Supporting Information

Mechanistic Investigations *via* DFT Support the Cooperative Heterobimetallic C-H and O-H Bond Activation Across Ta=Ir Multiple Bonds

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Content

A. Experimental characterizations data

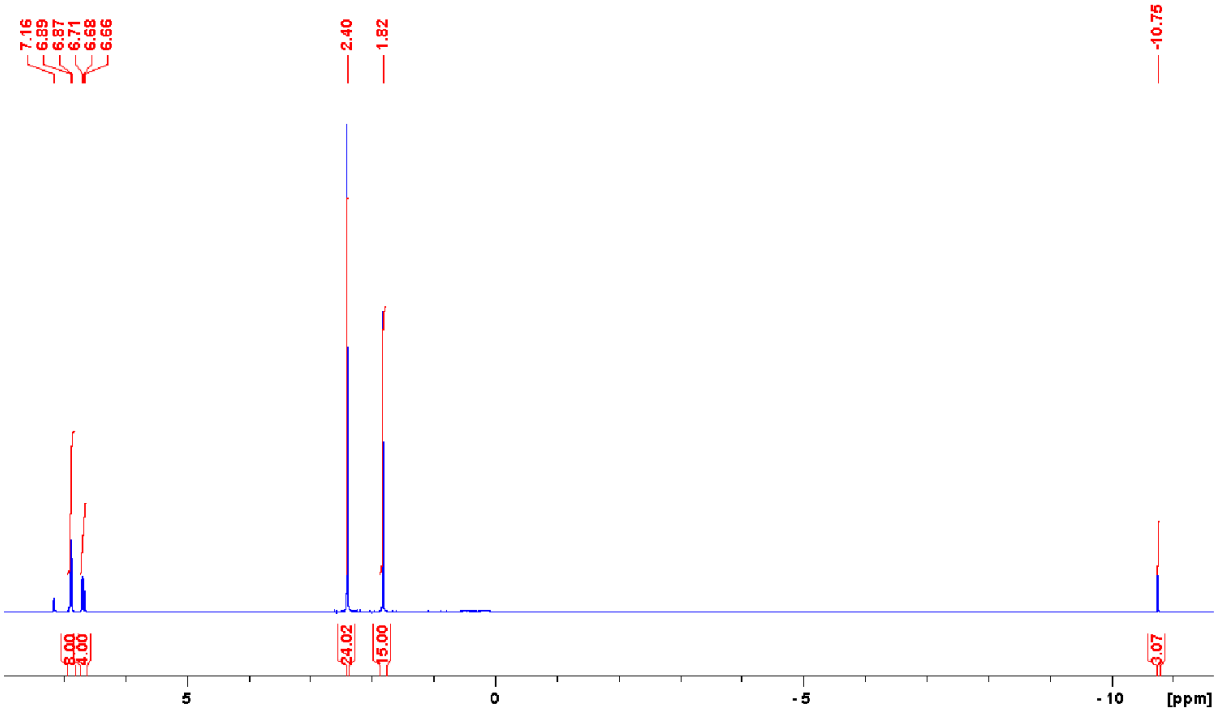

Figure S1. ^{1}H NMR spectrum (293K, 500 MHz, C_6D_6) of compound **4.**

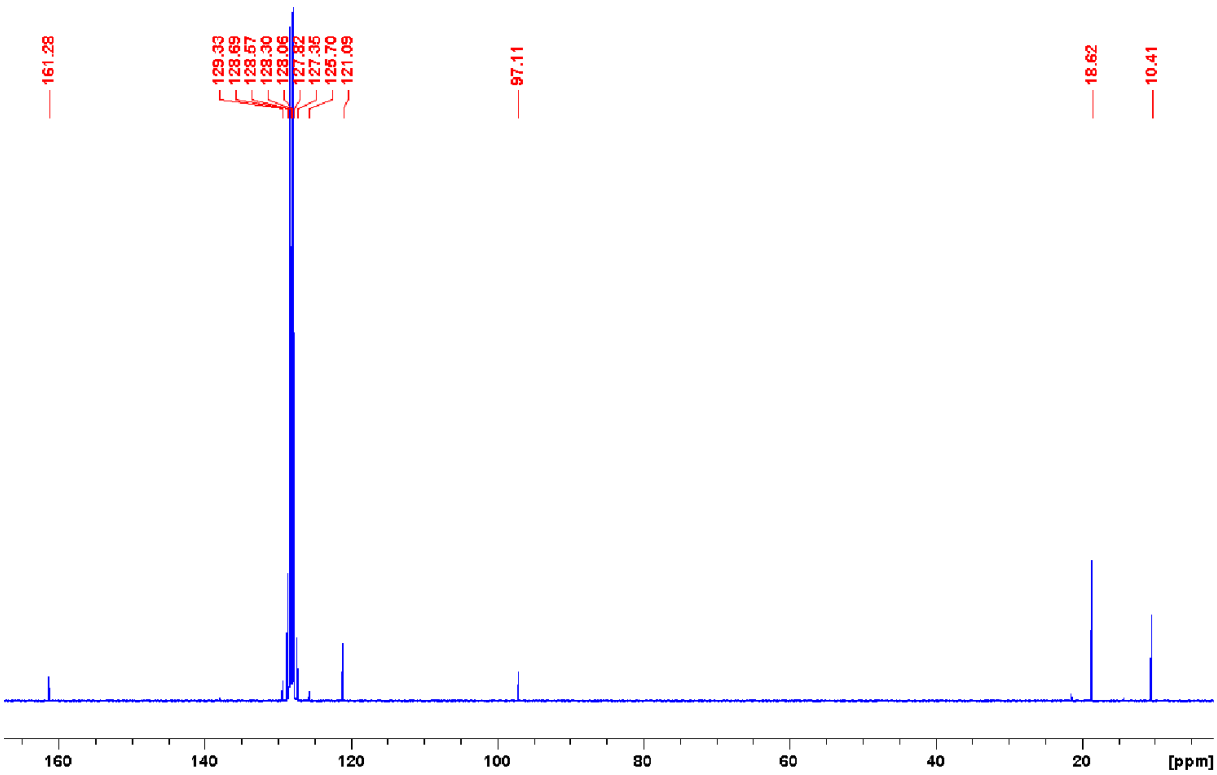

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum (293K, 125 MHz, C_6D_6) of compound **4.**

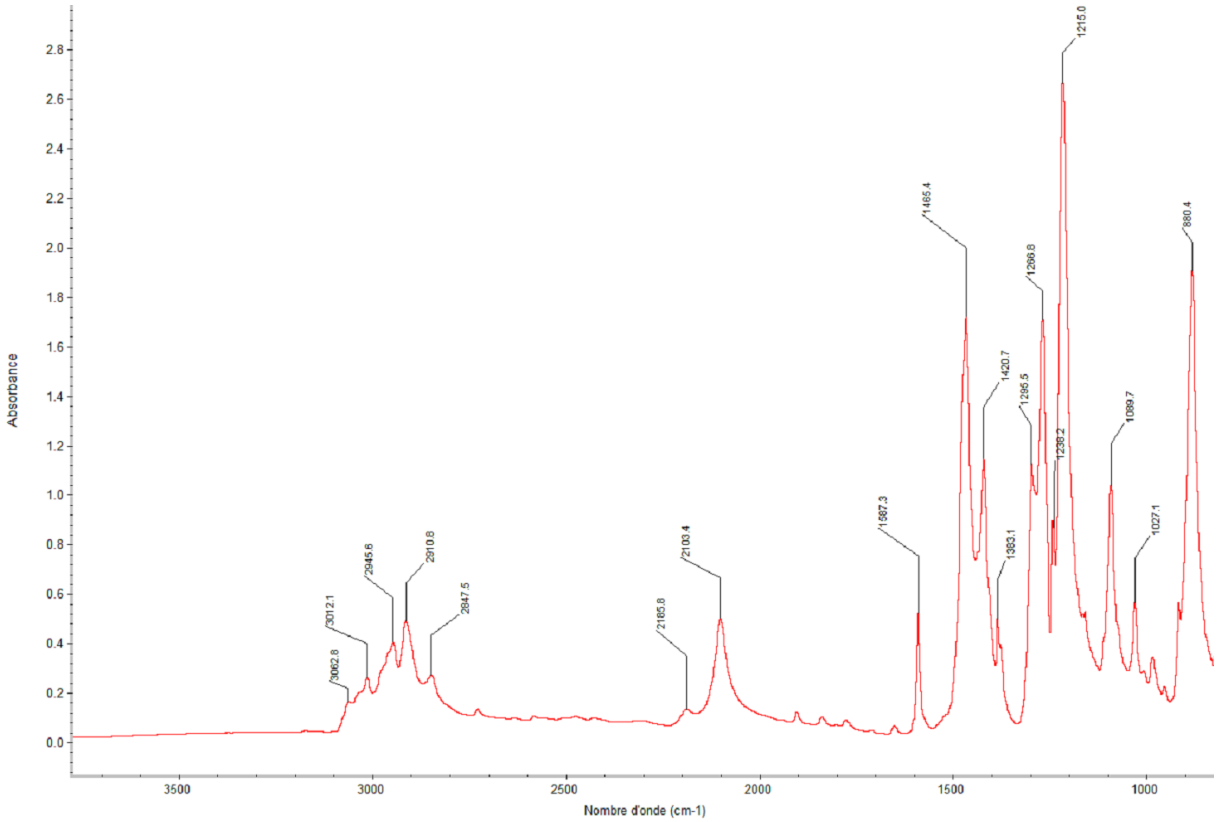

Figure S3. FTIR spectrum (295K, KBr pellet) of compound **4.**

XRD data. The X-ray structural determination was performed at the centre de diffractométrie Henri Longchambon, Université de Lyon. A suitable colorless plate-shaped crystal 0.20×0.09×0.05 mm^3 coated in Parabar oil was selected and mounted on a nylon loop on an Xcalibur, Eos, Nova diffractometer. The crystal was kept at a steady T = 150 K during data collection. Data were measured using ω scans using MoK_α radiation. The total number of runs and images was based on the strategy calculation from the program **CrysAlisPro** (Rigaku, V1.171.39.46, 2018). The maximum resolution that was achieved was Θ = 29.723° (0.72 Å). The total number of runs and images was based on the strategy calculation from the program **CrysAlisPro** and the unit cell was refined using **CrysAlisPro** on 30605 reflections. Data reduction, scaling and absorption corrections were performed using **CrysAlisPro.** The final completeness is 99.80 % out to 29.723° in Θ. An analytical absorption correction was performed using **CrysAlisPro**. Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid[1] using spherical harmonicsas implemented in SCALE3 ABSPACK. The absorption coefficient μ of this material is 5.523 mm^{-1} at this wavelength (□ = 0.711Å) and the minimum and maximum transmissions are 0.425 and 0.779. The structure was solved and the space group $P2_1/n$ (# 14) determined by the **ShelXT**[2] structure solution program using Intrinsic Phasing and refined by Least Squares using version 2018/3 of **ShelXL**.[3] All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model. There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. CCDC 2018001 contains the supplementary crystallographic data for this paper. These data are provided free of charge by the Cambridge Crystallographic Data Centre.

Table S1. Crystallographic parameters.

Compound	[**4**•toluene]
Formula	$C_{49}H_{59}IrO_4Ta$
$D_{calc.}$/ g cm^{-3}	1.631
μ/mm^{-1}	5.523
Formula Weight	1085.11
Colour	colourless
Shape	plate
Size/mm^3	0.20×0.09×0.05
T/K	150
Crystal System	monoclinic
Space Group	$P2_1/n$
a/Å	11.14450(10)
b/Å	21.29120(10)
c/Å	18.95870(10)
α/°	90
β/°	100.7350(10)
γ/°	90
V/Å^3	4419.79(5)
Z	4
Z'	1
Wavelength/Å	0.71073
Radiation type	MoK
Θ_{min}/°	3.418
Θ_{max}/°	29.723
Measured Refl.	60033
Independent Refl.	11121
Reflections with I > 2(I)	9897
R_{int}	0.0337
Parameters	511
Restraints	0
Largest Peak	2.144
Deepest Hole	-2.220
GooF	1.079
wR_2 (all data)	0.0570
wR_2	0.0537
R_1 (all data)	0.0336
R_1	0.0266

B. Computational details

All DFT calculations were carried out with the Gaussian 09 suite of programs.[11] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional.[12] The nature of the extrema was verified by analytical frequency calculations. The calculation of electronic energies and enthalpies of the extrema of the potential energy surface (minima and transition states) were performed at the same level of theory as the geometry optimizations. IRC calculations were performed to confirm the connections of the optimized transition states. Iridium and Tantalum atoms were treated with a small-core effective core potential (60 MWB), associated with its adapted basis set[13] augmented with a polarization function (ζ_f = 0.938 and 0.790 respectively for Ir and Ta). Si atoms were treated with a Stuttgart effective core potential [14] augmented with a polarization function (ζ_d = 0.284).[15] For the other elements (H, C and O), Pople's double-ζ basis set 6-31G(d,p) was used.[16] The electronic charges (at the DFT level) were computed using the natural population analysis (NPA) technique.[17] zeta 6-31G basis set11 augmented by a polarization and diffuse function were used. Some reactant intermediates and transition states were additionally optimized including solvent effect and dispersion corrections (Table S2). More precisely, dispersion corrections were treated with the D3 version of Grimme's dispersion with Becke-Johnson damping.[18] Solvent effect was evaluated by using SMD solvation model.[19] Benzene was used as solvent.

Table S2. Comparison of computed enthalpy values with or without dispersion effects.

	$\Delta H^{\ddagger}$ ($\Delta G^{\ddagger}$) / kcal.mol^{-1}		ΔH_r (ΔG_r) / kcal.mol^{-1}	
	Without dispersion	With dispersion	Without dispersion	With dispersion
Complex **1**	38.8 (53.8)	27.3 (43.1)	27.1 (40.9)	15.5 (28.6)
Complex **2**	29.1 (46.6)	14.4 (26.2)	17.5 (35.4)	10.1 (18.9)
Complex **3**	19.2 (34.6)	13.1 (30.8)	5.5 (18.9)	0.7 (19.5)

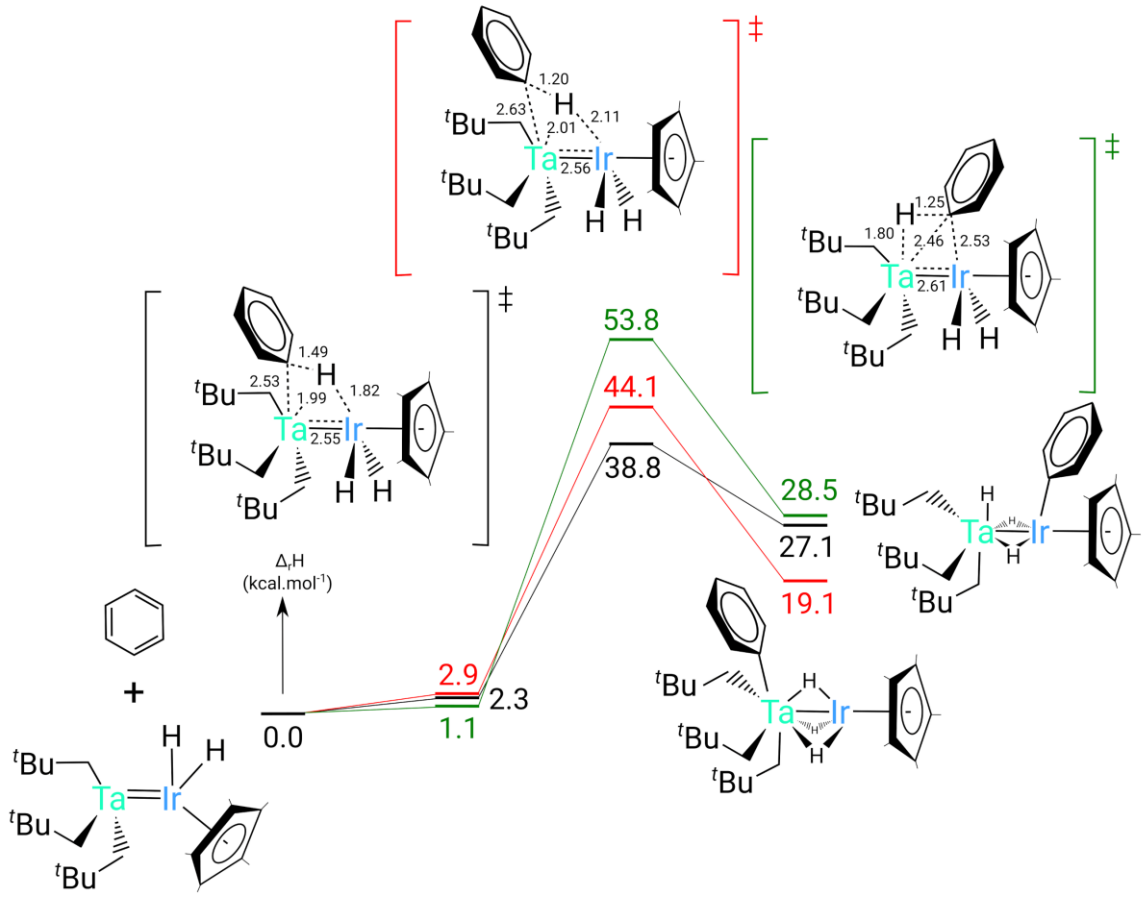

Figure S4. Computed Enthalpy profile at room temperature of all investigated reactions for the C-H activation of benzene catalyzed by complex **1**.

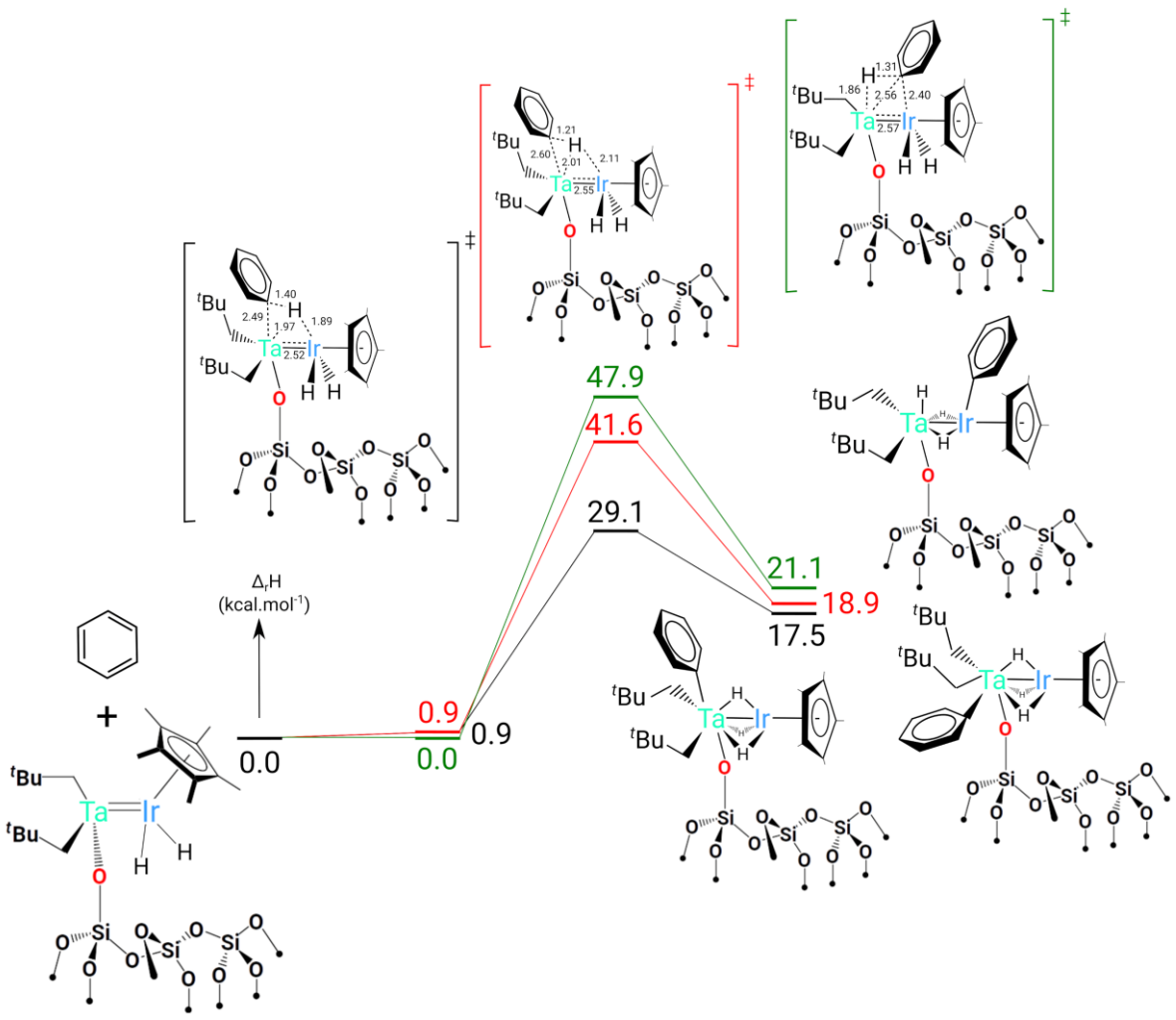

Figure S5. Computed Enthalpy profile at room temperature of all investigated reactions for the C-H activation of benzene catalyzed by complex **2**.

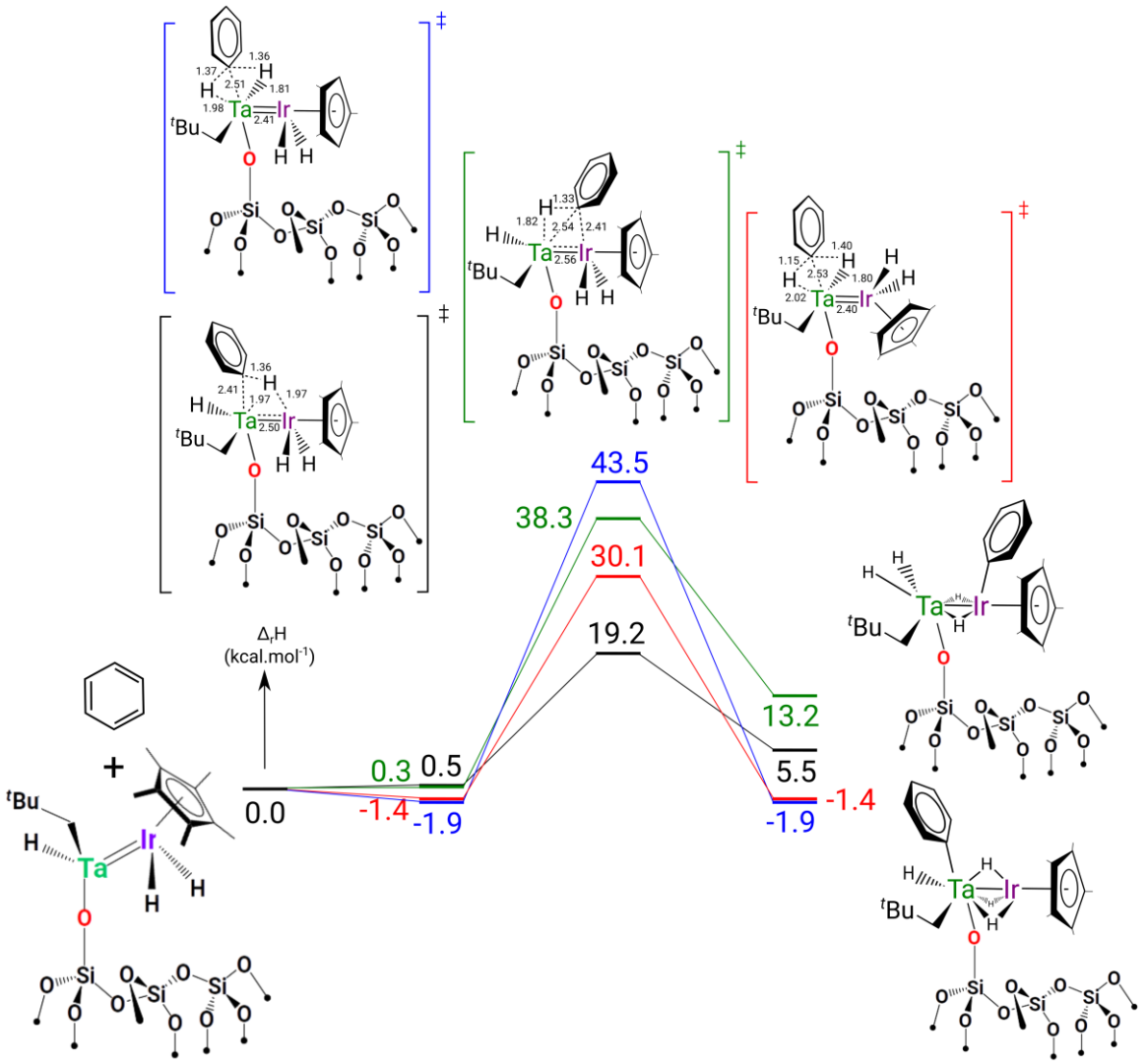

Figure S6. Computed Enthalpy profile at room temperature of all investigated reactions for the C-H activation of benzene catalyzed by complex **3**.

