Electronic Supplementary Information

Mechanistic Aspects of Acetone Addition to Metalloaromatic Complexes of Iridium: A DFT Investigation

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Computational Details:

All calculations were carried out using Gaussian 98 Revision A11[1] running on Compaq ES40 and XP1000 workstations in our group, on the SGI Origin computers of the Faculty of Chemistry and the (Israel) Inter-University Computing Center and on a mini-farm belonging to our group consisting of four Intel Pentium IV and four Intel dual Xeon 2.0 GHz PC's running Red Hat Linux 7.2.

The mPW1K (modified Perdew-Wang 1-parameter for kinetics) DFT exchange-correlation functional of Truhlar and coworkers[2] was used to investigate the reaction. This functional is based on the Perdew-Wang exchange functional[3] with Adamo and Barone's modified enhancement factor[4] and the Perdew-Wang correlation functional.[3] A larger percentage of Hatree-Fock exchange has been introduced[2] to circumvent the underestimated barrier heights typical of standard exchange-correlation functionals. It has been shown (e.g., refs[2, 5-7]) that this functional generally yields much more reliable reaction barrier heights than B3LYP or other "conventional" exchange-correlation functionals. With this functional, two basis set-RECP (relativistic effective core potential) combinations were used. The first, denoted SDD, is the combination of the Huzinaga-Dunning double-ζ basis set on lighter elements with the Stuttgart-Dresden basis set-RECP combination[8] on transition metals. The second, denoted SDB-cc-pVDZ, combines the Dunning cc-pVDZ basis set[9] on the main group elements and the Stuttgart-Dresden basis set-RECP on the transition metals with an added *f*-type polarisation exponent taken as the geometric average of the two *f*-exponents given in the Appendix to Ref.[10] Geometry optimisations were carried out using the former basis set while the energetics of the reaction were calculated at these geometries with the latter basis set; this level of theory is conventionally denoted as mPW1K/SDB-cc-pVDZ//mPW1K/SDD. We have previously recommended this level of theory as better suited than the more popular B3LYP[11, 12]/LANL2DZ[13] to investigate reaction mechanisms.[7] Since Gaussian 98 uses the same number of radial grid points throughout the periodic table, the "ultrafine" grid, i.e., a pruned (99,590) grid, was used throughout the calculations as recommended in Ref.[14] The identities of the transition states were confirmed by performing intrinsic reaction coordinate(IRC) calculations.[15-17]

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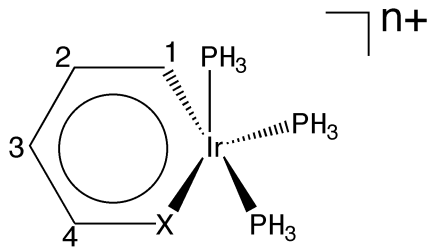
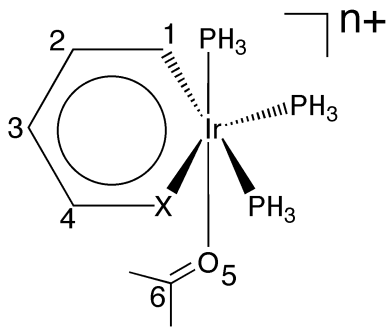
Key Geometric Data for Calculated Structures:



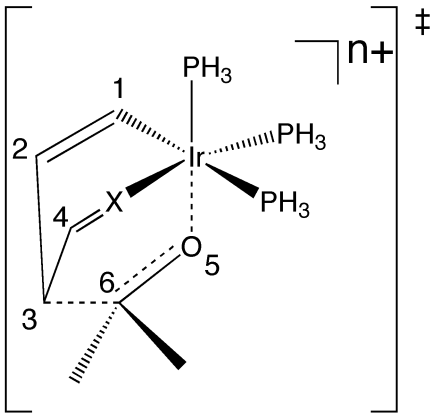
3C: X = CH, n = 0
3O: X= O, n = 1
3S: X = S, n = 1

Bond Length (Å) / Angle (°)	**3C**	**3O**	**3S**
Ir—C1	1.970	1.957	1.985
C1—C2	1.395	1.395	1.380
C2—C3	1.398	1.407	1.421
C3—C4	1.398	1.382	1.366
C4—X	1.395	1.308	1.375
Ir—X	1.970	1.997	2.310
Ir—C3	3.465	3.400	3.602
Ir—C1—C2	130.2	125.2	131.2
C1—C2—C3	123.8	126.8	129.0
C2—C3—C4	123.2	123.0	126.8
C3—C4—X	123.8	124.2	126.5
C4—X—Ir	130.2	129.9	112.7
C1—Ir—X	87.5	89.8	92.6



