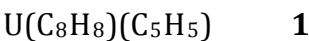


Reductive Coupling of Carbon Monoxide by U(III) Complexes – a Computational Study.

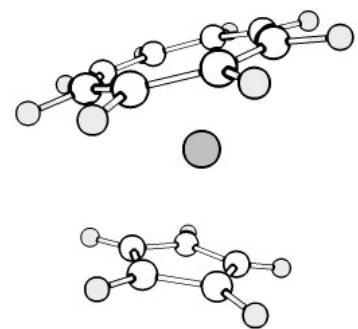
Georgina Aitken,^a Alistair S. P. Frey^b, F. Geoffrey N. Cloke^b, O. Summerscales^b and
Jennifer C. Green^{a*}.

Electronic supplementary information

Structural information



ADF BP86/TZP



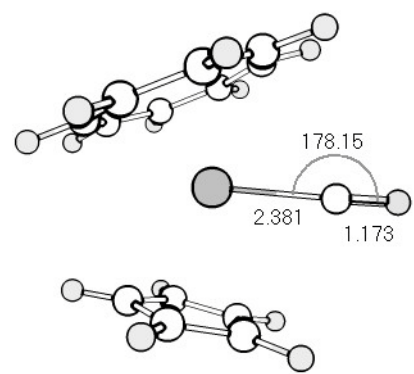
27

U	-1.54195323	2.19787729	-0.63287467
C	0.32504766	3.80729173	0.39243528
C	1.01356277	3.04622318	-0.59095763
C	0.75539679	2.69112154	-1.94050968
C	-0.29905462	2.94360209	-2.85897980
H	-0.17659797	2.39130432	-3.79381049
C	-1.52180443	3.67419896	-2.82038421
C	-2.19163628	4.46383584	-1.84651106
C	-1.93266145	4.82117964	-0.49786558
C	-0.89352378	4.54168950	0.43163301
H	-1.11561524	4.92583876	1.43019433
H	-2.75800155	5.37441984	-0.04469409
H	-3.17544493	4.79655989	-2.18437336
H	-2.10769880	3.55224457	-3.73447078
H	1.49806643	1.99490199	-2.33802936
H	1.91542482	2.57029556	-0.19696531
C	-2.92310801	0.24231507	0.56605339
C	-3.53597646	1.43665704	1.05035482
C	-4.21663326	2.05140591	-0.03444836
C	-4.03082569	1.24533333	-1.19112921
C	-3.23349740	0.12181281	-0.82500078
H	-2.95926499	-0.70646272	-1.47578400
H	-4.44560590	1.44124401	-2.17764913
H	-4.78677827	2.97649932	0.01324436
H	-3.50944572	1.79927622	2.07601678
H	-2.37104957	-0.47985083	1.16657186

H 0.81382600 3.76220064 1.36914696

U(C₈H₈)(C₅H₅)CO **2**

ADF BP86/TZP

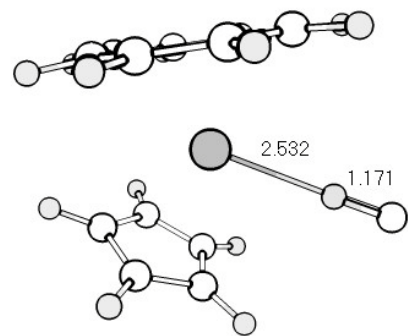


29

U	0.02510765	0.08413464	-0.34520168
C	0.21121246	-2.49089884	0.35717186
H	1.00770449	-3.19456426	0.10499261
C	-0.80994681	-2.45156738	-0.62967108
C	-1.97951015	-1.67807328	-0.83004859
C	-2.58863376	-0.58646772	-0.16100640
H	-3.43841241	-0.18059312	-0.71355030
C	-2.28531884	0.16880582	0.99913495
C	-1.27596362	0.11137396	1.99773106
C	-0.15938224	-0.72691139	2.25602424
C	0.46170890	-1.79599640	1.57104235
H	1.40392362	-2.09665038	2.03501124
H	0.41144115	-0.40110470	3.12789573
H	-1.35185264	0.93586150	2.71022644
H	-2.94816933	1.02799773	1.12534532
H	-2.47514291	-1.91286502	-1.77453712
H	-0.61312238	-3.13316488	-1.46046442
C	2.03355655	1.47351090	-1.64268805
C	1.20752127	2.47975932	-1.06767283
C	1.31527298	2.38450750	0.34329116
C	2.21388684	1.31917391	0.64691828
C	2.65592614	0.75800278	-0.58686550
H	3.37091261	-0.05446849	-0.69944263
H	2.53774165	1.01921797	1.64007726
H	0.82325452	3.02971932	1.06796364
H	0.60922327	3.20087337	-1.61920790
H	2.17720106	1.30131380	-2.70652397
C	-0.79919212	0.57337617	-2.52491317
O	-1.22750347	0.78379704	-3.59640112

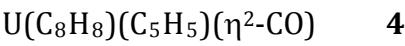
U(C₈H₈)(C₅H₅)OC **3**

ADF BP86/TZP

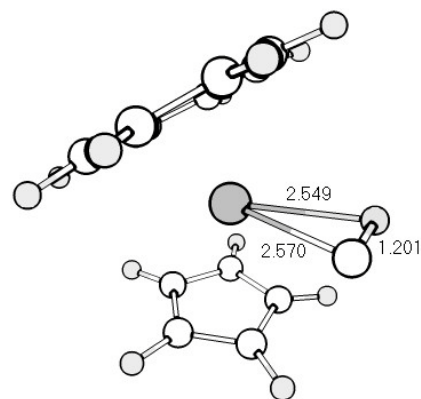


29

C	0.51351626	-0.92790253	-0.35389796
O	-0.16957911	0.01244035	-0.49650851
U	-1.50789656	2.15837041	-0.60865942
C	0.31023896	3.88929475	0.35118340
C	1.00788143	3.17718624	-0.65687360
C	0.73473334	2.79780077	-1.99365541
C	-0.35632373	2.97699863	-2.88160540
H	-0.23088355	2.42078689	-3.81422870
C	-1.60437132	3.65230999	-2.81523654
C	-2.27065856	4.42983233	-1.83293020
C	-1.99622520	4.80858417	-0.49699900
C	-0.94046725	4.56220001	0.41812562
H	-1.15642041	4.94181418	1.41938388
H	-2.83463653	5.33181140	-0.03295306
H	-3.26916044	4.73355095	-2.15416408
H	-2.21301263	3.49638827	-3.70869257
H	1.50569323	2.14437744	-2.40826874
H	1.93408590	2.73362342	-0.28362038
C	-3.06187324	0.27086465	0.52595016
C	-3.58723272	1.50536364	1.00047158
C	-4.18429380	2.18225766	-0.09971643
C	-4.02933269	1.36759334	-1.25429501
C	-3.33500180	0.18756248	-0.87168303
H	-3.08320773	-0.64625945	-1.52372026
H	-4.39425282	1.60124971	-2.25226166
H	-4.68889601	3.14400518	-0.06014897
H	-3.56750526	1.85620098	2.03091501
H	-2.57734752	-0.49413602	1.12922325
H	0.83310570	3.87969029	1.31050201