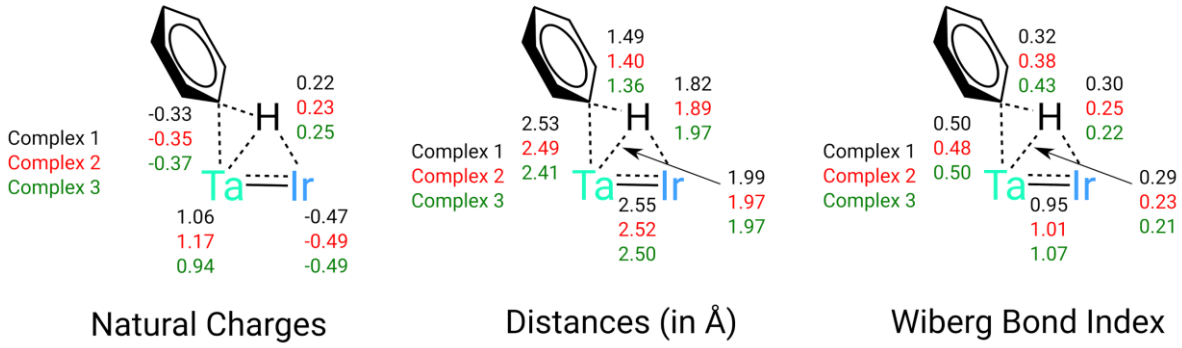

Figure S7. Main parameters of the C-H activation TS.

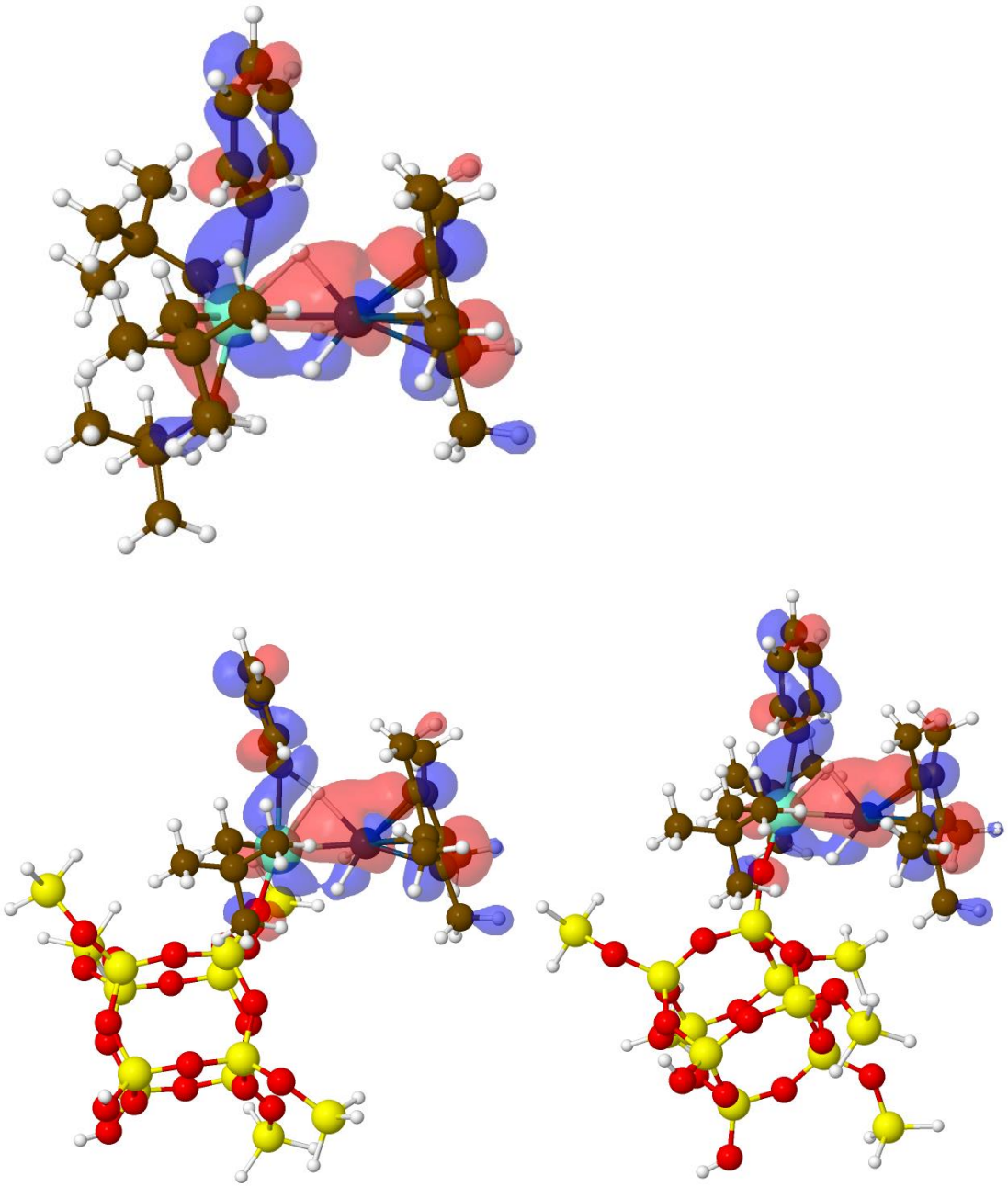

Figure S8. HOMO of the C-H activation transition states from species **1**, **2** and **3.**

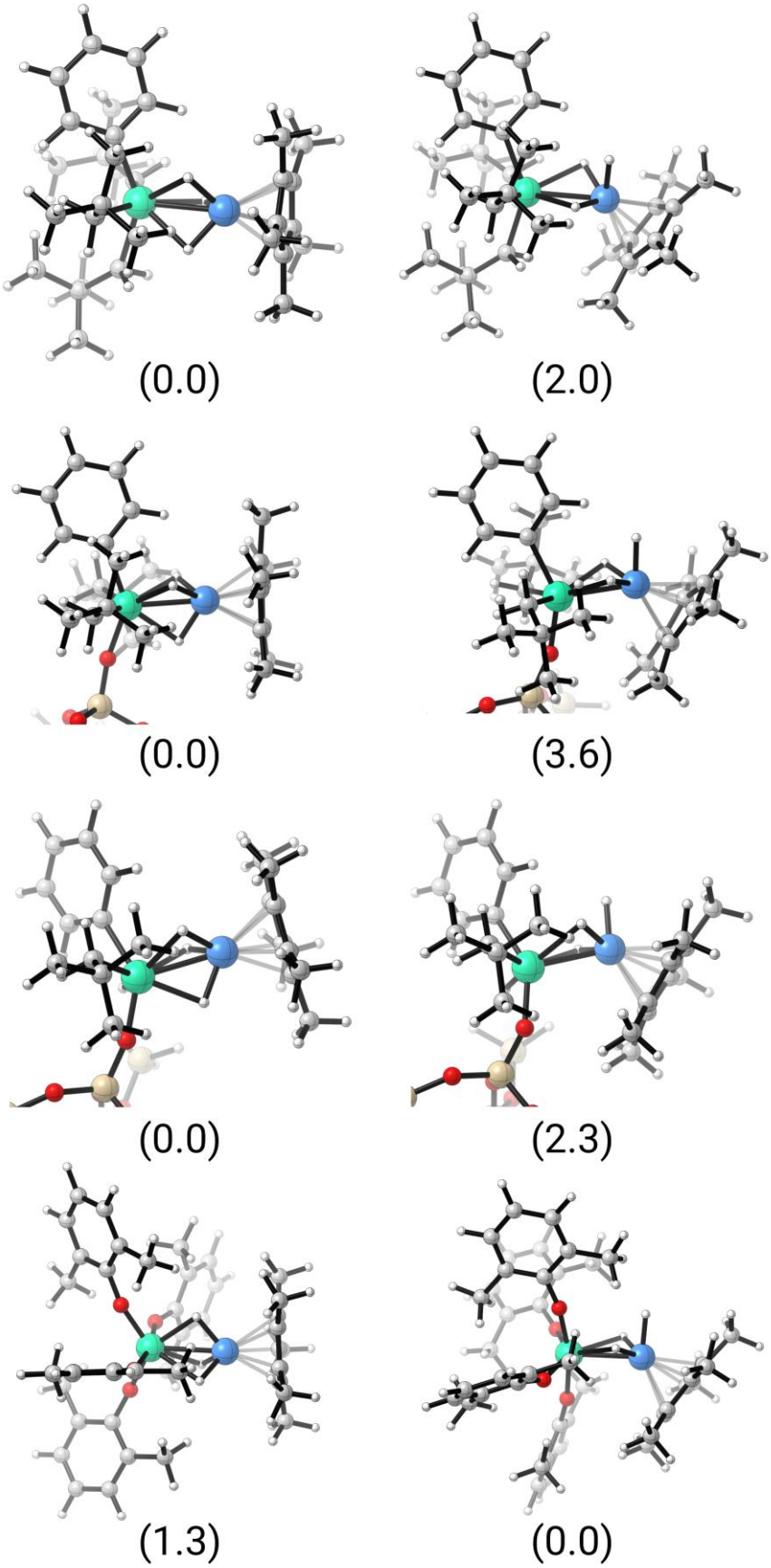

Figure S9. Optimized structures for the CH activation products catalyzed by **1**, **2** and **3** as well as complex **4.**

77
Complex 1
C 11.47992 7.99322 13.83632
C 11.08398 8.01858 12.44138
C 11.76858 9.11888 11.81189
C 12.49511 9.82474 12.83598
C 12.33463 9.08986 14.07565
Ir 10.25188 9.99161 13.20577
Ta 8.67016 11.45604 12.21687
C 7.52788 10.23737 10.82746
C 6.80176 10.72487 9.55045
C 7.80600 10.88234 8.39979
C 10.32351 6.93436 11.74007
C 11.84956 9.37639 10.33712
C 13.46153 10.94916 12.61858
C 12.99155 9.44700 15.37302
C 11.05493 6.95611 14.82914
C 9.76037 12.99894 11.15770
C 10.00404 14.48031 11.53103
C 10.92409 15.12321 10.47727
C 7.25703 12.28271 13.61778
C 6.57417 11.77155 14.90514
C 5.88224 10.42806 14.63125
C 10.68691 14.57334 12.90341
C 8.68107 15.25903 11.55510
C 7.59564 11.60451 16.03729
C 5.51061 12.79418 15.34662
C 5.75303 9.67578 9.13724
C 6.08339 12.06047 9.79650
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H 9.21122 12.96624 10.19251
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H 11.62168 14.00299 12.91634
H 10.92200 15.61504 13.15296
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H 11.89424 14.61472 10.43960
H 10.47782 15.06726 9.47766
H 7.80012 13.22481 13.84727
H 6.46536 12.58959 12.90174
H 7.09952 11.25743 16.95155
H 8.08495 12.55882 16.26689
H 8.37227 10.88462 15.76756
H 5.00755 12.46659 16.26454
H 5.96280 13.77296 15.54464
H 4.74341 12.92965 14.57475
H 5.33794 10.08262 15.51816
H 6.61192 9.65672 14.36303
H 5.15815 10.51516 13.81165
H 8.07370 9.30929 10.60701
H 6.76176 9.92846 11.57330
H 5.23508 9.97242 8.21662
H 4.99722 9.54388 9.92001
H 6.22205 8.70147 8.95946
H 5.53217 12.38188 8.90476
H 6.78883 12.86175 10.04894
H 5.36208 11.97567 10.61793

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H       8.58341     11.61742      8.63345
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H      12.65704      8.78383      9.88635
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12
Benzene
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C       1.21221      0.00000      2.09404
C       2.42030     -0.00000      1.39725
C       2.42095      0.00000      0.00251
C       1.21342      0.00000     -0.69529
H      -0.93670      0.00000      1.93932
H       1.21172     -0.00000      3.18082
H       3.36118      0.00000      1.94112
H       3.36237      0.00000     -0.54043
H       1.21373     -0.00000     -1.78206
H      -0.93531      0.00000     -0.54284
89
Complex 1 - C-H activation - adduct
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C       3.58882     -2.15157     -0.14564
C       2.72132     -3.22828     -0.43029
C       1.53318     -3.07920      0.38390
C       1.71121     -1.91825      1.21654
Ir      1.51756     -1.17215     -0.89450
Ta      0.01677      0.61789     -1.38826
C       0.63997      2.33925     -0.22865
C      -0.09807      3.19000      0.83243
C       0.78065      4.39752      1.20778
C       4.94136     -1.91419     -0.74270
C       2.97449     -4.35621     -1.38199
C       0.48077     -4.13219      0.55033
C       0.83545     -1.52498      2.36632
C       3.62892     -0.16741      1.56255
C      -3.71652     -0.09330      5.00673
C      -3.02757      0.87389      5.73860
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C	-2.95591	-1.05541	-1.28809
C	-2.51525	-2.27001	-0.46665
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C	-4.40984	-0.70044	-0.92976
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C	1.19746	3.16302	-4.17744
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H	0.85856	2.98503	-1.10976
H	1.74703	4.07156	1.60870
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H	0.19302	-4.57557	-0.40700

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H       0.73000     -1.63242     -2.21995
89
Complex 1 - C-H activation - TS
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C      10.53537      7.52672     13.36729
C      10.62425      8.32674     14.55565
Ir     10.38218      9.69479     12.78286
Ta      8.78227     11.54604     12.04937
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C       9.03899     15.46566     14.22668
C      13.76045      9.39504     12.73805
C      12.04329      7.14345     11.25727
C       9.54720      6.43279     13.10498
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C       7.51101     11.96415     17.24382
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C       7.02234     11.10374     15.03477
C       6.68970     11.02108     11.72861
C       6.00490      9.69346     11.31337
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H       8.82584     12.68464      6.53724
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H       6.31874     10.59014     14.38834
H       9.43364      9.52901     11.47890
89
Complex 1 - C-H activation - product
C       2.82804     -1.81973      1.63428
C       3.35897     -1.81538      0.28014
C       2.66075     -2.81026     -0.47273
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C	1.67781	-3.42877	0.39018
C	1.80378	-2.81693	1.69389
Ir	1.18324	-1.24987	0.20145
Ta	-0.55679	0.69565	-0.39523
C	0.28307	2.68375	0.05311
C	-0.12648	4.13520	0.43513
C	-0.35695	4.25319	1.95002
C	4.51984	-0.99771	-0.19427
C	2.94532	-3.20953	-1.88700
C	0.83934	-4.62292	0.05684
C	1.04187	-3.22263	2.91699
C	3.36631	-1.02546	2.78331
C	-1.82628	1.20607	1.34243
C	-1.27628	0.90635	2.60771
C	-1.94020	1.20188	3.80002
C	-3.18522	1.82626	3.76998
C	-3.75470	2.14659	2.53659
C	-3.08783	1.83246	1.35314
C	-2.49792	-0.22002	-1.05526
C	-3.19913	-1.52587	-0.57646
C	-3.34418	-1.64964	0.94491
C	-0.28566	1.06437	-2.55617
C	-0.85079	2.02514	-3.63283
C	-0.76056	1.34395	-5.01182
C	-4.61201	-1.55091	-1.19343
C	-2.42917	-2.74619	-1.10219
C	-2.32013	2.38988	-3.37104
C	-0.00529	3.30577	-3.68582
C	-1.39678	4.61376	-0.28258
C	1.03218	5.08092	0.06300
H	0.89872	2.30582	0.89687
H	1.00183	2.73301	-0.78688
H	-1.19104	3.63371	2.28345
H	0.53702	3.94993	2.50848
H	-0.57841	5.29353	2.21829
H	0.80576	6.11490	0.35201
H	1.95750	4.78598	0.57207
H	1.22630	5.07107	-1.01590
H	-3.20731	0.61453	-0.93813
H	-2.39036	-0.34421	-2.14095
H	-3.88561	-2.57062	1.19676
H	-3.89633	-0.80586	1.36812
H	-2.37020	-1.68445	1.44229
H	-5.13755	-2.48174	-0.94415
H	-5.21729	-0.71573	-0.82242
H	-4.56734	-1.47346	-2.28614
H	-2.93688	-3.67728	-0.82099
H	-1.41306	-2.77049	-0.69792
H	-2.35549	-2.72399	-2.19677
H	0.81831	1.16905	-2.54073
H	-0.43884	0.02900	-2.90536
H	-1.10219	2.01573	-5.80937
H	-1.38127	0.44082	-5.04632
H	0.27116	1.05089	-5.23926
H	-2.69398	3.06743	-4.14873
H	-2.44055	2.88918	-2.40489

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H      -2.95814      1.50086     -3.37008
H      -0.40761      4.01124     -4.42277
H       0.02234      3.81008     -2.71765
H       1.02834      3.07728     -3.97269
H       3.71401     -0.04040      2.46289
H       4.21557     -1.54315      3.24797
H       2.60912     -0.87265      3.55577
H       4.54640     -0.01954      0.29164
H       5.46596     -1.50722      0.02886
H       4.47672     -0.83007     -1.27270
H       3.66542     -4.03704     -1.91035
H       3.36784     -2.38203     -2.46092
H       2.03868     -3.54069     -2.39823
H       0.56336     -4.63827     -1.00005
H      -0.08645     -4.63711      0.63632
H       1.38356     -5.55162      0.27328
H       1.56275     -4.03890      3.43290
H       0.93902     -2.39378      3.62055
H       0.03831     -3.57261      2.66600
H      -1.63593      5.64292      0.01359
H      -2.25226      3.98509     -0.02219
H      -1.28140      4.60613     -1.36961
H       1.46857      0.34657      0.18809
H      -0.29305     -1.05632      0.84886
H      -0.30044      0.42753      2.67337
H      -1.48194      0.94562      4.75278
H      -3.70696      2.06064      4.69417
H      -4.72513      2.63632      2.49661
H      -3.57545      2.08927      0.41477
H       0.45869     -1.12752     -1.23497
89
Complex 1 - C-H activation - rot. TS
C      -3.77590      0.86820     -0.47757
C      -2.68041      0.16948      0.07177
C      -3.00956     -0.92744      0.89689
C      -4.33051     -1.30460      1.14942
C      -5.38444     -0.58535      0.59170
C      -5.09882      0.51087     -0.22366
Ta     -0.55642      0.71710     -0.26311
C       0.67048      2.33674     -1.11865
C       0.40685      3.72633     -1.76055
C       0.68872      4.81981     -0.71766
Ir      1.19801     -1.15946      0.47191
C       2.38709     -2.97713     -0.12898
C       1.54235     -3.32431      0.97776
C       1.94611     -2.50693      2.10871
C       3.02143     -1.66485      1.68524
C       3.29550     -1.94011      0.28890
C       0.54208     -4.43729      1.01410
C       1.40363     -2.62029      3.49948
C       3.80437     -0.72903      2.55243
C       4.43125     -1.38037     -0.51007
C       2.38387     -3.64254     -1.46932
C      -0.91609      1.95458      1.53329
C      -1.96384      2.85415      2.23966
C      -1.24418      3.65009      3.34697
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C	-1.23751	0.44999	-2.39135
C	-1.51172	-0.86449	-3.18549
C	-0.18922	-1.42491	-3.73157
C	-3.05996	2.01054	2.90874
C	-2.62896	3.85191	1.28267
C	-2.20986	-1.95703	-2.36648
C	-2.40891	-0.51666	-4.38913
C	1.37156	3.93255	-2.94249
C	-1.03212	3.88914	-2.27458
H	-0.72671	1.09770	2.21385
H	0.04818	2.49518	1.52710
H	-3.64927	1.45330	2.17887
H	-2.62652	1.29158	3.61456
H	-3.74237	2.65888	3.47235
H	-1.94986	4.27808	3.90522
H	-0.75846	2.97522	4.06195
H	-0.47138	4.30562	2.92798
H	-2.15361	1.05760	-2.41645
H	-0.51206	1.00959	-2.99783
H	-2.39464	-2.83965	-2.99276
H	-3.16995	-1.61375	-1.97268
H	-1.59632	-2.26931	-1.51448
H	-2.57628	-1.39421	-5.02661
H	-3.38724	-0.15438	-4.05372
H	-1.95355	0.26574	-5.00762
H	-0.36589	-2.32967	-4.32622
H	0.49965	-1.68563	-2.92150
H	0.31306	-0.69376	-4.37665
H	1.42570	2.47027	-0.32465
H	1.18402	1.68430	-1.85061
H	1.25160	4.93029	-3.38332
H	1.18956	3.19440	-3.73247
H	2.41472	3.83073	-2.62116
H	-1.18164	4.89568	-2.68488
H	-1.75755	3.74765	-1.46742
H	-1.26051	3.17144	-3.06749
H	0.47327	5.81585	-1.12273
H	0.07833	4.68153	0.17896
H	1.74137	4.80393	-0.41050
H	-0.27392	-4.22104	1.70773
H	1.01455	-5.37365	1.33854
H	0.09974	-4.61052	0.03054
H	0.34619	-2.89447	3.49524
H	1.94574	-3.39224	4.06037
H	1.49982	-1.68003	4.04684
H	4.67795	-1.24379	2.97183
H	3.20541	-0.35471	3.38537
H	4.16556	0.13295	1.98710
H	4.64763	-0.34717	-0.22805
H	4.20944	-1.38796	-1.57976
H	5.34589	-1.96759	-0.35495
H	3.05056	-4.51381	-1.45687
H	1.38576	-3.98837	-1.74623
H	2.73192	-2.96770	-2.25413
H	-3.34288	4.48516	1.82437
H	-3.17784	3.33063	0.49417

