Supplementary Material (ESI) for Chemical Communications

A DFT study of the single electron reduction and silylation of the U-O bond of the uranyl dication in a macrocyclic environment

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Supporting Information

Computational details :

Uranium was treated with a Stuttgart–Dresden pseudopotential in combination with the appropriate basis set.[24,25] In all cases, the basis set was augmented by a set of polarization function (g for U).[26] Carbon, oxygen, nitrogen and hydrogen atoms were described with a 6–31G(d,p) polarized double–ζ basis set.[27] Calculations were carried out at the DFT level of theory using the hybrid functional B3PW91.[28,29] Geometry optimisations were carried out without any symmetry restrictions and the nature of the *extrema* (*minima*) was verified with analytical frequency calculations. For all transition states, the intrinsic reaction coordinate was followed to verify the direct connection between the transition state and the adducts. All these computations were performed with the Gaussian 03[30] suite of programs. Gibbs free energies were obtained at 298.15 K within the harmonic approximation. The electronic density was analyzed using the Natural Bonding Analysis (NBO) technique.[31]. The solvent effect was taken into account by applying the polarisable continuum model available in the Gaussian 03 program.

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Cartesian coordinates of the optimized structures.

Complex 1P:

E= -2497.4912275

C	6.583802	9.401024	10.576963
N	6.937233	8.092421	10.274316
C	6.181578	7.731049	9.217283
C	5.333020	8.792019	8.829924
C	5.589964	9.852959	9.693591
U	8.246708	6.961747	12.041800
O	9.511691	7.339379	14.194118
C	8.834640	7.519717	15.466861
C	9.904125	8.043287	16.410897
C	11.156927	7.329463	15.898519
C	10.957547	7.366344	14.390318
C	6.339978	6.383618	8.543977
C	5.247911	6.184059	7.485632
C	7.250046	10.103941	11.593586
N	8.206707	9.563509	12.308786
C	8.813690	10.373841	13.288022
C	8.060821	11.003265	14.285258
C	8.637960	11.825986	15.255658
C	10.033302	12.026416	15.232004
C	10.785954	11.404870	14.234866
C	10.209221	10.591268	13.247323
C	7.778920	12.472548	16.309119
C	10.708196	12.888647	16.265803
N	10.937025	9.943879	12.251992
C	11.984723	10.481833	11.729449
C	12.765155	9.779935	10.755281
N	12.388501	8.543802	10.284193
C	13.298871	8.082513	9.380244
C	14.297336	9.049124	9.271534
C	13.960696	10.115036	10.127092
C	13.155680	6.738418	8.687472
C	11.743036	6.605250	8.077031
N	7.066848	5.278147	10.670431
C	6.824507	4.079824	11.328744
C	5.878456	3.319569	10.622079
C	5.538255	4.074359	9.503023
C	6.290643	5.268339	9.567586
C	7.547192	3.740975	12.483912
N	8.453428	4.533427	13.003644
C	9.129773	4.065501	14.147763
C	10.537326	3.947338	14.127077
C	11.182882	3.462384	15.275009
C	10.488226	3.072110	16.420635
C	9.082411	3.174245	16.431552
C	8.435792	3.669797	15.296720
N	11.207935	4.365201	12.980067
C	12.284886	3.783186	12.578305
C	13.002497	4.271958	11.439345
C	14.212619	3.874389	10.879351
C	14.464425	4.720105	9.782552
C	13.401374	5.615818	9.680919
N	12.534483	5.328734	10.693224
C	8.284641	2.770715	17.642531
C	11.235913	2.558820	17.622666
O	6.848859	7.037117	13.077814
O	9.720964	6.896647	11.066274
C	7.717869	6.344262	7.837932
C	14.184015	6.643153	7.552550
H	11.041003	3.166506	18.514741