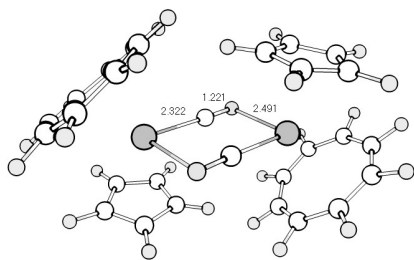
ADF BP86/TZP



29

C	-0.10557827	0.17027568	0.08938136
O	-0.31696590	-0.03951833	-1.07417778
U	-1.53238422	2.16592161	-0.67670970
C	0.21145877	3.86558275	0.45880780
C	0.96303280	3.21792040	-0.55495547
C	0.75663664	2.93088680	-1.92430894
C	-0.28950767	3.15951029	-2.85203726
H	-0.11412929	2.66349043	-3.80909961
C	-1.54461001	3.82019339	-2.80121217
C	-2.26336364	4.53110186	-1.80683230
C	-2.05402565	4.82451531	-0.43827601
C	-1.03828337	4.53382230	0.50655368
H	-1.30817956	4.84294964	1.51875439
H	-2.91277586	5.32185395	0.01644377
H	-3.24802039	4.85025402	-2.15453390
H	-2.11052381	3.71222939	-3.72961149
H	1.53733779	2.28700720	-2.33442428
H	1.86822793	2.75015723	-0.16302500
C	-3.07624045	0.39613202	0.68682471
C	-3.54859093	1.67433061	1.09469608
C	-4.18902111	2.28463120	-0.01779436
C	-4.10765285	1.38784788	-1.11843898
C	-3.41991360	0.22202297	-0.68498596
H	-3.19779005	-0.65221559	-1.29322762
H	-4.51673422	1.55715998	-2.11266040
H	-4.66974490	3.25872413	-0.02234165
H	-3.45582411	2.10148850	2.09163325
H	-2.56578835	-0.32620752	1.31804280
H	0.67687710	3.77374967	1.44304233

[U(C₈H₈)(C₅H₅)CO]₂ 5



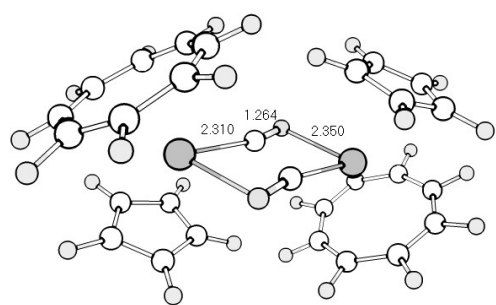
ADF BP86/TZP

58

U	0.00393158	0.01910370	2.21325671
C	2.34494140	0.00505206	3.62963239
H	3.11162666	0.78221839	3.60265431
C	2.53395718	-0.98771611	2.63961218
C	1.80184352	-2.10894892	2.19276373
C	0.52600668	-2.66029441	2.45223170
H	0.26426902	-3.46019539	1.75650730
C	-0.50557170	-2.37776662	3.37872196
C	-0.64203241	-1.45615802	4.43794618
C	0.14360947	-0.40085376	4.96115255
C	1.36483063	0.22270371	4.62153337
H	1.54917277	1.12769045	5.20487068
H	-0.37938713	0.13433533	5.75672826
H	-1.61611800	-1.52596733	4.92559244
H	-1.40204965	-2.97981946	3.21545445
H	2.31035706	-2.62454108	1.37811983
H	3.42383428	-0.80855309	2.03309315
C	-1.70587920	1.93583797	1.31396669
C	-2.55702285	1.01869718	1.99338104
C	-2.26648437	1.10706014	3.37602024
C	-1.24690018	2.08355588	3.55440278
C	-0.89973992	2.59336047	2.27764968
H	-0.15073607	3.35343716	2.07180726
H	-0.82310145	2.39575069	4.50460223
H	-2.75329366	0.54676480	4.16836915
H	-3.31292564	0.38760886	1.53460896
H	-1.68272673	2.10369402	0.24665812
C	-0.94703300	-0.85476711	0.28414150
O	-1.47147473	-1.34783888	-0.70181321
U	-0.00393158	-0.01910370	-2.21325671
C	0.50557170	2.37776662	-3.37872196
H	1.61611800	1.52596733	-4.92559244
C	-0.52600668	2.66029441	-2.45223170
C	-1.80184352	2.10894892	-2.19276373
C	-2.53395718	0.98771611	-2.63961218
H	-2.31035706	2.62454108	-1.37811983
C	-2.34494140	-0.00505206	-3.62963239

C	-1.36483063	-0.22270371	-4.62153337
C	-0.14360947	0.40085376	-4.96115255
C	0.64203241	1.45615802	-4.43794618
H	-1.54917277	-1.12769045	-5.20487068
H	0.37938713	-0.13433533	-5.75672826
H	-3.11162666	-0.78221839	-3.60265431
H	-3.42383428	0.80855309	-2.03309315
H	-0.26426902	3.46019539	-1.75650730
H	1.40204965	2.97981946	-3.21545445
C	2.55702285	-1.01869718	-1.99338104
C	1.70587920	-1.93583797	-1.31396669
C	0.89973992	-2.59336047	-2.27764968
C	1.24690018	-2.08355588	-3.55440278
C	2.26648437	-1.10706014	-3.37602024
H	2.75329366	-0.54676480	-4.16836915
H	0.82310145	-2.39575069	-4.50460223
H	0.15073607	-3.35343716	-2.07180726
H	1.68272673	-2.10369402	-0.24665812
H	3.31292564	-0.38760886	-1.53460896
C	0.94703300	0.85476711	-0.28414150
O	1.47147473	1.34783888	0.70181321