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H      -1.89538      4.51343      0.81262
H       1.44112      0.43398      0.59798
H      -0.28160     -0.96876      1.09373
H      -2.22233     -1.51913      1.35817
H      -4.53360     -2.16302      1.78599
H      -6.41411     -0.87322      0.78709
H      -5.90878      1.08549     -0.66741
H      -3.60356      1.72621     -1.12509
H       0.58272     -0.93856     -1.01666
89
Complex 1 - C-H activation - product Ben.
Ir      1.30620     -1.03765      0.02363
Ta     -0.61637      0.72169     -0.46831
C      -1.79022      1.25506      1.31667
C      -2.56716     -0.28422     -0.97153
C       0.21701      2.74668     -0.18048
C      -0.49385      1.00895     -2.62588
C      -1.13516      1.86804     -3.74062
C      -2.59468      2.22474     -3.41851
C      -3.05064      1.88465      1.35675
C      -3.69723      2.18318      2.55415
C      -3.10480      1.84697      3.77317
C      -1.86225      1.21852      3.77337
C      -1.21808      0.93559      2.56623
C       2.40225     -2.82978     -0.82514
C       3.13852     -2.41415      0.33562
C       3.58764     -1.07255      0.12394
C       3.18729     -0.66559     -1.20984
C       2.45612     -1.74952     -1.79410
C       1.84966     -4.19987     -1.07320
C       3.42130     -3.25565      1.54127
C       4.46353     -0.27970      1.04493
C       3.63184      0.58657     -1.89956
C       1.98104     -1.83472     -3.21084
C      -0.18165      4.19160      0.22245
C      -1.49181      4.64652     -0.43632
C      -3.20892     -1.58324     -0.39196
C      -4.70916     -1.56366     -0.74473
C      -0.32841      3.16157     -3.92821
C      -1.10423      1.09103     -5.06988
C       0.94325      5.14861     -0.21906
C      -0.32979      4.31494      1.74662
C      -2.58591     -2.81707     -1.06629
C      -3.07409     -1.73624      1.12792
H       0.94646      2.39861      0.58183
H       0.81795      2.80113     -1.10690
H      -1.13136      3.68110      2.12914
H       0.59978      4.03060      2.25460
H      -0.55445      5.35246      2.02295
H       0.72228      6.18162      0.07744
H       1.89943      4.86731      0.23821
H       1.07542      5.13477     -1.30752
H      -3.27596      0.54501     -0.82071
H      -2.55370     -0.44118     -2.05849
H      -3.57477     -2.65549      1.45800
H      -3.52533     -0.89516      1.66072
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H      -2.02472     -1.79838      1.43271
H      -5.20414     -2.48981     -0.42570
H      -5.21527     -0.72654     -0.25065
H      -4.85974     -1.45736     -1.82564
H      -3.07544     -3.73568     -0.72074
H      -1.51843     -2.90553     -0.83790
H      -2.69701     -2.76956     -2.15676
H       0.60662      1.14536     -2.65416
H      -0.63444     -0.06276     -2.86302
H      -1.51501      1.69288     -5.88999
H      -1.69540      0.17029     -5.00281
H      -0.07880      0.81335     -5.34120
H      -3.02783      2.83293     -4.22220
H      -2.66564      2.79621     -2.48783
H      -3.21233      1.32817     -3.30964
H      -0.78836      3.80062     -4.69122
H      -0.26795      3.73633     -3.00102
H       0.69600      2.94126     -4.25268
H       3.52079     -2.64706      2.44278
H       4.35909     -3.80930      1.40665
H       2.62709     -3.98440      1.71750
H       4.28524     -0.53753      2.09146
H       5.52255     -0.47137      0.82966
H       4.29231      0.79361      0.93435
H       4.64022      0.45800     -2.31423
H       3.66222      1.43804     -1.21533
H       2.96759      0.84844     -2.72610
H       1.71477     -0.85271     -3.60707
H       1.10158     -2.47655     -3.30136
H       2.76667     -2.25477     -3.85185
H       2.60889     -4.84995     -1.52675
H       1.51874     -4.67169     -0.14498
H       0.99218     -4.16881     -1.74911
H      -1.72413      5.68057     -0.15222
H      -2.32767      4.01773     -0.11934
H      -1.43104      4.61320     -1.52806
H       0.61592     -1.53279      1.35797
H      -0.24821      0.44591      2.61516
H      -1.38901      0.94605      4.71399
H      -3.60905      2.07118      4.70952
H      -4.66829      2.67292      2.53789
H      -3.55404      2.15219      0.42944
H      -0.18827     -1.44415     -0.40588
H       1.15089      0.28968      0.90498
89
Complex 1 - SI C-H activation Red Profil - adduct
C       2.22950     -1.48106      1.03747
C       1.47622     -2.70661      1.10729
C       2.07068     -3.64330      0.17752
C       3.13203     -2.99551     -0.48930
C       3.22555     -1.63671      0.01003
Ir      1.15662     -1.67108     -0.92544
Ta     -0.13779      0.17784     -1.68932
C      -2.00163      0.38803     -0.63132
C      -3.08774     -0.60631     -0.16750
C      -2.53933     -1.50635      0.94332
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C	0.48421	-3.06846	2.16950
C	1.62885	-5.06203	-0.00803
C	4.03679	-3.59526	-1.52093
C	4.33182	-0.67523	-0.30191
C	2.11377	-0.33033	1.98949
C	-0.64095	-0.25905	-3.76255
C	-1.11154	0.72640	-4.85773
C	-2.22920	1.64170	-4.33967
C	1.08628	1.95346	-1.45957
C	0.75775	3.34163	-0.85890
C	-0.53712	3.91724	-1.44892
C	0.06444	1.58130	-5.35005
C	-1.65599	-0.08350	-6.04920
C	1.91056	4.31194	-1.17630
C	0.61585	3.23774	0.66628
C	-4.29731	0.17938	0.37030
C	-3.54592	-1.47643	-1.34635
H	2.04342	1.60295	-1.04320
H	1.29421	2.07739	-2.54688
H	-0.20291	2.56781	0.95050
H	1.53539	2.85622	1.12336
H	0.40869	4.22085	1.10520
H	1.72195	5.30492	-0.74971
H	2.85806	3.94465	-0.76606
H	2.03906	4.43097	-2.25822
H	-1.66412	0.98746	0.23963
H	-2.47802	1.12827	-1.31024
H	-4.35706	-2.14803	-1.04094
H	-2.72334	-2.09422	-1.72239
H	-3.91994	-0.86108	-2.17347
H	-3.30092	-2.22192	1.27571
H	-1.66408	-2.05834	0.59001
H	-2.23766	-0.91226	1.81467
H	-5.08464	-0.49873	0.72125
H	-4.73085	0.82139	-0.40567
H	-4.00846	0.82082	1.21103
H	0.12662	-0.92424	-4.18159
H	-1.48216	-0.94439	-3.51820
H	-1.99302	0.57643	-6.85833
H	-2.50635	-0.70501	-5.74626
H	-0.88597	-0.74836	-6.45640
H	-2.59164	2.30722	-5.13214
H	-1.88249	2.27456	-3.51503
H	-3.08407	1.05720	-3.97997
H	-0.24524	2.23544	-6.17381
H	0.46028	2.21995	-4.55329
H	0.88499	0.95191	-5.71325
H	-0.03458	-2.18883	2.55601
H	0.98738	-3.55473	3.01652
H	-0.27503	-3.76200	1.79855
H	1.07770	-0.16639	2.29518
H	2.70580	-0.51487	2.89612
H	2.47639	0.59745	1.54174
H	5.21976	-0.88228	0.31077
H	4.03246	0.35758	-0.10615
H	4.63258	-0.73526	-1.35117

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H        4.93848     -4.01351     -1.05479
H        4.36113     -2.84964     -2.25138
H        3.54403     -4.40203     -2.06962
H        2.09832     -5.72004      0.73503
H        0.54593     -5.16061      0.10476
H        1.89342     -5.44196     -0.99810
H       -0.73321      4.92045     -1.05242
H       -1.40573      3.29518     -1.20488
H       -0.47206      4.00100     -2.53984
H       -0.18170     -2.32918     -1.52942
H       -2.00977      2.32520      4.79314
C       -2.47773      2.79185      5.65606
C       -1.91857      3.94019      6.21629
C       -2.51811      4.53819      7.32447
C       -3.67668      3.98789      7.87224
C       -4.23587      2.83970      7.31177
C       -3.63649      2.24159      6.20356
H       -1.01563      4.36878      5.78956
H       -2.08247      5.43292      7.76123
H       -4.14387      4.45392      8.73573
H       -5.13875      2.41102      7.73853
H       -4.07222      1.34691      5.76682
H        1.52798     -1.44955     -2.46452
89
Complex 1 - SI C-H activation Red Profil - TS
C       11.94909      9.92974     14.28331
C       11.26769      8.66144     14.35798
C       11.68391      7.87288     13.22155
C       12.57636      8.65067     12.43537
C       12.73432      9.94187     13.07937
Ir      10.57139      9.79449     12.51637
Ta       8.63965     11.28571     11.74678
C        6.60752     12.18316     11.90457
C        5.13121     11.82668     12.23453
C        4.79455     12.15100     13.69516
C       10.46858      8.16712     15.52331
C       11.27226      6.45912     12.95065
C       13.29850      8.20845     11.20139
C       13.72624     10.98789     12.67252
C       11.94471     10.97981     15.34979
C        7.98736     10.19060      9.94820
C        8.10050     10.62288      8.45901
C        7.28482     11.88532      8.15055
C        9.59620     13.10040     11.05974
C        9.99599     14.42453     11.75934
C        8.78034     15.15186     12.34761
C        9.56613     10.84163      8.05716
C        7.53450      9.47461      7.59977
C       10.64377     15.34705     10.70904
C       11.02123     14.15230     12.86671
C        4.20136     12.67505     11.34494
C        4.82891     10.34356     11.97139
H       10.49716     12.70056     10.57077
H        8.89025     13.34777     10.24207
H       10.60961     13.50303     13.64591
H       11.90692     13.65364     12.46036
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H	11.34302	15.08989	13.33619
H	10.95632	16.29712	11.15946
H	11.52879	14.87829	10.26421
H	9.94243	15.57540	9.89840
H	6.85272	13.11442	12.45055
H	6.62204	12.48971	10.83861
H	3.78709	10.10808	12.22256
H	5.47609	9.69799	12.57415
H	4.97553	10.08260	10.91750
H	3.73756	11.94004	13.90006
H	5.39342	11.56304	14.39083
H	4.96857	13.21209	13.90865
H	3.14595	12.47166	11.56690
H	4.36635	12.46352	10.28200
H	4.37743	13.74532	11.50440
H	8.48083	9.21502	10.02735
H	6.92223	10.01052	10.16461
H	7.58848	9.71880	6.53141
H	6.48514	9.27676	7.84660
H	8.09728	8.54849	7.76203
H	7.32886	12.11997	7.08017
H	7.65870	12.76163	8.69007
H	6.23078	11.75112	8.41864
H	9.64688	11.03841	6.98115
H	10.00930	11.69262	8.58302
H	10.17087	9.95726	8.28580
H	9.91682	8.97722	16.00588
H	11.12026	7.70863	16.27970
H	9.73914	7.41203	15.21838
H	10.96711	11.06029	15.83249
H	12.68091	10.73975	16.12872
H	12.19896	11.96211	14.94544
H	14.73424	10.72629	13.02199
H	13.47597	11.96433	13.09326
H	13.77223	11.09799	11.58581
H	14.28701	7.80014	11.45068
H	13.45016	9.04099	10.50983
H	12.74458	7.43240	10.66721
H	11.94104	5.75510	13.46274
H	10.25624	6.26386	13.30237
H	11.30278	6.22900	11.88277
H	9.07738	16.12603	12.75374
H	8.31669	14.58424	13.16027
H	8.01318	15.32802	11.58519
H	9.20915	9.04077	12.06815
H	9.07409	10.76747	13.64439
C	8.09786	11.00139	14.30162
C	8.08561	12.13559	15.12611
C	7.38332	12.12588	16.32996
C	6.69360	10.97956	16.72921
C	6.71575	9.83824	15.92508
C	7.42887	9.84565	14.72809
H	8.63660	13.02675	14.83712
H	7.37786	13.01058	16.96134
H	6.14939	10.97267	17.66956
H	6.19045	8.94043	16.23996

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H       7.49748      8.94298     14.12566
H      10.56925     10.48537     11.04888
89
Complex 1 - SI C-H activation Red Profil - product
C       3.08578     -0.78540      1.85682
C       2.31682     -1.98629      2.00507
C       2.41252     -2.71743      0.75597
C       3.24462     -1.96996     -0.13982
C       3.66295     -0.76022      0.53417
Ir      1.43833     -0.75481      0.34573
Ta     -0.87182      0.54489     -0.39021
C      -2.78560      1.65483     -0.65240
C      -4.30194      1.43308     -0.39884
C      -4.66090      1.68493      1.07312
C       1.63742     -2.46217      3.25009
C       1.83330     -4.07360      0.49952
C       3.69361     -2.40685     -1.49912
C       4.64770      0.24005      0.01528
C       3.31581      0.23774      2.92479
C      -1.43290     -0.79546     -2.03679
C      -1.17222     -0.62130     -3.55634
C      -1.82688      0.65034     -4.11315
C       0.09098      2.41979     -1.03107
C       0.54123      3.70284     -0.28828
C      -0.64368      4.44261      0.34709
C       0.33200     -0.58243     -3.85930
C      -1.78371     -1.83391     -4.28455
C       1.19539      4.64396     -1.31914
C       1.57901      3.38888      0.79800
C      -5.08843      2.44872     -1.25218
C      -4.76628      0.02388     -0.78959
H       0.97485      2.01807     -1.55242
H      -0.60951      2.72792     -1.82775
H       1.15386      2.78221      1.60397
H       2.42715      2.83491      0.38135
H       1.96149      4.31665      1.24125
H       1.52380      5.57892     -0.84834
H       2.07158      4.17466     -1.78141
H       0.49233      4.90065     -2.11982
H      -2.53716      2.63836     -0.21943
H      -2.66196      1.81327     -1.74373
H      -5.84507     -0.08650     -0.62290
H      -4.25858     -0.74054     -0.19325
H      -4.57918     -0.18201     -1.85020
H      -5.74791      1.62907      1.21165
H      -4.19785      0.95516      1.73931
H      -4.33757      2.68375      1.38931
H      -6.16960      2.35223     -1.08897
H      -4.89692      2.30111     -2.32189
H      -4.80216      3.47675     -1.00090
H      -1.02281     -1.77117     -1.74093
H      -2.52145     -0.86587     -1.88092
H      -1.62750     -1.76511     -5.36833
H      -2.86278     -1.89863     -4.10440
H      -1.33051     -2.76998     -3.93851
H      -1.68969      0.70750     -5.19970
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H      -1.38827      1.55639     -3.68161
H      -2.90379      0.66719     -3.91204
H       0.50649     -0.54563     -4.94156
H       0.80973      0.29689     -3.41424
H       0.83817     -1.46956     -3.46345
H       1.31735     -1.62620      3.87585
H       2.31066     -3.09191      3.84682
H       0.74679     -3.05100      3.01856
H       2.46739      0.29552      3.60999
H       4.20644     -0.02006      3.51159
H       3.47125      1.23187      2.50032
H       5.67678     -0.06361      0.24935
H       4.48522      1.22588      0.45725
H       4.57283      0.34934     -1.06955
H       4.64920     -2.94245     -1.43232
H       3.83490     -1.55392     -2.16684
H       2.96809     -3.07722     -1.96524
H       2.51715     -4.85644      0.85194
H       0.88098     -4.20502      1.01859
H       1.65707     -4.23934     -0.56575
H      -0.30514      5.37091      0.82280
H      -1.13723      3.83830      1.11480
H      -1.39561      4.70887     -0.40434
H      -0.09870     -1.29819      0.30725
H       0.81669      0.69225      0.81057
C      -1.69806      0.10805      1.58794
C      -1.55759      1.03446      2.63438
C      -2.08547      0.79595      3.90413
C      -2.77504     -0.38848      4.16337
C      -2.91732     -1.33242      3.14554
C      -2.37821     -1.08711      1.88192
H      -1.02683      1.97104      2.46615
H      -1.96215      1.53759      4.69022
H      -3.19269     -0.57655      5.14889
H      -3.44633     -2.26337      3.33697
H      -2.49152     -1.85335      1.11504
H       1.11147     -0.22657     -1.15479
89
Complex 1 - SI C-H activation Green Profil - adduct
C       2.84996      0.26966      2.10511
C       2.55999     -0.93151      1.36305
C       3.44128     -0.96300      0.22533
C       4.33860      0.17286      0.33035
C       3.98014      0.91848      1.47174
Ir      2.01630      0.78865      0.03723
Ta     -0.15577      0.86427     -0.94281
C      -1.69627      1.66852      0.31409
C      -1.89181      1.85439      1.82966
C      -3.29285      2.43147      2.10069
C       1.64898     -2.03812      1.79864
C       3.59757     -2.09980     -0.73883
C       5.46059      0.46788     -0.61638
C       4.64594      2.16142      1.97567
C       2.30673      0.62829      3.45421
C      -0.72206     -1.19624     -1.33604
C      -1.71002     -1.70689     -2.41303
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C	-3.02962	-0.92231	-2.36752
C	-0.19593	2.04498	-2.76119
C	0.28213	3.47931	-3.09309
C	-0.23609	3.86647	-4.49000
C	-1.08447	-1.57689	-3.80891
C	-2.01537	-3.19257	-2.14957
C	1.81359	3.56340	-3.09608
C	-0.27932	4.47201	-2.06478
C	-1.76910	0.49490	2.53040
C	-0.83748	2.81803	2.38663
H	0.28790	1.33794	-3.46534
H	-1.27919	1.98488	-2.99948
H	-1.37497	4.42840	-2.02719
H	0.10780	4.26091	-1.06174
H	0.00147	5.50046	-2.32138
H	2.13967	4.57447	-3.36826
H	2.22752	3.31789	-2.11489
H	2.24370	2.86647	-3.82538
H	-1.78827	2.65311	-0.19361
H	-2.54789	1.07821	-0.08859
H	-0.97171	2.95726	3.46610
H	-0.91546	3.80331	1.91150
H	0.16955	2.43390	2.20203
H	-3.46057	2.57246	3.17549
H	-3.41933	3.40500	1.61296
H	-4.07645	1.76346	1.72411
H	-1.92277	0.59516	3.61169
H	-0.77433	0.06812	2.36486
H	-2.51271	-0.21650	2.15236
H	0.20915	-1.77898	-1.39707
H	-1.13328	-1.43421	-0.33188
H	-2.69455	-3.59774	-2.91014
H	-2.48760	-3.33079	-1.17070
H	-1.09671	-3.79000	-2.16916
H	-3.74355	-1.31317	-3.10231
H	-2.87669	0.13967	-2.59601
H	-3.49902	-0.99378	-1.37965
H	-1.75377	-1.98373	-4.57608
H	-0.88394	-0.53157	-4.06542
H	-0.13709	-2.12517	-3.86740
H	0.81344	-1.66028	2.39236
H	2.19381	-2.76410	2.41730
H	1.23174	-2.57814	0.94528
H	2.93654	0.20983	4.25124
H	2.27164	1.71124	3.59906
H	1.29426	0.24555	3.59892
H	5.37876	1.92401	2.75803
H	3.92104	2.85730	2.40626
H	5.17553	2.68779	1.17751
H	6.37051	-0.07406	-0.32703
H	5.70332	1.53340	-0.63579
H	5.21147	0.16783	-1.63762
H	4.36251	-2.80800	-0.39226
H	2.66455	-2.65671	-0.85652
H	3.89760	-1.74770	-1.72939
H	0.08724	4.87803	-4.76458

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H      -1.33176      3.84353     -4.52686
H       0.13957      3.17588     -5.25381
H       2.15299      1.12613     -1.52591
H       1.51525      2.31633      0.16806
C      -4.24187     -3.87135      2.59667
C      -4.94715     -2.70655      2.90025
C      -5.96603     -2.26741      2.05432
C      -6.28057     -2.99377      0.90568
C      -5.57603     -4.15909      0.60279
C      -4.55659     -4.59787      1.44805
H      -4.70535     -2.14307      3.79734
H      -6.51726     -1.36167      2.29265
H      -7.07635     -2.65351      0.24845
H      -5.82290     -4.72657     -0.29046
H      -4.01012     -5.50744      1.21350
H      -3.45056     -4.21519      3.25745
89
Complex 1 - SI C-H activation Green Profil - TS
C      11.97815      9.23585     14.50358
C      11.55017      8.19912     13.59246
C      12.16472      8.45339     12.32307
C      12.95382      9.66139     12.43141
C      12.82805     10.13406     13.79011
Ir     10.82127     10.16693     12.71293
Ta      8.68374     11.39597     11.85795
C       6.82434     12.64051     12.14313
C       5.54828     12.46704     13.00003
C       4.48061     13.46966     12.52112
C      10.75071      6.99300     13.96771
C      12.10391      7.56341     11.12071
C      13.86921     10.21385     11.38410
C      13.54879     11.30989     14.37186
C      11.71811      9.25464     15.97249
C       7.76476      9.97067     10.49794
C       7.81232      9.89612      8.95383
C       7.25107     11.17929      8.32526
C       9.48575     13.09145     10.72896
C      10.36926     14.29919     11.13465
C      10.14759     15.44156     10.12596
C       9.24957      9.66974      8.46506
C       6.94633      8.70820      8.49423
C      11.85649     13.91977     11.10738
C      10.00210     14.80486     12.53823
C       4.97371     11.04960     12.86713
C       5.84398     12.75461     14.47896
H       9.98499     12.55932      9.89817
H       8.54317     13.48783     10.31256
H       8.94779     15.09631     12.59593
H      10.18360     14.03314     13.29587
H      10.60340     15.68204     12.80689
H      12.47798     14.77451     11.40029
H      12.06924     13.09042     11.78779
H      12.16141     13.61280     10.09998
H       7.22999     13.64560     12.35523
H       6.51121     12.70782     11.08069
H       4.92825     12.68304     15.07821
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H       6.24660     13.76671     14.60746
H       6.56709     12.05027     14.90115
H       3.56229     13.39011     13.11660
H       4.84574     14.50012     12.60336
H       4.21566     13.29318     11.47177
H       4.04369     10.94781     13.43974
H       5.67591     10.29767     13.24496
H       4.74324     10.81103     11.82155
H       8.08307      8.99849     10.90731
H       6.71121     10.09727     10.81007
H       6.94736      8.61836      7.40104
H       5.90690      8.82846      8.81985
H       7.31993      7.76480      8.90898
H       7.23779     11.10181      7.23169
H       7.85377     12.05493      8.58696
H       6.22330     11.36505      8.65799
H       9.27428      9.55367      7.37489
H       9.90152     10.50949      8.72766
H       9.67788      8.76425      8.90927
H       9.93841      7.25448     14.64981
H      11.38520      6.24875     14.46666
H      10.30884      6.51639     13.08907
H      12.49285      8.67543     16.49308
H      11.73358     10.26912     16.37548
H      10.74741      8.82195     16.21845
H      14.53262     11.00790     14.75342
H      12.98985     11.74906     15.20133
H      13.70940     12.09218     13.62606
H      14.86574      9.75824     11.45669
H      13.99008     11.29475     11.48829
H      13.48813     10.02249     10.37802
H      12.92004      6.83028     11.14913
H      11.16187      7.01221     11.07717
H      12.19941      8.13372     10.19397
H      10.78353     16.30460     10.35909
H       9.10504     15.78013     10.13605
H      10.38460     15.11612      9.10642
H      10.24089     10.09256     11.20833
H      10.68923     11.78268     12.52395
C       8.76028     10.50080     14.14833
C       9.10316     11.23170     15.33448
C       8.79599     10.75790     16.60115
C       8.13297      9.53941     16.78448
C       7.78345      8.80269     15.64762
C       8.07326      9.26020     14.36895
H       9.59533     12.19514     15.23015
H       9.07762     11.35620     17.46528
H       7.88956      9.17984     17.77906
H       7.26908      7.84983     15.75631
H       7.78126      8.65957     13.51127
H       8.01032     11.27959     13.52064
89
Complex 1 - SI C-H activation Green Profil - product
C       2.52050     -2.16232      1.80136
C       2.67953     -2.42251      0.40119
C       3.29766     -1.24808     -0.19960
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C	3.46687	-0.27424	0.82778
C	2.95367	-0.82189	2.07074
Ir	1.25541	-0.69871	0.58288
Ta	-0.87389	0.79445	-0.43176
C	-2.54247	2.24613	-0.45954
C	-3.58450	2.59876	0.63132
C	-4.71165	3.43612	-0.00231
C	2.45509	-3.73283	-0.28760
C	3.79330	-1.16264	-1.60990
C	4.19690	1.02712	0.72024
C	3.06021	-0.18542	3.42161
C	2.04304	-3.13505	2.83028
C	-2.26531	-0.77843	-1.07680
C	-2.56146	-1.20565	-2.53847
C	-3.20695	-0.08078	-3.35967
C	0.03152	1.80750	-2.11446
C	0.86178	3.10394	-2.25740
C	1.16104	3.33816	-3.74986
C	-1.28024	-1.67999	-3.24014
C	-3.55159	-2.38643	-2.49485
C	2.18954	2.95218	-1.50853
C	0.12093	4.33184	-1.71203
C	-4.20185	1.33874	1.25240
C	-2.93498	3.43617	1.74231
H	0.61502	0.98122	-2.55969
H	-0.87307	1.89538	-2.74917
H	-0.84595	4.47190	-2.20833
H	-0.05935	4.24856	-0.63527
H	0.71418	5.23851	-1.88103
H	2.82070	3.83836	-1.64611
H	2.02426	2.81039	-0.43623
H	2.74193	2.08117	-1.87719
H	-2.03674	3.18600	-0.73796
H	-3.08228	1.94664	-1.37861
H	-3.67541	3.71083	2.50336
H	-2.51123	4.36399	1.33857
H	-2.12875	2.88416	2.23497
H	-5.46011	3.72879	0.74508
H	-4.31427	4.35181	-0.45599
H	-5.22763	2.87173	-0.78827
H	-4.94331	1.60472	2.01619
H	-3.43652	0.71547	1.72790
H	-4.71480	0.73171	0.49701
H	-1.93038	-1.67149	-0.53635
H	-3.21234	-0.49739	-0.59017
H	-3.79383	-2.73693	-3.50621
H	-4.48833	-2.09683	-2.00554
H	-3.13224	-3.23132	-1.93720
H	-3.47816	-0.44057	-4.35954
H	-2.53304	0.77202	-3.49349
H	-4.12094	0.28580	-2.87897
H	-1.50312	-2.05801	-4.24537
H	-0.55186	-0.86910	-3.34611
H	-0.79944	-2.48697	-2.67560
H	1.65263	-4.30282	0.18662
H	3.36335	-4.34894	-0.25646