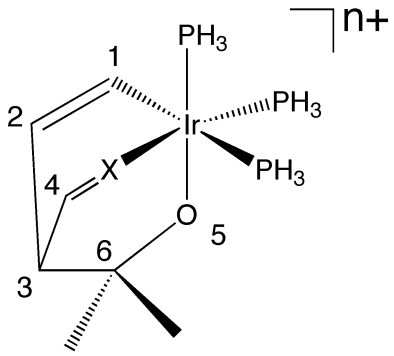
4C: X = CH, n = 0
4O: X= O, n = 1
4S: X = S, n = 1

Bond Length (Å) / Angle (º)	**4C**	**4O**	**4S**
Ir—C1	1.969	2.035	2.040
C1—C2	1.396	1.357	1.356
C2—C3	1.398	1.451	1.454
C3—C4	1.398	1.358	1.351
C4—X	1.396	1.345	1.777
Ir—X	1.969	2.030	2.392
Ir—O5	3.991	2.131	2.140
O5—C6	1.241	1.256	1.256
C3—C6	5.250	4.423	4.693
Ir—C1—C2	130.2	123.5	129.6
C1—C2—C3	123.9	126.3	129.0
C2—C3—C4	123.2	124.7	128.1
C3—C4—X	123.9	126.8	128.5
C4—X—Ir	130.2	124.7	108.3
C1—Ir—X	87.7	91.6	93.8
Ir—O5—C6	76.9	137.4	138.0
C3—C6—O5	126.4	76.2	76.4
C1—Ir—O5	100.1	92.6	93.2
X—Ir—O5	100.1	91.4	92.3



5C: X = CH, n = 0
5O: X = O, n = 1
5S: X = S, n = 1

Bond Length (Å) / Angle (°)	**5C**	**5O**	**5S**
Ir—C1	2.012	2.026	2.033
C1—C2	1.371	1.347	1.342
C2—C3	1.419	1.464	1.477
C3—C4	1.419	1.391	1.392
C4—X	1.371	1.301	1.718
Ir—X	2.011	2.056	2.411
Ir—O5	2.411	2.107	2.092
O5—C6	1.277	1.313	1.325
C3—C6	2.689	2.258	2.090
Ir—C1—C2	124.1	119.6	122.2
C1—C2—C3	125.1	124.0	125.2
C2—C3—C4	122.0	120.8	121.0
C3—C4—X	125.1	125.2	126.3
C4—X—Ir	124.1	119.8	102.1
C1—Ir—X	90.4	89.7	89.9
Ir—O5—C6	128.0	129.6	131.1
C3—C6—O5	101.0	102.7	105.3
C1—Ir—O5	83.0	89.9	90.0
X—Ir—O5	83.0	81.0	82.7



6C: X = CH, n = 0
6O: X = O, n = 1
6S: X = S, n = 1

Bond Length (Å) / Angle (°)	**6C**	**6O**	**6S**
Ir—C1	2.036	2.028	2.034
C1—C2	1.340	1.341	1.339
C2—C3	1.515	1.519	1.520
C3—C4	1.515	1.489	1.482
C4—X	1.340	1.255	1.667
Ir—X	2.356	2.088	2.399
Ir—O5	2.052	2.038	2.045
O5—C6	1.434	1.433	1.426
C3—C6	1.563	1.579	1.585
Ir—C1—C2	118.4	117.5	120.1
C1—C2—C3	119.8	120.3	121.7
C2—C3—C4	109.0	107.1	108.8
C3—C4—X	119.8	122.2	124.8
C4—X—Ir	118.4	117.9	101.2
C1—Ir—X	86.5	85.8	87.7
Ir—O5—C6	121.9	121.8	124.4
C3—C6—O5	111.2	110.8	111.5
C1—Ir—O5	87.6	89.9	90.6
X—Ir—O5	87.6	85.3	85.9

Cartesian Coordinates of Calculated Structures:

