Supplemental information to accompany, Oxidative Addition to U(V)-U(V) Dimers:

Facile Routes to Uranium(VI) Bis(imido) Complexes

Liam P. Spencer, Ping Yang, Brian L. Scott, Enrique R. Batista, James M. Boncella*

Los Alamos National Laboratory, MS J514, Los Alamos NM, 87545

Email: boncella@lanl.gov

Contents:

	Page
Crystallographic data for $[U(N^tBu)_2(SPh)(^tBu_2bpy)]_2$ (**2**)	S2
Crystallographic data for $U(N^tBu)_2(Cl)(I)(^tBu_2bpy)$ (**4**)	S3
Crystallographic data for $U(N^tBu)_2(SePh)(I)(^tBu_2bpy)$ (**8**)	S4
Crystallographic data for $[(U(N^tBu)_2(I)(^tBu_2bpy))_2(\mu\text{-}O)]$ (**13**)	S5
Crystallographic data for $[U(N^tBu)_2(I)(^tBu_2bpy)]_2(\mu\text{-}\eta^2\text{:}\ \eta^2\text{-}Se_4)$ (**17**)	S6
^1H NMR studies of the equilbrium between $U(N^tBu)_2(SePh)(I)(^tBu_2bpy)$ (**8**) and $U(N^tBu)_2(SePh)_2(^tBu_2bpy)$ (**9**) / $U(N^tBu)_2(I)_2(^tBu_2bpy)$ (**3**)	S7
Comparison of theoretical and experimental bond parameters in $[(U(N^tBu)_2(I)(^tBu_2bpy))_2(\mu\text{-}E)]$ (E =O(**13**); S(**14**); Se(**15**) and model complexes $[U(N^tBu)_2(I)(bpy)]_2(\mu\text{-}E)$] (**13'**-**15'**)	S8
Geometry Optimization for $[U(N^tBu)_2(I)(bpy)]_2(\mu\text{-}E)$] (**13'**)	S9
Geometry Optimization for $[U(N^tBu)_2(I)(bpy)]_2(\mu\text{-}S)$] (**14'**)	
Geometry Optimization for $[U(N^tBu)_2(I)(bpy)]_2(\mu\text{-}Se)$] (**15'**)	

Table S1. Crystal data and structure refinement for $[U(N^tBu)_2(SPh)(^tBu_2bpy)]_2$ (**2**).

Identification code	apx682a	
Empirical formula	$C_{66}H_{98}Cl_4N_8S_2U_2$	
Formula weight	1685.50	
Temperature	120(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\ 2_1/c$	
Unit cell dimensions	a = 12.359(2) Å	α= 90°.
	b = 26.174(4) Å	β= 98.713(2)°.
	c = 11.2726(19) Å	γ = 90°.
Volume	3604.3(11) $Å^3$	
Z	2	
Density (calculated)	1.553 Mg/m^3	
Absorption coefficient	4.736 mm^{-1}	
F(000)	1668	
Crystal size	0.16 x 0.14 x 0.14 mm^3	
Theta range for data collection	1.84 to 28.32°.	
Index ranges	-16<=h<=16, -34<=k<=33, -14<=l<=14	
Reflections collected	40293	
Independent reflections	8498 [R(int) = 0.0688]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5569 and 0.5179	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8498 / 0 / 380	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0367, wR2 = 0.0769	
R indices (all data)	R1 = 0.0613, wR2 = 0.0857	
Largest diff. peak and hole	1.425 and -1.121 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement for $U(N^tBu)_2(Cl)(I)(^tBu_2bpy)$ (**4**).