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H       2.18661     -3.59187     -1.33748
H       2.90393     -3.64097      3.28542
H       1.48324     -2.63658      3.62460
H       1.39229     -3.89778      2.39930
H       4.00187     -0.46061      3.91513
H       2.23998     -0.49686      4.07308
H       3.03048      0.90489      3.35255
H       5.21334      0.91411      1.11868
H       3.70412      1.81635      1.29296
H       4.28020      1.36590     -0.31293
H       4.78134     -1.63250     -1.70179
H       3.11886     -1.67183     -2.30275
H       3.88671     -0.12613     -1.94147
H       1.77295      4.23733     -3.89284
H       0.23593      3.46812     -4.32310
H       1.70497      2.48972     -4.18108
H       0.43667     -0.89732     -0.81577
H       0.76000      0.86238      0.76882
C      -0.39800     -1.27009      1.71000
C      -0.77901     -0.56212      2.86765
C      -1.70463     -1.07903      3.77871
C      -2.28825     -2.32540      3.56120
C      -1.93107     -3.04959      2.42314
C      -1.00533     -2.52829      1.51926
H      -0.33580      0.40992      3.06300
H      -1.96728     -0.50072      4.66171
H      -3.01040     -2.72754      4.26668
H      -2.37310     -4.02604      2.23736
H      -0.74376     -3.11895      0.64324
H      -0.99929      1.49971      1.14920
111
Complex 2
O       0.01792      0.20141      3.96360
Si      1.10614      0.75691      5.13144
Si     -0.26711      0.56126      2.39401
O      -1.87254      0.91572      2.21911
Si     -2.86031      1.87107      1.30039
O      -3.39885      1.02717     -0.01319
Si     -2.96176     -0.22720     -1.00104
O      -4.30823     -1.03608     -1.46131
O       0.65574      1.86352      1.95291
Si      1.43427      2.46156      0.62669
O       0.44604      3.49252     -0.21356
Si     -1.16150      3.76206     -0.47968
O      -1.41251      5.37018     -0.64892
Si     -1.91514      6.36464     -1.91871
O       0.11773     -0.74950      1.46333
Si     -0.35275     -1.52591      0.08249
O      -1.96812     -1.27251     -0.18857
O       2.75016      3.25682      1.20731
O       1.90669      1.23853     -0.38445
Si      1.35495      0.37765     -1.67715
O       2.69318     -0.04376     -2.53548
O      -0.07407     -3.13231      0.23382
Si     -0.96595     -4.43890      0.82494
O       0.53647     -0.98160     -1.19909
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O	-2.04066	3.22553	0.81514
O	-4.17407	2.30548	2.17501
Si	-4.50417	3.53022	3.29207
O	-1.65087	2.98484	-1.85921
Si	-1.26144	1.66671	-2.77733
O	-1.55583	2.04424	-4.34277
Si	-2.19339	1.23160	-5.67775
O	0.34241	1.30724	-2.60240
O	-2.18596	0.36274	-2.33916
H	3.34417	3.60532	0.53599
H	2.55792	-0.74796	-3.17620
H	0.01916	-5.47646	1.23903
H	-1.79762	-4.02116	1.99109
H	-1.84287	-4.97229	-0.25765
H	0.86229	-0.06984	6.34666
H	2.50937	0.57674	4.66013
H	0.84791	2.19516	5.42965
H	-1.93800	2.10350	-6.85823
H	-1.50751	-0.08233	-5.85881
H	-3.65722	1.01950	-5.49870
H	-1.82725	7.76175	-1.40940
H	-1.01887	6.19026	-3.09820
H	-3.32179	6.04426	-2.29748
H	-5.65663	3.05916	4.10946
H	-3.31776	3.77201	4.16421
H	-4.86640	4.78237	2.56784
Ta	-6.20155	-1.32855	-1.38730
Ir	-6.99597	-2.45314	-3.33488
C	-7.55290	-4.61673	-3.71444
C	-8.19961	-3.91951	-4.80994
C	-7.20227	-3.27862	-5.57802
C	-5.91195	-3.55547	-4.97635
C	-6.13192	-4.43608	-3.85594
C	-9.67295	-3.91728	-5.07593
C	-7.41664	-2.46180	-6.81406
C	-4.58195	-3.20569	-5.57138
C	-5.06684	-5.15038	-3.08027
C	-8.23555	-5.55912	-2.77051
C	-7.18153	0.54268	-1.01908
C	-7.76582	1.66017	-1.90990
C	-8.97454	1.15819	-2.70960
C	-6.43884	-2.67430	0.30234
C	-7.55365	-2.70814	1.37660
C	-8.93993	-2.78778	0.72160
C	-8.21651	2.82781	-1.01313
C	-6.67988	2.16637	-2.87132
C	-7.47273	-1.46637	2.27646
C	-7.35435	-3.95574	2.25673
H	-6.38642	-3.66244	-0.18571
H	-5.46705	-2.55362	0.81842
H	-9.16225	-1.89226	0.13066
H	-9.00821	-3.64852	0.04797
H	-9.72412	-2.88763	1.48169
H	-8.11097	-4.00607	3.04936
H	-7.43071	-4.87329	1.66206
H	-6.36805	-3.94715	2.73469