H	12.315136	2.560729	17.448398
H	10.941753	1.532046	17.872330
H	8.433376	1.712573	17.890341
H	7.214841	2.926703	17.481318
H	8.575020	3.344356	18.531387
H	11.329379	8.289834	13.941778
H	11.372920	6.507384	13.861543
H	11.183103	6.294943	16.255984
H	12.086176	7.822212	16.197367
H	8.004435	8.209498	15.308741
H	8.447929	6.544947	15.783624
H	10.006044	9.127775	16.300598
H	9.674122	7.818359	17.456076
H	8.523226	6.484483	8.561273
H	7.782096	7.140029	7.087910
H	7.861531	5.378721	7.341012
H	10.538643	12.514448	17.282888
H	10.328310	13.917275	16.243054
H	11.788376	12.930663	16.102835
H	6.727106	12.204261	16.180709
H	7.850271	13.566564	16.273269
H	8.078338	12.171883	17.320714
H	5.383917	5.226239	6.975130
H	5.304521	6.970606	6.727618
H	4.247574	6.201369	7.928459
H	10.952680	6.660239	8.829543
H	11.646477	5.643854	7.563583
H	11.570387	7.407935	7.353744
H	14.015335	7.442074	6.825350
H	14.087670	5.682448	7.039290
H	15.208429	6.730191	7.924831
H	7.352243	3.766989	15.298107
H	14.520934	11.026892	10.285385
H	15.170414	8.984918	8.638757
H	5.133763	10.835102	9.690661
H	4.625809	8.780405	8.012387
H	6.977063	11.151395	11.755426
H	5.508286	2.340030	10.898130
H	12.269475	3.407506	15.274395
H	12.323716	11.495358	11.984940
H	15.325095	4.686779	9.130792
H	14.838022	3.068386	11.239386
H	12.696688	2.890297	13.068494
H	4.839022	3.799868	8.725493
H	7.365607	2.758470	12.930666
H	6.987393	10.827334	14.303818
H	11.865507	11.540048	14.230238
H	11.631325	5.752303	10.875593
H	11.511851	8.113620	10.557934

Complex 1:

E= -809.520568

C	-0.164954	0.173904	1.642637
N	-0.324629	-0.449781	0.449789
U	1.756164	0.408093	-0.287548
O	1.607296	2.150516	-0.169382
C	1.075641	0.221118	2.319186
N	2.242736	-0.479218	1.990995
C	3.474169	0.056924	1.725855
C	4.656359	-0.748639	1.215586
C	4.949182	-0.508775	-0.253573
N	4.050854	0.090876	-0.940439
C	3.817877	0.539756	-2.234487
C	2.629659	0.511640	-2.942176
N	1.461088	-0.298352	-2.726340

C	0.176640	0.094847	-2.565473
C	-0.877281	-0.791993	-1.945872
C	-1.045370	-0.083520	-0.599231
O	1.995627	-1.349431	-0.471350
H	2.545834	1.204405	-3.774922
H	4.547656	1.243173	-2.636973
H	1.205002	1.019450	3.046123
H	-0.938263	0.826886	2.054108
H	5.867712	-0.915860	-0.690661
H	3.630093	1.072413	2.088154
H	-0.068881	1.114325	-2.861071
H	-1.732813	0.766395	-0.556936
H	-1.805008	-0.781995	-2.525547
H	-0.541639	-1.825222	-1.821971
H	4.504395	-1.833789	1.329094
H	5.555389	-0.527710	1.808728
H	2.105168	-1.451147	1.700125
H	1.644693	-1.286068	-2.541524

Complex 1A :