Geometry of complex: 3C

23
Stoichiometry = C5H14IrP3

H	-0.838610	0.471205	-2.436350
C	-1.187523	0.466486	-1.397894
C	-2.643063	0.631178	1.151141
Ir	0.141352	0.079413	0.004256
C	-2.569353	0.631729	-1.307149
C	-3.268035	0.690204	-0.097835
C	-1.269150	0.465876	1.324442
H	-0.639229	-2.820341	-1.095796
H	-3.138572	0.769474	-2.219768
H	-4.340779	0.836015	-0.129968
H	-0.983083	0.470124	2.381939
H	-3.265940	0.768521	2.028078
H	1.167537	-3.115991	0.034329
P	0.044882	-2.233584	0.000841
H	-0.703742	-2.820820	1.054225
P	1.833647	0.406172	-1.672475
P	1.730139	0.405391	1.779518
H	2.762676	1.471534	-1.503028
H	1.329859	0.769680	-2.951374
H	2.785946	-0.567432	-2.113463
H	2.667643	1.470812	1.666519
H	2.654314	-0.568429	2.276332
H	1.150626	0.768332	3.026098

Geometry of complex: 3O

22
Stoichiometry = C4H13IrOP3

H	1.155675	0.395500	3.088293
O	-1.153335	0.432837	-1.423041
C	-2.614369	0.708352	1.049711
Ir	0.140448	0.106568	0.063170
C	-2.455241	0.553478	-1.390568
C	-3.192563	0.709335	-0.232590
C	-1.282999	0.435087	1.365165
H	-0.694861	-2.703450	-1.030800
H	-2.932136	0.567588	-2.361349
H	-4.253250	0.871440	-0.332564
H	-1.081535	0.397584	2.433984
H	-3.279254	0.946382	1.870920
H	1.331822	-2.904118	-0.199049
P	0.126671	-2.189690	-0.003197
H	-0.398836	-2.822066	1.143222
P	1.778549	0.348755	-1.766158
P	1.706774	0.307274	1.789012
H	2.714043	1.408840	-1.702327
H	1.090858	0.667766	-2.957982
H	2.635961	-0.686003	-2.220714
H	2.528398	1.457490	1.763079
H	2.686427	-0.697974	1.980396

Geometry of complex: 3S

22
Stoichiometry = C4H13IrP3S1

H	0.728697	0.871484	2.840339
S	-0.832485	1.453733	-1.299236
C	-2.691574	0.269595	1.101673
Ir	0.115507	-0.238322	-0.045047
C	-2.333960	2.017494	-0.638420
C	-3.050674	1.430127	0.365146
C	-1.516893	-0.453450	1.064177
H	0.780462	-3.416691	-0.197043
H	-2.712399	2.898967	-1.131325
H	-3.997907	1.887811	0.613618
H	-1.506874	-1.261585	1.795471
H	-3.455938	-0.086357	1.781837
H	2.140858	-2.532959	1.246034
P	0.829260	-2.358277	0.739926
H	0.060536	-2.899655	1.796589
P	1.902155	-0.164566	-1.741294
P	1.213298	1.005207	1.522627
H	3.245926	0.116646	-1.386427
H	1.691972	0.807732	-2.746879
H	2.105532	-1.319301	-2.533946
H	1.129653	2.396835	1.307929
H	2.603102	0.810085	1.695886

Geometry of complex: 4C

33
Stoichiometry = C8H20IrOP3

C	0.290834	1.467296	-1.227760
Ir	0.559063	0.003244	0.061799
O	-2.831133	-2.033174	-0.473398
C	-3.216117	-0.854675	-0.422035
C	-3.295123	0.000856	-1.653404
C	-0.006642	1.252445	1.475267
C	-0.227947	2.630062	1.425519
C	-0.190155	3.383470	0.248039
C	0.040393	2.823863	-1.012593
P	2.857392	0.078117	0.320794
P	0.075499	-1.796039	1.591790
P	0.448763	-1.526587	-1.798176
C	-3.574043	-0.200736	0.881305
H	0.261801	-0.903596	-3.062847
H	3.329777	0.696009	1.508470
H	-0.478797	3.151302	2.343102
H	-0.386305	4.446794	0.310972
H	0.432074	1.236413	-2.289649
H	-0.015114	3.486182	-1.869813
H	3.724465	-1.056798	0.324451
H	3.564155	0.868275	-0.623462
H	-0.983661	-2.674777	1.240665
H	-0.391008	-1.374917	2.867522
H	1.007606	-2.781242	2.045393
H	-0.645833	-2.431229	-1.825888
H	1.473860	-2.444590	-2.187600
H	-4.243466	0.533378	-1.703279
H	-3.164693	-0.603702	-2.545762
H	-2.496571	0.743052	-1.601092

```
H   -3.629396  -0.939433   1.675074
H   -4.519633   0.333905   0.807557
H   -2.795785   0.526496   1.119487
H   -0.094282   0.856238   2.493208
```

