432,0.3856733815,1.5441919407	-1627.702763
I17	O,0,-0.3082550956,2.5226398628,0.1805366481 O,0,1.7826740427,1.9089910856,2.6867105815 Ru,0,1.7784898379,-0.1285045031,0.1415994153 Ru,0,-1.4331952373,-0.663537517,1.1718389719 O,0,-1.2710083705,0.7269861744,2.4492330113 Ru,0,0.229708006,1.2887471142,-1.244224464 Ru,0,-1.2790285322,-0.3665499483,-1.167156559 Ru,0,0.3314335003,-1.7779877225,0.1682196128 O,0,1.4109150867,1.2627189989,-2.719248887 Ti,0,0.1293313878,1.3178232524,1.4243126242 H,0,2.244325812,0.7809495824,-2.6325149712 H,0,2.1718926417,2.7920894111,2.6988100688 H,0,3.0308444125,0.0745232739,1.2519384656 H,0,2.443375508,1.2722289351,2.3056664816	-1627.705353
T16	O,0,-0.083190664,1.1734958853,-2.4189253417 Ti,0,0.5553576169,-0.4816222012,-2.1944170649 O,0,-0.3921365232,-1.5983444628,-3.8107606643 Ru,0,-0.8017062702,-1.301956388,-0.4294478759 Ru,0,-1.0570634669,1.1574532753,-0.7093571957 O,0,-2.8914029811,1.4116140464,-0.3447827671 Ru,0,0.2470163808,1.3765920336,1.031552458 Ru,0,1.8126011527,-0.4122384352,0.1247554447 O,0,2.287726367,-0.7300189661,-1.6840759448 Ru,0,0.1788029876,-0.871918173,1.7244991332 H,0,-3.394084548,0.5872207546,-0.2849124596 H,0,-1.0758287152,-2.1483917004,-3.3935262096 H,0,-2.2491830654,-1.8133778682,-1.0847371686 H,0,-0.8317542709,-1.0614968003,-4.4851783437	-1627.686117
I18	O,0,-0.5936955802,0.8708656318,-2.5732328313 Ti,0,0.0406506341,-0.7483246787,-2.1098089318 O,0,0.0325127953,-1.8178600772,-4.0287449232 Ru,0,-1.3422511287,-1.3991227593,-0.0795540136 Ru,0,-1.3471501731,1.0405272777,-0.7906099278 O,0,-3.063440424,1.4440441031,-0.1232205565 Ru,0,0.2929944094,1.3572864029,0.6624220696 Ru,0,1.6469909526,-0.5214066338,-0.3192691446	-1627.691890

	O,0,1.8501974915,-1.183889782,-2.066056339 Ru,0,0.1265128193,-0.8039587027,1.5512111105 H,0,-3.5597722976,0.6609009955,0.1580330939 H,0,0.9609617821,-2.0570654226,-4.1678964399 H,0,-2.9261175367,-1.1950571933,0.1201575059 H,0,-0.2894409841,-1.3746894714,-4.8234870122	
T17	O,0,-0.5831724527,0.8386350455,-2.5158662196 Ti,0,0.0594873425,-0.779268335,-2.0733361056 O,0,0.0077026305,-1.7884061746,-4.0244358992 Ru,0,-1.2826370221,-1.4549782203,-0.0457765437 Ru,0,-1.3387854455,0.9910607874,-0.7246202847 O,0,-3.135362452,1.4758030516,-0.2462078986 Ru,0,0.3354267644,1.3100769962,0.6565090558 Ru,0,1.7180119988,-0.5469236549,-0.3171451482 O,0,1.8747263779,-1.2087359579,-2.0662983548 Ru,0,0.2336499661,-0.8534310123,1.5580198311 H,0,-3.3583187027,1.7264570137,0.6563627177 H,0,0.9302359856,-2.0187009972,-4.2081332547 H,0,-2.8133795952,-1.0950551772,0.1776186703 H,0,-0.3424323957,-1.309523365,-4.7860065657	-1627.677795
I19	O,0,-0.6237185359,0.8675777748,-2.4325842977 Ti,0,0.0511572262,-0.7642123526,-2.0563497602 O,0,-0.0124383173,-1.7362919904,-4.0250066904 Ru,0,-1.2555852451,-1.5087699629,-0.0160139289 Ru,0,-1.3588761169,0.9467008068,-0.6435151335 O,0,-3.1570162875,1.265539536,-0.077919739 Ru,0,0.3583026796,1.2555634864,0.7223647357 Ru,0,1.727721447,-0.5667920813,-0.3281425157 O,0,1.861911213,-1.1935701858,-2.0963393518 Ru,0,0.2720361695,-0.9261499497,1.5708454867 H,0,-3.2919591198,2.2066263103,0.1114911803 H,0,0.9142850362,-1.9480139921,-4.211425459 H,0,-2.7917879718,-1.2119178689,0.2514753671 H,0,-0.374632007,-1.2597745107,-4.7821037537	-1627.682617
T18	O,0,-0.3831948629,0.9088338676,-2.7879907019 Ti,0,0.0038676902,-0.7205715328,-2.0955409949 O,0,0.0727467994,-1.8787566748,-3.9780416913 Ru,0,-1.7487145823,-1.0810151858,-0.3334893593 Ru,0,-1.3617911616,1.2360487455,-1.1438136142 O,0,-3.1731501241,1.4680570607,-0.1580847033 Ru,0,0.1925349631,1.4580387958,0.4403752997 Ru,0,1.5770457855,-0.4904972369,-0.258239745 O,0,1.7674036844,-1.3230366821,-1.9369981731 Ru,0,-0.2054310451,-0.6693372004,1.3216053576 H,0,-3.1303682917,1.9030684595,0.705126723 H,0,1.0129174482,-2.1173302129,-3.9801964956 H,0,-2.925813439,0.1793728137,-0.0413865646 H,0,-0.106497864,-1.3733100171,-4.7807843371	-1627.657661