[UCotCp]C₂O₂ **6***

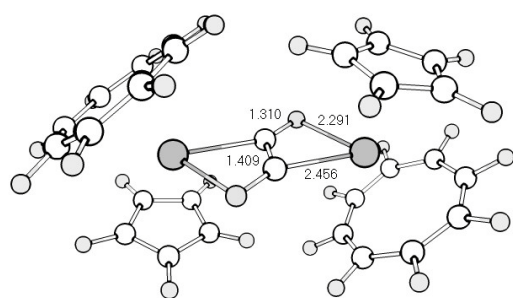


58

C	-0.95831727	0.00023669	0.00109561
C	0.95831727	-0.00023669	-0.00109561
O	1.46687512	1.15743654	-0.00238223
O	-1.46687512	-1.15743654	0.00238223
U	0.59554644	-2.27867461	0.11753216
C	-0.68181467	-3.93024409	1.88373871
H	-1.72550239	-4.24841683	1.83689517
C	-0.51091802	-2.71704496	2.59309333
C	0.56856323	-1.84226158	2.83620115
C	1.92372540	-1.75873816	2.43222332
H	2.39263888	-0.81806560	2.72718632
C	2.78516742	-2.59385687	1.68508634
C	2.63876319	-3.85687386	1.06832272
C	1.57218544	-4.76714862	0.87865826
C	0.19545274	-4.79761585	1.19514493

H	-0.32185045	-5.64425570	0.73830478
H	1.86501042	-5.60766068	0.24597003
H	3.54433080	-4.16666624	0.54350779
H	3.76294588	-2.14138973	1.50507022
H	0.25809653	-0.96777162	3.40809109
H	-1.45616522	-2.31817358	2.96662516
C	0.48174489	-1.67454154	-2.52203527
C	1.85516124	-1.98334711	-2.31545260
C	1.95068787	-3.37367375	-2.06686265
C	0.64207909	-3.92674210	-2.12297050
C	-0.26696894	-2.87557806	-2.40325337
H	-1.34411496	-2.97151067	-2.51622100
H	0.38696244	-4.97429814	-1.98576440
H	2.86527653	-3.92766407	-1.87766920
H	2.68067105	-1.27684003	-2.35403587
H	0.07963556	-0.69502282	-2.74664174
U	-0.59554644	2.27867461	-0.11753216
C	-2.78516742	2.59385687	-1.68508634
H	-3.54433080	4.16666624	-0.54350779
C	-1.92372540	1.75873816	-2.43222332
C	-0.56856323	1.84226158	-2.83620115
C	0.51091802	2.71704496	-2.59309333
H	-0.25809653	0.96777162	-3.40809109
C	0.68181467	3.93024409	-1.88373871
C	-0.19545274	4.79761585	-1.19514493
C	-1.57218544	4.76714862	-0.87865826
C	-2.63876319	3.85687386	-1.06832272
H	0.32185045	5.64425570	-0.73830478
H	-1.86501042	5.60766068	-0.24597003
H	1.72550239	4.24841683	-1.83689517
H	1.45616522	2.31817358	-2.96662516
H	-2.39263888	0.81806560	-2.72718632
H	-3.76294588	2.14138973	-1.50507022
C	-1.85516124	1.98334711	2.31545260
C	-0.48174489	1.67454154	2.52203527
C	0.26696894	2.87557806	2.40325337
C	-0.64207909	3.92674210	2.12297050
C	-1.95068787	3.37367375	2.06686265
H	-2.86527653	3.92766407	1.87766920
H	-0.38696244	4.97429814	1.98576440
H	1.34411496	2.97151067	2.51622100
H	-0.07963556	0.69502282	2.74664174
H	-2.68067105	1.27684003	2.35403587

[UCotCp]C₂O₂

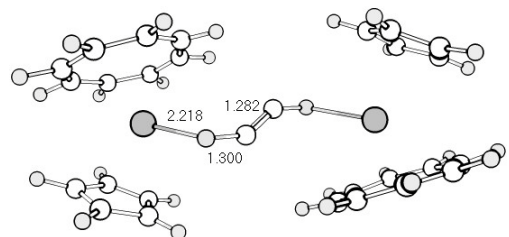


58

U	-0.00515546	0.08326844	2.44978407
C	2.33501981	-0.02087867	3.79604251
H	3.10067729	0.75722977	3.80474223
C	2.51309346	-0.95035838	2.74518683
C	1.75785582	-2.02135252	2.22053380
C	0.49217771	-2.59885354	2.48595882
H	0.20152708	-3.33432963	1.73312379
C	-0.50878830	-2.39208458	3.46223308
C	-0.62930352	-1.53898077	4.58321202
C	0.15189220	-0.50276835	5.14387129
C	1.36054374	0.14816931	4.80962906
H	1.55345211	1.02146466	5.43457828
H	-0.35902429	-0.01288715	5.97417883
H	-1.58907178	-1.65359061	5.08892891
H	-1.39900205	-3.00102225	3.29176194
H	2.22288305	-2.44658407	1.33009196
H	3.38477456	-0.72086929	2.12912700
C	-1.74857580	2.04176893	1.60693580
C	-2.58688060	1.09145775	2.24951105
C	-2.30491272	1.13273438	3.63754339
C	-1.29004980	2.10537595	3.85305908
C	-0.94802958	2.66687772	2.59566130
H	-0.19943157	3.43380333	2.41441651
H	-0.86669002	2.38373491	4.81324310
H	-2.78916442	0.53617338	4.40444053
H	-3.31816435	0.45260577	1.75864187
H	-1.71469891	2.24028460	0.54093275
C	-0.52780992	-0.45296933	0.11071786
O	-1.15157826	-1.16554110	-0.79453020
U	0.00515546	-0.08326844	-2.44978407
C	0.50878830	2.39208458	-3.46223308
H	1.58907178	1.65359061	-5.08892891
C	-0.49217771	2.59885354	-2.48595882
C	-1.75785582	2.02135252	-2.22053380
C	-2.51309346	0.95035838	-2.74518683
H	-2.22288305	2.44658407	-1.33009196
C	-2.33501981	0.02087867	-3.79604251
C	-1.36054374	-0.14816931	-4.80962906
C	0.52780992	0.45296933	-0.11071786
C	-0.15189220	0.50276835	-5.14387129
C	0.62930352	1.53898077	-4.58321202