E= -1077.798264

C	0.370380	3.460901	-0.966912
C	-0.427128	2.852979	-0.023506
N	0.423989	2.049964	0.802187
C	1.747281	2.178836	0.310694
C	1.715960	3.027971	-0.764449
C	2.861946	1.315452	0.865593
C	2.788860	-0.091629	0.308282
N	1.830837	-1.012442	0.800535
C	1.886250	-2.181780	-0.024468
C	2.866086	-1.971723	-0.968686
C	3.412676	-0.668142	-0.767197
C	0.767058	-3.103270	-0.050311
N	-0.379644	-2.700246	0.393557
C	-1.638007	-3.441495	0.338366
C	-2.727623	-2.612439	-0.361110
O	-2.804361	-1.288539	0.245946
C	-3.755729	-0.367405	-0.364707
C	-3.678001	0.998772	0.336260
N	-2.296160	1.471264	0.396420
C	-1.854850	2.602818	-0.050266
H	1.847297	-1.181582	1.809634
H	0.305840	2.176301	1.810871
H	3.115690	-2.642937	-1.781293
H	4.168024	-0.202009	-1.386566
H	2.561761	3.297846	-1.383507
H	0.023795	4.087231	-1.779808
H	2.837265	1.302637	1.963915
H	3.821682	1.755822	0.584805
H	0.905463	-4.082211	-0.518749
H	-2.507338	3.343546	-0.522020
H	-1.539342	-4.396158	-0.193461
H	-1.945237	-3.656747	1.368352
H	-3.695602	-3.109770	-0.244379
H	-2.507766	-2.490717	-1.428447
H	-3.514262	-0.278526	-1.430611
H	-4.764272	-0.777777	-0.253407
H	-4.045150	0.905209	1.364813
H	-4.335989	1.695605	-0.197989
U	-0.615488	-0.282837	0.583726
O	-0.443719	-0.200880	-1.145257
O	-0.675606	-0.317379	2.323145

Complex 2P:

E= -2553.06805855

C	6.309284	9.398954	10.642371
N	6.674825	8.101530	10.306750
C	5.856508	7.728553	9.294877
C	4.964728	8.771094	8.971512
C	5.251662	9.833840	9.829510
U	7.941398	6.945189	12.134367
O	9.581324	7.256434	13.905282
C	9.302972	7.432124	15.321143
C	10.590431	7.990983	15.902807
C	11.656395	7.287828	15.058174
C	11.041052	7.278668	13.668163
C	5.996502	6.382873	8.611013
C	4.880646	6.192714	7.576172
C	7.040932	10.105409	11.621305
N	8.074833	9.577509	12.227701
C	8.725933	10.389062	13.197157
C	7.998338	10.889627	14.281436
C	8.570562	11.702937	15.259637
C	9.940055	12.020437	15.137178
C	10.666909	11.519692	14.059621
C	10.103488	10.709747	13.047783
C	7.746083	12.212050	16.410993
C	10.618860	12.887713	16.165001
N	10.771498	10.181122	11.960095
C	12.044753	10.444272	11.721819
C	12.850890	9.730412	10.814673
N	12.416357	8.637259	10.079404
C	13.510973	8.092797	9.546825
C	14.687743	8.834480	9.887253
C	14.264404	9.880012	10.682819
C	13.458899	6.756943	8.805287
C	12.111419	6.601018	8.088346
N	6.801931	5.239860	10.693804
C	6.547617	4.050154	11.364035
C	5.541545	3.325414	10.707442
C	5.173127	4.094698	9.602734
C	5.966299	5.259638	9.628978
C	7.329486	3.694830	12.484143
N	8.308260	4.453240	12.911325
C	9.018313	3.996380	14.054520
C	10.422976	3.787025	13.982695
C	11.046413	3.337945	15.168812
C	10.355144	3.074991	16.348836
C	8.959223	3.275039	16.396107
C	8.325863	3.735384	15.241554
N	11.054904	4.068533	12.786981
C	12.346888	3.857307	12.607576
C	13.095688	4.373339	11.532376
C	14.516422	4.307108	11.415260
C	14.853127	5.138142	10.365537
C	13.620173	5.669426	9.867800
N	12.573263	5.198332	10.547201
C	8.169446	3.014048	17.650206
C	11.100152	2.589784	17.564676
O	6.632875	7.042083	13.286196
O	9.289172	6.853671	11.003997
C	7.355753	6.344049	7.867862
C	14.583547	6.669766	7.763476
H	10.982568	3.274520	18.413628
H	12.169799	2.491807	17.361710
H	10.733269	1.611497	17.898721
H	8.242520	1.966284	17.968253
H	7.109767	3.240338	17.502768