I20	O,0,-0.581545896,0.6501102944,-2.9477589745 Ti,0,0.0786937217,-0.8233459897,-2.1524932912 O,0,0.3347781572,-2.0151699918,-4.0022505612 Ru,0,-1.8020530274,-1.1435645552,-0.5190168928 Ru,0,-1.5881929515,1.0545757632,-1.3374554211 O,0,-3.0290687572,1.840721413,0.3299931816 Ru,0,0.0300202894,1.4570182056,0.3038374148 Ru,0,1.5668126073,-0.2945840429,-0.309337773 O,0,1.9051801702,-1.1503750993,-1.9623799805	-1627.671484

	Ru,0,-0.3209368029,-0.7183018004,1.1308153623 H,0,-2.6238159663,1.31778224,1.0454493744 H,0,1.29776861,-2.1305904352,-3.9770295095 H,0,-3.871239694,1.4065447441,0.140085451 H,0,0.1177505394,-1.5215777459,-4.8035493801	
T19	O,0,0.027395716,0.1193997296,0.0441899336 Ru,0,0.1351579054,0.0384289998,1.9717154099 Ru,0,2.3108735069,0.0701205978,2.7019884529 Ru,0,2.2788275138,-2.0892507605,3.3119707159 Ru,0,2.6955578374,-1.7970194495,0.9119483505 O,0,2.2961163864,-2.0996834743,-0.928680961 Ti,0,0.6833490277,-1.5563306969,-0.1178409853 Ru,0,0.198587625,-2.333308882,2.3035352053 O,0,-0.1092189561,-2.2819922135,-2.0602697823 O,0,-0.3935190505,0.309127488,4.2331202569 H,0,0.3873489136,-0.1422537878,4.6031925778 H,0,0.7618169348,-2.462805498,-2.4536467137 H,0,-1.1409286835,-0.2791601177,4.4001100655 H,0,-0.601576677,-1.701041935,-2.6522665261	-1627.645820
I21	O,0,-1.212506949,1.7708263715,-1.6823199187 Ru,0,-1.0826704003,1.3588150052,0.1831989617 Ru,0,1.0829398257,1.1182805402,0.8894762069 Ru,0,0.8528764844,-1.0121635125,1.519539331 Ru,0,1.0883293305,-0.6993154859,-0.9654159652 O,0,0.8649785882,-0.4196699457,-2.9416738063 Ti,0,-0.686413082,0.0942639307,-2.1528462261 Ru,0,-1.1319781412,-1.0712196606,0.3429929006 O,0,-1.5994869645,-0.9683900863,-3.8662609864 O,0,-1.6242571598,1.4262483184,2.4448734143 H,0,-0.9371973459,0.7946434038,2.736606373 H,0,-0.7314812666,-1.2099470943,-4.2395669712 H,0,-2.4693973091,0.9785677705,2.5785054781 H,0,-2.1608596102,-0.6242895552,-4.5706337918	-1627.652956
T20	O,0,0.0750752708,0.3797604244,0.152554246 Ru,0,0.4960452644,0.0265794392,2.0913752975 Ru,0,2.5506240937,-0.2413058675,3.0190543081 Ru,0,2.2833901123,-2.4325155096,3.3830065939 Ru,0,2.4469662159,-1.8050006418,0.9557908302 O,0,2.2376362723,-1.5899497321,-1.0030458286 Ti,0,0.5824091437,-1.2425749041,-0.3417486923 Ru,0,0.2821479618,-2.3509749385,2.219940068 O,0,-0.1345846566,-2.4091667108,-2.0709342459 O,0,-0.3393103616,0.4083807239,4.1907066515 H,0,0.2387516717,-0.2174995108,4.6605357778 H,0,0.7497767911,-2.6154377514,-2.4209828014 H,0,-1.2307998126,0.0380117141,4.2351309183 H,0,-0.7083419669,-2.1540767351,-2.8023171231	-1627.646475
I22	O,0,-1.692095193,2.0943001458,-1.377822189 Ru,0,-0.7790039603,0.943266266,0.0564425314 Ru,0,1.3212184002,0.5390173764,1.0704738944 Ru,0,1.0504601057,-1.6572834562,0.8511200302 Ru,0,1.0156833263,-0.210948921,-1.2893443045 O,0,0.6889563361,0.8056151137,-3.0118327828 Ti,0,-0.9630075117,0.7820061043,-2.3795546106 Ru,0,-0.9484758758,-1.379089668,-0.1709987491 O,0,-1.9747177147,-0.8388893379,-3.4229467764 O,0,-2.3158825296,2.1345216118,1.2768074079	-1627.676746

	H,0,-3.0190186307,1.6147726088,1.6817564091 H,0,-1.594073085,-1.501031027,-2.7895638492 H,0,-2.6714793029,2.5290930259,0.4595071003 H,0,-1.6558963647,-1.0756908428,-4.3056501119	