Identification code	apx594	
Empirical formula	C26 H42 Cl I N4 U	
Formula weight	811.02	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 19.096(8) Å	α = 90°.
	b = 14.268(6) Å	β = 95.921(5)°.
	c = 22.477(9) Å	γ = 90°.
Volume	6092(4) $Å^3$	
Z	8	
Density (calculated)	1.769 Mg/m^3	
Absorption coefficient	6.450 mm^{-1}	
F(000)	3104	
Crystal size	0.14 x 0.14 x 0.12 mm^3	
Theta range for data collection	1.79 to 26.10°.	
Index ranges	-23<=h<=23, -17<=k<=15, -27<=l<=19	
Reflections collected	15452	
Independent reflections	6020 [R(int) = 0.0574]	
Completeness to theta = 25.00°	99.7 %	
Max. and min. transmission	0.5116 and 0.4654	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6020 / 0 / 310	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0474, wR2 = 0.1118	
R indices (all data)	R1 = 0.0718, wR2 = 0.1216	
Largest diff. peak and hole	2.155 and -1.593 $e.Å^{-3}$	

Table S3. Crystal data and structure refinement for $U(N^tBu)_2(SePh)(I)(^tBu_2bpy)$ (**8**).

Identification code	apx659s	
Empirical formula	$C_{39}\ H_{57}\ I\ N_4\ Se\ U$	
Formula weight	1025.78	
Temperature	120(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\ 2_1/n$	
Unit cell dimensions	a = 13.928(3) Å	α= 90°.
	b = 14.961(3) Å	β= 96.152(2)°.
	c = 20.327(4) Å	γ = 90°.
Volume	4211.3(15) $Å^3$	
Z	4	
Density (calculated)	1.618 Mg/m^3	
Absorption coefficient	5.481 mm^{-1}	
F(000)	1992	
Crystal size	0.20 x 0.10 x 0.08 mm^3	
Theta range for data collection	1.87 to 25.17°.	
Index ranges	-16<=h<=16, -17<=k<=17, -24<=l<=24	
Reflections collected	39036	
Independent reflections	7505 [R(int) = 0.0805]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6682 and 0.4070	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7505 / 231 / 505	
Goodness-of-fit on F^2	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0464, wR2 = 0.1166	
R indices (all data)	R1 = 0.0709, wR2 = 0.1252	
Largest diff. peak and hole	0.986 and -1.454 $e.Å^{-3}$	

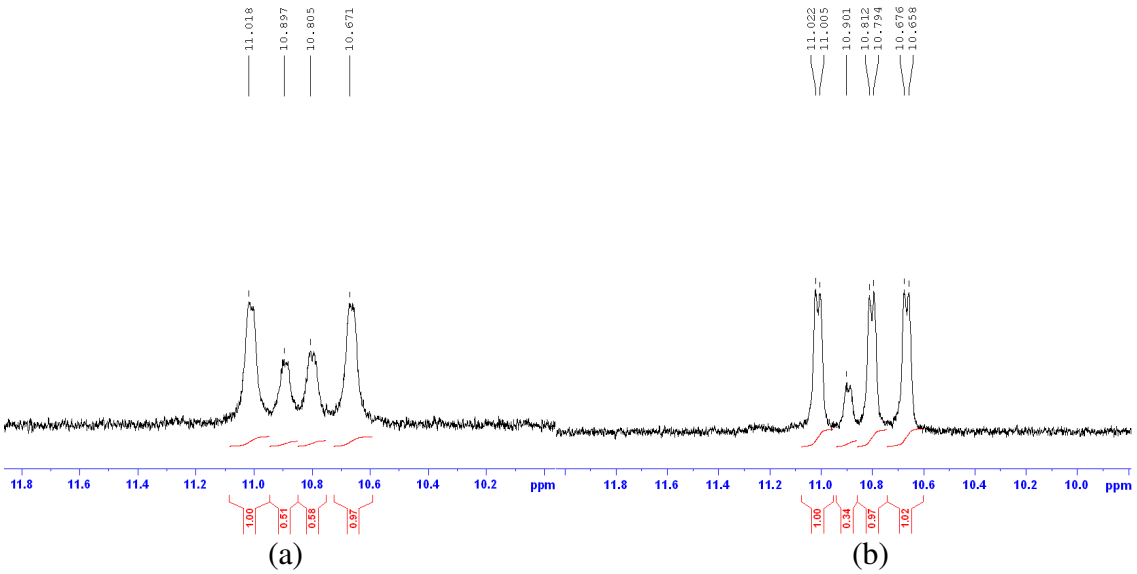
Table S4. Crystal data and structure refinement for [(U(N^{t}Bu)$_2$(I)(^{t}Bu$_2$bpy))$_2$(μ-O)] (**13**).