H	8.523240	3.621382	18.492895
H	11.249020	8.184200	13.097275
H	11.286157	6.398091	13.074726
H	11.813217	6.264859	15.415302
H	12.618274	7.806880	15.063740
H	8.446288	8.103137	15.410204
H	9.054062	6.449069	15.735877
H	10.631166	9.074745	15.754760
H	10.678585	7.779387	16.972160
H	8.181428	6.481073	8.571699
H	7.401962	7.138786	7.114239
H	7.485192	5.382874	7.356913
H	10.548300	12.456560	17.171098
H	10.160809	13.883057	16.218238
H	11.678804	13.021963	15.933732
H	6.714922	11.853697	16.346333
H	7.714013	13.308621	16.437016
H	8.148642	11.888557	17.379225
H	5.000262	5.237545	7.056731
H	4.918532	6.985550	6.823620
H	3.892527	6.208956	8.044539
H	11.297912	6.658211	8.814190
H	12.062727	5.634981	7.571304
H	11.981366	7.393346	7.341242
H	14.477888	7.464356	7.016816
H	14.556719	5.702846	7.249277
H	15.571571	6.774315	8.217881
H	7.253916	3.923579	15.259100
H	14.875206	10.643077	11.152293
H	15.705778	8.608929	9.597143
H	4.766093	10.800914	9.870157
H	4.204557	8.750087	8.202999
H	6.751205	11.138099	11.838976
H	5.142118	2.364581	11.007258
H	12.122502	3.188203	15.170391
H	12.575547	11.231163	12.274888
H	15.849481	5.359208	10.005247
H	15.187332	3.744147	12.054544
H	12.936600	3.285901	13.337218
H	4.423229	3.845645	8.864757
H	7.129283	2.736692	12.973678
H	6.949095	10.611912	14.365214
H	11.722457	11.770605	14.003478
K	10.028113	4.321103	10.281360
K	9.806384	9.170626	9.626859

Complex 2:

E= -865.213173

C	-0.184452	-0.132596	1.768468
N	-0.290426	-0.161815	0.387709
U	1.864262	-0.503489	-0.371612
O	1.883193	1.255361	-0.321747
C	1.030542	-0.167968	2.475251
N	2.280635	-0.233414	1.883578
C	3.506835	0.030458	2.237532
C	4.714965	0.134119	1.303157
C	4.932670	0.091001	-0.211422
N	4.026828	-0.166666	-1.112696
C	3.923360	-0.051884	-2.489351
C	2.708781	-0.019171	-3.196168
N	1.457354	-0.094313	-2.608104
C	0.238423	0.221334	-2.944764
C	-0.967703	0.299095	-2.005606
C	-1.189609	0.167629	-0.496763

O	1.844695	-2.374236	-0.424151
H	2.785498	0.164290	-4.269212
H	4.825166	0.112151	-3.081729
H	0.956497	-0.049047	3.557539
H	-1.082613	0.013863	2.370940
H	5.946387	0.388935	-0.493347
H	3.758106	0.288430	3.270056
H	-0.004442	0.549743	-3.959130
H	-2.197419	0.469142	-0.198002
H	-1.334803	1.324422	-2.197085
H	-1.757981	-0.307617	-2.480268
H	5.487661	-0.523764	1.737073
H	5.111219	1.134259	1.558334
K	3.193602	-3.405029	-2.650836
K	0.466015	-3.504450	1.732412

Complex 2A :