T21	O,0,1.8960691486,-1.298984033,-0.1354361374 Ru,0,1.4873096162,0.489845286,-0.1088070995 Ru,0,-0.0689893398,0.6953495397,1.5146677735 Ru,0,-1.6316898765,1.525513072,-0.0026413546 Ru,0,-0.1272927404,1.0209582975,-1.6454213411 Ru,0,-1.3785135355,-0.7989870624,-0.0500982892 O,0,-1.1616259477,-2.6481675209,-0.0734991103 O,0,0.6425299607,-2.5614993153,2.381682071 Ti,0,0.517283346,-2.3180074074,0.7670266108 O,0,2.7029063684,1.6580671437,-0.0519391233	-1625.305769
I23	O,0,1.9029905023,-1.6038135056,-0.01149024 Ru,0,1.7515573124,0.2983752281,-0.3591010642 Ru,0,0.204908174,0.3432169109,1.3752112065 Ru,0,-1.5961784975,1.3191383294,0.217143457 Ru,0,-0.0241803461,0.5551569113,-1.7723536106 Ru,0,-1.2118773307,-0.9059636672,-0.3182684755 O,0,-1.0124209489,-2.7287855327,0.3346680024 O,0,0.3085164996,-1.1529555967,2.5878307596 Ti,0,0.5365273149,-2.1743111382,1.0874789647 O,0,2.98512932,1.4340360607,-0.3213030001	-1625.331227
T22	O,0,1.7628936434,-1.4125807534,-0.3128925125 Ru,0,1.6059878685,0.5187148382,-0.5794211459 Ru,0,0.0897795201,0.8029136172,1.251653652 Ru,0,-1.524890682,1.7040206315,0.0356533897 Ru,0,-0.2233460569,0.7611384174,-1.8926124526 Ru,0,-1.4424141303,-0.6582057511,-0.4102654784 O,0,-1.0966701611,-2.4060943426,0.3131627331 O,0,0.4944258259,-0.8154486288,2.3075966884 Ti,0,0.5397323398,-1.9296098788,0.9196105709 O,0,2.2662798327,1.6628188504,0.5626575553	-1625.296308
I24	O,0,2.0060772284,-1.7461259693,-0.1950513411 Ru,0,1.7028796183,0.0985852517,-0.4264419247 Ru,0,0.5157852225,0.7281295388,1.5132372361 Ru,0,-1.3101603412,1.1631720993,0.2710294078 Ru,0,-0.1103250436,0.5253167374,-1.6893822523 Ru,0,-1.4803457666,-1.1489227795,-0.5309222147 O,0,-1.0159106457,-2.7856404502,0.2859888734 O,0,0.3637528444,-0.8702015678,2.4946490501 Ti,0,0.4178983299,-1.7823401624,0.8350950558 O,0,2.0096435537,1.5844123019,0.7125461095	-1625.365943
T23	O,0,1.8771204871,-1.8362843254,-0.3439324202 Ru,0,1.7804388987,0.0323145359,-0.6108092852 Ru,0,0.6610575292,0.8762604379,1.3662354224 Ru,0,-1.255200975,1.151346683,0.2254589797 Ru,0,-0.158237389,0.193568839,-1.7824129715 Ru,0,-1.5081592603,-1.1515730607,-0.5064645857 O,0,-1.169213261,-2.7583326258,0.4249893026 O,0,0.4752540638,-0.8480480175,2.2755181411 Ti,0,0.4244231059,-1.8907674364,0.8089770539 O,0,1.9718118005,1.99789997,1.413188363	-1625.318265
T4E	O,0,1.9865229051,-0.4015355593,1.8134712266 Ru,0,1.2014159234,0.6542803126,0.4606374092 Ru,0,-0.46235591,2.1035765521,0.2294876419	-1661.929644

	<p>Ru,0,-1.3069744595,0.9152661327,-1.5629277585 Ru,0,0.2450055551,-0.7150919081,-1.4671874135 N,0,1.7971177906,-1.0098150938,-2.405922491 N,0,2.812093985,-1.7191732769,-2.112188305 Ru,0,-1.0691132257,-0.3538329294,0.6851705608 O,0,-0.8737436282,-1.7866460531,1.9670021418 O,0,1.3597816582,-2.9905338348,0.2690179468 H,0,2.8145069003,-2.2907773401,-1.2595330457 H,0,3.5807575322,-1.7834667653,-2.7705193762 Ti,0,0.889045023,-1.8930177172,1.5137890249 H,0,0.4173129867,-2.6456263829,-0.8732084451 H,0,-0.1022890362,-2.4805801365,-1.5667611169</p>	
I4E	<p>O,0,1.7494828778,-0.6103789605,1.7674875052 Ru,0,1.1923316027,0.738350526,0.5350181961 Ru,0,-0.4019971756,2.2635614177,0.1881576731 Ru,0,-1.2384300126,1.1291988351,-1.6324999455 Ru,0,0.3462670018,-0.5329753361,-1.4237285923 N,0,1.7606577357,-0.8301479336,-2.483319313 N,0,2.9369581969,-1.3189504369,-2.6243403277 Ru,0,-1.1549655889,-0.1278526512,0.5998977334 O,0,-1.0191466544,-1.6719481636,1.8170289478 O,0,1.2556423676,-3.6492672412,1.2987641428 H,0,3.3763607559,-1.875896323,-1.8987745318 H,0,3.4389590145,-1.1674152969,-3.4900975304 Ti,0,0.6175943776,-1.9319904853,1.1834733282 H,0,0.8974022269,-4.5344929999,1.3882296989 H,0,0.2294392741,-2.1110479507,-0.886217985</p>	-1661.989853