Identification code	apx685s	
Empirical formula	C_{58} H_{98} I_2 N_8 O U_2	
Formula weight	1653.30	
Temperature	120(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/c	
Unit cell dimensions	a = 13.114(2) Å	α= 90°.
	b = 19.609(3) Å	β= 101.454(2)°.
	c = 26.552(4) Å	γ = 90°.
Volume	6691.8(19) Å^3	
Z	4	
Density (calculated)	1.641 Mg/m^3	
Absorption coefficient	5.797 mm^{-1}	
F(000)	3200	
Crystal size	0.20 x 0.14 x 0.08 mm^3	
Theta range for data collection	1.88 to 25.22°.	
Index ranges	-15<=h<=15, -23<=k<=23, -31<=l<=31	
Reflections collected	62450	
Independent reflections	12016 [R(int) = 0.0945]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6542 and 0.3902	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12016 / 36 / 535	
Goodness-of-fit on F^2	0.799	
Final R indices [I>2sigma(I)]	R1 = 0.0508, wR2 = 0.1388	
R indices (all data)	R1 = 0.1009, wR2 = 0.1648	
Largest diff. peak and hole	1.549 and -1.439 e.Å^{-3}	

Table S5. Crystal data and structure refinement for $[U(N^tBu)_2(I)(^tBu_2bpy)]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}Se_4)$ (**17**).

Identification code	apx674	
Empirical formula	$C_{80}\ H_{116}\ I_2\ N_8\ Se_4\ U_2$	
Formula weight	2235.51	
Temperature	120(1) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P\ 2_1/n$	
Unit cell dimensions	a = 12.291(3) Å	α= 90°.
	b = 21.472(5) Å	β= 103.485(2)°.
	c = 16.935(4) Å	γ = 90°.
Volume	4346.4(16) $Å^3$	
Z	2	
Density (calculated)	1.708 Mg/m^3	
Absorption coefficient	6.150 mm^{-1}	
F(000)	2156	
Crystal size	0.28 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.86 to 25.16°.	
Index ranges	-14<=h<=14, -25<=k<=25, -20<=l<=20	
Reflections collected	40322	
Independent reflections	7754 [R(int) = 0.0635]	
Completeness to theta = 25.00°	100.0 %	
Max. and min. transmission	0.5783 and 0.2778	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7754 / 31 / 440	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0353, wR2 = 0.0836	
R indices (all data)	R1 = 0.0536, wR2 = 0.0913	
Largest diff. peak and hole	2.748 and -1.626 e.$Å^{-3}$	

Figure S1. ^{1}H NMR studies of the equilbrium between U(N^{t}Bu)$_2$(SePh)(I)(^{t}Bu$_2$bpy) (**8**) (δ 10.67, 11.01 *o*-H$_{bpy}$) and U(N^{t}Bu)$_2$(SePh)$_2$(^{t}Bu$_2$bpy) (**9** (δ 10.90 *o*-H$_{bpy}$)) / U(N^{t}Bu)$_2$(I)$_2$(^{t}Bu$_2$bpy) (**3**) (δ 10.80 *o*-H$_{bpy}$).[a]



(a) (b)

[a] (a) before the addition of U(N^{t}Bu)$_2$(I)$_2$(^{t}Bu$_2$bpy) (**3**); (b) represents after the addition of U(N^{t}Bu)$_2$(I)$_2$(^{t}Bu$_2$bpy) (**3**).