Geometry of complex: 4O

```
32
Stoichiometry = C7H19IrO2P3
H    0.733211  -1.450958  -3.000050
O   -0.014408   1.181015   1.379862
C    0.126814   2.506930  -1.300303
Ir   0.339386  -0.217139  -0.049168
C    0.066090   2.509902   1.188409
C    0.139679   3.157767  -0.003010
C    0.179376   1.170781  -1.528865
H    2.609962   1.838689   0.321564
H    0.048460   3.069030   2.115226
H    0.177614   4.235143   0.024487
H    0.152416   0.843014  -2.565127
H    0.056207   3.170216  -2.154501
H    3.411426  -0.127358   0.943709
P    2.534565   0.465646   0.006221
H    3.277149   0.365686  -1.188418
P    0.418150  -1.695587   1.922258
P    0.588837  -1.897066  -1.664564
H   -0.538021  -2.731126   2.062113
H    0.173403  -0.939025   3.091054
H    1.586924  -2.401089   2.302463
H   -0.520350  -2.765937  -1.778092
H    1.653063  -2.825311  -1.577658
O   -1.731088  -0.710631  -0.155524
C   -2.830702  -0.119685  -0.016343
C   -4.079924  -0.910622  -0.205591
C   -2.940476   1.318908   0.340837
H   -3.950250   1.685437   0.191801
H   -2.232903   1.915817  -0.227494
H   -2.670068   1.442432   1.389832
H   -3.865689  -1.960385  -0.368345
H   -4.629002  -0.514722  -1.060859
H   -4.730719  -0.791718   0.660042
```

Geometry of complex: 4S

```
32
Stoichiometry = C7H19IrOP3S1
C    0.027080   0.914902  -1.685891
Ir   0.324518  -0.296804  -0.072395
O   -1.750098  -0.797825   0.085319
C   -2.853855  -0.200494   0.141698
C   -2.999336   1.275960   0.044873
S    0.112884   1.486498   1.507055
C    0.248917   3.027226   0.632338
C    0.220802   3.243234  -0.700999
C    0.045121   2.268128  -1.764653
P    2.514036   0.374862  -0.247500
P    0.581590  -1.692993   1.934063
P    0.439199  -2.140642  -1.554838
```

```
C   -4.084447  -1.022957   0.329415
H    0.379359  -1.828047  -2.934455
H    2.632982   1.775610  -0.351734
H    0.352053   3.863045   1.308093
H    0.306694   4.273334  -1.019777
H   -0.148148   0.411524  -2.635659
H   -0.106994   2.707233  -2.744223
H    3.382560   0.059200   0.821060
H    3.248843  -0.085900  -1.363677
H   -0.318487  -2.771653   2.111895
H    0.402332  -0.992848   3.150876
H    1.807347  -2.351778   2.200484
H   -0.619223  -3.071752  -1.437620
H    1.557218  -3.008198  -1.530136
H   -3.992099   1.543394  -0.304918
H   -2.236152   1.712465  -0.589084
H   -2.864253   1.701261   1.041201
H   -3.842002  -2.060648   0.526811
H   -4.699141  -0.961047  -0.569525
H   -4.684250  -0.617074   1.142852
```