H	-1.55345211	-1.02146466	-5.43457828
H	0.35902429	0.01288715	-5.97417883
H	-3.10067729	-0.75722977	-3.80474223
H	-3.38477456	0.72086929	-2.12912700
H	-0.20152708	3.33432963	-1.73312379
H	1.39900205	3.00102225	-3.29176194
C	2.58688060	-1.09145775	-2.24951105
C	1.74857580	-2.04176893	-1.60693580
C	0.94802958	-2.66687772	-2.59566130
C	1.29004980	-2.10537595	-3.85305908
C	2.30491272	-1.13273438	-3.63754339
H	2.78916442	-0.53617338	-4.40444053
H	0.86669002	-2.38373491	-4.81324310
H	0.19943157	-3.43380333	-2.41441651
H	1.71469891	-2.24028460	-0.54093275
H	3.31816435	-0.45260577	-1.75864187
O	1.15157826	1.16554110	0.79453020

[UCotCp]₂C₂O₂ **8***

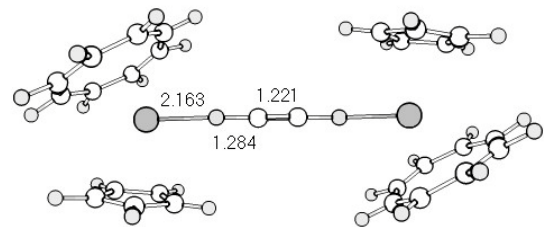


58

U	-3.05447925	-1.59580001	-0.22075537
O	-0.83945683	-1.66023747	-0.12928225
C	-0.16415416	-0.55779276	-0.26943647
C	0.16415416	0.55779276	0.26943647
O	0.83945683	1.66023747	0.12928225
U	3.05447925	1.59580001	0.22075537
C	-3.66332063	-2.71570344	2.12560945
H	-3.35681341	-3.70408403	2.47579862
C	-2.72550815	-1.70525218	2.45473013
C	-2.58118317	-0.33621753	2.13621382
C	-3.28464304	0.59228128	1.33448125
H	-2.74055895	1.53194494	1.21508997
C	-4.46889518	0.54458480	0.55580456
C	-5.46002078	-0.43808892	0.30779722
C	-5.63522858	-1.79296088	0.67187386
C	-4.87920125	-2.74578245	1.39550450
H	-5.29673799	-3.75265463	1.32398627
H	-6.50458525	-2.23985783	0.18627136
H	-6.22317992	-0.09240603	-0.39214608
H	-4.63428727	1.46321757	-0.01266847
H	-1.61625529	0.06111853	2.46023516
H	-1.85586352	-2.10134258	2.98348445

C	-2.24752229	-2.50209159	-2.64748702
C	-3.11337209	-1.41378754	-2.93650250
C	-4.43675869	-1.79948050	-2.58241351
C	-4.38544289	-3.12079408	-2.06557065
C	-3.03000885	-3.55324325	-2.09780873
H	-2.65979574	-4.52689946	-1.78340106
H	-5.23376939	-3.70437423	-1.71887130
H	-5.33166963	-1.19447783	-2.69916410
H	-2.81953810	-0.46299336	-3.37624549
H	-1.17249227	-2.52299678	-2.80135285
C	4.46889518	-0.54458480	-0.55580456
H	6.22317992	0.09240603	0.39214608
C	3.28464304	-0.59228128	-1.33448125
C	2.58118317	0.33621753	-2.13621382
C	2.72550815	1.70525218	-2.45473013
H	1.61625529	-0.06111853	-2.46023516
C	3.66332063	2.71570344	-2.12560945
C	4.87920125	2.74578245	-1.39550450
C	5.63522858	1.79296088	-0.67187386
C	5.46002078	0.43808892	-0.30779722
H	5.29673799	3.75265463	-1.32398627
H	6.50458525	2.23985783	-0.18627136
H	3.35681341	3.70408403	-2.47579862
H	1.85586352	2.10134258	-2.98348445
H	2.74055895	-1.53194494	-1.21508997
H	4.63428727	-1.46321757	0.01266847
C	3.11337209	1.41378754	2.93650250
C	2.24752229	2.50209159	2.64748702
C	3.03000885	3.55324325	2.09780873
C	4.38544289	3.12079408	2.06557065
C	4.43675869	1.79948050	2.58241351
H	5.33166963	1.19447783	2.69916410
H	5.23376939	3.70437423	1.71887130
H	2.65979574	4.52689946	1.78340106
H	1.17249227	2.52299678	2.80135285
H	2.81953810	0.46299336	3.37624549

[UCotCp]₂C₂O₂ **9**

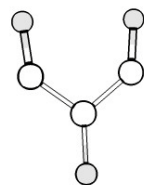
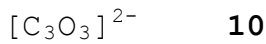


58

U	-0.18551124	-0.07061721	4.05125822
C	2.24881081	-0.13762644	5.15741221

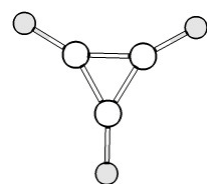
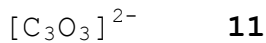
H	3.00089647	0.65496044	5.13887278
C	2.34902946	-1.00946739	4.04131865
C	1.58663180	-2.09195566	3.54741051
C	0.37066515	-2.71225546	3.91336002
H	0.02075931	-3.42112532	3.15954104
C	-0.55688863	-2.54629623	4.97506117
C	-0.60587632	-1.74028657	6.14172750
C	0.21111507	-0.72410122	6.69015211
C	1.37691254	-0.04036911	6.27241831
H	1.61896795	0.80844608	6.91563707
H	-0.22668269	-0.28314033	7.58769972
H	-1.52444658	-1.89169751	6.71238015
H	-1.45041497	-3.16306797	4.85105963
H	1.94057175	-2.42870314	2.57058098
H	3.15500592	-0.72352621	3.36152439
C	-1.86539042	1.87128999	3.17869809
C	-2.69238718	0.93705868	3.85901047
C	-2.38811137	1.01168385	5.24795578
C	-1.36307793	1.97904087	5.42152147
C	-1.03445923	2.50615877	4.13986830
H	-0.29765842	3.28035602	3.93470997
H	-0.91896905	2.27569987	6.36814338
H	-2.86455659	0.43795204	6.03835340
H	-3.44274195	0.29754866	3.39930542
H	-1.85399714	2.04989163	2.10688486
C	0.00861906	-0.01025874	-0.61047142
O	0.03747243	0.02841597	-1.89376969
U	0.18551124	0.07061721	-4.05125822
C	0.55688863	2.54629623	-4.97506117
H	1.52444658	1.89169751	-6.71238015
C	-0.37066515	2.71225546	-3.91336002
C	-1.58663180	2.09195566	-3.54741051
C	-2.34902946	1.00946739	-4.04131865
H	-1.94057175	2.42870314	-2.57058098
C	-2.24881081	0.13762644	-5.15741221
C	-1.37691254	0.04036911	-6.27241831
C	-0.00861906	0.01025874	0.61047142
C	-0.21111507	0.72410122	-6.69015211
C	0.60587632	1.74028657	-6.14172750
H	-1.61896795	-0.80844608	-6.91563707
H	0.22668269	0.28314033	-7.58769972
H	-3.00089647	-0.65496044	-5.13887278
H	-3.15500592	0.72352621	-3.36152439
H	-0.02075931	3.42112532	-3.15954104
H	1.45041497	3.16306797	-4.85105963
C	2.69238718	-0.93705868	-3.85901047
C	1.86539042	-1.87128999	-3.17869809
C	1.03445923	-2.50615877	-4.13986830
C	1.36307793	-1.97904087	-5.42152147
C	2.38811137	-1.01168385	-5.24795578
H	2.86455659	-0.43795204	-6.03835340