Table S2. Comparison of theoretical and experimental bond parameters in $[(U(N^tBu)_2(I)(^tBu_2bpy)]_2(\mu\text{-}E)]$ (E =O(**13**); S(**14**); Se(**15**) and model complexes $[U(N^tBu)_2(I)(bpy)]_2(\mu\text{-}E)]$ (**13'-15'**).

	U-N_{imido} (avg)	**U-N_{bpy} (avg)**	**U-I (avg)**	**U-O (avg)**	**U-O-U**	**N_{imido}-U-N_{imido} (avg)**
Expt.	1.869	2.532	3.112	2.104	173.3	165.4
Theoretical	1.879	2.620	3.144	2.128	173.8	165.1

Table S3. Geometry Optimization for [U(N^{t}Bu)$_2$(I)(bpy)]$_2$(μ-O)] (**13'**) expressed as Cartesian coordinates.

U	2.095624	0.345559	0.073284
U	-2.100294	-0.333056	0.057331
I	-2.521084	-3.192599	1.284430
I	2.405061	3.380109	0.854761
N	4.623094	-0.280328	-0.253429
N	2.678981	-2.116293	-0.590813
N	-4.592945	0.383645	-0.354217
N	-2.361948	0.508599	1.709354
N	2.384791	-0.267047	1.824206
N	2.261363	0.798188	-1.745640
N	-2.304468	-1.061740	-1.669997
N	-2.544429	2.071888	-0.870143
C	-5.558830	-0.514610	-0.114780
H	-5.226438	-1.466787	0.293693
C	3.950602	-2.535276	-0.790400
C	-3.795739	2.551823	-1.056803
C	-4.915701	1.592333	-0.859708
C	-6.247123	1.908452	-1.166339
H	-6.502213	2.867772	-1.601411
C	-7.247827	0.973447	-0.919587
C	5.019310	-1.511449	-0.640159
C	-6.903576	-0.262431	-0.373597
H	-7.651171	-1.019771	-0.161425
C	4.222603	-3.871293	-1.105527
H	5.240752	-4.207724	-1.261452
C	-2.565921	1.169926	3.001755
C	7.319310	-0.780169	-0.696236
C	2.551183	-0.796146	3.183338
C	5.534722	0.686866	-0.081305
H	5.143746	1.653962	0.229619
C	1.673471	-2.996434	-0.685097
H	0.678335	-2.606422	-0.500483
C	-1.498594	2.902021	-0.989008
H	-0.520198	2.470530	-0.809176
C	6.374072	-1.786362	-0.874076
H	6.694337	-2.770661	-1.195127
C	-4.008271	3.898342	-1.376300
H	-5.013134	4.284185	-1.503439
C	1.871689	-4.342314	-0.994050
H	1.017330	-5.008094	-1.053347
C	6.897201	0.484300	-0.290038
H	7.598182	1.298266	-0.137072
C	3.173405	-4.783262	-1.209059