T5E	<p>O,0,1.6790294906,-0.3240486799,2.1040914809 Ru,0,1.1285138436,0.8369234015,0.6332998987 Ru,0,-0.5537767995,2.20002508,0.0207888674 Ru,0,-1.2282739769,0.8129182376,-1.6576108381 Ru,0,0.5152514092,-0.6864356641,-1.2127317216 N,0,1.9523065415,-1.1269861238,-2.1378511062 N,0,3.0913774266,-1.5087546752,-2.590719595 Ru,0,-1.1789824515,-0.1635978663,0.6731011608 O,0,-1.0858043543,-1.5595915045,2.1178172054 O,0,0.9855026024,-3.3038267221,0.4423251706 H,0,3.6732969308,-2.147270986,-2.0613661249 H,0,3.4383832132,-1.1468944986,-3.470251855 Ti,0,0.5670146609,-1.6388028687,1.519993513 H,0,0.337503945,-4.0192217342,0.3901496259 H,0,0.6652125184,-2.4556893956,-0.431955682</p>	-1661.941997
I5E	<p>O,0,1.4252603051,-1.1224528689,2.4527511534 Ru,0,1.2845431944,0.2590810302,1.0458291583 Ru,0,-0.0851497742,1.9723570357,0.4868366623 Ru,0,-0.7863622061,0.9231352488,-1.3764787173 Ru,0,0.6041716502,-0.9189859959,-0.9734716044 N,0,1.9154593378,-1.585175013,-1.9442619197 N,0,2.8023116589,-1.7251347564,-2.8987454135 Ru,0,-1.1802833116,-0.2920469051,0.8162093286 O,0,-1.4533948299,-1.8723375664,2.0418947114 O,0,0.9950643078,-3.9114561665,0.5848424197 H,0,3.5168537166,-2.4334215274,-2.7814487052 H,0,3.0868350237,-0.8897148866,-3.3981441757 Ti,0,0.2206702064,-2.1219336412,1.5682834063 H,0,1.8020795398,-4.3660363345,0.8599514227 H,0,1.137143181,-3.5651416529,-0.322416727</p>	-1661.945628

T6E	O,0,1.0115133683,-0.7476831396,2.7338541003 Ru,0,1.0144698359,0.6351861847,1.2944021706 Ru,0,-0.4654636985,2.2212570308,0.4915303783 Ru,0,-0.5745279985,1.2463547996,-1.467680332 Ru,0,0.9247095917,-0.5044988618,-0.7576272826 N,0,2.0927420777,-1.3596151423,-1.7490042872 N,0,2.6673251516,-1.9724817142,-2.7862909755 Ru,0,-1.2750391528,-0.1753947598,0.5176945116 O,0,-1.6034840744,-1.8148130591,1.6449804169 O,0,1.1890519827,-3.6240213268,0.8833772601 H,0,3.55276392,-1.5620950143,-3.0678155609 H,0,2.0523564239,-2.1559419081,-3.5743632793 Ti,0,0.1616082809,-1.8325481374,1.594897681 H,0,2.1225276562,-3.4004564952,0.7380690358 H,0,0.8500536352,-3.8017014565,-0.008999837	-1661.941801
I6E	O,0,1.3156392665,-0.7649712876,2.430413126 Ru,0,1.0123329082,0.7138791853,1.226748903 Ru,0,-0.7493733085,2.1015415335,0.680977387 Ru,0,-0.9258113168,1.2440884531,-1.3593228429 Ru,0,0.8280355386,-0.3413586159,-0.9242758081 N,0,2.0192900192,-1.3670383563,-1.7332028776 N,0,2.3761493021,-2.7037561581,-1.9936737454 Ru,0,-1.1719303498,-0.3875426462,0.5655599498 O,0,-1.0885320042,-2.1967746573,1.4735118182 O,0,1.6832696155,-3.5426437016,0.3615426075 H,0,3.3559244651,-2.7427816743,-2.2745244874 H,0,1.8201748457,-3.0739137666,-2.7656161293 Ti,0,0.6303537238,-1.9534317434,1.2292854245 H,0,2.0237688882,-3.3457879522,-0.6199153611 H,0,1.4619394066,-4.4759506124,0.4441810358	-1661.950217
T7E	O,0,1.3350647993,-0.7750280787,2.4058983761 Ru,0,1.0142180168,0.7124648444,1.22686802 Ru,0,-0.7498110215,2.0971410575,0.7008607524 Ru,0,-0.934416015,1.2465340772,-1.3504037398 Ru,0,0.8163583672,-0.3270348624,-0.9349189379 N,0,2.0086555499,-1.3537847153,-1.757407457 N,0,2.3603047683,-2.7154510528,-1.9420905336 Ru,0,-1.1689180146,-0.3923339505,0.5691509712 O,0,-1.0782030802,-2.2008509208,1.4669446536 O,0,1.6729998647,-3.5209880218,0.3367566296 H,0,3.3501739264,-2.7763606652,-2.1830006615 H,0,1.8315664104,-3.1127910886,-2.7202881333 Ti,0,0.641948483,-1.9695461897,1.2095280011 H,0,2.0321992521,-3.2937066042,-0.71586072 H,0,1.4590896934,-4.4547058291,0.4296517792	-1661.952104
I7E	O,0,1.19076612,-0.9559236994,2.2822235697 Ru,0,0.8529849858,0.5750744587,1.1930290764 Ru,0,-0.9382784772,1.8914204088,0.6313797875 Ru,0,-0.9032170507,1.171864805,-1.5000012609 Ru,0,0.8741305744,-0.2941772517,-1.0493214379 N,0,2.1723606892,-1.1918283089,-1.9257661468 N,0,2.5191835218,-2.5873728089,-2.0996583412 Ru,0,-1.2061110579,-0.595849853,0.2886657955 O,0,-1.0934899939,-2.4197783977,1.1108944315 O,0,1.7262681515,-3.5881033225,0.2748906546 H,0,3.5194273291,-2.6664741873,-2.2969713554 H,0,2.0109365475,-2.9917695184,-2.8903919638	-1661.954529