H	0.91896905	-2.27569987	-6.36814338
H	0.29765842	-3.28035602	-3.93470997
H	1.85399714	-2.04989163	-2.10688486
H	3.44274195	-0.29754866	-3.39930542
O	-0.03747243	-0.02841597	1.89376969



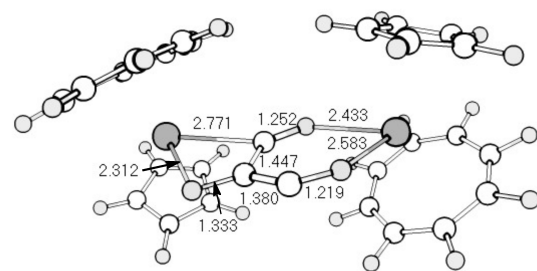
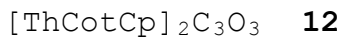
6

C	0.00000000	0.00000000	0.00020783
O	0.00000000	0.00000000	-1.32408230
C	0.00000000	1.15113668	0.88515473
O	0.00000000	1.29496290	2.13131497
C	0.00000000	-1.15113668	0.88515473
O	0.00000000	-1.29496290	2.13131497



6

C	0.14026688	-0.14268116	-0.00198927
C	1.59025796	-0.11591153	-0.00183332
C	0.84293657	1.12564414	-0.00466375
O	0.82021039	2.42765554	-0.00648172
O	-0.97523774	-0.81331042	0.00655386
O	2.73047946	-0.74325514	-0.00097750



60

Th	-0.31416502	-0.05789505	3.13625746
C	2.24103233	0.13647945	4.09584786
H	2.93163509	0.97265432	3.97089885
C	2.32091135	-0.80709582	3.03542905
C	1.61771458	-1.99165560	2.70334356
C	0.51184556	-2.69562234	3.24299295
H	0.18635962	-3.51075680	2.59376354
C	-0.35424410	-2.51547654	4.35019826
C	-0.42229627	-1.58189928	5.41967979
C	0.34698362	-0.45633191	5.81048427
C	1.44228538	0.25524795	5.26248718
H	1.66394221	1.16709992	5.81992688
H	-0.07300307	0.04344457	6.68586959
H	-1.28420381	-1.74774445	6.06854521
H	-1.18210222	-3.22647955	4.35679545
H	1.93517771	-2.40188152	1.74289014
H	3.04744451	-0.52341083	2.27227185
C	-1.68702358	2.23197011	2.18803710
C	-2.65586033	1.53528651	2.95528650
C	-2.28180407	1.62595711	4.32235702
C	-1.08033253	2.38060141	4.39895064
C	-0.71061446	2.75222271	3.07759379
H	0.15198125	3.35467452	2.79891798
H	-0.54653680	2.64067953	5.30850846
H	-2.82889399	1.21070322	5.16625252
H	-3.53476341	1.02779868	2.56667258
H	-1.69026713	2.34835701	1.10820324
C	-1.24304975	-1.46046583	-0.71702056
O	-1.35635635	-1.91054750	-1.96628907
Th	-0.09234336	-0.37868550	-3.14954072
C	0.58403507	2.28969662	-3.64669427
H	1.60926644	1.87216987	-5.41613723
C	-0.38195999	2.31708529	-2.60597503
C	-1.68906999	1.78591983	-2.45083475
C	-2.53550172	0.95434797	-3.22448026
H	-2.11326748	2.00505775	-1.46881944
C	-2.42783163	0.27750847	-4.46398218
C	-1.44111461	0.21050682	-5.48389001
C	-0.25381347	-0.45805379	-0.38486101
C	-0.17798670	0.82441874	-5.68227729
C	0.64711296	1.69729768	-4.93046106
H	-1.70479434	-0.48574819	-6.28265962
H	0.30777537	0.48520496	-6.59981555
H	-3.26775469	-0.39518777	-4.64592845
H	-3.44201181	0.67527410	-2.68338279
H	-0.03378208	2.84878359	-1.71861257
H	1.50489839	2.81091969	-3.37816033
C	2.69002081	-0.97722969	-2.75028628
C	1.98489904	-2.08791734	-2.21105253

C	1.39285990	-2.79908505	-3.28816053
C	1.72179071	-2.12380958	-4.49131267
C	2.52751097	-0.99737040	-4.15783543
H	2.95527575	-0.28935766	-4.86234680
H	1.43262330	-2.42598885	-5.49593137
H	0.78244840	-3.69433315	-3.20240162
H	1.92707067	-2.35880101	-1.16047216
H	3.26434113	-0.24655637	-2.18387822
O	-0.00965130	0.06527976	0.72561990
O	-1.96036280	-1.31977119	1.59690064
C	-1.96798818	-1.68829278	0.43464550