E= -1133.496256

C	0.180448	3.668855	0.432617
C	-0.277486	2.677069	-0.461048
N	0.732771	1.829547	-0.777565
C	1.840657	2.211836	0.000780
C	1.510923	3.380323	0.724865
C	-1.687927	2.435713	-0.965968
C	-2.322774	1.186028	-0.384478
N	-1.847531	-0.047181	-0.689902
C	-2.507004	-0.955870	0.158259
C	-3.473069	-0.256560	0.917371
C	-3.353841	1.087460	0.574351
C	-1.942793	-2.237867	0.379651
N	-0.828950	-2.606891	-0.232570
U	0.491405	-0.538321	-0.485084
O	0.383426	-0.304708	1.237339
C	2.895912	1.287652	0.208007
N	2.872355	0.090789	-0.356350
C	3.794033	-0.961474	0.086236
C	3.317131	-2.327589	-0.404357
O	1.946324	-2.513232	0.007282
C	1.333392	-3.772825	-0.339943
C	-0.090103	-3.792892	0.214554
O	0.614192	-0.791882	-2.258614
H	2.160006	3.918663	1.404064
H	-0.405715	4.488599	0.827193
H	-3.928746	1.911480	0.976457
H	-4.144918	-0.684537	1.650797
H	-2.308317	3.299505	-0.716206
H	-1.675315	2.362153	-2.062415
H	3.684148	1.562035	0.915748
H	-2.407459	-2.876430	1.137197
H	4.808086	-0.805033	-0.307411
H	3.865254	-0.972889	1.181066
H	3.937811	-3.118619	0.030997
H	3.371833	-2.399002	-1.499555
H	1.336390	-3.879341	-1.433610
H	1.915533	-4.592804	0.095159
H	-0.052886	-3.830959	1.310449
H	-0.565510	-4.721466	-0.131003
K	-2.198599	-1.825054	-2.963907
K	2.435509	1.545516	-3.123294

Adduct of $TMSNMe_2$ (3):

E= -1123.398635

C	4.002532	1.268375	0.368436
Si	2.212910	1.816976	0.112455
C	2.201414	3.726243	-0.043972
C	1.522821	1.100495	-1.493545
O	1.038801	6.740546	-2.710223
U	1.233085	8.480057	-2.662170
N	3.497757	8.066728	-2.229326
C	4.197693	8.506597	-3.319903
C	3.558075	8.621113	-4.566963
N	2.256994	8.260284	-4.739559
C	1.240479	8.683311	-5.475443
C	-0.142537	8.029803	-5.360994
C	-0.959604	8.893358	-4.391699
N	-1.048481	8.581571	-3.108938
C	-1.626217	9.131707	-2.003574
C	-1.035139	9.027794	-0.731929
N	0.167769	8.395571	-0.582152
C	1.208998	8.465107	0.210244
C	2.444298	7.570223	-0.036379
C	3.523490	8.223509	-0.930572
O	1.450922	10.344352	-2.592574
N	1.238018	1.249120	1.461501
K	3.822461	11.673256	-3.479436
K	-0.537332	12.118172	-1.560551
H	-2.589253	9.644322	-2.088252
H	-1.563176	9.436288	0.133616
H	5.263062	8.739317	-3.244293
H	4.141293	8.985503	-5.417987
H	1.252852	9.174667	1.043128
H	4.280149	8.845159	-0.439656
H	-1.416318	9.805363	-4.790245
H	1.339487	9.545442	-6.142623
H	-0.057505	7.003954	-4.988705
H	-0.629387	7.992280	-6.341252
H	2.900627	7.350701	0.934113
H	2.134082	6.610106	-0.466634
H	4.059796	0.188841	0.536465
H	4.588988	1.498162	-0.527891
H	4.485992	1.769917	1.212439
H	1.446215	0.010893	-1.432104
H	0.535127	1.497600	-1.747475
H	2.195258	1.342166	-2.323947
H	2.594668	4.187264	0.869035
H	2.825098	4.036657	-0.891621
H	1.181609	4.090990	-0.211353
C	1.727917	1.244557	2.824231
C	-0.203090	1.136269	1.381009
H	1.360420	2.103073	3.412776
H	1.405742	0.333306	3.348680
H	2.820471	1.264545	2.846917
H	-0.725046	1.984361	1.857485
H	-0.533271	1.080560	0.340428
H	-0.548849	0.221770	1.884463