C	-2.450680	-1.880208	-2.877749
C	2.097869	0.265460	4.202776
H	1.043052	0.515822	4.054553
H	2.682808	1.183924	4.093878
H	2.222501	-0.109606	5.226620
C	-1.634955	4.254382	-1.300262
H	-0.751060	4.880961	-1.357607
C	-2.917266	4.756332	-1.502515
C	1.709143	-2.076337	3.333452
H	0.649367	-1.878372	3.147517
H	1.811442	-2.487513	4.345734
H	2.038831	-2.841163	2.621388
C	-1.629696	2.388905	3.102512
H	-1.868786	3.126313	2.328543
H	-0.583599	2.095415	2.972126
H	-1.734055	2.876233	4.080318
C	-4.036195	1.626306	3.083075
H	-4.260443	2.337862	2.280425
H	-4.237509	2.118731	4.042729
H	-4.712408	0.770496	2.983206
C	-1.310986	-2.915090	-2.932009
H	-1.354875	-3.562576	-2.050194
H	-0.337539	-2.413457	-2.954881
H	-1.397143	-3.540606	-3.829531
C	4.042601	-1.119591	3.401758
H	4.388241	-1.867617	2.678835
H	4.206327	-1.519604	4.410321
H	4.655094	-0.218842	3.286295
C	2.379943	1.157353	-3.158112
C	-2.397318	-0.964135	-4.114615
H	-3.189788	-0.208667	-4.069030
H	-2.532102	-1.547373	-5.034494
H	-1.435895	-0.445317	-4.175652
C	-3.808720	-2.610609	-2.829533
H	-3.867945	-3.246249	-1.940889
H	-3.939661	-3.238952	-3.719672
H	-4.633595	-1.889788	-2.798039
C	0.991286	1.545960	-3.702791
H	0.273167	0.740804	-3.524836
H	1.036639	1.747233	-4.780702
H	0.621011	2.448572	-3.202973
C	-2.262589	0.162967	4.123792
H	-2.884805	-0.730963	4.018466
H	-2.450482	0.612977	5.107238
H	-1.216218	-0.155030	4.083690
C	3.350136	2.342926	-3.305284

H	4.349067	2.074357	-2.943655
H	3.004192	3.202914	-2.723055
H	3.437273	2.643196	-4.357727
C	2.927209	-0.064329	-3.924494
H	2.255797	-0.922300	-3.817682
H	3.909547	-0.348699	-3.530108
H	3.037147	0.160499	-4.992818
O	0.013356	-0.070088	-0.020094
H	3.378048	-5.822443	-1.449043
H	8.371080	-0.984163	-0.875050
H	-8.282219	1.208270	-1.153312
H	-3.073679	5.805144	-1.737598

Table S4. Geometry Optimization for $[U(N^tBu)_2(I)(bpy)]_2(\mu\text{-}S)$ (**14'**) expressed as Cartesian coordinates.

U	2.651967	0.300850	0.032306
U	-2.646004	-0.294020	0.036285
I	-3.280049	-3.329031	0.441228
I	3.258446	3.350253	0.351585
N	5.101220	-0.586627	-0.149026
N	3.003274	-2.283083	-0.229467
N	-5.095848	0.590178	-0.160809
N	-2.873610	0.058089	1.843068
N	2.882098	0.010432	1.850630
N	2.799318	0.453090	-1.812759
N	-2.795203	-0.513506	-1.802316
N	-2.993756	2.278484	-0.308374
C	-6.092853	-0.303795	-0.090475
H	-5.791958	-1.336887	0.066953
C	4.234903	-2.833996	-0.331307
C	-4.225221	2.830090	-0.407710
C	-5.381739	1.895945	-0.352864
C	-6.710300	2.324067	-0.487960
H	-6.942329	3.369394	-0.651192
C	-7.743331	1.394023	-0.415798
C	5.389151	-1.895559	-0.314302
C	-7.434277	0.050876	-0.210455
H	-8.205402	-0.709277	-0.145938
C	4.395020	-4.221623	-0.436634
H	5.381863	-4.662173	-0.511267
C	-2.887173	0.208605	3.302586
C	7.747806	-1.387135	-0.418784
C	2.905681	-0.095035	3.314481
C	6.095399	0.312265	-0.111892
H	5.792119	1.347810	0.024016
C	1.924056	-3.082417	-0.226591
H	0.967077	-2.578338	-0.135481
C	-1.912596	3.074646	-0.341348
H	-0.955540	2.570703	-0.250653
C	6.717360	-2.322246	-0.456710
H	6.951033	-3.370211	-0.599580
C	-4.383127	4.215151	-0.546393
H	-5.369664	4.656597	-0.619844
C	2.009866	-4.470086	-0.329743
H	1.103397	-5.065968	-0.320034
C	7.436578	-0.040579	-0.240192
H	8.205805	0.723312	-0.202780
C	3.272378	-5.046318	-0.437062