	Ti,0,0.6441664419,-2.1517764481,0.9964965723 H,0,2.2830787137,-3.1316073324,-1.2140378999 H,0,1.5151705047,-4.5221855442,0.3641865183	
I8E	O,0,1.415241636,-0.7799811637,2.448481322 Ru,0,1.0558120251,0.5055680642,1.1022228694 Ru,0,-0.8256299087,1.7937868916,0.7211263069 Ru,0,-0.9014177429,1.3080848899,-1.4357791938 Ru,0,0.9420284561,-0.1439030681,-1.219496758 N,0,2.2727590589,-0.1793289662,-2.1287926648 Ru,0,-1.126419511,-0.623808594,0.4397889376 O,0,-1.1998668388,-2.1755570231,1.6315380797 O,0,1.5027630064,-3.6504392094,1.1044534393 Ti,0,0.5746160133,-2.1523134339,1.5725867491 H,0,1.3449248056,-4.5023073875,0.6919669125	-1605.437122
⁵(Ru₆-TiO₂)	Ru,0,-1.1080956169,0.58307076,-0.6647317959 Ru,0,-1.2512023812,0.6696550193,1.6318176546 Ru,0,1.2194365939,0.7117564362,1.785806183 Ru,0,0.0433809842,-1.372876027,1.7965390465 Ru,0,0.1526516265,-1.4663661271,-0.4860528528 Ru,0,1.3492101836,0.67041017,-0.5049075397 Ti,0,0.56831921,-0.2181416664,-2.7934012316 O,0,0.5916296802,-1.9249999743,-2.4468603374 O,0,2.0625797197,0.6133724092,-2.4015321267	-1569.700039
⁵(Ru₆-TiO₂-N₂)	Ru,0,-1.35424021,0.6581595782,-0.1057120507 Ru,0,-0.9770909472,0.2614120119,2.121372989 Ru,0,1.3938372182,0.5366234308,1.7717101551 Ru,0,0.5362187286,-1.7176383968,1.5662052626 Ru,0,0.1652670755,-1.3885959853,-0.6650197218 Ru,0,1.0396266883,0.8825448163,-0.444531895 Ti,0,-0.3467847143,0.2071362057,-2.6707594387 O,0,-0.0493303155,-1.5165805035,-2.7123902298 O,0,1.0745291249,1.221438744,-2.4729921746 N,0,-2.1138989803,1.2344332397,-2.1114809208 N,0,-2.3997046682,1.9772058591,-1.2478829753	-1679.292114
⁵I₁	Ru,0,-1.3469498009,0.6540633745,-0.1129496179 Ru,0,-0.9848464071,0.2495439281,2.1168701413 Ru,0,1.379431718,0.5421911231,1.790478411 Ru,0,0.5386574415,-1.7212640967,1.5749631931 Ru,0,0.1892242296,-1.3879990455,-0.6562387742 Ru,0,1.0327095616,0.8793157485,-0.435470851 Ti,0,-0.3656772184,0.2024720212,-2.731501189 O,0,-0.031514654,-1.533297656,-2.6951062224 O,0,1.0405934984,1.219788932,-2.4927567133 N,0,-2.1034993203,1.2564161044,-2.1017435568 N,0,-2.3797000421,1.9949088559,-1.2280243752 O,0,-0.4863790464,0.133619719,-4.9198877204 H,0,-0.1959351141,-0.7628829006,-5.1445113812 H,0,0.0810381541,0.753859892,-5.3960073442	-1755.769345
⁵T₁	Ru,0,0.0769681758,0.1313795132,0.0301480023 Ru,0,0.0108853219,-0.0659600816,2.3551378731 Ru,0,2.3672997627,-0.0185618644,2.4169325867	-1755.747057

	<p>Ru,0,1.3255463189,-2.1845586033,2.2391045361 Ru,0,1.3661716173,-2.1257835305,-0.0401026775 Ru,0,2.4280152484,0.1441610191,0.1139189489 Ti,0,1.9922279379,-1.0000436725,-2.2474879 O,0,2.0729678449,-2.7250509744,-1.755678725 O,0,3.2926402676,0.0520022849,-1.7286580588 N,0,-0.8637529825,0.1290449071,-1.7993718867 N,0,-0.930206547,1.2159390223,-1.2918190842 O,0,0.6450918936,-0.4891754637,-3.6186596032 H,0,-0.4382632429,-0.1450739853,-2.8569932037 H,0,0.7398363835,0.0873494288,-4.3828828081</p>	
⁵ I ₂	<p>Ru,0,-1.3792641579,0.916411473,-0.5179994844 Ru,0,-1.1788431184,0.6372573486,1.7816436964 Ru,0,1.168441409,0.6188340984,1.5553172215 Ru,0,0.0675007832,-1.4935055708,1.3836623504 Ru,0,-0.1159787299,-1.3616753531,-0.853801415 Ru,0,0.9393701215,0.8991564871,-0.7148268142 Ti,0,1.2898764112,-0.5240972267,-3.135368309 O,0,0.8502521041,-2.0799997357,-2.3659367744 O,0,2.0883819624,0.8275852946,-2.3436063205 N,0,-2.9033547429,0.9768568334,-1.9094566211 N,0,-2.6844444551,2.0727101283,-1.4055641541 O,0,0.5958512871,-0.233677186,-4.8044208706 H,0,-3.4939154204,0.884725491,-2.7457714705 H,0,0.6200355463,0.5542079178,-5.3551420343</p>	-1755.758158