TS TMS (4):

E= -1028.663967

C	2.809069	4.364802	0.787591
Si	1.505912	3.956757	-0.521179
C	-0.308419	4.166364	-0.019094
O	1.627378	2.137358	-0.432225
U	1.701120	0.179400	-0.427639
O	1.896286	-1.736520	-0.370035
N	-0.330005	-0.094514	0.715076

C	-1.019501	-0.499024	-0.334850
C	-0.878992	0.211840	-1.701168
C	0.137678	-0.511312	-2.610580
N	1.366507	-0.041436	-2.734125
C	2.508593	-0.451800	-3.364754
C	3.767278	-0.309264	-2.770611
N	3.847332	0.121362	-1.465992
C	4.701126	0.089297	-0.480852
C	4.336330	0.711178	0.898198
C	3.480117	-0.061314	1.938680
N	2.182384	0.031584	1.902804
C	1.120879	-0.492266	2.603947
C	-0.130972	-0.561134	1.993640
C	1.997008	4.181193	-2.337425
C	1.291901	6.696126	-0.763159
H	2.449473	-0.861772	-4.374892
H	4.666879	-0.528226	-3.350892
H	1.242479	-0.839669	3.630715
H	-0.974450	-0.962262	2.562048
H	5.710226	-0.324736	-0.587271
H	4.007658	-0.660687	2.686740
H	-0.181706	-1.442398	-3.084954
H	-1.677186	-1.375454	-0.304357
H	-0.592002	1.261917	-1.560254
H	-1.857181	0.241603	-2.194899
H	5.287311	0.935369	1.391130
H	3.853569	1.684492	0.718836
H	2.810290	5.408516	1.106063
H	2.630055	3.745234	1.673924
H	3.807777	4.139923	0.396065
H	-0.434483	4.938144	0.743568
H	-0.932631	4.440233	-0.874843
H	-0.682153	3.224640	0.397623
H	2.746146	4.964012	-2.473875
H	2.418735	3.238712	-2.704791
H	1.132572	4.433633	-2.958386
H	0.568759	6.700027	-1.570746
H	0.939531	6.924281	0.236185
H	2.324059	6.925267	-1.002137
K	0.362436	-3.421432	1.068906
K	3.825872	-3.106637	-1.686606

TS SN NMe_2 of $TMSNMe_2$ (4):

E= -1123.313553

C	3.410674	3.850207	-0.320551
Si	1.582295	4.090381	-0.704454
C	0.384189	4.355543	0.735407
C	0.964052	3.115975	-2.193649
O	1.618008	5.757029	-1.392388
U	1.523266	7.582716	-2.134181
N	3.846728	7.991564	-1.787949
C	4.544667	8.023062	-2.967177
C	3.950582	7.526227	-4.131981
N	2.676100	7.017378	-4.105016
C	1.644640	6.968446	-4.920247
C	0.277996	6.408582	-4.438420
C	-0.655573	7.474440	-3.820666
N	-0.788277	7.559781	-2.508659
C	-1.439913	8.402680	-1.649292
C	-0.855057	8.827640	-0.453280
N	0.456245	8.495616	-0.194273
C	1.444252	8.942420	0.527295
C	2.837066	8.252350	0.456337