[ThCotCp]₂C₃O₃ **13***



60

Th	-0.29682600	-0.06277400	3.05756000
C	2.27206000	0.27821500	3.97970000
H	2.91710000	1.14788000	3.83828000
C	2.38374000	-0.66698700	2.92391000
C	1.74514000	-1.89334000	2.61706000
C	0.68926900	-2.65092000	3.18370000
H	0.40113600	-3.49333000	2.55145000
C	-0.16876600	-2.50545000	4.30156000
C	-0.27190000	-1.56726000	5.36467000
C	0.44254100	-0.40084200	5.73283000
C	1.48982000	0.36245800	5.15905000
H	1.67745000	1.28607000	5.71032000
H	0.01602220	0.08270420	6.61418000
H	-1.11210000	-1.77683000	6.02954000
H	-0.95794600	-3.25880000	4.32570000
H	2.07314000	-2.29844000	1.65793000
H	3.08019000	-0.34929500	2.14594000
C	-1.87377000	2.11883000	2.15741000
C	-2.74955000	1.37814000	2.99182000
C	-2.30182000	1.51787000	4.33157000
C	-1.14981000	2.34964000	4.32487000
C	-0.88384700	2.71910000	2.97977000
H	-0.07929810	3.36913000	2.64149000
H	-0.58187400	2.66013000	5.19721000
H	-2.76994000	1.08304000	5.21173000
H	-3.61041000	0.80214300	2.66284000
H	-1.94548000	2.21432000	1.07788000
C	-1.44429000	-1.54071000	-0.85537200
O	-1.60090000	-1.92780000	-2.09557000

Th	-0.14193200	-0.36789200	-3.12482000
C	0.67174900	2.26488000	-3.44919000
H	1.80603000	1.86769000	-5.15651000
C	-0.36684300	2.29644000	-2.48017000
C	-1.70050000	1.81370000	-2.43633000
C	-2.52208000	1.04400000	-3.29816000
H	-2.17997000	2.00857000	-1.47502000
C	-2.35431000	0.41767800	-4.55697000
C	-1.30289000	0.35736500	-5.51197000
C	-0.53886400	-0.56229100	-0.31023000
C	-0.00456967	0.92049800	-5.59612000
C	0.80389900	1.71998000	-4.74912000
H	-1.53843000	-0.29318700	-6.35673000
H	0.52896000	0.59581300	-6.49158000
H	-3.20407000	-0.21178900	-4.82701000
H	-3.47296000	0.77905500	-2.83156000
H	-0.05915720	2.76953000	-1.54605000
H	1.59274000	2.72937000	-3.09013000
C	2.56012000	-1.13657000	-2.58413000
C	1.76368000	-2.21239000	-2.10538000
C	1.19260000	-2.87069000	-3.22757000
C	1.62553000	-2.19667000	-4.39698000
C	2.47474000	-1.12498000	-3.99878000
H	2.98160000	-0.43235100	-4.66443000
H	1.37600000	-2.46661000	-5.42117000
H	0.53124300	-3.73263000	-3.19315000
H	1.64046000	-2.50009000	-1.06442000
H	3.14642000	-0.45373200	-1.97287000
O	0.01639630	0.10403100	0.63681700
O	-1.95823000	-1.37208000	1.63785000
C	-1.77240000	-1.47805000	0.40981000

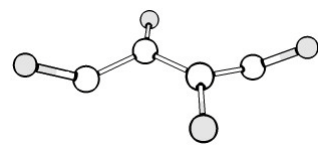
[UCotCp]₂C₃O₃ **14**

60

U	-0.00000000	0.09740550	-3.53307000
O	1.74893000	0.15688500	-1.74892000
C	0.73946000	0.09131550	-1.00558000
C	-0.73946000	0.09131550	-1.00558000
O	-1.74893000	0.15688500	-1.74892000
C	0.00000000	0.02770550	0.19208900
O	0.00000000	-0.00433450	1.45815000
U	0.00000000	-0.07165450	3.70498000
C	1.69427000	1.99760000	4.13259000
C	0.70398000	2.54942000	3.31243000
C	-0.70398000	2.54942000	3.31243000
C	-1.69427000	1.99760000	4.13259000
H	-2.70393000	2.16078000	3.73835000
C	-1.70136000	1.24542000	5.32549000
C	-0.70446000	0.76095500	6.19563000
C	0.70446000	0.76095500	6.19563000
C	1.70136000	1.24542000	5.32549000
H	2.71388000	0.97069500	5.64562000

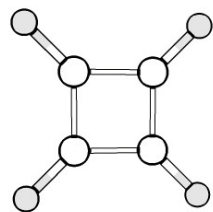
H	1.12340000	0.19916500	7.04037000
H	-1.12340000	0.19916500	7.04037000
H	-2.71388000	0.97069500	5.64562000
H	-1.11842000	3.04156000	2.42245000
H	1.11842000	3.04156000	2.42245000
C	0.69285000	-2.57522000	3.07920000
C	1.11670000	-2.42451000	4.37823000
C	0.00000000	-2.33907000	5.18589000
C	-1.11670000	-2.42451000	4.37823000
C	-0.69285000	-2.57522000	3.07920000
H	-1.31463000	-2.67766000	2.21943000
H	-2.12737000	-2.42029000	4.71096000
H	0.00000000	-2.25025000	6.24727000
H	2.12737000	-2.42029000	4.71096000
H	1.31463000	-2.67766000	2.21943000
C	-1.68388000	-2.05521000	-3.96064000
H	-2.68849000	-2.21708000	-3.56942000
C	-0.69712000	-2.56142000	-3.11383000
C	0.69712000	-2.56142000	-3.11383000
C	1.68388000	-2.05521000	-3.96064000
H	2.68849000	-2.21708000	-3.56942000
C	1.68812000	-1.31422000	-5.14575000
C	0.69897000	-0.79714400	-5.98871000
C	-0.69897000	-0.79714400	-5.98871000
C	-1.68812000	-1.31422000	-5.14575000
H	-2.69543000	-1.06035000	-5.47896000
H	-1.11507000	-0.22388400	-6.81949000
H	1.11507000	-0.22388400	-6.81949000
H	2.69543000	-1.06035000	-5.47896000
H	1.11559000	-3.03195000	-2.22157000
H	-1.11559000	-3.03195000	-2.22157000
C	-0.00000000	2.67906000	-2.77915000
C	1.13530000	2.54723000	-3.59257000
C	0.70116000	2.32380000	-4.90548000
C	-0.70116000	2.32380000	-4.90548000
C	-1.13530000	2.54723000	-3.59257000
H	-2.16075000	2.60489000	-3.25757000
H	-1.33512000	2.20110000	-5.77407000
H	1.33512000	2.20110000	-5.77407000
H	2.16075000	2.60489000	-3.25757000
H	-0.00000000	2.87778000	-1.71322000
H	2.70393000	2.16078000	3.73835000