C	-2.762635	-0.922897	-3.212643
C	2.092123	1.066854	3.912527
H	1.058345	1.028171	3.555336
H	2.521430	2.028394	3.614241
H	2.087235	1.005932	5.008058
C	-1.996254	4.459510	-0.477864
H	-1.087992	5.052453	-0.494997
C	-3.258574	5.036526	-0.582360
C	2.291665	-1.447920	3.719400
H	1.264480	-1.527559	3.349877
H	2.279275	-1.553647	4.811289
H	2.872060	-2.278372	3.300996
C	-2.252215	1.563885	3.664344
H	-2.827171	2.390525	3.230928
H	-1.228679	1.620553	3.281230
H	-2.225862	1.698163	4.752833
C	-4.352153	0.159701	3.777109
H	-4.934186	0.967007	3.317259
H	-4.407282	0.273555	4.866972
H	-4.810108	-0.797042	3.504930
C	-1.611636	-1.924725	-3.418807
H	-1.776357	-2.822218	-2.814080
H	-0.660309	-1.475713	-3.116780
H	-1.545530	-2.219213	-4.473804
C	4.371787	-0.010537	3.780077
H	4.964102	-0.822899	3.343288
H	4.433062	-0.089425	4.872697
H	4.814066	0.944104	3.476484
C	2.741718	0.768982	-3.245197
C	-2.543917	0.331010	-4.080035
H	-3.357122	1.050931	-3.932904
H	-2.512278	0.061759	-5.143238
H	-1.600016	0.819918	-3.819000
C	-4.108493	-1.586146	-3.562969
H	-4.281552	-2.457645	-2.923612
H	-4.111412	-1.913659	-4.610176
H	-4.936533	-0.881503	-3.423494
C	1.584960	1.753929	-3.496213
H	0.641430	1.328354	-3.139900
H	1.494258	1.972903	-4.567661
H	1.762960	2.692360	-2.961086
C	-2.087359	-0.947503	3.929645
H	-2.527633	-1.910698	3.653021
H	-2.082920	-0.860417	5.023413
H	-1.052579	-0.929592	3.573049
C	4.080354	1.409478	-3.659758

H	4.912168	0.716863	-3.485544
H	4.261433	2.321743	-3.082694
H	4.067123	1.666910	-4.726342
C	2.512720	-0.540091	-4.023327
H	1.572615	-1.009189	-3.716682
H	3.328115	-1.248124	-3.836205
H	2.467854	-0.344185	-5.101896
H	3.388531	-6.123363	-0.516584
H	8.779227	-1.709539	-0.528278
H	-8.774957	1.717692	-0.519481
H	-3.373210	6.111577	-0.687264
S	0.003338	0.005938	0.036054

Table S5. Geometry Optimization for $[U(N^tBu)_2(I)(bpy)]_2(\mu\text{-Se})]$ (**15'**) expressed as Cartesian coordinates.