C	3.863984	8.627007	-0.649090
O	1.489708	9.406385	-2.776861
N	1.375147	1.569081	0.571410
K	2.830106	10.218609	-4.947721
K	0.148294	11.419113	-1.619856
H	-2.455770	8.730568	-1.879876
H	-1.445024	9.404661	0.262817
H	5.560251	8.419375	-3.008884
H	4.522849	7.531483	-5.063647
H	1.338362	9.784336	1.221818
H	4.583835	9.419910	-0.426362
H	-1.149817	8.169240	-4.504168
H	1.688683	7.347109	-5.948297
H	0.435570	5.584863	-3.729459
H	-0.227641	5.955996	-5.298864
H	3.328853	8.449443	1.414051
H	2.673172	7.165774	0.416403
H	3.664983	2.790346	-0.263041
H	4.011150	4.302262	-1.115882
H	3.692133	4.321390	0.626825
H	1.069432	2.041669	-2.033048
H	-0.088887	3.331276	-2.404251
H	1.556995	3.378599	-3.076326
H	0.865652	4.161821	1.697265
H	0.022467	5.389773	0.729035
H	-0.482271	3.694338	0.658381
C	2.198804	1.148944	1.649593
C	0.218485	0.759910	0.409063
H	1.635916	1.036662	2.595677
H	2.617845	0.139941	1.459467
H	3.032968	1.836604	1.804602
H	-0.367064	0.665002	1.343349
H	-0.428558	1.144315	-0.383064
H	0.493738	-0.282690	0.151588

Product O=U-O-SiMe$_3$ (5):

E= -988.9384224

C	3.394061	3.574769	0.111258
Si	1.677096	3.878746	-0.593066
C	0.376120	4.028626	0.756412
C	1.207697	2.579317	-1.872284
O	1.729188	5.403734	-1.423627
U	1.760614	7.171884	-2.471438
N	4.063109	7.625146	-2.063886
C	4.937538	7.138069	-2.974081
C	4.430865	6.462233	-4.119089
N	3.090971	6.340451	-4.264807
C	2.205376	6.003529	-5.177832
C	0.688117	5.879230	-4.795389
C	-0.216813	7.095382	-4.475400
N	-0.570501	7.332954	-3.256870
C	-1.264668	8.410297	-2.699443
C	-0.779015	9.051759	-1.591638
N	0.423887	8.640739	-1.011941
C	1.459868	9.309817	-0.633771
C	2.733961	8.563348	-0.161945
C	4.038643	8.431474	-1.025244
O	1.870464	8.880395	-3.516470
K	4.153864	9.337313	-4.918907
K	0.276008	11.009045	-3.944364
H	-2.223383	8.711403	-3.124263
H	-1.353112	9.859806	-1.135505

H	6.016820	7.249532	-2.849246
H	5.127706	6.058413	-4.857170
H	1.491470	10.406909	-0.622691
H	4.922836	8.939708	-0.638049
H	-0.532718	7.719419	-5.320731
H	2.473976	5.673228	-6.182435
H	0.576834	5.164048	-3.963300
H	0.215709	5.384103	-5.650717
H	3.047271	9.076250	0.753658
H	2.415657	7.562454	0.173839
H	3.424631	2.610154	0.629102
H	4.151357	3.552114	-0.678482
H	3.674128	4.345430	0.836412
H	1.179083	1.587380	-1.408708
H	0.215292	2.768302	-2.294813
H	1.936397	2.537820	-2.688235
H	0.294087	3.086706	1.309239
H	0.631473	4.811731	1.477367
H	-0.609620	4.253799	0.337445

Product O=U-O-Si(Me)$_2$NMe$_2$ (5):