[C₄O₄]²⁻ **15**



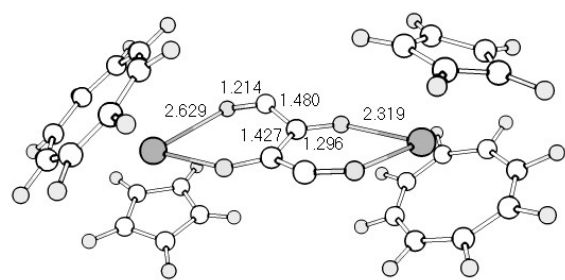
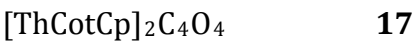
8

C	0.57010010	0.45081341	0.03881535
O	1.81333578	0.04247715	-0.00088274
C	-0.58768002	-0.44468851	-0.06534330
O	-1.83484444	-0.05260938	0.00240732
C	0.34979833	1.87383762	-0.08448610
O	0.59201978	2.91573125	0.53691691
C	-0.34242540	-1.80207676	-0.49548030
O	-0.55176081	-2.95945656	-0.11369228



8

C	0.32419026	0.58959382	0.81434753
O	0.71046410	1.29785305	1.79521731
C	-0.32959231	-0.74903133	0.66645821
O	-0.72832610	-1.64784749	1.47027700
C	0.33201236	0.74984080	-0.67339382
O	0.72771500	1.64996487	-1.47702641
C	-0.31917465	-0.58923069	-0.82156557
O	-0.70451258	-1.29657466	-1.80334119



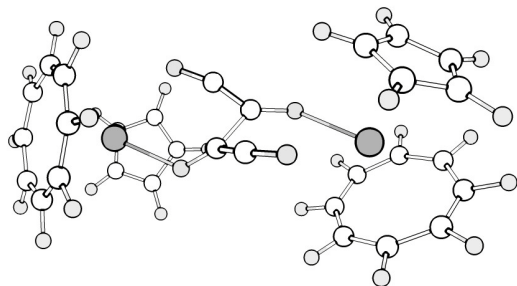
62

Th	-0.21205771	0.00158477	3.73857598
C	2.24368658	-0.24061348	4.93561434
H	3.03389295	0.51184523	4.97208378
C	2.32957826	-1.07253044	3.78893489
C	1.52826500	-2.10365611	3.23929549
C	0.29190182	-2.70964191	3.57230638
H	-0.05725650	-3.39615137	2.79839907

C	-0.64829515	-2.55918350	4.62525784
C	-0.69634870	-1.77991133	5.81225875
C	0.14282235	-0.80256465	6.39971081
C	1.34405354	-0.14835628	6.03032455
H	1.60554921	0.66070970	6.71515068
H	-0.29850205	-0.37067705	7.30023191
H	-1.62419021	-1.92592476	6.36881126
H	-1.54563589	-3.16301960	4.47811911
H	1.89903939	-2.43649225	2.26734015
H	3.15915284	-0.79685538	3.13559209
C	-1.74738133	2.28484686	3.05529281
C	-2.65543511	1.46986265	3.77944597
C	-2.24486590	1.45408405	5.13846151
C	-1.08167992	2.26087160	5.25342358
C	-0.77367177	2.77388801	3.96474964
H	0.05171807	3.43813263	3.71711558
H	-0.53341086	2.46173173	6.17007917
H	-2.74145778	0.92992859	5.95155961
H	-3.51801411	0.95408179	3.36513133
H	-1.78837864	2.49931188	1.99026456
C	-0.53899877	-0.34659885	-0.34090388
O	-0.54438647	-0.59417700	-1.61972364
Th	0.18085545	-0.04845597	-3.73862421
C	0.32179983	2.46413209	-4.85138842
H	1.47086597	1.81525792	-6.48037250
C	-0.68809707	2.57708551	-3.86040078
C	-1.84666906	1.83709706	-3.51921657
C	-2.47375940	0.66108732	-4.00019970
H	-2.30911927	2.20041481	-2.59880528
C	-2.21587604	-0.24856907	-5.05843713
C	-1.25293575	-0.31172698	-6.10134670
C	0.40054150	0.48754085	0.33516089
C	-0.12959268	0.46456690	-6.47942335
C	0.54013854	1.59577081	-5.95328880
H	-1.36916310	-1.20519427	-6.71794272
H	0.41426739	0.01876771	-7.31460541
H	-2.89832494	-1.10064820	-5.05936450
H	-3.29221853	0.33306732	-3.35694091
H	-0.47454928	3.36895205	-3.14020983
H	1.12284500	3.19448838	-4.72158185
C	2.82425555	-1.10632825	-3.56713903
C	2.02445714	-1.98328423	-2.78956312
C	1.17698602	-2.70412762	-3.67161494
C	1.45689516	-2.27448870	-4.99644234
C	2.47460237	-1.28620848	-4.93188900
H	2.91584795	-0.76821350	-5.77998359
H	0.98378076	-2.64532870	-5.90235016
H	0.45257821	-3.46257615	-3.38260357
H	2.05348422	-2.08753787	-1.70794119
H	3.58239524	-0.42687731	-3.18483510
O	0.50907378	0.61244365	1.62077022

O	-1.73464730	-0.76202244	1.74848572
C	-1.63172799	-0.77154853	0.53747361
C	1.16854620	1.35816754	-0.58324739
O	1.34811296	1.25993782	-1.77988968

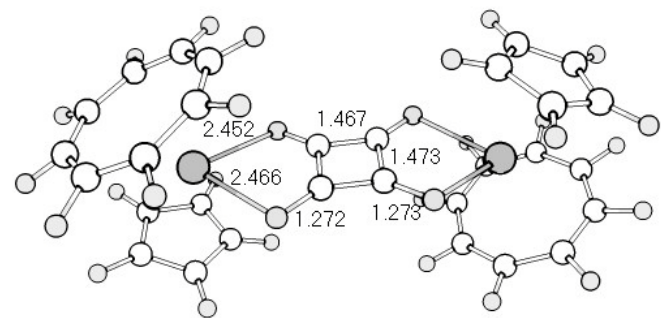
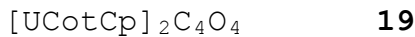
[ThCotCp]₂C₄O₄ **18***