⁵ T ₂	<p>O,0,0.0414050016,-0.0237073257,-0.0659524344 Ti,0,-0.0407793632,-0.129331924,1.7085692697 O,0,1.5543892805,-0.2329518006,2.5940092642 Ru,0,-0.8509870963,1.6987881411,-0.2411858039 Ru,0,-2.1742758452,1.7087346407,1.9351557666 O,0,-1.5301053151,-0.0029190347,2.6609247418 Ru,0,-0.983435641,3.6189934061,1.3555959737 N,0,-0.1664284771,5.0385526661,2.3401266668 N,0,0.9089675405,5.2071682476,1.7837845308 Ru,0,-2.8505425388,4.4413089955,0.1970924343 Ru,0,-2.7291314044,2.5034696848,-1.2721338772 Ru,0,-3.9969771522,2.4497822664,0.7444780179 H,0,1.5454265331,5.8399173039,2.3019559008 H,0,1.7727537339,-0.2250546575,3.5300529406</p>	-1755.753776
⁵ I ₃	<p>O,0,1.7905741148,-2.615211375,-0.4163125902 Ti,0,2.0626881372,-1.9031448014,1.1768874426 O,0,3.7356329735,-2.035762508,1.8926452446 Ru,0,0.5473532728,-1.2049123196,-1.0474963486 Ru,0,-0.4231263042,-0.609797618,1.2048928334 O,0,0.5862314184,-1.9571191278,2.1978081877 Ru,0,1.1147205891,0.8886967578,0.1217434918 N,0,2.0541316966,1.8554201866,1.3198318662 N,0,2.9017223629,2.2390108596,2.0958812664 Ru,0,-0.738326963,1.9071908215,-0.9195442255 Ru,0,-1.1922420145,-0.1597704137,-2.0861325482</p>	-1755.763846

	Ru,0,-2.1855969571,0.4252965448,0.1844605675 H,0,2.7053730912,3.1948070511,2.4437623209 H,0,4.1518015822,-1.955907058,2.7537524916	
⁵ T ₃	O,0,0.3679558561,0.1094406729,0.3387079613 Ti,0,-0.1833384999,-0.1074229145,2.0531246894 O,0,1.0141467123,-0.6962106465,3.1437248034 Ru,0,0.8357766545,1.9943764893,0.4692749148 Ru,0,-0.4028342275,2.6957153148,2.4148183882 O,0,-1.3431790554,1.0634814879,2.8347258961 Ru,0,2.074657407,2.7276264765,2.4291681702 N,0,2.5119462134,1.9310762085,4.0056557884 N,0,2.4330979101,0.7897832761,4.5053623738 Ru,0,2.0095045561,5.0276681126,1.9589548601 Ru,0,0.8455138551,4.1689481394,-0.2670223006 Ru,0,-0.3693874068,4.8493037033,1.6789235896 H,0,2.8091020461,0.7114281338,5.4548976738 H,0,1.7517306443,-0.0930203144,3.8849629533	-1755.760706
⁵ I ₄	O,0,-0.3452417719,-2.8854252714,-1.3331421481 Ti,0,-1.0288710169,-3.1703432361,0.3642668204 O,0,0.038141573,-3.9138655073,1.3981722314 Ru,0,0.1059491331,-1.0395296846,-1.1343534421 Ru,0,-1.1493679167,-0.3554970924,0.803373254 O,0,-2.1038042323,-1.9280370464,1.2522224223 Ru,0,1.333444895,-0.2785844355,0.8024071806 N,0,1.7624020236,-1.0937146427,2.3627013968 N,0,1.6573636076,-2.2407190101,2.8938498465 Ru,0,1.2084658256,2.002817072,0.2781413469 Ru,0,0.0162637869,1.1153895534,-1.9217914463 Ru,0,-1.1793330729,1.7830795037,0.0272672093 H,0,1.9535995897,-2.3472924643,3.8596396241 H,0,1.1510155763,-3.0181127381,2.4136447044	-1755.761449
⁵ I ₄ WT	O,0,-0.3605199948,-2.9463256552,-1.2094581522 Ru,0,0.1593824754,-1.1225276591,-1.083417684 Ru,0,0.0684584361,0.9677669314,-2.0094881799 Ru,0,-1.1313961967,1.7841571315,-0.1247879588 Ru,0,1.261745272,1.9761227402,0.137162852 Ru,0,1.3312029308,-0.2632663017,0.8301523045 N,0,1.8022010212,-1.0454384786,2.4005716878 N,0,1.6981409823,-2.1869258095,2.95537919 Ti,0,-1.0646695464,-3.1505678921,0.4905524092 O,0,-2.1727961456,-1.8950642205,1.2582065765 Ru,0,-1.1520494268,-0.2722029163,0.8223138773 O,0,-2.1711295799,0.1702946632,2.8775399554 O,0,-0.026321569,-3.8493288504,1.5928710669 H,0,2.0401816055,-2.2866112755,3.9062695836 H,0,1.1615220842,-2.9643992807,2.5073907136 H,0,-1.4850367741,0.1977176749,3.5551264167 H,0,-2.5028725744,-0.7497868017,2.8446293415	-1832.219023
⁵ T ₄	O,0,-0.3506659061,-2.8584882546,-1.175378921 Ru,0,0.2337196254,-1.0815042816,-0.980293477	-1832.189475