Geometry of complex: 5C

```
33
Stoichiometry = C8H20IrOP3
C    0.337815   1.064590   1.448017
Ir  -0.598502   0.049423  -0.014556
O    1.412519  -1.279238   0.021996
C    2.622202  -0.873135   0.056793
C    3.414600  -0.856690  -1.221735
C    1.553816   1.680670   1.298167
C    2.266147   1.792494   0.076184
C    1.616327   1.707061  -1.182227
C    0.409747   1.094959  -1.406198
P   -1.185788  -1.422957  -1.820219
P   -1.275207  -1.460699   1.727519
P   -2.285925   1.545210  -0.041176
C    3.349210  -0.884301   1.373659
H    2.153715   2.108787  -2.036164
H    2.047297   2.063859   2.186435
H   -0.109008   1.104317   2.444149
H    3.251016   2.241935   0.105787
H    4.248660  -0.275289   1.354341
H    3.713222  -1.881633  -1.466568
H    4.311607  -0.248705  -1.144212
H    2.788179  -0.488312  -2.029339
H    3.635670  -1.914377   1.611374
H    2.682724  -0.532835   2.156346
H   -0.318869  -2.542548  -1.931207
H   -1.033442  -0.896021  -3.131060
H   -2.425220  -2.105039  -2.008518
H   -3.647910   1.140560  -0.079752
H   -2.280801   2.466983  -1.116964
H   -2.335417   2.443972   1.052802
H   -0.414390  -2.582870   1.858198
H   -2.522192  -2.145952   1.838608
H   -1.189353  -0.961836   3.055277
H    0.013640   1.156098  -2.422500
```

Geometry of complex: 5O

32
Stoichiometry = C7H19IrO2P3

H	-2.192533	-0.118313	-2.762347
C	-1.648741	-0.456929	-1.887799
C	-1.494108	-2.148097	-0.077191
H	-1.960277	-3.092271	0.173943
C	-0.273193	-1.846366	0.405047
O	-0.435622	0.005250	-1.795158
C	-2.275358	-1.262531	-0.942415
Ir	0.535719	-0.029665	0.016712
P	1.165918	2.266193	-0.593142
H	0.241743	-2.587823	1.010659
C	-2.500757	0.509803	0.438429
H	-3.283065	-1.567245	-1.183242
H	-4.108968	-0.699976	1.227355
P	1.325170	0.038957	2.197103
P	2.323989	-1.106564	-0.953154
O	-1.258598	0.893467	0.622149
C	-3.172809	-0.252951	1.546889
C	-3.373366	1.458261	-0.345574
H	-3.695035	2.251902	0.332698
H	-4.264804	0.970526	-0.728355
H	-2.823187	1.920159	-1.158629
H	-3.396495	0.466415	2.338981
H	-2.519426	-1.013949	1.957314
H	0.449950	3.259308	0.113736
H	0.795017	2.566251	-1.923827
H	2.473619	2.810373	-0.553796
H	3.602983	-0.504616	-0.935809
H	2.115274	-1.323628	-2.332113
H	2.613975	-2.406923	-0.485505
H	0.446024	0.740778	3.051216
H	2.567290	0.640404	2.506453
H	1.445136	-1.202867	2.862131

Geometry of complex: 5S

32
Stoichiometry = C7H19IrOP3S1

H	-2.699071	-0.400588	-2.608848
C	-1.985547	-0.629068	-1.829410
C	-1.521498	-2.125804	0.115833
H	-1.956656	-3.072852	0.409749
C	-0.256054	-1.832574	0.451391
S	-0.396960	-0.057023	-2.146496
C	-2.421228	-1.250216	-0.661835
Ir	0.576927	-0.019799	0.058715
P	1.264204	2.264438	-0.489614
H	0.308666	-2.592139	0.988264
C	-2.476746	0.472801	0.519078
H	-3.461505	-1.550084	-0.671929
H	-3.971671	-0.652082	1.615789
P	1.193703	0.102774	2.313378
P	2.464685	-1.115315	-0.701519
O	-1.228341	0.917130	0.547744
C	-3.010198	-0.173378	1.777490
C	-3.444106	1.396025	-0.186928

```
H   -3.658461   2.232759   0.480210
H   -4.385906   0.904046  -0.414806
H   -3.005403   1.798103  -1.094288
H   -3.153746   0.626489   2.507585
H   -2.310790  -0.892256   2.188023
H    0.211852   3.164857  -0.211542
H    1.523404   2.562726  -1.848146
H    2.357633   2.925018   0.124301
H    3.743385  -0.616452  -0.359054
H    2.568415  -1.217004  -2.106309
H    2.577635  -2.468280  -0.309853
H    0.260502   0.841273   3.074060
H    2.415556   0.699325   2.705647
H    1.244242  -1.118187   3.024682
```