62

Th	-0.15715200	0.08207870	3.68440000
C	2.05913000	-1.07182000	4.81307000
H	3.03388000	-0.60489800	4.96768000
C	1.94752000	-1.71102000	3.55043000
C	0.90336300	-2.35716000	2.84682000
C	-0.47489300	-2.59717000	3.07445000
H	-0.97518700	-3.02021000	2.20079000
C	-1.37680000	-2.33450000	4.13952000
C	-1.24147000	-1.77865000	5.44082000
C	-0.17649200	-1.20659000	6.17678000
C	1.17824000	-0.88536000	5.91039000
H	1.63548000	-0.30607300	6.71471000
H	-0.50757800	-0.81266100	7.13949000
H	-2.19391000	-1.72920000	5.97266000
H	-2.40531000	-2.61034000	3.89997000
H	1.20356000	-2.62747000	1.83253000
H	2.84846000	-1.59540000	2.94550000
C	-0.99147100	2.76676000	3.41105000
C	-2.05537000	2.16027000	4.12988000
C	-1.58702000	1.85206000	5.43216000
C	-0.23104900	2.26992000	5.52038000
C	0.13505900	2.83879000	4.27215000
H	1.10324000	3.26468000	4.02013000
H	0.40524000	2.18581000	6.39781000
H	-2.16647000	1.38900000	6.22716000
H	-3.05330000	1.96657000	3.74501000
H	-1.03415000	3.11944000	2.38343000
C	-0.59050500	-0.02160350	-0.40828500
O	-0.40475800	-0.71866200	-1.51374000
Th	0.16910000	-0.04370430	-3.67645000
C	-0.37454400	2.24844000	-5.08881000
H	0.99289500	1.78560000	-6.60968000
C	-1.42293000	2.17372000	-4.13696000
C	-2.33012000	1.16707000	-3.72112000
C	-2.56333000	-0.18808100	-4.06124000
H	-2.92494000	1.48243000	-2.86106000
C	-1.99422000	-1.09787000	-4.98954000
C	-1.00023000	-0.99600900	-5.99924000

C	0.33855600	0.82086400	0.42717100
C	-0.13813600	0.03074960	-6.46010000
C	0.14145500	1.36242000	-6.07279000
H	-0.81595000	-1.94918000	-6.49863000
H	0.55465200	-0.32863700	-7.22375000
H	-2.39597000	-2.10856000	-4.89276000
H	-3.28406000	-0.66649600	-3.39588000
H	-1.47927000	3.06588000	-3.51182000
H	0.17362400	3.19120000	-5.03870000
C	2.99756000	-0.20186200	-3.35429000
C	2.47621000	-1.19146000	-2.48142000
C	1.93062000	-2.23507000	-3.27379000
C	2.11825000	-1.89157000	-4.63899000
C	2.77651000	-0.63369800	-4.68983000
H	3.07481000	-0.10605400	-5.59199000
H	1.82404000	-2.49192000	-5.49642000
H	1.45812000	-3.14005000	-2.89832000
H	2.48493000	-1.15746000	-1.39536000
H	3.49750000	0.71558500	-3.05217000
O	0.80723300	0.67432700	1.65149000
O	-2.02752000	0.36000300	1.61079000
C	-1.49574000	0.21045900	0.52732000
C	0.46707700	1.58268000	-0.64297900
O	0.60955300	1.96982000	-1.78646000



62

U	0.99459492	-2.84081328	-2.96240405
O	0.46162384	-0.65825530	-1.98096676
C	0.22175303	-0.90291556	-0.75515186
C	0.45914751	-2.16992585	-0.04291468
O	0.93724031	-3.24277570	-0.53053307
C	-0.05650603	-1.57141641	1.19360919
O	-0.29637684	-1.81607667	2.41942409
C	-0.29390051	-0.30440612	0.48137201
O	-0.77199331	0.76844372	0.96899040
U	-0.82934792	0.36648131	3.40086138
C	0.77527514	-4.62485027	-5.03000281
C	0.40999283	-5.33751763	-3.86373661
C	-0.47669480	-5.07689270	-2.76427431
C	-1.38505374	-4.03591701	-2.45608067

C	-1.71570770	-2.78998673	-3.03403093
C	-1.27578801	-2.03538813	-4.15860702
C	-0.37592216	-2.27326520	-5.22023732
C	0.45464463	-3.36002055	-5.58640252
H	1.06252332	-3.13603793	-6.46805520
H	-0.24316466	-1.40125425	-5.86899167
H	-1.67312511	-1.01777704	-4.15445512
H	-2.38450701	-2.20720046	-2.39615131
H	-1.85188805	-4.17453028	-1.47850904
H	-0.39938290	-5.82701957	-1.97149547
H	0.99596786	-6.25038325	-3.71638427
H	1.56843736	-5.12915979	-5.59064785
C	-0.61002814	2.15051829	5.46846014
C	-0.24474583	2.86318566	4.30219394
C	0.64194180	2.60256073	3.20273165
C	1.55030074	1.56158504	2.89453800
C	1.88095470	0.31565476	3.47248826
C	1.44103501	-0.43894385	4.59706436
C	0.54116916	-0.20106677	5.65869465
C	-0.28939763	0.88568858	6.02485986
H	-0.89727632	0.66170596	6.90651253
H	0.40841166	-1.07307773	6.30744900
H	1.83837211	-1.45655493	4.59291246
H	2.54975401	-0.26713151	2.83460864
H	2.01713505	1.70019831	1.91696637
H	0.56462990	3.35268760	2.40995280
H	-0.83072086	3.77605127	4.15484160
H	-1.40319036	2.65482782	6.02910518
C	3.59656595	-3.27300977	-2.20630626
C	3.56761399	-3.59977104	-3.58888795
C	3.34619869	-2.39548263	-4.31756734
C	3.23897777	-1.32701650	-3.38953697
C	3.39305697	-1.87130900	-2.08619561
H	3.35739028	-1.30892401	-1.15312765
H	3.06112156	-0.27797377	-3.62760228
H	3.28993376	-2.30982264	-5.40246730
H	3.70704430	-4.59220266	-4.01745618
H	3.73656042	-3.96873756	-1.37884417
C	-3.43131895	0.79867780	2.64476360
C	-3.40236699	1.12543906	4.02734528
C	-3.18095169	-0.07884934	4.75602467
C	-3.07373077	-1.14731548	3.82799430
C	-3.22780997	-0.60302297	2.52465294
H	-3.19214328	-1.16540796	1.59158498
H	-2.89587456	-2.19635820	4.06605961
H	-3.12468676	-0.16450933	5.84092463
H	-3.54179730	2.11787069	4.45591351
H	-3.57131342	1.49440559	1.81730150