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H      -7.99088      0.12702     -0.37672
H      -6.46709      0.99892     -0.30546
H      -9.38480      1.96593     -3.32753
H      -9.77272      0.81450     -2.04035
H      -8.70279      0.32478     -3.36228
H      -8.63628      3.64388     -1.61374
H      -8.98673      2.50579     -0.30257
H      -7.37615      3.23262     -0.43725
H      -7.05092      3.00692     -3.46985
H      -6.36532      1.37507     -3.55997
H      -5.79695      2.51274     -2.32126
H      -8.40884     -2.00381     -6.82778
H      -7.32486     -3.08322     -7.71446
H      -6.68090     -1.65747     -6.89383
H      -9.97606     -3.04223     -5.65623
H      -9.97095     -4.80961     -5.64203
H     -10.24763     -3.91136     -4.14604
H      -8.35994     -6.55069     -3.22653
H      -9.22918     -5.19785     -2.49242
H      -7.66339     -5.69078     -1.84861
H      -4.77635     -6.07943     -3.58905
H      -5.41078     -5.41835     -2.07804
H      -4.16975     -4.53607     -2.97022
H      -4.27392     -3.95176     -6.31664
H      -4.61150     -2.23319     -6.06954
H      -3.80297     -3.15709     -4.80676
H      -6.49748     -1.40376      2.77335
H      -8.24277     -1.50105      3.05593
H      -7.61811     -0.53976      1.71150
H      -6.72704     -0.91234     -3.72357
H      -8.21628     -1.88862     -2.42282
123
Complex 2 - C-H activation - adduct
C      -2.06530     -2.88388      2.40649
C      -3.03465     -2.08005      3.04049
C      -4.14131     -1.88769      2.12337
C      -3.86011     -2.64404      0.93075
C      -2.54261     -3.20880      1.07498
Ir     -2.38478     -0.94933      0.98451
Ta     -2.21565      0.47239     -0.90986
C      -2.87868     -0.63936     -2.64174
C      -2.29446     -0.41154     -4.05722
C      -0.86379     -0.96621     -4.11996
C      -2.97013     -1.52858      4.43095
C      -5.46142     -1.28160      2.49020
C      -4.83456     -2.95045     -0.16452
C      -1.89130     -4.18292      0.14015
C      -0.76404     -3.34355      2.98781
C      -6.19872     -5.19333     -4.38157
C      -6.83159     -5.84138     -3.32087
C      -6.15956     -6.83660     -2.61122
C      -4.85453     -7.18309     -2.96132
C      -4.22137     -6.53505     -4.02183
C      -4.89395     -5.54077     -4.73259
O      -0.44373      1.18142     -1.14663
Si      1.10120      1.24289     -0.58845
```

O	1.77967	-0.26285	-0.65816
Si	3.24154	-0.98741	-0.89855
O	4.00985	-1.22559	0.54597
Si	4.08967	-0.59749	2.07105
O	2.66324	0.14450	2.45054
Si	1.95512	1.63251	2.37844
O	0.94463	1.76133	3.65651
Si	-0.33100	2.76804	4.11088
C	-3.48711	2.21851	-0.81591
C	-4.89706	2.43973	-0.23259
C	-5.85349	1.35973	-0.75655
O	1.12656	1.82183	0.95963
O	1.94281	2.27621	-1.57275
Si	3.18996	3.35590	-1.48783
O	3.27744	4.00455	0.03335
Si	4.04166	3.75454	1.47715
O	5.50448	3.02548	1.22130
Si	6.18006	1.51324	1.19088
O	6.20073	0.97419	-0.37472
Si	5.34657	1.13166	-1.77709
O	4.19641	-0.05544	-1.88289
O	3.11318	2.81768	2.47626
O	4.27506	5.22427	2.16093
Si	4.61508	5.78073	3.71766
O	2.94507	4.55507	-2.57673
Si	2.27768	6.10421	-2.49670
O	4.61343	2.61281	-1.88341
O	6.45019	0.97870	-2.98880
O	2.96632	-2.43147	-1.62012
Si	3.90535	-3.50398	-2.52328
O	5.33490	0.49186	2.17201
O	4.35669	-1.82410	3.11966
Si	5.37468	-2.06418	4.44533
O	7.71387	1.54673	1.78367
C	-5.41861	3.81959	-0.67243
C	-4.85130	2.39064	1.29910
C	-3.16210	-1.15414	-5.08791
C	-2.27831	1.08358	-4.41134
H	8.36711	1.91712	1.18270
H	6.13000	1.24243	-3.85657
H	3.85892	-3.11626	-3.96332
H	5.31846	-3.49808	-2.04426
H	3.30667	-4.85637	-2.34291
H	4.92858	-3.33297	5.08672
H	6.78860	-2.19100	3.98883
H	5.25066	-0.93277	5.41016
H	0.98363	6.07826	-1.75351
H	3.22970	7.03467	-1.82476
H	2.04970	6.53432	-3.90492
H	5.49751	4.81759	4.43878
H	5.30487	7.09223	3.56187
H	3.34054	5.96253	4.47118
H	-1.41974	1.90894	4.65085
H	0.15866	3.69188	5.17601
H	-0.81697	3.56060	2.94502
H	-2.79674	2.97490	-0.39672

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H      -3.51362      2.45046     -1.90232
H      -4.46260      1.42820      1.64282
H      -4.19782      3.17739      1.69470
H      -5.85133      2.54350      1.72246
H      -6.41917      4.01078     -0.26564
H      -4.75661      4.62005     -0.32274
H      -5.48192      3.89076     -1.76491
H      -2.86151     -1.71244     -2.40515
H      -3.95514     -0.36672     -2.63871
H      -1.90777      1.23895     -5.43158
H      -1.62388      1.65157     -3.73885
H      -3.28505      1.51543     -4.35695
H      -0.44060     -0.83974     -5.12351
H      -0.20417     -0.45534     -3.41115
H      -0.84711     -2.03586     -3.88172
H      -2.76005     -1.03544     -6.10175
H      -4.18931     -0.77134     -5.08740
H      -3.20450     -2.22597     -4.86486
H      -2.21985     -4.03010     -0.89068
H      -2.13801     -5.21715      0.41578
H      -0.80275     -4.08530      0.15536
H      -4.33084     -3.17188     -1.10784
H      -5.43892     -3.82966      0.09494
H      -5.52096     -2.11835     -0.34113
H      -6.08260     -2.00443      3.03676
H      -6.02157     -0.96819      1.60638
H      -5.34024     -0.40397      3.13059
H      -3.49102     -2.18800      5.13763
H      -3.44231     -0.54464      4.49336
H      -1.93863     -1.42404      4.77641
H      -0.87036     -4.33325      3.45094
H       0.01167     -3.42080      2.22183
H      -0.39934     -2.65598      3.75496
H      -6.87046      1.51481     -0.37688
H      -5.52199      0.36378     -0.44193
H      -5.90355      1.37224     -1.85243
H      -0.82226     -0.78742      0.68779
H      -6.72280     -4.42000     -4.93681
H      -7.84886     -5.57256     -3.04900
H      -6.65336     -7.34364     -1.78647
H      -4.33189     -7.95953     -2.40903
H      -3.20561     -6.80682     -4.29642
H      -4.40352     -5.03992     -5.56304
H      -2.23776      0.53922      1.58090
123
Complex 2 - C-H activation - TS
C      -9.26600     -3.06712     -3.64168
C      -9.06001     -2.27434     -2.49712
C     -10.20989     -1.96544     -1.73969
C     -11.48894     -2.33692     -2.14645
C     -11.66319     -3.07442     -3.31886
C     -10.54223     -3.45051     -4.05641
Ta     -6.93464     -1.06960     -2.01138
C      -8.29512      0.62752     -1.70560
C      -8.52557      1.52968     -0.46681
C      -9.40107      0.81249      0.57079
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Ir	-6.71310	-2.92639	-0.31653
C	-5.99495	-5.04456	-0.09085
C	-5.62017	-4.34792	1.12679
C	-6.81676	-3.91237	1.76619
C	-7.94316	-4.31842	0.95768
C	-7.42750	-5.05536	-0.17237
C	-4.22323	-4.19377	1.64075
C	-6.90505	-3.19553	3.07714
C	-9.38946	-4.17534	1.31661
C	-8.25711	-5.77822	-1.18587
C	-5.04604	-5.77648	-0.98852
C	-6.53155	-1.36744	-4.15485
C	-5.44501	-2.24636	-4.82724
C	-4.06740	-2.00360	-4.19951
O	-5.39181	0.11114	-1.87773
Si	-3.88240	0.66370	-1.61250
O	-3.28202	1.30342	-3.02123
Si	-2.29449	2.50149	-3.57727
O	-0.76338	1.91445	-3.79476
Si	0.25724	0.76931	-3.17187
O	1.30869	0.26975	-4.33537
C	-5.78365	-3.73808	-4.70157
C	-5.37142	-1.88466	-6.32235
O	-2.88965	-0.56127	-1.09676
Si	-1.32478	-1.05805	-1.20566
O	-1.31061	-2.69941	-1.20283
Si	-0.08438	-3.84653	-1.02486
O	-3.90000	1.85222	-0.45755
Si	-2.98072	2.47332	0.76080
O	-2.09845	3.75402	0.19404
Si	-1.41995	4.30735	-1.21090
O	-1.43470	5.94439	-1.21058
Si	-1.95843	7.12372	-0.12111
O	-0.44520	-0.51413	0.09105
Si	-0.43385	0.73964	1.16784
O	0.11686	0.19714	2.61116
Si	1.50574	0.48590	3.52886
O	-0.63603	-0.50433	-2.60480
O	-1.96959	1.31398	1.37802
O	0.56047	1.94844	0.62697
Si	1.12475	2.56253	-0.79788
O	2.63527	3.12287	-0.46841
O	-3.95179	3.02345	1.95905
Si	-4.25253	2.55655	3.55208
C	-9.26026	2.80513	-0.92137
C	-7.20528	1.93535	0.19491
O	-2.28109	3.77770	-2.51967
O	-2.83731	3.01828	-5.03440
Si	-3.72057	4.35717	-5.56135
O	0.14303	3.78363	-1.33100
O	1.19685	1.39228	-1.96630
H	3.13300	3.41587	-1.23753
H	0.89487	0.00168	-5.16120
H	0.12323	-4.13600	0.42368
H	-0.54657	-5.07859	-1.72486
H	1.18757	-3.35760	-1.63221

H	1.40259	-0.40270	4.72078
H	2.72724	0.14774	2.74267
H	1.55351	1.91328	3.95811
H	-4.12630	4.06326	-6.96452
H	-4.92969	4.55443	-4.70920
H	-2.86762	5.58017	-5.52196
H	-1.22626	6.99575	1.17238
H	-1.65131	8.43697	-0.75429
H	-3.42634	6.99720	0.11110
H	-4.64940	1.11971	3.61308
H	-3.03845	2.77966	4.39056
H	-5.36873	3.41627	4.03604
H	-7.80645	1.25142	-2.48519
H	-9.27324	0.35915	-2.12414
H	-10.39298	0.58262	0.16488
H	-8.93756	-0.12397	0.89999
H	-9.54621	1.44662	1.45376
H	-7.39068	2.62207	1.02975
H	-6.67153	1.06434	0.58828
H	-6.53821	2.43840	-0.51029
H	-7.49052	-1.54413	-4.65967
H	-6.28274	-0.31139	-4.38112
H	-3.29896	-2.58477	-4.72404
H	-4.04942	-2.30607	-3.14764
H	-3.78556	-0.94807	-4.25780
H	-4.97790	-4.35143	-5.12313
H	-5.91684	-4.02261	-3.65231
H	-6.70022	-3.99046	-5.24723
H	-4.63222	-2.50568	-6.84390
H	-5.08339	-0.83597	-6.45864
H	-6.34018	-2.03204	-6.81377
H	-5.45690	-5.89816	-1.99303
H	-4.83117	-6.77703	-0.59099
H	-4.09699	-5.24373	-1.08319
H	-7.68632	-5.99093	-2.09265
H	-8.60566	-6.73612	-0.77858
H	-9.13664	-5.19862	-1.47798
H	-9.74410	-5.05193	1.87494
H	-10.01262	-4.07293	0.42434
H	-9.56031	-3.29417	1.94003
H	-7.01042	-3.91443	3.89948
H	-7.76712	-2.52534	3.10980
H	-6.01116	-2.59768	3.26891
H	-3.90291	-5.09704	2.17623
H	-3.51532	-4.01759	0.82752
H	-4.14260	-3.35185	2.33219
H	-9.47667	3.46124	-0.06908
H	-10.21160	2.56104	-1.40813
H	-8.65437	3.37465	-1.63562
H	-5.42585	-2.33499	-1.10521
H	-8.03250	-2.66485	-1.63880
H	-10.09470	-1.42239	-0.80627
H	-12.35098	-2.05733	-1.54512
H	-12.65858	-3.36771	-3.64176
H	-10.65919	-4.04684	-4.95839
H	-8.41383	-3.39608	-4.22602

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H      -7.01816     -1.42424      0.21903
123
Complex 2 - C-H activation - product
C      -5.05403      0.32124     -2.35360
C      -4.60921     -0.77257     -1.58069
C      -5.55358     -1.80216     -1.38546
C      -6.84024     -1.75034     -1.92788
C      -7.24011     -0.65455     -2.68834
C      -6.33617      0.38828     -2.89550
Ta     -2.60401     -0.77003     -0.59060
C      -3.74770      0.74751      0.58757
C      -3.62390      0.97893      2.11857
C      -4.49247     -0.04496      2.86569
Ir     -2.42413     -3.15851      0.47597
C      -1.07371     -4.91119      0.82660
C      -1.48177     -4.36553      2.11075
C      -2.90344     -4.49553      2.21240
C      -3.39655     -5.10170      0.99341
C      -2.25298     -5.37370      0.15577
C      -0.55604     -3.85875      3.17206
C      -3.73967     -4.14514      3.40248
C      -4.80577     -5.53165      0.72953
C      -2.29185     -6.08844     -1.15793
C       0.33692     -5.07214      0.35247
C      -1.97913     -0.63891     -2.73013
C      -1.89817     -1.74651     -3.81457
C      -0.82197     -2.77675     -3.43661
O      -1.05845      0.37328     -0.25443
Si      0.46703      0.92941     -0.18682
O       1.12077      0.97114     -1.70995
Si      2.14557      1.86166     -2.64644
O       3.65544      1.18481     -2.60398
Si      4.60838      0.29884     -1.58124
O       5.64888     -0.62974     -2.45514
C      -3.23005     -2.46505     -4.05602
C      -1.46782     -1.07768     -5.13579
O       1.38889     -0.07361      0.76722
Si      2.93807     -0.61862      0.87422
O       2.90694     -2.14528      1.48876
Si      4.02154     -2.97171      2.45659
O       0.49256      2.45842      0.45237
Si      1.42635      3.44363      1.38681
O       2.37486      4.39725      0.41949
Si      3.08402      4.36998     -1.07644
O       3.14566      5.89179     -1.67576
Si      2.60825      7.40318     -1.14785
O       3.83681      0.32917      1.89579
Si      3.89747      1.88545      2.45299
O       4.41365      1.87166      4.00623
Si      5.77193      2.48404      4.80396
O       3.64573     -0.64871     -0.62036
O       2.38676      2.55265      2.40279
O       4.94961      2.77856      1.53810
Si      5.54410      2.79865     -0.00253
O       7.07868      3.37488      0.12658
O       0.45098      4.40838      2.27887
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Si	0.37724	4.85109	3.90662
C	-4.16799	2.38683	2.43003
C	-2.18670	0.88965	2.64696
O	2.20347	3.43033	-2.11406
O	1.62688	1.84045	-4.19924
Si	0.96402	2.99682	-5.23826
O	4.62440	3.77921	-0.96822
O	5.55764	1.27456	-0.64837
H	7.58030	3.37709	-0.69408
H	5.23639	-1.14242	-3.15667
H	3.88788	-2.53399	3.87566
H	3.67813	-4.41789	2.33927
H	5.41388	-2.73810	1.97585
H	5.63070	2.07322	6.22932
H	7.01725	1.90430	4.22358
H	5.80420	3.97144	4.70071
H	0.64511	2.28251	-6.50535
H	-0.27627	3.57703	-4.64665
H	1.95715	4.07940	-5.49803
H	3.30390	7.78600	0.11530
H	2.95183	8.36617	-2.23143
H	1.13305	7.38178	-0.92862
H	0.08406	3.66159	4.75598
H	1.66874	5.46820	4.33076
H	-0.72356	5.84820	4.01758
H	-3.38434	1.65078	0.05848
H	-4.81527	0.69370	0.36134
H	-5.53483	0.00187	2.52948
H	-4.13264	-1.06533	2.69866
H	-4.47754	0.14651	3.94591
H	-2.16453	1.09836	3.72416
H	-1.75954	-0.10763	2.49365
H	-1.53617	1.61470	2.15040
H	-2.58313	0.19001	-3.13149
H	-0.95942	-0.23683	-2.64010
H	-0.71287	-3.53249	-4.22469
H	-1.07403	-3.29099	-2.50333
H	0.15265	-2.29293	-3.29947
H	-3.13173	-3.18105	-4.88216
H	-3.56098	-3.01340	-3.16918
H	-4.02365	-1.75649	-4.31201
H	-1.34415	-1.82075	-5.93410
H	-0.51592	-0.54782	-5.01752
H	-2.21875	-0.35185	-5.46875
H	0.39587	-5.04465	-0.73801
H	0.74843	-6.03286	0.68767
H	0.98223	-4.27888	0.73541
H	-1.44747	-5.81227	-1.79232
H	-2.24787	-7.17232	-0.99368
H	-3.20947	-5.87067	-1.70871
H	-4.98295	-6.54580	1.11051
H	-5.02706	-5.53471	-0.34025
H	-5.52429	-4.86507	1.21242
H	-3.85788	-5.02336	4.04933
H	-4.73664	-3.81029	3.10761
H	-3.28365	-3.35094	3.99683

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H      -0.20006     -4.68744      3.79724
H       0.31576     -3.36532      2.73700
H      -1.05319     -3.13695      3.82354
H      -4.16572      2.58333      3.51013
H      -5.19714      2.49922      2.06990
H      -3.55789      3.15841      1.94671
H      -1.25844     -2.01936      0.44641
H      -2.77615     -2.82870     -1.08379
H      -5.28056     -2.67424     -0.79643
H      -7.53089     -2.57351     -1.75523
H      -8.23973     -0.61092     -3.11310
H      -6.62958      1.25523     -3.48368
H      -4.38775      1.16437     -2.53559
H      -3.53911     -2.02877      0.86202
123
Complex 2 - C-H activation - rot. TS
C      -7.08855     -2.37930     -4.34992
C      -7.90914     -2.03150     -3.25975
C      -9.26094     -2.41084     -3.33151
C      -9.77542     -3.08252     -4.44065
C      -8.95017     -3.38483     -5.52381
C      -7.60184     -3.02930     -5.47274
Ta     -7.05487     -1.01647     -1.49250
C      -8.11159     -0.22875      0.30355
C      -9.44665     -0.64355      0.97541
C      -9.47019     -2.12850      1.35645
Ir     -6.13402     -3.39875     -0.53058
C      -6.34174     -5.60576     -0.89315
C      -4.95516     -5.23093     -1.02946
C      -4.51192     -4.73550      0.25502
C      -5.61856     -4.78786      1.16197
C      -6.75861     -5.33494      0.45179
C      -4.09292     -5.46286     -2.23075
C      -3.11159     -4.32888      0.59281
C      -5.58213     -4.45672      2.62112
C      -8.07644     -5.69419      1.06258
C      -7.17585     -6.23846     -1.96333
C      -8.21374      0.65867     -2.46929
C      -8.15802      1.29714     -3.88832
C      -6.73243      1.32340     -4.45612
O      -5.49522      0.05785     -1.70335
Si     -3.93350      0.54286     -1.64851
O      -3.04772     -0.34463     -2.72703
Si     -1.76536     -0.17414     -3.75285
O      -0.37873     -0.66866     -2.99363
Si      0.27192     -0.71885     -1.47073
O       1.35321     -1.95583     -1.37348
C      -9.08911      0.60143     -4.89145
C      -8.64189      2.75657     -3.75434
O      -3.33429      0.33399     -0.11961
Si     -1.90457     -0.01258      0.63055
O      -2.20244     -0.87433      1.99384
Si     -2.06307     -0.50254      3.63737
O      -3.87308      2.14577     -2.04907
Si     -3.02057      3.52098     -1.71543
O      -1.81292      3.71107     -2.82835
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Si	-0.85017	2.80123	-3.82117
O	-0.51984	3.64730	-5.18201
Si	-0.95559	5.17627	-5.75672
O	-1.12542	1.38790	1.05310
Si	-0.99326	2.96502	0.57220
O	-0.77459	3.89425	1.90064
Si	0.37671	5.03821	2.37322
O	-0.95190	-0.91732	-0.37211
O	-2.38535	3.43244	-0.18783
O	0.29898	3.14800	-0.44730
Si	1.17216	2.25385	-1.52563
O	2.71100	2.82370	-1.42915
O	-3.99997	4.82608	-1.82502
Si	-5.07579	5.60766	-0.78241
C	-10.64421	-0.34261	0.06365
C	-9.60534	0.18919	2.26220
O	-1.61822	1.39927	-4.24788
O	-2.01163	-1.13191	-5.05805
Si	-1.94402	-0.88898	-6.72919
O	0.56876	2.43581	-3.05653
O	1.13031	0.64683	-1.12963
H	3.35641	2.33907	-1.95226
H	1.02653	-2.80335	-1.68904
H	-2.86095	0.71315	3.96771
H	-2.60376	-1.68262	4.37015
H	-0.63219	-0.29107	4.00010
H	-0.10679	5.59768	3.66668
H	1.70322	4.38361	2.56033
H	0.47965	6.12031	1.35203
H	-2.20327	-2.21921	-7.34851
H	-2.98641	0.08854	-7.15317
H	-0.59176	-0.39750	-7.12476
H	-0.46435	6.23519	-4.82818
H	-0.29922	5.31724	-7.08673
H	-2.43668	5.27051	-5.90122
H	-5.86400	4.60897	-0.00317
H	-4.31537	6.49114	0.14825
H	-5.97857	6.42396	-1.64024
H	-7.31306	-0.32025	1.06111
H	-8.18383	0.84748	0.09311
H	-9.39842	-2.77421	0.47557
H	-8.63115	-2.37849	2.01562
H	-10.39986	-2.37312	1.88488
H	-10.54730	-0.04782	2.77241
H	-8.78544	-0.00749	2.96255
H	-9.60553	1.26223	2.03946
H	-9.27467	0.52104	-2.20931
H	-7.86053	1.44867	-1.78183
H	-6.71266	1.84380	-5.42220
H	-6.35175	0.31030	-4.61819
H	-6.04500	1.84355	-3.78196
H	-9.12113	1.17070	-5.82927
H	-8.76248	-0.41168	-5.12853
H	-10.11311	0.54486	-4.50358
H	-8.64889	3.26170	-4.72895
H	-7.98990	3.33023	-3.08499

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H      -9.65945      2.79720     -3.34771
H      -8.23888     -6.03638     -1.81579
H      -7.03626     -7.32689     -1.96290
H      -6.90615     -5.86439     -2.95342
H      -8.87024     -5.72305      0.31253
H      -8.02857     -6.68462      1.53407
H      -8.37431     -4.97556      1.82958
H      -5.36606     -5.35424      3.21523
H      -6.53916     -4.05532      2.96350
H      -4.81093     -3.71593      2.84350
H      -2.53924     -5.19430      0.95110
H      -3.08602     -3.56166      1.36875
H      -2.59454     -3.92458     -0.28007
H      -3.61849     -6.45242     -2.18789
H      -4.67490     -5.41246     -3.15391
H      -3.29982     -4.71481     -2.30329
H     -11.58495     -0.58283      0.57344
H     -10.61107     -0.93050     -0.85924
H     -10.67563      0.71585     -0.21681
H      -5.14716     -2.18214     -0.89038
H      -7.05532     -3.03230     -1.81371
H      -9.93973     -2.17671     -2.51267
H     -10.82731     -3.35805     -4.46422
H      -9.35151     -3.89580     -6.39477
H      -6.94435     -3.26593     -6.30630
H      -6.02372     -2.14960     -4.32560
H      -6.98713     -2.26825      0.26534
123
Complex 2 - C-H activation - product Ben.
C      -4.85448      0.73249     -2.34506
C      -4.61393     -0.46258     -1.63391
C      -5.67195     -1.39576     -1.63395
C      -6.88480     -1.14945     -2.28300
C      -7.08525      0.04510     -2.96921
C      -6.05645      0.98798     -3.00093
Ta     -2.64002     -0.95137     -0.72588
C      -2.22273     -1.08376     -2.91881
C      -1.17664     -1.94619     -3.67521
C      -1.57785     -3.42801     -3.62294
Ir     -2.90485     -3.18640      0.56520
C      -2.47527     -3.90933      2.69374
C      -2.82291     -5.06670      1.92764
C      -1.88258     -5.19163      0.85172
C      -0.89374     -4.13856      0.99909
C      -1.26157     -3.34299      2.13349
C      -3.95136     -6.00614      2.22056
C      -1.81243     -6.32191     -0.12861
C       0.38313     -4.04096      0.22519
C      -0.44753     -2.25033      2.75294
C      -3.13805     -3.46670      3.96108
O      -0.79121     -0.40559     -0.50077
Si      0.54864      0.50980     -0.33265
O       1.83653     -0.49891     -0.04975
Si      3.45617     -0.60254     -0.34172
O       4.31580      0.00237      0.94024
Si      4.16395      1.10226      2.16536
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O	4.95977	0.54919	3.48416
Si	6.40660	0.95207	4.25862
O	0.38369	1.52502	0.96897
Si	1.26133	2.21931	2.17724
O	2.57014	1.28030	2.56718
O	0.82562	1.41583	-1.68946
Si	1.46702	2.86190	-2.16391
O	3.05953	2.66557	-2.56392
Si	4.37139	1.73167	-2.18100
O	5.37762	1.61782	-3.47747
O	0.29548	2.36213	3.49282
Si	0.56356	2.36804	5.16000
O	1.77543	3.72470	1.71447
Si	2.16618	4.56029	0.33769
O	1.79060	6.14032	0.53946
Si	1.19040	7.06415	1.81965
C	-1.18936	-1.50132	-5.15184
C	0.25282	-1.79142	-3.14741
O	0.67291	3.38877	-3.49444
Si	-0.41491	4.64267	-3.81045
O	1.30932	3.98051	-0.95205
O	3.84942	0.22984	-1.71488
O	3.82342	-2.18788	-0.53466
Si	5.23747	-3.10040	-0.39750
O	5.27129	2.42569	-0.98421
Si	5.06718	3.42259	0.32177
O	6.44172	4.28296	0.59206
O	3.78409	4.42631	0.02983
O	4.80977	2.55417	1.70278
C	-3.11062	0.92554	0.38981
H	6.79276	4.73688	-0.17986
H	4.95971	1.30536	-4.28554
H	5.43992	-3.49655	1.02638
H	5.04436	-4.31425	-1.23979
H	6.41435	-2.32071	-0.88020
H	6.63183	-0.10381	5.28562
H	7.53346	0.96669	3.28172
H	6.28132	2.28542	4.91451
H	-0.88866	4.43837	-5.20760
H	-1.56451	4.58337	-2.86181
H	0.27596	5.95914	-3.69013
H	2.08237	6.93982	3.00923
H	1.16994	8.47416	1.34000
H	-0.18922	6.62035	2.17204
H	-0.62856	3.01029	5.77982
H	0.70541	0.96742	5.65312
H	1.79505	3.14472	5.48824
H	-3.17811	-1.25257	-3.42516
H	-1.99791	-0.01321	-3.10286
H	0.95119	-2.37798	-3.75763
H	0.34289	-2.13465	-2.11431
H	0.57509	-0.74612	-3.18578
H	-0.90243	-4.03728	-4.23633
H	-1.54431	-3.81306	-2.59841
H	-2.59750	-3.57518	-3.99793
H	-0.49222	-2.10110	-5.75115

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H      -0.89465     -0.44983     -5.24681
H      -2.18861     -1.60885     -5.58883
H      -2.80570     -6.71336     -0.36065
H      -1.21264     -7.14760      0.27514
H      -1.35402     -6.00818     -1.06891
H      -4.33910     -6.46705      1.30945
H      -3.60930     -6.81167      2.88244
H      -4.78082     -5.49805      2.71732
H      -2.70970     -3.99681      4.82126
H      -4.21161     -3.66834      3.94527
H      -3.00391     -2.39673      4.13180
H       0.18379     -2.65625      3.55397
H      -1.07944     -1.47347      3.18912
H       0.20776     -1.77595      2.02076
H       1.14222     -4.69126      0.67919
H       0.25415     -4.36309     -0.81026
H       0.78104     -3.02536      0.21238
H      -4.38970     -3.53916      0.15852
H      -2.92996     -3.15042     -1.04524
H      -4.07748      1.49416     -2.40377
H      -6.19284      1.92548     -3.53575
H      -8.02781      0.24084     -3.47405
H      -7.67492     -1.89652     -2.24738
H      -5.55999     -2.34196     -1.11160
H      -3.76439     -1.87510      0.95446
H      -2.13233      1.23932      0.77965
H      -3.33766      1.62920     -0.42782
C      -4.11518      1.18664      1.54612
C      -4.16064      2.70770      1.79418
C      -5.54110      0.70499      1.25717
C      -3.61023      0.51273      2.83122
H      -6.20682      0.98111      2.08495
H      -5.93752      1.14794      0.33899
H      -5.58453     -0.38190      1.13900
H      -4.27636      0.73216      3.67474
H      -3.56829     -0.57519      2.71162
H      -2.60645      0.86828      3.09232
H      -4.81071      2.95021      2.64456
H      -3.16146      3.10304      2.01012
H      -4.54939      3.23503      0.91545
123
Complex 2 - C-H activation Red profile - adduct
C      -2.06530     -2.88388      2.40649
C      -3.03465     -2.08005      3.04049
C      -4.14131     -1.88769      2.12337
C      -3.86011     -2.64404      0.93075
C      -2.54261     -3.20880      1.07498
Ir     -2.38478     -0.94933      0.98451
Ta     -2.21565      0.47239     -0.90986
C      -2.87868     -0.63936     -2.64174
C      -2.29446     -0.41154     -4.05722
C      -0.86379     -0.96621     -4.11996
C      -2.97013     -1.52858      4.43095
C      -5.46142     -1.28160      2.49020
C      -4.83456     -2.95045     -0.16452
C      -1.89130     -4.18292      0.14015
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C	-0.76404	-3.34355	2.98781
C	-6.19872	-5.19333	-4.38157
C	-6.83159	-5.84138	-3.32087
C	-6.15956	-6.83660	-2.61122
C	-4.85453	-7.18309	-2.96132
C	-4.22137	-6.53505	-4.02183
C	-4.89395	-5.54077	-4.73259
O	-0.44373	1.18142	-1.14663
Si	1.10120	1.24289	-0.58845
O	1.77967	-0.26285	-0.65816
Si	3.24154	-0.98741	-0.89855
O	4.00985	-1.22559	0.54597
Si	4.08967	-0.59749	2.07105
O	2.66324	0.14450	2.45054
Si	1.95512	1.63251	2.37844
O	0.94463	1.76133	3.65651
Si	-0.33100	2.76804	4.11088
C	-3.48711	2.21851	-0.81591
C	-4.89706	2.43973	-0.23259
C	-5.85349	1.35973	-0.75655
O	1.12656	1.82183	0.95963
O	1.94281	2.27621	-1.57275
Si	3.18996	3.35590	-1.48783
O	3.27744	4.00455	0.03335
Si	4.04166	3.75454	1.47715
O	5.50448	3.02548	1.22130
Si	6.18006	1.51324	1.19088
O	6.20073	0.97419	-0.37472
Si	5.34657	1.13166	-1.77709
O	4.19641	-0.05544	-1.88289
O	3.11318	2.81768	2.47626
O	4.27506	5.22427	2.16093
Si	4.61508	5.78073	3.71766
O	2.94507	4.55507	-2.57673
Si	2.27768	6.10421	-2.49670
O	4.61343	2.61281	-1.88341
O	6.45019	0.97870	-2.98880
O	2.96632	-2.43147	-1.62012
Si	3.90535	-3.50398	-2.52328
O	5.33490	0.49186	2.17201
O	4.35669	-1.82410	3.11966
Si	5.37468	-2.06418	4.44533
O	7.71387	1.54673	1.78367
C	-5.41861	3.81959	-0.67243
C	-4.85130	2.39064	1.29910
C	-3.16210	-1.15414	-5.08791
C	-2.27831	1.08358	-4.41134
H	8.36711	1.91712	1.18270
H	6.13000	1.24243	-3.85657
H	3.85892	-3.11626	-3.96332
H	5.31846	-3.49808	-2.04426
H	3.30667	-4.85637	-2.34291
H	4.92858	-3.33297	5.08672
H	6.78860	-2.19100	3.98883
H	5.25066	-0.93277	5.41016
H	0.98363	6.07826	-1.75351

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H       3.22970      7.03467     -1.82476
H       2.04970      6.53432     -3.90492
H       5.49751      4.81759      4.43878
H       5.30487      7.09223      3.56187
H       3.34054      5.96253      4.47118
H      -1.41974      1.90894      4.65085
H       0.15866      3.69188      5.17601
H      -0.81697      3.56060      2.94502
H      -2.79674      2.97490     -0.39672
H      -3.51362      2.45046     -1.90232
H      -4.46260      1.42820      1.64282
H      -4.19782      3.17739      1.69470
H      -5.85133      2.54350      1.72246
H      -6.41917      4.01078     -0.26564
H      -4.75661      4.62005     -0.32274
H      -5.48192      3.89076     -1.76491
H      -2.86151     -1.71244     -2.40515
H      -3.95514     -0.36672     -2.63871
H      -1.90777      1.23895     -5.43158
H      -1.62388      1.65157     -3.73885
H      -3.28505      1.51543     -4.35695
H      -0.44060     -0.83974     -5.12351
H      -0.20417     -0.45534     -3.41115
H      -0.84711     -2.03586     -3.88172
H      -2.76005     -1.03544     -6.10175
H      -4.18931     -0.77134     -5.08740
H      -3.20450     -2.22597     -4.86486
H      -2.21985     -4.03010     -0.89068
H      -2.13801     -5.21715      0.41578
H      -0.80275     -4.08530      0.15536
H      -4.33084     -3.17188     -1.10784
H      -5.43892     -3.82966      0.09494
H      -5.52096     -2.11835     -0.34113
H      -6.08260     -2.00443      3.03676
H      -6.02157     -0.96819      1.60638
H      -5.34024     -0.40397      3.13059
H      -3.49102     -2.18800      5.13763
H      -3.44231     -0.54464      4.49336
H      -1.93863     -1.42404      4.77641
H      -0.87036     -4.33325      3.45094
H       0.01167     -3.42080      2.22183
H      -0.39934     -2.65598      3.75496
H      -6.87046      1.51481     -0.37688
H      -5.52199      0.36378     -0.44193
H      -5.90355      1.37224     -1.85243
H      -0.82226     -0.78742      0.68779
H      -6.72280     -4.42000     -4.93681
H      -7.84886     -5.57256     -3.04900
H      -6.65336     -7.34364     -1.78647
H      -4.33189     -7.95953     -2.40903
H      -3.20561     -6.80682     -4.29642
H      -4.40352     -5.03992     -5.56304
H      -2.23776      0.53922      1.58090
123
Complex 2 - C-H activation Red profile - TS
C      -5.50594     -3.88169      1.82127
```

C	-6.32729	-2.98395	2.55479
C	-7.69369	-3.14965	2.10482
C	-7.70550	-4.20030	1.11593
C	-6.35104	-4.63162	0.91484
Ir	-6.53340	-2.44431	0.31763
Ta	-6.74887	-0.99700	-1.76987
C	-7.03124	-0.69766	-3.96349
C	-6.22012	-1.22356	-5.18736
C	-7.04179	-2.25718	-5.96957
C	-5.87673	-2.06480	3.64648
C	-8.89854	-2.52553	2.73846
C	-8.92664	-4.82661	0.51944
C	-5.90552	-5.80448	0.09684
C	-4.03316	-4.07988	1.99713
C	-8.02585	-3.13216	-2.51550
C	-9.35472	-3.07740	-2.96110
C	-9.85829	-4.06051	-3.81069
C	-9.04751	-5.12274	-4.21453
C	-7.73189	-5.20429	-3.75548
C	-7.23280	-4.22416	-2.89976
O	-5.07571	-0.06266	-1.91694
Si	-3.56610	0.21432	-1.34748
O	-2.76190	-1.21369	-1.13531
Si	-1.25981	-1.87899	-1.24081
O	-0.51002	-1.81658	0.23265
Si	-0.52693	-0.93209	1.62673
O	-2.01518	-0.24445	1.84388
Si	-2.81139	1.16218	1.51178
O	-3.85791	1.44154	2.74040
Si	-5.25489	2.37229	2.91696
C	-7.93943	0.73170	-1.18174
C	-9.47542	0.88694	-1.06747
C	-10.13432	0.80181	-2.45095
O	-3.63156	1.05323	0.08006
O	-2.76499	1.12931	-2.47386
Si	-1.59092	2.28640	-2.55927
O	-1.58471	3.19048	-1.17093
Si	-0.84097	3.24032	0.30276
O	0.67293	2.58288	0.19347
Si	1.44352	1.13655	0.43375
O	1.53994	0.33550	-1.01196
Si	0.71861	0.19678	-2.43649
O	-0.33722	-1.07872	-2.36262
O	-1.73244	2.41942	1.43091
O	-0.72153	4.81448	0.73822
Si	-0.58993	5.64726	2.20009
O	-1.87387	3.26242	-3.84335
Si	-2.71580	4.70749	-4.07613
O	-0.11355	1.58141	-2.79577
O	1.86536	-0.07016	-3.58663
O	-1.42548	-3.44315	-1.70133
Si	-0.45548	-4.51511	-2.57296
O	0.63564	0.24683	1.56482
O	-0.21904	-1.93360	2.88408
Si	0.83387	-1.88745	4.20433
O	2.95527	1.37191	1.03724

C	-9.77702	2.27880	-0.48069
C	-10.07005	-0.17314	-0.13254
C	-5.91415	-0.04663	-6.13187
C	-4.88514	-1.85672	-4.76315
H	3.60299	1.66715	0.39043
H	1.55324	0.02111	-4.49184
H	-0.60971	-4.26397	-4.03532
H	0.97632	-4.36439	-2.18153
H	-0.93672	-5.88568	-2.24032
H	0.42722	-3.00905	5.09715
H	2.23954	-2.08183	3.74627
H	0.70732	-0.58750	4.92495
H	-4.00640	4.68865	-3.32696
H	-1.88178	5.85671	-3.61989
H	-2.97393	4.81386	-5.53956
H	0.29299	4.90763	3.14868
H	-0.00046	6.97759	1.88009
H	-1.94397	5.82196	2.80174
H	-6.44493	1.57810	2.50023
H	-5.35533	2.72193	4.36218
H	-5.16322	3.61579	2.09619
H	-7.49050	1.01178	-0.21747
H	-7.57286	1.48093	-1.90552
H	-9.90270	-1.18834	-0.50765
H	-9.60805	-0.12083	0.85804
H	-11.15069	-0.02556	-0.01532
H	-10.85815	2.44857	-0.40555
H	-9.35034	2.38425	0.52315
H	-9.35574	3.07151	-1.10938
H	-8.10323	-0.78611	-4.19787
H	-6.83770	0.38999	-3.89707
H	-4.32379	-2.20894	-5.63802
H	-5.04830	-2.71983	-4.10740
H	-4.25709	-1.13689	-4.23042
H	-6.47285	-2.63457	-6.82859
H	-7.31696	-3.11061	-5.34672
H	-7.96558	-1.80818	-6.35315
H	-5.38031	-0.38703	-7.02854
H	-5.29024	0.70500	-5.63450
H	-6.83871	0.44410	-6.45784
H	-6.60112	-6.01160	-0.71925
H	-5.84402	-6.70873	0.71727
H	-4.91629	-5.63818	-0.33873
H	-8.73348	-5.21750	-0.48247
H	-9.27401	-5.66063	1.14363
H	-9.74713	-4.10894	0.44026
H	-9.22002	-3.10118	3.61714
H	-9.74102	-2.48341	2.04451
H	-8.69412	-1.50431	3.07022
H	-5.89894	-2.57728	4.61724
H	-6.52606	-1.18923	3.72158
H	-4.85780	-1.70811	3.47989
H	-3.83321	-4.88234	2.71955
H	-3.55020	-4.35466	1.05635
H	-3.54689	-3.17388	2.36527
H	-11.21910	0.94079	-2.37364