Geometry of complex: 6C

```
33
Stoichiometry = C8H20IrOP3
C   -0.619212   1.722629   0.543293
Ir  -0.428771  -0.278997   0.220756
O    1.563521   0.057438  -0.138334
C    2.014117   1.162204  -0.934016
C    2.806716   0.597768  -2.116484
C    0.022925   2.564123  -0.278620
C    0.810522   2.015464  -1.450831
C   -0.104461   1.158852  -2.301968
C   -0.763270   0.133197  -1.745200
P    0.185165  -2.514256  -0.464247
P    0.371346  -0.459182   2.494477
P   -2.705046  -0.528310   0.537221
C    2.935951   2.022551  -0.065079
H   -0.202708   1.401197  -3.353575
H    0.000018   3.637732  -0.133362
H   -1.194392   2.119824   1.380022
H    1.215590   2.834341  -2.045064
H    3.353271   2.860011  -0.628003
H    3.628991  -0.009506  -1.738960
H    3.220184   1.393155  -2.740008
H    2.167067  -0.033398  -2.729407
H    3.757566   1.408211   0.302316
H    2.388844   2.411580   0.790795
H    1.582605  -2.550543  -0.688414
H   -0.280556  -2.977764  -1.723543
H    0.018044  -3.724976   0.268255
H   -3.269843  -1.584076   1.306005
H   -3.494983  -0.665942  -0.634815
H   -3.383298   0.565189   1.137928
H    1.782383  -0.343750   2.487528
H    0.214961  -1.559034   3.386778
H    0.041346   0.582070   3.402476
H   -1.429601  -0.475565  -2.356857
```

Geometry of complex: 6O

32
Stoichiometry = C7H19IrO2P3

H	-0.304165	1.298046	-3.338569
C	-0.133179	1.122412	-2.280128
C	-0.025886	2.559722	-0.336969
H	-0.096156	3.635989	-0.270354
C	-0.609632	1.739050	0.547876
O	-0.753950	0.161809	-1.762942
C	0.782003	1.991523	-1.490845
Ir	-0.402058	-0.256914	0.252630
P	0.182584	-2.550946	-0.392915
H	-1.166675	2.163272	1.378137
C	2.009227	1.138216	-0.981219
H	1.158246	2.784643	-2.129042
H	3.308300	2.863793	-0.695295
P	0.333362	-0.464613	2.427803
P	-2.699496	-0.573052	0.616974
O	1.564101	0.019338	-0.204954
C	2.911221	2.023032	-0.126816
C	2.782136	0.590748	-2.183905
H	3.626646	0.007205	-1.826000
H	3.164259	1.391535	-2.816638
H	2.161638	-0.071781	-2.788221
H	3.747855	1.425015	0.228104
H	2.374010	2.406348	0.736770
H	1.500102	-2.906028	-0.028298
H	0.248277	-2.710670	-1.795738
H	-0.525326	-3.725402	-0.036024
H	-3.173093	-1.786775	1.168017
H	-3.474111	-0.492616	-0.563080
H	-3.362013	0.367658	1.439120
H	1.743007	-0.410580	2.449592
H	0.044923	-1.623343	3.185152
H	-0.040581	0.557872	3.327101

Geometry of complex: 6S

32
Stoichiometry = C7H19IrOP3S1

H	0.050196	1.699456	-3.399942
C	0.050772	1.378634	-2.366078
C	0.035502	2.575558	-0.238455
H	-0.046784	3.647531	-0.124088
C	-0.599210	1.721853	0.574033
S	-0.926009	0.075669	-2.009875
C	0.905344	2.088137	-1.384882
Ir	-0.399908	-0.283937	0.302892
P	0.212219	-2.600983	-0.201392
H	-1.200143	2.126360	1.384521
C	2.069049	1.142082	-0.872461
H	1.376087	2.933360	-1.879546
H	3.370603	2.803693	-0.326307
P	0.474631	-0.385859	2.464255
P	-2.650604	-0.608531	0.878306
O	1.551952	-0.035366	-0.255530
C	2.918598	1.922730	0.128672
C	2.924219	0.696815	-2.060409
H	3.732908	0.066252	-1.699027

H	3.362072	1.547493	-2.582369
H	2.339860	0.108540	-2.766635
H	3.718126	1.274795	0.482518
H	2.325910	2.240752	0.982910
H	1.567713	-2.848227	0.108315
H	0.193202	-2.947294	-1.571993
H	-0.412662	-3.744726	0.354910
H	-3.008043	-1.717361	1.681790
H	-3.560201	-0.762364	-0.193990
H	-3.265970	0.445590	1.593594
H	1.883715	-0.409061	2.399802
H	0.181866	-1.469649	3.325949
H	0.215627	0.715958	3.309120