	<p>Ru,0,0.0897174859,0.9757228219,-1.9843930174 Ru,0,-1.025409885,1.8379052974,-0.0412598588 Ru,0,1.3490672878,2.0876223404,0.0747142713 Ru,0,1.5269293254,-0.1393404879,0.8156881066 N,0,1.7818894905,-0.7587625555,2.4565221845 N,0,0.9387562704,-1.605252848,3.2236957233 Ti,0,-1.215605263,-3.0784653113,0.4705094849 O,0,-2.2687379893,-1.7409191383,1.0187754216 Ru,0,-1.0089747664,-0.1646357152,0.9450937758 O,0,-1.2248571046,-0.2913288015,2.9583385394 O,0,-0.2122994291,-3.5691073663,1.7245775658 H,0,1.3581530352,-1.7840155765,4.1348288002 H,0,0.6789023751,-2.5025111647,2.7236314902 H,0,-0.0467938996,-1.0414825856,3.2999989692 H,0,-2.0027276525,-0.8587433729,3.0707629412</p>	
⁵ I ₅	<p>O,0,-0.411290096,-2.9250432326,-1.2637005614 Ru,0,0.1819560546,-1.1514501376,-1.0649634758 Ru,0,0.0393551842,0.907945009,-2.062811549 Ru,0,-1.0719211107,1.7744675245,-0.1162528525 Ru,0,1.3004234894,2.0187327657,-0.0063229651 Ru,0,1.4770099968,-0.210279612,0.7307377205 N,0,1.7422313574,-0.8416609206,2.3660741596 N,0,0.8968556701,-1.6992339119,3.1293640253 Ti,0,-1.2677334157,-3.1415344204,0.3861359338 O,0,-2.3203911642,-1.807125871,0.9341789948 Ru,0,-1.0596697869,-0.228994887,0.8677078144 O,0,-1.2867939212,-0.3365440435,2.8657035934 O,0,-0.2549586389,-3.6282766072,1.6379834256 H,0,1.3284755092,-1.901884442,4.0299739865 H,0,0.6176528658,-2.5883127195,2.6120067687 H,0,-0.0516080878,-1.1442234493,3.2383335627 H,0,-2.0767669061,-0.8854100447,2.9843204184</p>	-1832.188223
⁵ T ₅	<p>O,0,-0.3510544049,-3.0171842896,-1.3324552476 Ru,0,0.286320177,-1.2364343694,-1.0805956788 Ru,0,0.3325782624,0.9265087013,-1.9244364386 Ru,0,-1.3018837212,1.6581183906,-0.1570018568 Ru,0,1.0084738882,2.2837784718,-0.036507634 Ru,0,1.4361008785,0.007966021,0.7343876751 N,0,1.9922727717,-0.8053328072,2.0764853478 N,0,0.9132972438,-1.8833206328,3.3213418843 Ti,0,-1.3196868487,-3.233476319,0.2240720471 O,0,-2.3216699126,-1.7823914116,0.7699451354 Ru,0,-1.0997924551,-0.3053757649,0.8731373251 O,0,-1.3063207876,-0.1087605933,2.8162301356 O,0,-0.4918032966,-3.926676924,1.4731721094 H,0,1.4801322306,-2.0715856954,4.1358898106 H,0,0.6357241796,-2.7260620746,2.8132578115 H,0,0.1113247271,-1.2729250608,3.4947977075 H,0,-2.2211859323,-0.295673642,3.0667488664</p>	-1832.166173

5I_6	O,0,0.1756901581,-3.1573425707,-0.7040561081 Ru,0,0.5752091294,-1.3416365538,-0.6274797561 Ru,0,0.1543550019,0.4381656135,-1.918322148 Ru,0,-1.4789212897,1.2783908559,-0.3515810918 Ru,0,0.6401932699,2.2861608041,-0.1628746534 Ru,0,1.7158829109,0.4041846339,0.8799614148 N,0,2.5141378188,0.4488348844,2.2664693245 Ti,0,-1.4147056239,-3.316554461,0.2950566832 O,0,-2.0640426686,-1.8795797407,1.2561040299 Ru,0,-0.8673502305,-0.3871385056,1.1307415484 O,0,-0.8811830465,-0.1327175031,3.0322535446 O,0,-2.5348008424,-4.3624145507,-0.2507818681 H,0,-1.5555535876,-0.7037699064,3.4290000801	-1775.637438
5T_6	O,0,0.2715957745,-3.267985084,-0.4598337332 Ru,0,0.5091973093,-1.4150052861,-0.353641002 Ru,0,-0.0497745371,0.2599947052,-1.7517537563 Ru,0,-1.4766872159,1.3296434431,0.0214970144 Ru,0,0.7140864477,2.0645689216,-0.2412070318 Ru,0,1.6028595178,0.3236111842,1.0841862738 N,0,1.6079119595,0.6443149666,2.7304075208 Ti,0,-1.5150033815,-3.2568400002,0.1341903231 O,0,-2.1787424165,-1.8406390166,1.1750628955 Ru,0,-0.9345847669,-0.4315739664,1.3781110984 O,0,-0.6310409663,-0.0936248836,3.0945945452 O,0,-2.5960235636,-3.8999377223,-0.8964305041 H,0,0.5687612791,0.2631820586,3.2724701563	-1775.626483