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H      -9.95444     -0.16378     -2.93270
H      -9.74384      1.57658     -3.12059
H      -5.26785     -2.27437     -0.68328
H      -7.71100     -2.72803     -1.41490
H     -10.00919     -2.27322     -2.63745
H     -10.88890     -4.00412     -4.15142
H      -9.44405     -5.89044     -4.87319
H      -7.10045     -6.03621     -4.05632
H      -6.22536     -4.30925     -2.49981
H      -6.49137     -0.84226      0.48065
123
Complex 2 - C-H activation Red profile - product
C      -1.43709     -2.91377      2.62145
C      -2.33563     -2.06246      3.35114
C      -3.68201     -2.39890      2.97909
C      -3.61449     -3.50499      2.03546
C      -2.24333     -3.82300      1.81939
Ir     -2.59660     -1.70805      1.15530
Ta     -2.63414     -0.31540     -1.20705
C      -2.93897      0.38691     -3.29404
C      -2.21558      0.04794     -4.62809
C      -2.88606     -1.12870     -5.35140
C      -1.93657     -1.04737      4.37540
C      -4.93262     -1.84756      3.58861
C      -4.78984     -4.22924      1.45838
C      -1.71685     -4.94238      0.97839
C       0.04742     -2.98455      2.79492
C      -3.05430     -2.25068     -2.16116
C      -4.37718     -2.57192     -2.51270
C      -4.70874     -3.79171     -3.10398
C      -3.71270     -4.72837     -3.38037
C      -2.39115     -4.43613     -3.04162
C      -2.07390     -3.22262     -2.42867
O      -0.90866      0.52656     -1.19726
Si      0.62569      0.74700     -0.68344
O       1.37218     -0.71358     -0.46671
Si      2.85791     -1.41314     -0.60205
O       3.64094     -1.35786      0.85462
Si      3.69018     -0.46440      2.24247
O       2.23049      0.27347      2.49177
Si      1.47415      1.70156      2.15365
O       0.45167      2.01764      3.39534
Si     -0.77614      3.15170      3.64359
C      -4.11913      1.20501     -0.64013
C      -5.66805      1.24046     -0.62242
C      -6.25525      1.15914     -2.03799
O       0.62684      1.59703      0.73929
O       1.43693      1.62247     -1.83134
Si      2.63814      2.74896     -1.95204
O       2.69603      3.66189     -0.57046
Si      3.47910      3.70386      0.88234
O       4.96663      2.99309      0.74664
Si      5.69780      1.52604      0.98325
O       5.73365      0.70537     -0.45395
Si      4.87688      0.58724     -1.85971
O       3.77340     -0.64535     -1.75060
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O	2.58784	2.92450	2.04129
O	3.66005	5.27780	1.29473
Si	4.00239	6.11999	2.71665
O	2.35667	3.72053	-3.23836
Si	1.52888	5.17295	-3.48079
O	4.09029	2.00037	-2.20890
O	5.98691	0.26606	-3.03110
O	2.63891	-2.97690	-1.04090
Si	3.54216	-4.07641	-1.95121
O	4.89004	0.67315	2.14321
O	3.99254	-1.46441	3.50208
Si	5.15340	-1.50781	4.72908
O	7.22996	1.72000	1.54830
C	-6.10003	2.58528	-0.00462
C	-6.25199	0.11010	0.23489
C	-2.31295	1.28114	-5.54829
C	-0.72990	-0.27271	-4.41281
H	7.87307	1.97875	0.88153
H	5.65723	0.34964	-3.93087
H	3.31242	-3.83616	-3.40522
H	4.99496	-3.94621	-1.63797
H	3.05507	-5.43365	-1.57607
H	4.74857	-2.61568	5.63967
H	6.50071	-1.78448	4.15316
H	5.17113	-0.21461	5.47205
H	0.25070	5.18084	-2.71073
H	2.38577	6.31627	-3.05313
H	1.25041	5.26118	-4.94135
H	4.95865	5.35042	3.56506
H	4.60613	7.41957	2.30940
H	2.73738	6.35900	3.47030
H	-2.07255	2.60086	3.15701
H	-0.84282	3.39506	5.11227
H	-0.46296	4.42220	2.92638
H	-3.77192	1.41416	0.38508
H	-3.77455	2.06148	-1.24488
H	-6.04284	-0.87504	-0.19514
H	-5.82894	0.12519	1.24482
H	-7.34057	0.21607	0.31845
H	-7.19313	2.67393	0.02376
H	-5.72810	2.68534	1.02166
H	-5.71033	3.42915	-0.58547
H	-4.02258	0.37175	-3.48573
H	-2.70925	1.44855	-3.07477
H	-0.22728	-0.43400	-5.37493
H	-0.60757	-1.18528	-3.82028
H	-0.21470	0.54307	-3.89661
H	-2.40721	-1.29596	-6.32447
H	-2.81658	-2.05516	-4.77897
H	-3.94745	-0.92297	-5.53469
H	-1.85003	1.08419	-6.52375
H	-1.80509	2.14617	-5.10501
H	-3.35887	1.55951	-5.72348
H	-2.34100	-5.10975	0.09791
H	-1.68234	-5.87443	1.55716
H	-0.70398	-4.73098	0.62851

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H      -4.55659     -4.65001      0.47803
H      -5.09563     -5.05176      2.11776
H      -5.64816     -3.56405      1.33794
H      -5.23407     -2.44178      4.46141
H      -5.76306     -1.85810      2.87876
H      -4.79522     -0.81590      3.92172
H      -1.85418     -1.51887      5.36288
H      -2.67461     -0.24543      4.44926
H      -0.97254     -0.59337      4.13792
H       0.30920     -3.70665      3.57953
H       0.54362     -3.30067      1.87477
H       0.46676     -2.01751      3.07881
H      -7.34605      1.26670     -2.00589
H      -6.03349      0.20139     -2.51918
H      -5.85922      1.95440     -2.67933
H      -1.56265     -1.73592     -0.11399
H      -3.83256     -1.26270      0.16015
H      -5.18079     -1.85867     -2.33046
H      -5.74406     -4.00494     -3.36054
H      -3.96338     -5.67458     -3.85254
H      -1.60443     -5.15868     -3.24731
H      -1.03695     -3.04087     -2.14973
H      -2.22586     -0.13620      1.18141
123
Complex 2 - C-H activation Green profile - adduct
C      -3.68582      1.85383     -0.93968
C      -2.85364      2.47376     -1.95314
C      -2.90935      1.68110     -3.11814
C      -3.78392      0.55322     -2.86358
C      -4.31115      0.69878     -1.53127
Ir     -2.11796      0.25703     -1.30846
Ta     -1.46242     -1.55146      0.07643
C      -1.27119     -3.43120     -0.96812
C      -2.00950     -4.02566     -2.18366
C      -1.60015     -5.49943     -2.35623
C      -2.08545      3.74590     -1.77012
C      -2.20964      1.94529     -4.41559
C      -4.28235     -0.39550     -3.91030
C      -5.44761     -0.08138     -0.94439
C      -4.03697      2.46659      0.38219
O       0.26306     -1.27018      0.88587
Si      1.65742     -0.40263      0.83503
O       2.67323     -1.02837      1.98866
Si      4.29348     -1.23042      2.25479
O       4.91767      0.06458      3.06976
Si      4.67678      1.68363      3.29055
O       3.07751      2.05043      3.08510
Si      2.03992      2.51439      1.87896
O       0.85964      3.44943      2.52303
Si      0.38928      3.82683      4.10037
C      -3.02562     -1.83281      1.54951
C      -2.76465     -2.40554      2.96411
C      -1.96376     -3.71430      2.89036
O       1.36170      1.18737      1.17187
O       2.35963     -0.56600     -0.65218
Si      3.25276      0.29785     -1.73979
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O	2.98750	1.91551	-1.52851
Si	3.61796	3.20003	-0.70887
O	5.23464	2.96033	-0.44678
Si	6.25903	2.37690	0.71547
O	6.58849	0.78610	0.39342
Si	5.88534	-0.52937	-0.32971
O	5.09708	-1.42192	0.82141
O	2.84440	3.40630	0.74245
O	3.42048	4.54475	-1.62205
Si	2.92891	6.12797	-1.30310
O	2.81132	-0.12963	-3.25456
Si	3.63463	-0.65620	-4.63109
O	4.86294	-0.04028	-1.52772
O	7.02728	-1.45994	-1.06388
O	4.52796	-2.57750	3.15811
Si	3.49942	-3.74182	3.81993
O	5.60229	2.54418	2.22051
O	5.09647	2.08992	4.81897
Si	6.42513	2.86224	5.52028
O	7.65091	3.25400	0.74661
C	-1.98736	-1.38012	3.80264
C	-4.11264	-2.68924	3.64961
C	-3.52478	-3.95469	-1.95456
C	-1.64114	-3.25345	-3.45568
C	-9.63637	-2.02449	-0.30919
C	-9.77794	-1.97840	-1.69606
C	-9.26110	-3.00638	-2.48460
C	-8.60310	-4.08085	-1.88620
C	-8.46161	-4.12716	-0.49903
C	-8.97817	-3.09878	0.28951
H	8.11333	3.30596	-0.09511
H	7.56759	-1.97971	-0.46147
H	4.37296	-4.68842	4.56852
H	2.52095	-3.10450	4.74806
H	2.77393	-4.46651	2.73592
H	6.30732	2.63927	6.98879
H	7.69817	2.27472	5.01158
H	6.38193	4.32248	5.22015
H	4.74435	0.28373	-4.96492
H	4.17989	-2.02687	-4.41041
H	2.63336	-0.67595	-5.73393
H	3.68996	6.68718	-0.14780
H	3.22253	6.91169	-2.53581
H	1.46700	6.16304	-1.01085
H	-0.87093	4.61280	3.98004
H	0.14321	2.58201	4.88459
H	1.44037	4.64847	4.76770
H	-0.18063	-3.45719	-1.15639
H	-1.41142	-4.11033	-0.09972
H	-2.16210	-3.66872	-4.32679
H	-0.56370	-3.31194	-3.65042
H	-1.90465	-2.19727	-3.35333
H	-2.10604	-5.95055	-3.21861
H	-0.51977	-5.59176	-2.51614
H	-1.85879	-6.09032	-1.46931
H	-4.07350	-4.39462	-2.79581

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H      -3.84916     -2.91399     -1.84501
H      -3.81516     -4.49939     -1.04759
H      -3.58875     -0.89201      1.63750
H      -3.70173     -2.51512      0.99277
H      -3.96733     -3.07749      4.66528
H      -4.69273     -3.42961      3.08671
H      -4.71547     -1.77690      3.72280
H      -1.83079     -4.14698      3.88900
H      -0.96322     -3.55209      2.47119
H      -2.47706     -4.46039      2.27194
H      -1.82153     -1.75347      4.82012
H      -1.00888     -1.16252      3.36177
H      -2.53988     -0.43645      3.87911
H      -5.48360     -1.10210     -1.33169
H      -6.40649      0.39469     -1.18818
H      -5.38002     -0.14343      0.14454
H      -5.11044      0.05278     -4.47623
H      -3.49847     -0.65384     -4.62683
H      -4.64878     -1.32693     -3.47316
H      -2.86853      2.47511     -5.11602
H      -1.89816      1.01505     -4.89788
H      -1.31587      2.55812     -4.27469
H      -2.71953      4.61836     -1.97569
H      -1.22458      3.79780     -2.44143
H      -1.71233      3.84453     -0.74754
H      -4.83287      3.21563      0.27084
H      -4.39127      1.71246      1.08936
H      -3.17534      2.96324      0.83580
H      -0.92426      0.81564     -0.40584
H      -0.91324     -0.45322     -2.10294
H     -10.29264     -1.14243     -2.16225
H      -9.37281     -2.97122     -3.56503
H      -8.20308     -4.88342     -2.50009
H      -7.95275     -4.96658     -0.03260
H      -8.87079     -3.13645      1.37030
H     -10.04095     -1.22456      0.30521
123
Complex 2 - C-H activation Green profile - TS
C      -9.31702     -2.20702     -3.13220
C      -8.91059     -1.47595     -1.96206
C      -9.99104     -1.15382     -1.06796
C     -11.29083     -1.59598     -1.28187
C     -11.63340     -2.35028     -2.40624
C     -10.62363     -2.62594     -3.33567
Ta     -6.56608     -1.16417     -0.99350
Ir     -7.67868      0.47144     -2.63235
C      -7.46899      2.54315     -3.37855
C      -7.36861      1.65308     -4.49746
C      -8.62590      0.95338     -4.63341
C      -9.51983      1.46171     -3.62307
C      -8.81098      2.41396     -2.82988
C      -6.19219      1.53027     -5.41363
C      -9.01160      0.03761     -5.75153
C     -10.95763      1.09152     -3.48470
C      -9.37872      3.25387     -1.72861
C      -6.43676      3.53512     -2.94256
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O	-4.85864	-0.56405	-0.26069
Si	-3.34350	0.01981	-0.23839
O	-3.33262	1.54390	0.41438
Si	-2.38306	2.52183	1.34127
O	-1.47190	3.50049	0.36238
Si	-0.81211	3.49430	-1.15625
O	-0.79319	5.02291	-1.74390
Si	-1.21837	6.53830	-1.13486
O	-2.74243	0.07957	-1.78578
Si	-1.74731	0.99522	-2.72699
O	-2.32274	0.99679	-4.26373
Si	-1.60064	0.67861	-5.75908
O	-0.21581	0.36260	-2.73110
Si	0.75277	-0.55619	-1.75900
O	1.66874	-1.47883	-2.76806
O	-0.13520	-1.53762	-0.76600
Si	-0.81807	-1.52543	0.74087
O	-0.79673	-3.06752	1.29188
Si	-1.75756	-3.97658	2.34187
O	0.08406	-0.57455	1.75217
Si	0.12970	0.97562	2.32229
O	1.14644	1.89056	1.38735
Si	1.69532	1.94411	-0.16812
O	3.22284	2.54769	-0.07308
O	0.67268	0.97350	3.86608
Si	2.16326	1.28107	4.59934
O	-1.39016	1.62556	2.31858
O	-2.37028	-0.96633	0.67730
O	1.71494	0.42982	-0.83824
O	-1.71268	2.55465	-2.17456
O	-3.34393	3.46556	2.27305
Si	-3.39662	3.82994	3.92149
O	0.74014	2.92680	-1.09843
C	-7.45451	-1.64722	0.95424
C	-7.47366	-0.80728	2.26051
C	-8.24559	0.50399	2.05389
C	-5.51855	-2.88413	-1.83225
C	-5.80891	-4.09079	-2.74286
C	-7.08660	-4.82384	-2.31552
C	-5.90131	-3.63507	-4.20619
C	-4.63019	-5.07970	-2.63071
C	-8.18401	-1.62735	3.35408
C	-6.05754	-0.47914	2.75059
H	3.65884	2.67859	-0.92029
H	2.04619	-2.26258	-2.35771
H	-0.95077	-5.17018	2.72114
H	-2.10004	-3.18140	3.55715
H	-3.00484	-4.40343	1.64518
H	2.04567	0.79122	6.00154
H	3.25378	0.55116	3.88997
H	2.44146	2.74612	4.59071
H	-0.35688	1.48573	-5.92101
H	-1.28970	-0.77414	-5.88374
H	-2.60061	1.07552	-6.79086
H	-0.44187	6.83929	0.10294
H	-0.88203	7.52325	-2.20111

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H      -2.68019      6.58567     -0.83969
H      -4.50593      4.81000      4.09219
H      -3.66950      2.60026      4.71874
H      -2.10645      4.44133      4.35627
H      -4.56254     -2.43820     -2.15947
H      -5.29816     -3.27534     -0.81248
H      -6.11292     -4.48276     -4.86870
H      -4.95510     -3.18551     -4.53040
H      -6.68442     -2.88581     -4.34854
H      -4.77763     -5.94334     -3.29077
H      -3.68313     -4.60233     -2.90777
H      -4.52868     -5.45594     -1.60599
H      -7.23954     -5.72325     -2.92436
H      -7.97582     -4.19624     -2.41823
H      -7.01880     -5.14104     -1.26803
H      -8.47292     -2.02436      0.78047
H      -6.84700     -2.55656      1.15260
H      -8.22914     -1.07260      4.29977
H      -7.65571     -2.56909      3.54345
H      -9.21029     -1.87477      3.05909
H      -6.09651      0.02153      3.72565
H      -5.53222      0.17850      2.05453
H      -5.45877     -1.38987      2.86807
H      -8.26718      1.09304      2.97898
H      -7.78244      1.11872      1.27419
H      -9.28467      0.31434      1.76196
H     -11.11656      0.02681     -3.66586
H     -11.55553      1.65608     -4.21199
H     -11.33816      1.31785     -2.48774
H      -9.46636      0.60544     -6.57353
H      -8.14479     -0.49217     -6.15437
H      -9.73416     -0.70923     -5.41604
H      -6.26141      2.27673     -6.21493
H      -6.15172      0.54364     -5.88006
H      -5.24913      1.68685     -4.88628
H      -6.59262      4.49612     -3.44974
H      -5.42663      3.19297     -3.17731
H      -6.48317      3.71524     -1.86618
H      -9.78318      4.19132     -2.13138
H     -10.18767      2.73858     -1.20651
H      -8.61724      3.51191     -0.98913
H      -7.11673      0.82541     -1.14670
H      -6.47275     -0.54920     -3.03105
H      -8.56752     -2.46654     -3.87121
H     -10.85456     -3.19006     -4.23747
H     -12.65061     -2.69414     -2.56442
H     -12.05695     -1.32382     -0.55820
H      -9.78849     -0.54082     -0.19779
H      -8.02733     -2.25115     -1.37946
123
Complex 2 - C-H activation Green profile - product
C      -6.31671     -2.19001     -1.39675
C      -5.71972     -1.04110     -0.84921
C      -6.43726     -0.36465      0.15233
C      -7.69289     -0.80503      0.57843
C      -8.26781     -1.94343      0.01693
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C	-7.57121	-2.63390	-0.97381
Ta	-2.22710	-1.60911	-0.14578
Ir	-3.93953	-0.28205	-1.60315
C	-2.95904	1.55357	-2.45585
C	-2.89653	0.51676	-3.44054
C	-4.26028	0.18010	-3.81966
C	-5.14367	1.05186	-3.10734
C	-4.36150	1.86391	-2.22446
C	-1.66323	0.00757	-4.11909
C	-4.65017	-0.77607	-4.90374
C	-6.63097	1.09955	-3.24309
C	-4.87990	2.97446	-1.36406
C	-1.79927	2.31157	-1.88895
O	-0.68487	-0.56528	0.42923
Si	0.86605	-0.07895	0.56652
O	0.90497	1.37495	1.35859
Si	1.85201	2.25200	2.38500
O	2.84571	3.24959	1.51346
Si	3.59965	3.33686	0.04230
O	3.72073	4.90521	-0.41192
Si	3.21719	6.37581	0.24676
O	1.51715	0.10680	-0.94880
Si	2.62875	1.01168	-1.76360
O	2.12226	1.14007	-3.31819
Si	2.93233	1.19786	-4.80109
O	4.11782	0.29064	-1.73480
Si	5.00913	-0.73705	-0.79843
O	5.93459	-1.62365	-1.83000
O	4.04161	-1.75145	0.07961
Si	3.27145	-1.82193	1.54111
O	3.20390	-3.40104	1.96242
Si	2.51171	-4.29495	3.21848
O	4.13569	-0.98368	2.67685
Si	4.24032	0.51650	3.36147
O	5.34675	1.43688	2.54285
Si	5.97895	1.59229	1.02658
O	7.52506	2.10789	1.24873
O	4.70991	0.36629	4.92137
Si	6.16233	0.59034	5.75503
O	2.75965	1.25102	3.34300
O	1.74739	-1.19579	1.41694
O	5.96661	0.14097	0.22930
O	2.72577	2.52443	-1.10139
O	0.88908	3.17655	3.33217
Si	0.73756	3.40977	4.99831
O	5.12041	2.69670	0.14036
C	-2.97546	-2.11160	1.84516
C	-2.87818	-1.21344	3.10565
C	-3.17335	0.26154	2.79353
C	-0.81844	-2.74712	-1.39579
C	-0.97164	-4.11562	-2.09625
C	-1.02413	-5.24839	-1.06097
C	-2.23017	-4.17184	-2.97108
C	0.26042	-4.33983	-2.99481
C	-3.91180	-1.70805	4.13473
C	-1.48035	-1.33402	3.72754

H	8.01490	2.27831	0.43879
H	6.18543	-2.48913	-1.49371
H	3.45517	-5.40612	3.52798
H	2.31539	-3.43666	4.42258
H	1.20472	-4.84591	2.76147
H	5.95978	-0.00137	7.10730
H	7.27860	-0.10532	5.05151
H	6.46233	2.04634	5.87289
H	4.12562	2.08861	-4.71062
H	3.34728	-0.17519	-5.20675
H	1.95836	1.74901	-5.78558
H	3.83670	6.58245	1.58785
H	3.67702	7.43203	-0.69804
H	1.73019	6.40813	0.36496
H	-0.32202	4.44201	5.17563
H	0.33545	2.13944	5.66679
H	2.02646	3.89908	5.56948
H	-0.52054	-1.98907	-2.14582
H	0.05563	-2.82232	-0.72401
H	-2.28670	-5.12381	-3.51314
H	-2.22969	-3.36574	-3.71493
H	-3.13362	-4.07260	-2.36147
H	0.21747	-5.31736	-3.49126
H	0.32800	-3.57130	-3.77432
H	1.18657	-4.30103	-2.40961
H	-1.09771	-6.22409	-1.55635
H	-1.88656	-5.13536	-0.39719
H	-0.11753	-5.25555	-0.44344
H	-4.04351	-2.24107	1.57409
H	-2.64280	-3.12517	2.11378
H	-3.84880	-1.13335	5.06773
H	-3.74763	-2.76403	4.37830
H	-4.93170	-1.61020	3.74590
H	-1.39987	-0.71955	4.63243
H	-0.70329	-1.01205	3.02985
H	-1.26864	-2.37229	4.00976
H	-3.16903	0.86153	3.71207
H	-2.42326	0.68842	2.11903
H	-4.16047	0.37381	2.33034
H	-7.02761	0.15995	-3.63251
H	-6.92120	1.90236	-3.93214
H	-7.11445	1.28476	-2.28108
H	-4.68068	-0.26851	-5.87638
H	-3.93934	-1.60164	-4.98279
H	-5.63803	-1.20564	-4.72170
H	-1.48603	0.57057	-5.04463
H	-1.75635	-1.04713	-4.38740
H	-0.77620	0.11654	-3.49209
H	-1.60640	3.21176	-2.48621
H	-0.88921	1.70983	-1.88893
H	-1.98758	2.62816	-0.86061
H	-4.93315	3.91234	-1.93159
H	-5.88365	2.75467	-0.99252
H	-4.23376	3.14593	-0.50008
H	-3.71605	0.00982	-0.03710
H	-3.64251	-1.87408	-1.72773