E= -1083.5744705

C	3.438698	3.679927	-0.123771
Si	1.612204	3.811428	-0.527058
O	0.780303	3.620946	0.975702
U	-0.622298	4.074353	2.410531
O	-1.955994	4.527562	3.836727
C	1.004927	2.456882	-1.671996
N	1.192265	5.397552	-1.164676
N	0.861203	3.820293	4.257656
C	0.647340	2.585322	4.655502
C	-0.077878	1.570583	3.703374
C	-1.600422	1.611008	3.413539
N	-2.030614	2.061187	2.283245
C	-3.320858	2.324640	1.817949
C	-3.596041	3.506288	1.180679
N	-2.587792	4.451566	0.985976
C	-2.552344	5.722974	1.209336
C	-1.223805	6.503777	1.046144
C	-0.366272	7.022497	2.257688
N	0.322469	6.178225	2.994588
C	1.228662	6.168415	4.000031
C	1.502422	4.940059	4.664627
K	-4.547669	4.005500	4.293967
K	-1.056777	5.992330	5.936092
H	-4.597344	3.690888	0.788303
H	-4.101708	1.569730	1.924942
H	2.225884	4.921774	5.482782
H	1.748891	7.076823	4.312847
H	-2.268553	1.243711	4.203391
H	1.051553	2.173295	5.581373
H	-3.435979	6.296248	1.517476
H	-0.281996	8.106313	2.352304
H	-0.566188	5.939248	0.352009
H	-1.494929	7.408171	0.490995
H	0.108830	0.582464	4.137365
H	0.438426	1.552689	2.729192
H	4.043399	3.805457	-1.027795
H	3.755100	4.435443	0.601250
H	3.664060	2.694611	0.295603
H	1.519807	2.502236	-2.636782
H	1.211143	1.476652	-1.231195
H	-0.070545	2.523323	-1.860950

C	2.059392	6.529394	-0.856379
C	0.454805	5.522511	-2.419250
H	1.567104	7.466473	-1.143048
H	2.256313	6.577384	0.220321
H	3.031837	6.503875	-1.371231
H	0.147929	6.565039	-2.563945
H	1.028261	5.229975	-3.311587
H	-0.453966	4.913254	-2.395624

TS SN Me of $TMSNMe_2$ (6):

E= -1123.307467

C	2.689091	4.381804	0.843686
Si	1.413957	3.910540	-0.476547
C	-0.448208	4.122503	-0.220388
N	1.925033	2.735848	-1.714528
O	1.656190	5.450541	-1.445060
U	1.838453	7.091845	-2.524624
N	4.182313	7.343734	-2.187281
C	4.870960	7.107829	-3.349022
C	4.236155	6.453307	-4.410466
N	2.931367	6.039020	-4.315634
C	1.893990	5.982268	-5.133358
C	0.488470	5.608824	-4.608434
C	-0.330109	6.862360	-4.238394
N	-0.457011	7.224975	-2.971434
C	-1.015168	8.290595	-2.323702
C	-0.402108	8.881043	-1.212318
N	0.860611	8.478737	-0.847391
C	1.875656	8.953979	-0.175141
C	3.193744	8.139529	-0.064663
C	4.247153	8.197754	-1.200880
O	1.998054	8.740163	-3.513268
K	3.323915	8.985197	-5.812408
K	1.030279	11.089397	-2.658191
C	1.221361	1.832470	0.583113
H	-1.980166	8.679709	-2.654642
H	-0.936688	9.649371	-0.647844
H	5.909650	7.422765	-3.459352
H	4.805622	6.263774	-5.324987
H	1.834341	9.910864	0.359074
H	5.022184	8.967285	-1.139927
H	-0.733732	7.462803	-5.057374
H	1.969222	6.242809	-6.195955
H	0.574965	4.942282	-3.740560
H	-0.043953	5.033192	-5.374720
H	3.695620	8.482717	0.845706
H	2.934438	7.084405	0.114210
H	2.970977	3.583902	1.530909
H	3.592789	4.769359	0.362485
H	2.250307	5.193084	1.437274
H	-0.594318	4.576994	0.766338
H	-0.860622	4.807362	-0.965929
H	-1.013646	3.189067	-0.230298
H	0.504263	1.224359	0.037899
H	2.213382	1.394253	0.656804
H	0.839352	2.230931	1.523739
C	3.300273	2.311493	-1.857888
C	0.992484	2.042091	-2.574009
H	3.393977	1.222465	-1.745850
H	3.682610	2.574095	-2.855626
H	3.937936	2.793674	-1.114494
H	1.050060	0.953781	-2.430759
H	-0.032832	2.362862	-2.378356
H	1.222140	2.238585	-3.632038