5I_7	O,0,0.2308516851,-3.0979111108,-0.3953777412 Ru,0,0.4428922584,-1.2535654301,-0.1589610854 Ru,0,-0.0230605274,0.3507587185,-1.6828465627 Ru,0,-1.5395957467,1.3861239582,-0.0977793791 Ru,0,0.672585376,2.1099826876,-0.0385170786 Ru,0,1.9535501255,0.3615140514,0.9395525956 N,0,1.9833794219,0.4515644028,2.65667484 Ti,0,-1.567569179,-3.2995933024,0.1106865579 O,0,-2.4734576358,-1.8962609019,0.9692912689 Ru,0,-1.2768359207,-0.495174713,1.3263464969 O,0,-0.9754781901,-0.0271827434,2.9236691308 O,0,-2.4776667315,-4.2852488241,-0.8041600275 H,0,1.1881004743,0.4668940073,3.3077975242	-1775.638902
5T_7	O,0,0.3238081933,-3.0092368018,-0.1119581561 Ru,0,0.4188554903,-1.1713948412,0.1904265972 Ru,0,-0.1909333218,0.3388538276,-1.4851233218 Ru,0,-1.6436561669,1.4200180605,-0.0184201662 Ru,0,0.7845542376,2.0960470614,-0.3203782195 Ru,0,1.6465067272,0.5605219284,1.2385906319 N,0,1.8128404031,0.8018819579,3.0421369754 Ti,0,-1.5423631093,-3.2785084261,0.0647394056 O,0,-2.685773,-1.9604500878,0.7352847013 Ru,0,-1.6140487202,-0.5217177265,1.3235031689 O,0,-1.4648534941,-0.136989743,2.9585420329	-1776.787547

	O,0,-2.2241307415,-4.2806005619,-1.0161505215 H,0,1.2804161884,0.1107961805,3.5897634125 H,0,3.2762582711,0.1020830806,1.2675415957 H,0,3.0020830427,0.1337730912,2.227962864	
⁵I_g	O,0,0.1953276423,-3.0867600392,-0.244143852 Ru,0,0.4771310642,-1.2705003593,0.1096432917 Ru,0,-0.1578441947,0.2938048479,-1.5203043569 Ru,0,-1.4653615783,1.4425184017,-0.0231645827 Ru,0,1.0188971506,1.938767056,-0.2906400621 Ru,0,1.842838588,0.3023733144,1.0915321074 N,0,1.9593898736,0.4072686632,2.9728480505 Ti,0,-1.6593957883,-3.2589069535,0.0431401937 O,0,-2.6817308285,-1.8588638002,0.7444225437 Ru,0,-1.5020168487,-0.5069840804,1.3283954284 O,0,-1.2190673204,-0.1819703281,2.9606428764 O,0,-2.460788075,-4.3206377528,-0.8894943957 H,0,1.1912726337,0.0132665916,3.5112241329 H,0,3.2740951752,0.0869153325,0.4429086592 H,0,2.3668177666,1.204786386,3.4494493456	-1776.870475
⁵T_g	O,0,0.1172484405,-3.1525183762,0.0067857755 Ru,0,0.3406300114,-1.2872498453,0.0823522353 Ru,0,0.1686175579,0.1511225748,-1.6534026231 Ru,0,-1.6940948078,1.2862846527,-0.6422132915 Ru,0,0.461162206,2.0233961038,0.0065411228 Ru,0,1.0371359014,0.4540971583,1.6046464187 N,0,2.5436342185,0.27005635,2.9577570221 Ti,0,-1.7494912394,-3.2927035339,0.0770806412 O,0,-2.8205479708,-1.827834723,0.5370921989 Ru,0,-1.7333389785,-0.3665469519,1.0267394374 O,0,-1.827520817,0.2414166069,2.6034130019 O,0,-2.4420277816,-4.4082717285,-0.8838919455 H,0,3.2733584163,-0.4291665499,2.9959954558 H,0,2.6728544375,0.4490414446,1.4935042034 H,0,2.8319454055,1.0939538177,3.4740603472	-1776.829632
⁵T_g	O,0,-0.5343508773,-2.8789382255,-1.4419615628 Ti,0,-1.0830124965,-3.2171399352,0.2560582139 O,0,0.2036670117,-3.7181068722,1.2851923519 Ru,0,0.0635051216,-1.0507545743,-1.1508862319 Ru,0,-1.1902726865,-0.4489146897,0.8227097919 O,0,-2.2072811134,-2.0643265872,1.1087823608 Ru,0,1.2511295943,-0.5228810594,0.9378512366 N,0,1.5275813803,-1.8815897604,2.3308966529 N,0,1.9956055642,-1.9623578285,3.4700911778 Ru,0,1.3244609415,1.7168906732,0.4982232461 Ru,0,0.1049712974,1.146424211,-1.7668028016 Ru,0,-1.0662312807,1.7383043737,0.22941208 H,0,2.3432826731,-1.0426903571,3.7982010253 H,0,0.9347378704,-2.9425153685,1.8731644591	-1755.738228
⁵I_g	O,0,-0.4243326289,-2.7025804635,-1.5979071518 Ti,0,-1.1946338991,-3.1296891316,0.0572901847	-1755.743453

O,0,-0.1381363328,-3.9327990942,1.0321117475
Ru,0,0.144268953,-0.9515122619,-1.1905074815
Ru,0,-1.1856897729,-0.3783822748,0.7429098154
O,0,-2.2247293479,-1.9240517517,1.0503671466
Ru,0,1.2459986873,-0.3892419584,0.9191786187
N,0,1.5738000746,-1.8156560751,2.3178244061
N,0,2.1011667778,-1.8652181824,3.4503008309
Ru,0,1.2507618988,1.8451962898,0.3985249594
Ru,0,0.0708305817,1.2303846565,-1.8575796482
Ru,0,-1.153575807,1.792601796,0.0858140708
H,0,2.5062470651,-0.943526803,3.6650494016
H,0,1.1402087503,-2.7247847458,2.0635970997