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H      -5.79191     -2.75392     -2.16360
H      -8.00041     -3.52875     -1.41894
H      -9.24156     -2.29148      0.35078
H      -8.21768     -0.25583      1.35706
H      -6.01071      0.52262      0.61423
H      -2.82604     -3.26423     -0.18477
96
Complex 3
C       0.02219     -1.41106     -0.98586
C       1.47163     -1.76935     -0.84899
C       2.52229     -0.89148     -0.40218
C       3.78947     -1.53137     -0.70114
C       3.52850     -2.80212     -1.25127
C       2.08977     -2.98957     -1.30554
Ir      2.42505     -2.75056      0.92857
Ta      0.89591     -3.16651      2.65349
C      -0.09270     -1.31609      3.11112
C      -0.70202     -1.04301      4.50470
C      -1.64941      0.16596      4.42360
C       2.35764      0.53332      0.03176
C       5.13253     -0.91329     -0.46382
C       4.53708     -3.80733     -1.71419
C       1.39461     -4.13336     -1.98046
H      -0.35259     -4.15236      1.85097
O       1.66642     -4.08986      4.14428
Si      2.92038     -4.99868      4.70753
O       3.13204     -6.31565      3.73398
Si      4.33923     -7.28076      3.14520
O       4.46163     -8.63264      4.09746
Si      4.17939     -9.08461      5.65858
O       3.72214    -10.66397      5.58950
O       2.50529     -5.50527      6.23120
Si      2.76430     -6.80068      7.22946
O       1.46053     -7.00431      8.20059
Si     -0.00888     -6.19506      8.39095
O       4.29489     -4.08788      4.77817
Si      5.68308     -3.91851      5.65689
O       6.89115     -4.82535      4.98569
Si      7.09217     -6.20481      4.09043
O       8.42491     -6.05408      3.15234
Si      9.26178     -4.74958      2.48207
O       4.09403     -6.54545      8.17621
Si      5.53125     -5.73083      8.17902
O       5.87635     -5.24413      9.70250
Si      6.92200     -5.78805     10.91307
O       2.97118     -8.18246      6.34461
O       5.41657     -4.38605      7.22385
O       6.74229     -6.71939      7.63240
Si      6.94022     -8.00650      6.61766
O       8.18113     -8.88106      7.25127
O       6.15236     -2.35083      5.63408
Si      6.11335     -1.08559      6.75121
C      -1.49576     -2.26545      4.99354
C       0.42485     -0.73247      5.50094
O       5.76648     -6.45201      3.13690
O       3.99294     -7.73126      1.61186
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Si      3.33212     -9.11465      0.90339
O       7.31686     -7.50601      5.08494
O       5.55698     -8.91590      6.56330
H       8.52355     -9.57054      6.67469
H       3.36435    -11.01456      6.41051
H      -0.73487     -6.90404      9.48159
H       0.22787     -4.77269      8.77375
H      -0.79935     -6.25576      7.12708
H       6.55188     -5.03878     12.14665
H       6.74864     -7.25341     11.13191
H       8.33460     -5.49178     10.53847
H       4.32077    -10.23052      0.94723
H       2.07980     -9.51539      1.60775
H       3.03224     -8.75602     -0.51135
H      10.08873     -4.08555      3.53070
H      10.14203     -5.31686      1.42214
H       8.31019     -3.76644      1.88760
H       6.47776      0.14718      5.99814
H       4.74717     -0.94545      7.33428
H       7.10503     -1.33212      7.83789
H       0.45025     -0.43485      2.74520
H      -0.91961     -1.47801      2.37582
H      -2.08403      0.39421      5.40453
H      -2.47470     -0.02474      3.72782
H      -1.11756      1.05892      4.07631
H      -1.96887     -2.06355      5.96168
H      -0.84846     -3.14125      5.13033
H      -2.28981     -2.53381      4.28624
H       0.01720     -0.50610      6.49312
H       1.10866     -1.58203      5.60534
H       1.01148      0.13370      5.17421
H      -0.62115     -2.29151     -0.91075
H      -0.16632     -0.94507     -1.96228
H      -0.29086     -0.69993     -0.21717
H       1.35134     -3.98107     -3.06749
H       1.91367     -5.07775     -1.79825
H       0.37112     -4.24855     -1.61651
H       4.68554     -3.74164     -2.79995
H       4.21791     -4.82764     -1.48666
H       5.50856     -3.65344     -1.23815
H       5.39761     -0.22949     -1.28067
H       5.91884     -1.66915     -0.39837
H       5.15038     -0.33687      0.46503
H       2.41089      1.21693     -0.82644
H       1.39370      0.69403      0.52135
H       3.13861      0.82799      0.73774
H       3.31665     -2.34989      2.19953
H       2.84737     -4.22744      1.37803
96
Complex 3 with 2 mu-H and one terminal H on Ir
C      -5.81336     -3.38679     -5.08937
C      -5.98736     -4.23740     -3.95851
C      -7.42033     -4.38377     -3.72566
C      -8.11089     -3.67322     -4.76000
C      -7.13695     -2.99840     -5.56466
Ir     -6.84116     -2.24062     -3.48470
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Ta	-5.95553	-0.39949	-1.95998
O	-4.11198	-0.17097	-1.49177
Si	-2.69962	0.38935	-0.88899
O	-2.04881	-0.74913	0.12001
Si	-0.56789	-1.30783	0.60541
O	-0.09877	-0.53070	1.98759
Si	-0.30285	0.91393	2.76494
O	0.92564	1.95026	2.36448
Si	1.96305	2.24959	1.11770
O	3.34473	2.80655	1.81300
C	-4.90971	-4.95162	-3.20421
C	-8.04357	-5.27681	-2.69864
C	-9.59441	-3.61459	-4.94446
C	-7.41218	-2.19475	-6.79735
C	-4.51909	-3.03906	-5.75586
C	-7.15802	1.06849	-1.03668
C	-8.64913	1.43294	-0.98387
C	-8.85577	2.67196	-0.09488
C	-9.15311	1.74311	-2.40071
C	-9.44303	0.25685	-0.39759
O	-1.65890	0.68388	-2.14535
Si	-0.42913	1.71260	-2.55399
O	-0.44601	1.95730	-4.17459
Si	-1.63300	1.85148	-5.37097
O	-2.97357	1.79409	-0.05851
Si	-2.41185	2.62159	1.25472
O	-1.26432	3.72286	0.78878
Si	-0.14480	3.94712	-0.40715
O	-0.01632	5.55051	-0.71335
Si	-0.26784	6.52194	-2.07063
O	1.03449	1.05827	-2.15812
Si	1.70303	0.03232	-1.04061
O	3.01112	-0.73096	-1.68286
O	-0.62387	3.16774	-1.78962
O	0.55288	-1.06807	-0.58440
O	2.27804	0.86980	0.25765
O	-0.65605	-2.91911	0.88428
Si	-1.81640	-3.93907	1.56642
O	-3.67859	3.40497	1.93234
Si	-3.87335	4.84650	2.78941
O	-1.76105	1.57103	2.35273
O	-0.28777	0.65659	4.38018
Si	0.78988	1.00426	5.63362
O	1.32516	3.37972	0.08727
H	4.08024	2.93379	1.20652
H	2.81444	-1.32838	-2.41029
H	-1.07940	-5.08531	2.16918
H	-2.59988	-3.22079	2.61279
H	-2.73057	-4.43220	0.49564
H	0.25400	0.31640	6.84188
H	2.15021	0.48626	5.30896
H	0.84671	2.47632	5.86658
H	-1.09390	2.57127	-6.55914
H	-1.87820	0.42037	-5.71460
H	-2.90064	2.48978	-4.91301
H	-0.00968	7.92233	-1.63309

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H       0.67839      6.14355     -3.16031
H      -1.67358      6.38677     -2.55229
H      -5.18263      4.74724      3.49266
H      -2.76992      5.01872      3.77924
H      -3.88738      5.99828      1.84168
H      -6.77036      0.88647     -0.00560
H      -6.56545      1.93310     -1.42335
H     -10.51154      0.49691     -0.34213
H      -9.09992      0.01723      0.61563
H      -9.32438     -0.64131     -1.01260
H      -9.91570      2.94979     -0.04296
H      -8.50693      2.48545      0.92735
H      -8.30183      3.53342     -0.48557
H     -10.21564      2.01369     -2.38502
H      -9.02907      0.87773     -3.06033
H      -8.59973      2.58136     -2.84005
H      -8.37922     -1.69013     -6.73735
H      -7.42431     -2.83898     -7.68609
H      -6.64987     -1.42763     -6.95127
H      -9.90765     -2.66081     -5.37519
H      -9.92852     -4.41255     -5.61947
H     -10.12125     -3.73863     -3.99555
H      -8.14245     -6.30052     -3.08226
H      -9.03960     -4.92687     -2.41792
H      -7.44108     -5.31769     -1.78840
H      -4.74073     -5.94983     -3.62839
H      -5.17440     -5.07709     -2.15194
H      -3.96494     -4.40527     -3.24387
H      -4.30042     -3.75082     -6.56240
H      -4.55180     -2.03903     -6.19404
H      -3.68544     -3.06413     -5.05079
H      -6.20164     -0.68056     -3.86407
H      -6.52434     -2.24845     -1.78791
H      -8.07435     -1.31967     -2.97528
108
Complex 3 - C-H activation - adduct
C      -6.06319      1.69442     -1.55529
C      -6.18731      0.30458     -1.57532
C      -7.39288     -0.28014     -1.96516
C      -8.47222      0.52269     -2.33360
C      -8.34690      1.91168     -2.31274
C      -7.14236      2.49755     -1.92378
C      -4.01871     -5.27158      0.14671
C      -2.87097     -5.06680      1.08962
C      -1.59798     -5.73883      1.03884
C      -0.91208     -5.47923      2.29081
C      -1.70935     -4.61365      3.06531
C      -2.91143     -4.30440      2.31281
Ir     -1.30163     -3.47055      0.93871
Ta     -1.62637     -2.13321     -0.95856
C      -1.61414     -3.42685     -2.66963
C      -1.33298     -2.86972     -4.08410
C       0.17437     -2.62401     -4.24504
C      -1.17402     -6.75055      0.01795
C       0.41293     -6.06164      2.67412
C      -1.40122     -4.09565      4.43601
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C	-4.09708	-3.56058	2.84982
O	-0.45163	-0.63271	-1.07092
Si	0.76491	0.37028	-0.59546
O	2.01895	-0.50672	0.01888
Si	3.67019	-0.49715	0.09466
O	4.16466	0.24175	1.49305
Si	3.64406	1.40193	2.55015
O	4.17668	1.00538	4.04527
Si	4.89961	1.86263	5.30944
O	0.17682	1.41517	0.54598
Si	0.73895	2.27008	1.85035
O	1.99196	1.45287	2.55083
O	1.25902	1.20533	-1.93347
Si	1.88090	2.67046	-2.37875
O	3.53062	2.59778	-2.40459
Si	4.78795	1.80687	-1.67103
O	6.06964	1.70459	-2.69692
O	-0.46804	2.47366	2.93596
Si	-1.83917	1.60248	3.40102
O	1.23906	3.77542	1.38346
Si	1.86213	4.57094	0.07220
O	1.31728	6.11441	0.06579
Si	0.48695	7.07932	1.17632
C	-1.79199	-3.89273	-5.13675
C	-2.09409	-1.55198	-4.30492
O	1.36286	3.03228	-3.88922
Si	0.24055	4.11969	-4.52960
O	1.36612	3.84396	-1.32847
O	4.27950	0.29752	-1.22007
O	4.22548	-2.03545	0.06532
Si	4.80434	-3.10863	1.23417
O	5.33728	2.65897	-0.36903
Si	4.76215	3.69797	0.78477
O	5.97062	4.68873	1.29577
O	3.51311	4.57335	0.13883
O	4.25019	2.88287	2.12482
H	-3.32583	-1.62210	-0.79192
H	6.47888	5.10088	0.59086
H	5.91173	1.18701	-3.49201
H	3.94660	-3.07302	2.45331
H	4.76362	-4.46328	0.61492
H	6.20908	-2.75468	1.59038
H	4.83863	0.97188	6.50234
H	6.31908	2.16908	4.97112
H	4.15314	3.12673	5.57375
H	0.10643	3.77556	-5.97297
H	-1.07655	3.97280	-3.84376
H	0.73775	5.51792	-4.38103
H	1.19608	7.09072	2.48849
H	0.46086	8.45073	0.59475
H	-0.90452	6.57254	1.35467
H	-1.45804	0.22016	3.80830
H	-2.42192	2.33785	4.55841
H	-2.81743	1.55572	2.27710
H	-1.08028	-4.37234	-2.51035
H	-2.69895	-3.68418	-2.58704

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H      -1.93876     -1.17555     -5.32269
H      -1.75164     -0.76460     -3.62041
H      -3.17335     -1.68451     -4.16266
H       0.40395     -2.25840     -5.25267
H       0.53506     -1.87750     -3.52942
H       0.74309     -3.54728     -4.08586
H      -1.59005     -3.53139     -6.15246
H      -2.86835     -4.08449     -5.05747
H      -1.26989     -4.84780     -5.00995
H      -1.62248     -6.54797     -0.95781
H      -1.47658     -7.76325      0.31710
H      -0.08881     -6.75618     -0.11408
H      -3.67690     -5.51055     -0.86363
H      -4.64727     -6.10591      0.48572
H      -4.65334     -4.38396      0.08479
H      -4.73246     -4.21928      3.45735
H      -4.71122     -3.15204      2.04421
H      -3.78900     -2.72404      3.48213
H      -1.88346     -4.71275      5.20532
H      -1.75844     -3.07100      4.56726
H      -0.32704     -4.09800      4.63727
H       0.28871     -7.05960      3.11426
H       1.06997     -6.16608      1.80673
H       0.93092     -5.43955      3.40809
H       0.22124     -3.29926      0.46825
H      -5.34606     -0.32001     -1.28593
H      -5.12480      2.15021     -1.25017
H      -7.04513      3.57991     -1.90726
H      -9.18797      2.53748     -2.59950
H      -9.41100      0.06641     -2.63659
H      -7.49111     -1.36263     -1.98024
H      -1.02550     -2.01434      1.54498
108
Complex 3 - C-H activation - TS
C      -8.14852     -5.27817     -0.43766
C      -6.83790     -5.85434     -0.50504
C      -6.17158     -5.60137      0.76138
C      -7.06005     -4.85676      1.58532
C      -8.27475     -4.61430      0.84218
Ir     -6.64430     -3.61422     -0.32495
Ta     -6.19291     -1.60178     -1.74361
O      -4.41825     -0.88050     -1.51016
Si     -3.15519      0.14492     -1.39458
O      -3.46218      1.30756     -0.25271
Si     -2.65121      2.22325      0.86020
O      -3.62026      2.50781      2.14918
Si     -5.09817      1.88981      2.68531
C      -6.30862     -6.73759     -1.59201
C      -4.81896     -6.11202      1.14741
C      -6.80020     -4.41967      2.99277
C      -9.52195     -3.97781      1.37267
C      -9.24504     -5.43509     -1.44294
C      -8.58942     -1.53393     -2.01061
C      -9.21985     -2.18765     -3.09126
C     -10.48871     -1.82035     -3.53139
C     -11.18606     -0.80284     -2.87822
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C	-10.61004	-0.17474	-1.77357
C	-9.33916	-0.54498	-1.33888
H	-6.78068	-0.17754	-0.88782
C	-6.11126	-1.65636	-3.93472
C	-5.28878	-2.67463	-4.76209
C	-5.19375	-2.18621	-6.21828
C	-3.86680	-2.83780	-4.20650
C	-5.99917	-4.03547	-4.73813
O	-2.90435	0.86571	-2.86657
Si	-2.37668	2.28574	-3.52235
O	-3.19197	2.56431	-4.91638
Si	-4.33991	3.70476	-5.39900
O	-1.80414	-0.70573	-0.95856
Si	-0.17611	-0.73261	-1.22368
O	0.16765	-0.05688	-2.69229
Si	0.59732	1.40127	-3.34677
O	1.40359	2.32597	-2.24357
Si	1.09235	3.46532	-1.08357
O	-0.24888	4.32759	-1.53143
Si	-1.87893	4.35948	-1.26395
O	-2.65267	3.54040	-2.47488
O	-0.76707	2.17423	-3.88239
O	1.65207	1.18934	-4.59184
O	0.34956	-2.28407	-1.23830
Si	1.18156	-3.24953	-0.13164
O	0.60493	0.09124	-0.01479
Si	0.32392	1.33596	1.03629
O	0.85209	2.76734	0.39196
O	-2.23364	3.68546	0.20555
O	-1.29150	1.43557	1.37281
O	-2.39396	5.91379	-1.28411
Si	-3.09449	6.94306	-0.14371
O	1.14727	1.02466	2.41622
Si	2.01665	1.96812	3.51498
O	2.39409	4.45454	-0.90739
H	2.74726	4.80443	-1.73076
H	1.33019	0.62517	-5.30119
H	0.55390	-3.15825	1.21878
H	1.08890	-4.64597	-0.64419
H	2.61066	-2.82908	-0.05627
H	2.22729	1.11601	4.71928
H	3.33026	2.35606	2.92602
H	1.24172	3.18926	3.88162
H	-4.79904	3.28420	-6.75263
H	-5.49050	3.71958	-4.44936
H	-3.72108	5.06028	-5.46846
H	-2.20631	7.08499	1.04630
H	-3.25696	8.26070	-0.82022
H	-4.42596	6.41733	0.27632
H	-5.05889	0.39969	2.71974
H	-5.29427	2.42786	4.06151
H	-6.20051	2.35519	1.79553
H	-7.11198	-1.57577	-4.37603
H	-5.65983	-0.64974	-4.06711
H	-3.28111	-3.51638	-4.83854
H	-3.87328	-3.25429	-3.19276

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H      -3.34389     -1.87663     -4.16987
H      -5.42830     -4.78787     -5.29579
H      -6.12158     -4.38717     -3.70747
H      -6.99398     -3.96795     -5.19559
H      -4.65106     -2.90630     -6.84361
H      -4.66603     -1.22750     -6.27615
H      -6.19036     -2.04707     -6.65286
H      -6.77579     -6.51625     -2.55382
H      -6.50362     -7.79279     -1.36046
H      -5.22923     -6.61950     -1.71521
H      -8.84984     -5.68243     -2.43087
H      -9.92224     -6.24555     -1.14330
H      -9.84003     -4.52346     -1.54129
H     -10.17262     -4.72681      1.84324
H     -10.09281     -3.49460      0.57602
H      -9.29461     -3.21704      2.12334
H      -7.14541     -5.18355      3.70093
H      -7.32374     -3.48983      3.22649
H      -5.73516     -4.25508      3.17177
H      -4.89122     -7.11696      1.58325
H      -4.15353     -6.17405      0.28302
H      -4.34125     -5.46269      1.88491
H      -5.22057     -3.39594     -1.09491
H      -7.90917     -2.43782     -1.26192
H      -8.90744     -0.05096     -0.47345
H     -11.15193      0.60904     -1.25014
H     -12.17606     -0.51201     -3.21934
H     -10.93725     -2.33089     -4.38010
H      -8.69948     -2.99848     -3.59500
H      -6.29081     -2.24781      0.47077
108
Complex 3 - C-H activation - product
C      -3.85507     -5.38407      0.76632
C      -2.45212     -5.53916      1.05542
C      -2.18166     -4.82020      2.28390
C      -3.39909     -4.21284      2.72738
C      -4.44671     -4.55743      1.78009
Ir     -2.87872     -3.36378      0.72952
Ta     -2.31536     -1.18460     -0.62286
O      -0.48191     -0.59459     -0.57392
Si      0.75959      0.45526     -0.40004
O       0.43627      1.55528      0.79662
Si      1.22584      2.43237      1.95510
O       0.25103      2.63145      3.25486
Si     -1.30226      2.11083      3.67120
C      -1.48699     -6.41653      0.32101
C      -0.86926     -4.79776      3.00319
C      -3.59878     -3.45269      4.00085
C      -5.89995     -4.23095      1.92733
C      -4.58696     -6.03681     -0.36411
C      -4.29934     -0.24981     -1.00602
C      -5.39007     -1.01860     -1.46989
C      -6.62570     -0.45062     -1.77880
C      -6.81135      0.92727     -1.66072
C      -5.75531      1.71927     -1.21493
C      -4.53380      1.13302     -0.87559
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H	-2.53153	0.19415	0.43757
C	-2.34498	-1.24321	-2.83028
C	-1.47940	-2.19612	-3.69836
C	-1.57449	-1.72587	-5.16237
C	-0.00002	-2.20384	-3.28997
C	-2.03119	-3.62747	-3.61327
O	0.99936	1.25006	-1.83251
Si	1.50626	2.70607	-2.42362
O	0.69382	3.03757	-3.80601
Si	-0.51933	4.13530	-4.22801
O	2.11726	-0.40302	0.00159
Si	3.74606	-0.38502	-0.25348
O	4.08544	0.36305	-1.68849
Si	4.49224	1.85613	-2.27669
O	5.28351	2.73707	-1.12767
Si	4.95486	3.82038	0.08031
O	3.60068	4.68020	-0.33058
Si	1.96937	4.67689	-0.06728
O	1.21127	3.90427	-1.31736
O	3.11854	2.63140	-2.78309
O	5.55118	1.71854	-3.52884
O	4.28353	-1.93172	-0.31727
Si	5.54813	-2.76330	0.42962
O	4.51417	0.40068	0.98843
Si	4.21530	1.58836	2.09898
O	4.72659	3.05501	1.52434
O	1.61945	3.93023	1.36806
O	2.59855	1.64770	2.43685
O	1.43310	6.22326	-0.01533
Si	0.73211	7.19012	1.17845
O	5.04070	1.22368	3.46470
Si	5.95033	2.11988	4.57064
O	6.24102	4.82077	0.30184
H	6.57828	5.22651	-0.50236
H	5.20571	1.25582	-4.29806
H	5.27812	-2.90897	1.88965
H	5.59842	-4.10693	-0.21347
H	6.84086	-2.04851	0.22162
H	6.16009	1.23341	5.75010
H	7.26355	2.49042	3.96950
H	5.21111	3.34953	4.97925
H	-1.00316	3.72288	-5.57513
H	-1.63576	4.08472	-3.24058
H	0.04356	5.51568	-4.28879
H	1.61765	7.26327	2.37659
H	0.57395	8.54337	0.57544
H	-0.60141	6.64462	1.56559
H	-1.36572	0.62132	3.66460
H	-1.54685	2.62377	5.04957
H	-2.30678	2.67756	2.72795
H	-3.37690	-1.30605	-3.19369
H	-2.04574	-0.19475	-3.03337
H	0.58363	-2.82363	-3.98190
H	0.14531	-2.60699	-2.28245
H	0.42109	-1.19342	-3.30599
H	-1.47413	-4.30008	-4.27698