U	2.722606	0.175841	0.042976
U	-2.766596	-0.348579	0.034890
I	-4.066049	-3.137599	0.561277
I	2.816694	3.295017	0.397171
N	5.302210	-0.195110	-0.159024
N	3.579167	-2.274442	-0.295530
N	-5.029148	0.932968	-0.268067
N	-2.930421	0.090532	1.822442
N	3.005860	-0.095837	1.853421
N	2.795089	0.360552	-1.801505
N	-2.890347	-0.619731	-1.792871
N	-2.660255	2.230326	-0.375088
C	-6.169368	0.226452	-0.241726
H	-6.060301	-0.836757	-0.043464
C	4.895668	-2.564674	-0.410808
C	-3.775538	2.985256	-0.506267
C	-5.074609	2.262101	-0.507606
C	-6.298223	2.905514	-0.741772
H	-6.333679	3.967331	-0.952724
C	-7.479239	2.169625	-0.713479
C	5.843071	-1.419430	-0.342371
C	-7.419631	0.801993	-0.454440
H	-8.312727	0.187252	-0.420972
C	5.327833	-3.886457	-0.583393
H	6.381905	-4.118196	-0.674613
C	-2.951624	0.198434	3.288424
C	8.059980	-0.461871	-0.384733
C	2.996119	-0.233223	3.316489
C	6.103350	0.878215	-0.086582
H	5.605103	1.833306	0.061612
C	2.679306	-3.270813	-0.346034
H	1.639409	-2.971211	-0.245299
C	-1.460080	2.832464	-0.355026
H	-0.602471	2.177432	-0.237336
C	7.231253	-1.577560	-0.460071
H	7.668017	-2.557307	-0.609831
C	-3.690939	4.378681	-0.618982
H	-4.586036	4.982533	-0.707440
C	3.039949	-4.606576	-0.514973
H	2.272299	-5.372275	-0.547848
C	7.489512	0.794573	-0.193681
H	8.094343	1.692638	-0.128247
C	4.391775	-4.915940	-0.636090

C	-2.878281	-1.130320	-3.172206
C	2.032884	0.810541	3.909715
H	1.019137	0.647546	3.530802
H	2.344800	1.821960	3.631200
H	2.015091	0.734143	5.004095
C	-1.300639	4.212946	-0.465812
H	-0.301788	4.635380	-0.434162
C	-2.442437	4.997251	-0.599709
C	2.531493	-1.656777	3.675114
H	1.529849	-1.842516	3.274419
H	2.503361	-1.787489	4.763958
H	3.215551	-2.404806	3.257544
C	-2.323279	1.545935	3.688107
H	-2.894280	2.381692	3.267618
H	-1.293656	1.614297	3.322890
H	-2.312356	1.653522	4.779786
C	-4.418175	0.127714	3.753878
H	-5.000106	0.952747	3.326856
H	-4.476319	0.195924	4.847325
H	-4.871448	-0.817468	3.438195
C	-1.867046	-2.287603	-3.270345
H	-2.166249	-3.112715	-2.616132
H	-0.872523	-1.950250	-2.961440
H	-1.813706	-2.659034	-4.301508
C	4.427627	0.011656	3.830763
H	5.125240	-0.715648	3.399588
H	4.463794	-0.084010	4.923020
H	4.765278	1.017892	3.560847
C	2.645659	0.626258	-3.237981
C	-2.471125	0.018561	-4.112577
H	-3.178947	0.851735	-4.037075
H	-2.456107	-0.326281	-5.154070
H	-1.473922	0.390280	-3.857135
C	-4.292972	-1.631664	-3.518420
H	-4.597940	-2.418674	-2.821556
H	-4.315323	-2.035759	-4.538205
H	-5.019600	-0.812888	-3.458846
C	1.524610	1.661147	-3.445609
H	0.582902	1.286972	-3.031240
H	1.383700	1.861730	-4.515165
H	1.772717	2.601019	-2.942406
C	-2.147286	-0.971079	3.885060
H	-2.598477	-1.927106	3.601211
H	-2.128988	-0.900346	4.979778
H	-1.118221	-0.953642	3.512489
C	3.981692	1.179137	-3.769345

H	4.789292	0.454636	-3.613482
H	4.243909	2.107947	-3.252069
H	3.910436	1.387960	-4.844062
C	2.291837	-0.694407	-3.946222
H	1.363672	-1.106769	-3.538598
H	3.088433	-1.434487	-3.808017
H	2.158825	-0.530197	-5.022810
H	4.719039	-5.943092	-0.768839
H	9.136289	-0.576567	-0.474669
H	-8.431025	2.660910	-0.894015
H	-2.369587	6.077944	-0.681897
Se	0.048602	-0.627460	0.133420