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H      -1.95774     -4.02055     -2.59350
H      -3.08611     -3.66051     -3.91117
H      -1.01090     -2.39069     -5.82950
H      -1.16914     -0.71403     -5.27618
H      -2.61591     -1.70888     -5.50367
H      -1.73902     -6.48932     -0.73934
H      -1.49033     -7.43281      0.73598
H      -0.46676     -6.03207      0.39022
H      -3.94491     -6.17003     -1.23733
H      -4.94336     -7.02724     -0.05523
H      -5.45527     -5.45074     -0.67208
H      -6.40606     -4.98655      2.54201
H      -6.40298     -4.19648      0.95858
H      -6.04420     -3.25927      2.40492
H      -3.91426     -4.13154      4.80322
H      -4.36727     -2.68448      3.89076
H      -2.67929     -2.95894      4.32177
H      -0.78684     -5.66812      3.66606
H      -0.02961     -4.82860      2.30549
H      -0.76041     -3.89935      3.61401
H      -1.38652     -2.75339      0.48802
H      -3.25337     -3.09595     -0.83905
H      -3.74276      1.77210     -0.48817
H      -5.88702      2.79391     -1.10949
H      -7.77043      1.37587     -1.90725
H      -7.44324     -1.08285     -2.11920
H      -5.27645     -2.09444     -1.59528
H      -3.42663     -1.85210      1.05032
108
Complex 3 - C-H activation - rot. TS
C      -7.10936     -4.38584      1.48672
C      -7.32269     -5.26075      0.36220
C      -6.02487     -5.57459     -0.18775
C      -5.02241     -4.90422      0.59188
C      -5.69731     -4.15965      1.63564
Ir     -6.33111     -3.36272     -0.35554
Ta     -6.85131     -1.27924     -1.97157
O      -5.43374     -0.01494     -1.81992
Si     -3.89547      0.54587     -1.75618
O      -3.94956      2.19853     -1.76749
Si     -3.11600      3.52146     -1.22479
O      -4.15502      4.75284     -0.94483
Si     -5.76235      4.87168     -0.43452
C      -8.63012     -5.84737     -0.07070
C      -5.77097     -6.51355     -1.32548
C      -3.53939     -5.03884      0.43694
C      -5.02754     -3.40198      2.73935
C      -8.17782     -3.86910      2.39897
C      -6.95119     -2.34467     -3.86750
C      -5.83937     -2.35749     -4.72975
C      -5.87081     -3.05400     -5.94039
C      -7.00832     -3.77148     -6.30674
C      -8.11564     -3.79047     -5.45537
C      -8.08419     -3.08413     -4.25554
H      -8.23827     -0.90461     -0.97524
C      -8.26104      0.17320     -2.95016
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C	-8.10960	0.94400	-4.29491
C	-8.99477	2.20394	-4.21007
C	-6.66349	1.39324	-4.54457
C	-8.59339	0.11568	-5.49276
O	-3.06860	-0.00823	-3.07767
Si	-1.90976	0.46476	-4.15526
O	-2.26125	-0.19361	-5.61267
Si	-2.29015	0.40790	-7.19310
O	-3.15238	0.01705	-0.37397
Si	-1.63286	-0.37259	0.13944
O	-0.74839	-0.96725	-1.12543
Si	0.35816	-0.45414	-2.24687
O	1.19467	0.84944	-1.68075
Si	1.13139	2.50447	-1.69972
O	0.36956	2.99010	-3.08745
Si	-1.13195	3.42865	-3.62058
O	-1.88067	2.11436	-4.29171
O	-0.43416	-0.09689	-3.65794
O	1.48893	-1.61763	-2.52222
O	-1.74451	-1.51936	1.31073
Si	-0.87302	-1.70799	2.75100
O	-0.86964	0.94798	0.78501
Si	-0.84400	2.59761	0.68137
O	0.33228	3.08350	-0.37725
O	-2.03465	4.02807	-2.36878
O	-2.31846	3.14629	0.17471
O	-0.97446	4.57776	-4.77450
Si	-1.45949	6.19094	-4.91247
O	-0.52324	3.19174	2.17067
Si	0.38675	4.48078	2.77596
O	2.64988	3.12788	-1.61311
H	3.26837	2.77984	-2.26226
H	1.14930	-2.42038	-2.92879
H	-1.35207	-0.73158	3.77020
H	-1.14143	-3.09962	3.21216
H	0.58663	-1.52441	2.50705
H	-0.01314	4.63653	4.20269
H	1.84058	4.16415	2.68175
H	0.08580	5.73101	2.01950
H	-2.51194	-0.77056	-8.07720
H	-3.40080	1.38855	-7.35182
H	-0.98593	1.05422	-7.52131
H	-0.86803	7.00488	-3.81131
H	-0.94794	6.66290	-6.22967
H	-2.94717	6.28653	-4.87483
H	-6.10552	3.73954	0.47410
H	-5.88358	6.16780	0.29011
H	-6.65870	4.86517	-1.62517
H	-9.28817	-0.22298	-2.90159
H	-8.25158	0.93837	-2.14844
H	-6.59897	2.00571	-5.45286
H	-5.99825	0.53435	-4.67977
H	-6.28236	1.99164	-3.71026
H	-8.58534	0.72609	-6.40479
H	-7.96240	-0.75728	-5.66772
H	-9.62057	-0.23576	-5.33782

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H      -8.95581      2.78132     -5.14299
H      -8.67026      2.86178     -3.39492
H     -10.04159      1.93536     -4.02492
H      -9.46005     -5.16590      0.13164
H      -8.83512     -6.78808      0.45759
H      -8.63485     -6.06084     -1.14230
H      -9.12117     -3.72240      1.86809
H      -8.35897     -4.58129      3.21379
H      -7.89523     -2.91366      2.84635
H      -4.74861     -4.07475      3.56094
H      -5.68400     -2.63046      3.14845
H      -4.12100     -2.90749      2.38369
H      -3.15752     -5.84879      1.07206
H      -3.02321     -4.11828      0.71783
H      -3.26694     -5.26875     -0.59578
H      -5.69643     -7.54533     -0.95914
H      -6.57741     -6.47638     -2.06136
H      -4.83971     -6.27361     -1.84296
H      -5.20940     -2.22709     -0.57825
H      -6.46773     -3.35179     -1.97788
H      -8.96401     -3.10722     -3.61290
H      -9.00571     -4.35014     -5.73308
H      -7.03263     -4.31585     -7.24709
H      -5.00245     -3.03856     -6.59459
H      -4.93061     -1.81689     -4.46892
H      -7.46663     -2.17257     -0.26864
108
Complex 3 - C-H activation - product Ben.
C      -3.07017     -5.27308      1.58377
C      -2.15562     -5.38910      0.48994
C      -1.08966     -4.42278      0.68470
C      -1.38288     -3.68681      1.87947
C      -2.62994     -4.19589      2.42402
Ir     -3.02698     -3.26999      0.39813
Ta     -2.44377     -1.13425     -0.94555
O      -0.52725     -0.88668     -0.75541
Si      0.67235      0.18885     -0.45489
O       0.26615      1.22828      0.76763
Si      0.91285      2.06792      2.03446
O      -0.17562      2.16775      3.25270
Si     -1.86319      2.19010      3.35401
C      -2.19460     -6.43501     -0.58108
C       0.16892     -4.33138     -0.12024
C      -0.48152     -2.70117      2.55688
C      -3.23577     -3.79609      3.73421
C      -4.26335     -6.14410      1.82682
C      -4.36300     -0.08172     -1.22988
C      -5.46916     -0.82664     -1.69956
C      -6.70511     -0.23625     -1.96051
C      -6.87435      1.13672     -1.77686
C      -5.80400      1.90403     -1.32014
C      -4.57835      1.29727     -1.04017
H      -2.40656      0.32949      0.02261
C      -2.37316     -1.14262     -3.13580
C      -1.54657     -2.05463     -4.07641
C      -1.71094     -1.53407     -5.51727
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C	-0.05260	-2.05536	-3.73024
C	-2.08428	-3.49204	-4.01719
O	1.00242	1.05741	-1.82515
Si	1.53487	2.54729	-2.29931
O	0.83553	2.93398	-3.72816
Si	-0.29571	4.09088	-4.21659
O	2.00714	-0.68490	0.00182
Si	3.65268	-0.60544	-0.09118
O	4.10057	0.21420	-1.45540
Si	4.51894	1.74227	-1.93792
O	5.19327	2.57804	-0.68514
Si	4.74433	3.60183	0.53611
O	3.41235	4.45706	0.04963
Si	1.76449	4.41414	0.17333
O	1.12819	3.68609	-1.16717
O	3.17316	2.51099	-2.52313
O	5.67957	1.68738	-3.10297
O	4.22809	-2.13820	-0.16138
Si	5.58019	-2.90901	0.49512
O	4.27955	0.14625	1.24527
Si	3.88822	1.27178	2.38988
O	4.41206	2.77109	1.92256
O	1.31701	3.59857	1.54268
O	2.25123	1.29707	2.62214
O	1.18628	5.94461	0.23865
Si	0.59942	6.94095	1.46883
O	4.62641	0.84378	3.78612
Si	5.28586	1.69728	5.08676
O	5.98793	4.61226	0.90509
H	6.39605	5.04139	0.14719
H	5.39547	1.30013	-3.93631
H	5.36359	-3.16546	1.94850
H	5.71778	-4.20150	-0.23387
H	6.80419	-2.07852	0.30169
H	5.32448	0.74833	6.23506
H	6.66691	2.14462	4.74659
H	4.43565	2.87614	5.42287
H	-0.61132	3.78459	-5.63980
H	-1.52877	3.99712	-3.38329
H	0.29181	5.45772	-4.10651
H	1.53670	6.94500	2.62950
H	0.49734	8.30817	0.88618
H	-0.74698	6.47080	1.90674
H	-2.38707	0.79601	3.30699
H	-2.18989	2.81193	4.66883
H	-2.44352	2.99986	2.24524
H	-3.41253	-1.14909	-3.49109
H	-2.04637	-0.08898	-3.26888
H	0.50967	-2.64781	-4.46252
H	0.13325	-2.47927	-2.73954
H	0.35508	-1.03918	-3.73482
H	-1.55230	-4.13770	-4.72653
H	-1.96626	-3.91951	-3.01550
H	-3.15096	-3.52639	-4.26866
H	-1.16685	-2.16619	-6.23027
H	-1.32437	-0.51293	-5.61177

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H      -2.76582     -1.52127     -5.81455
H      -3.21873     -6.74013     -0.80822
H      -1.64117     -7.32851     -0.26540
H      -1.74263     -6.07647     -1.50840
H      -4.69482     -6.50626      0.89099
H      -3.97863     -7.01969      2.42374
H      -5.04615     -5.61116      2.37090
H      -2.82214     -4.39879      4.55281
H      -4.31967     -3.93300      3.73241
H      -3.03672     -2.74641      3.96039
H       0.12842     -3.20834      3.31536
H      -1.04960     -1.91522      3.05940
H       0.19812     -2.22420      1.84882
H       0.94188     -4.98589      0.30270
H       0.00486     -4.64169     -1.15473
H       0.55835     -3.31205     -0.13716
H      -4.59975     -3.26561      0.23006
H      -3.29257     -3.22757     -1.19449
H      -3.76594      1.91112     -0.65755
H      -5.92751      2.97382     -1.16747
H      -7.83494      1.60221     -1.98312
H      -7.53555     -0.84593     -2.30951
H      -5.37238     -1.89928     -1.86387
H      -3.53749     -1.82408      0.89544
108
Complex 3 - SI C-H activation Red profile - adduct
C      -0.88954     -4.38451     -3.72643
C      -2.19470     -3.92835     -3.53623
C      -3.26756     -4.62591     -4.09238
C      -3.03565     -5.78048     -4.83987
C      -1.73160     -6.23625     -5.03142
C      -0.65935     -5.53857     -4.47511
Ta     -3.14669      0.87735     -0.43134
H      -3.66494      2.47133      0.15897
Ir     -3.73396     -0.66817      1.28932
C      -2.72374     -2.63359      1.49198
C      -2.51354     -1.90598      2.71726
C      -3.79437     -1.79123      3.38601
C      -4.78212     -2.38953      2.56924
C      -4.13864     -2.88591      1.36940
C      -1.18527     -1.56019      3.31718
C      -4.00508     -1.16487      4.72906
C      -6.24188     -2.51214      2.87698
C      -4.80331     -3.71866      0.31595
C      -1.64732     -3.15453      0.59055
C      -4.33618      0.45650     -2.16970
C      -3.95494      0.99646     -3.56655
C      -3.50029      2.46223     -3.47270
O      -1.27954      0.94916     -0.82103
Si      0.31696      1.03959     -0.43855
O       1.07901      1.89833     -1.63162
Si      2.33769      2.96387     -1.79371
O       3.72716      2.16145     -2.19045
Si      4.43911      0.68867     -1.93669
O       5.44081      0.32142     -3.18840
C      -2.82157      0.14927     -4.16225
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C	-5.17965	0.91689	-4.49422
O	0.95225	-0.48710	-0.35007
Si	2.40379	-1.24127	-0.59365
O	2.10082	-2.77843	-1.07262
Si	2.81441	-4.26705	-0.69997
O	0.48403	1.81825	1.00698
Si	1.42327	1.85033	2.36844
O	2.58591	3.01943	2.20406
Si	3.43978	3.77501	1.00701
O	3.73497	5.31497	1.47556
Si	5.12505	6.25908	1.64487
O	3.29096	-1.27529	0.80394
Si	3.50919	-0.43834	2.21356
O	3.85685	-1.51641	3.39262
Si	4.93536	-1.55575	4.69357
O	3.25115	-0.45376	-1.77488
O	2.12138	0.37090	2.59832
O	4.76133	0.63379	2.05366
Si	5.53337	1.47864	0.86405
O	7.11773	1.56385	1.29554
O	0.49962	2.17533	3.67759
Si	-0.13468	3.58321	4.36727
O	2.54470	3.79843	-0.38207
O	2.02603	4.00760	-3.01453
Si	0.71786	4.97109	-3.47642
O	4.87950	2.99697	0.74585
O	5.40355	0.71327	-0.59769
H	7.72618	1.66537	0.55756
H	5.02709	0.33585	-4.05659
H	2.31674	-5.23210	-1.71908
H	4.30070	-4.16299	-0.77492
H	2.40085	-4.70140	0.66470
H	6.31446	-1.83090	4.19786
H	4.90719	-0.25990	5.43168
H	4.47843	-2.66302	5.57919
H	-0.22672	5.15432	-2.33649
H	1.26936	6.28698	-3.90542
H	0.02067	4.31405	-4.61886
H	5.98790	5.71426	2.73265
H	5.88780	6.29298	0.36276
H	4.65670	7.62826	1.99784
H	-1.29278	3.16076	5.20252
H	0.90502	4.22664	5.22149
H	-0.57743	4.53031	3.30363
H	-4.68853	-0.58202	-2.22989
H	-5.21786	1.02742	-1.78735
H	-3.27898	2.86732	-4.46721
H	-2.58736	2.56478	-2.87236
H	-4.27553	3.09226	-3.02082
H	-2.55258	0.50648	-5.16321
H	-1.92112	0.19120	-3.53965
H	-3.12021	-0.90051	-4.25582
H	-4.93638	1.28186	-5.49979
H	-6.00698	1.52340	-4.10806
H	-5.53587	-0.11503	-4.58826
H	-2.03908	-3.40901	-0.39657

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H      -1.20479     -4.06620      1.01327
H      -0.84813     -2.42378      0.45164
H      -4.24491     -3.69745     -0.62263
H      -4.87777     -4.76751      0.63295
H      -5.81602     -3.36410      0.10572
H      -6.46340     -3.48229      3.34048
H      -6.84922     -2.43415      1.97154
H      -6.57469     -1.73191      3.56615
H      -3.82166     -1.89229      5.53051
H      -5.02605     -0.79308      4.84622
H      -3.32500     -0.32402      4.88624
H      -0.84604     -2.35302      3.99763
H      -0.41958     -1.43704      2.54877
H      -1.22753     -0.62978      3.88848
H      -3.53285      0.83363      1.86769
H      -2.37316     -3.02767     -2.95430
H      -4.28380     -4.27004     -3.94423
H      -3.87082     -6.32426     -5.27335
H      -1.55096     -7.13549     -5.61446
H       0.35646     -5.89452     -4.62518
H      -0.05606     -3.84146     -3.28935
H      -5.03305     -0.04992      0.52723
108
Complex 3 - SI C-H activation Red profile - TS
C      -5.07971     -3.63410     -2.96371
C      -6.42356     -3.23645     -2.79661
C      -7.39756     -3.95380     -3.51588
C      -7.05021     -4.96546     -4.40748
C      -5.70774     -5.29669     -4.60210
C      -4.72390     -4.63013     -3.87260
Ta     -6.55317     -1.09098     -1.71734
H      -7.11767      0.57247     -1.43494
Ir     -7.23978     -2.39138      0.32742
C      -6.89678     -4.45975      1.08616
C      -6.42896     -3.53179      2.07336
C      -7.57038     -2.77060      2.54904
C      -8.72615     -3.22439      1.84232
C      -8.32024     -4.25153      0.91486
C      -5.04170     -3.45053      2.63104
C      -7.54139     -1.75780      3.64936
C     -10.12979     -2.75125      2.05539
C      -9.22643     -5.08250      0.06094
C      -6.09012     -5.51993      0.40681
C      -8.16438     -0.76029     -3.21575
C      -7.84244      0.03632     -4.50969
C      -7.43858      1.48308     -4.19143
O      -4.72678     -0.58213     -2.01680
Si     -3.21000     -0.25239     -1.48597
O      -2.44292      0.69045     -2.60921
Si     -1.29259      1.87990     -2.67277
O       0.20399      1.22185     -2.92478
Si      1.05746     -0.15584     -2.59407
O       2.20122     -0.39957     -3.75107
C      -6.71341     -0.64246     -5.30151
C      -9.10393      0.06971     -5.39203
O      -2.39480     -1.68433     -1.30547
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Si	-0.86651	-2.29664	-1.41545
O	-0.98593	-3.85470	-1.90894
Si	-0.14922	-5.27356	-1.53333
O	-3.27478	0.54559	-0.04039
Si	-2.46031	0.67464	1.39116
O	-1.41811	1.96133	1.32509
Si	-0.54364	2.80911	0.20654
O	-0.46520	4.36823	0.69754
Si	0.77276	5.49575	0.91107
O	-0.11188	-2.24780	0.05869
Si	-0.13259	-1.37211	1.46169
O	0.21814	-2.38599	2.69745
Si	1.21583	-2.28912	4.05812
O	0.01143	-1.43790	-2.52245
O	-1.63428	-0.72381	1.69556
O	0.99873	-0.16450	1.39982
Si	1.79071	0.75673	0.28183
O	3.30608	1.01241	0.86758
O	-3.52234	0.90105	2.61670
Si	-4.26558	2.27191	3.27191
O	-1.29940	2.73946	-1.26020
O	-1.59690	2.87936	-3.93099
Si	-2.98934	3.56357	-4.60512
O	0.99091	2.19436	0.08487
O	1.89342	-0.01886	-1.17670
H	3.96986	1.17757	0.19136
H	1.87120	-0.38722	-4.65444
H	-0.48742	-6.25333	-2.60366
H	1.32150	-5.02434	-1.51114
H	-0.59753	-5.79118	-0.20822
H	2.64513	-2.41040	3.65117
H	0.99600	-0.99879	4.77337
H	0.83407	-3.43279	4.93363
H	-4.01428	3.80297	-3.54927
H	-2.57075	4.85393	-5.22159
H	-3.52710	2.64784	-5.65094
H	1.66336	5.07479	2.03111
H	1.56931	5.63604	-0.34307
H	0.10796	6.78701	1.24194
H	-5.47893	1.78957	3.98928
H	-3.33521	2.92903	4.23506
H	-4.64623	3.22934	2.19440
H	-8.60882	-1.71750	-3.52060
H	-8.96018	-0.22071	-2.68003
H	-7.29198	2.05346	-5.11749
H	-6.50959	1.52850	-3.61475
H	-8.21199	1.98688	-3.60078
H	-6.52837	-0.11634	-6.24659
H	-5.77072	-0.64785	-4.74061
H	-6.96326	-1.68265	-5.53597
H	-8.92635	0.62909	-6.31963
H	-9.93754	0.54811	-4.86510
H	-9.41827	-0.94402	-5.66653
H	-6.38904	-5.64856	-0.63659
H	-6.22286	-6.48314	0.91600
H	-5.02486	-5.28000	0.41823

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H      -8.71810     -5.42213     -0.84490
H      -9.56953     -5.97207      0.60548
H     -10.11077     -4.51970     -0.24759
H     -10.63259     -3.37616      2.80423
H     -10.71318     -2.80170      1.13333
H     -10.15601     -1.71853      2.41016
H      -7.66480     -2.24212      4.62681
H      -8.34162     -1.02228      3.53782
H      -6.59350     -1.21524      3.66487
H      -4.94994     -4.07643      3.52798
H      -4.29816     -3.79251      1.90796
H      -4.77999     -2.42749      2.90972
H      -6.17992     -1.13646      0.36269
H      -6.79791     -3.01454     -1.45274
H      -8.44974     -3.71607     -3.37501
H      -7.82622     -5.49694     -4.95329
H      -5.43340     -6.07911     -5.30470
H      -3.67604     -4.88859     -4.00185
H      -4.29277     -3.15740     -2.38436
H      -8.29595     -1.42433     -0.46922
108
Complex 3 - SI C-H activation Red Profile - product
C      -1.30544     -1.66767     -3.91761
C      -2.46440     -1.66791     -3.11217
C      -3.50831     -2.52203     -3.52771
C      -3.40864     -3.32193     -4.66592
C      -2.25264     -3.28590     -5.44536
C      -1.20130     -2.45264     -5.06726
Ta     -2.52754     -0.61369     -1.16746
H      -2.59996      1.06152     -0.62695
Ir     -3.16740     -2.10362      0.89247
C      -2.76603     -4.00667      2.00720
C      -2.49743     -2.88016      2.87815
C      -3.73975     -2.17037      3.05598
C      -4.75946     -2.82591      2.28615
C      -4.14845     -3.97415      1.63847
C      -1.21115     -2.60877      3.59452
C      -3.94207     -0.98785      3.95036
C      -6.21711     -2.48600      2.27200
C      -4.87053     -5.00035      0.82272
C      -1.77590     -5.06263      1.62765
C      -4.41628      0.26313     -1.90621
C      -4.49303      1.56394     -2.75011
C      -4.47148      2.80140     -1.84101
O      -0.65243     -0.17680     -1.35320
Si      0.80684      0.26623     -0.77406
O       1.74057      0.80415     -2.03563
Si      2.95786      1.88710     -2.31965
O       4.43244      1.14427     -2.20295
Si      5.17506     -0.08136     -1.37636
O       6.40809     -0.68432     -2.28506
C      -3.32156      1.64951     -3.74049
C      -5.81165      1.57005     -3.54374
O       1.53642     -1.04388     -0.06931
Si      3.02123     -1.71585      0.16858
O       2.86709     -3.34786      0.15752
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Si	3.63888	-4.59369	-0.67958
O	0.64494	1.47130	0.34784
Si	1.32020	1.99551	1.76140
O	2.44476	3.16695	1.43176
Si	3.47018	3.62078	0.21820
O	3.59387	5.25354	0.21099
Si	4.81878	6.35229	0.58553
O	3.61925	-1.24881	1.63757
Si	3.50612	0.00873	2.70282
O	3.66693	-0.58291	4.22066
Si	4.62112	-0.18174	5.55481
O	4.06745	-1.26591	-1.03702
O	2.03056	0.73922	2.56597
O	4.71321	1.10698	2.41377
Si	5.66185	1.63160	1.17027
O	7.12291	2.01340	1.82282
O	0.16213	2.60532	2.74443
Si	-1.03104	3.79042	2.57643
O	2.86740	3.13597	-1.24079
O	2.83780	2.46549	-3.84664
Si	1.55567	2.98412	-4.81918
O	4.97201	2.96324	0.46567
O	5.86859	0.45702	0.02157
H	7.85626	1.97554	1.20164
H	6.20238	-0.78330	-3.21938
H	3.39205	-4.46500	-2.14526
H	5.10609	-4.57302	-0.40952
H	3.04556	-5.86340	-0.17284
H	6.04541	-0.53869	5.29378
H	4.50779	1.27426	5.85843
H	4.09553	-0.98414	6.69550
H	0.47004	3.57077	-3.98218
H	2.11045	4.01416	-5.74201
H	1.03436	1.82661	-5.60103
H	5.31359	6.12796	1.97497
H	5.94750	6.21438	-0.38066
H	4.21194	7.70797	0.47019
H	-2.35839	3.14297	2.77694
H	-0.80477	4.81527	3.63605
H	-0.96167	4.42407	1.22870
H	-4.92564	-0.54487	-2.45634
H	-5.01024	0.40997	-0.98742
H	-4.53209	3.72063	-2.43667
H	-3.55513	2.83948	-1.24451
H	-5.32352	2.79446	-1.15027
H	-3.39981	2.54792	-4.36631
H	-2.36357	1.70451	-3.20653
H	-3.28944	0.77576	-4.39860
H	-5.92230	2.49430	-4.12527
H	-6.67445	1.49140	-2.87175
H	-5.85239	0.72684	-4.24296
H	-2.02331	-5.51849	0.66675
H	-1.76268	-5.85654	2.38478
H	-0.76585	-4.65462	1.55279
H	-4.20707	-5.47349	0.09575
H	-5.27636	-5.78727	1.47104

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H      -5.70493     -4.55934      0.27285
H      -6.74999     -3.03607      3.05824
H      -6.67871     -2.74201      1.31557
H      -6.38062     -1.41956      2.44182
H      -4.21222     -1.32397      4.95908
H      -4.74240     -0.34003      3.58674
H      -3.03399     -0.38689      4.02927
H      -1.18054     -3.14419      4.55228
H      -0.34954     -2.93038      3.00556
H      -1.08344     -1.54440      3.80308
H      -3.00606     -0.47057      0.90805
H      -1.80055     -2.22910      0.01483
H      -4.43163     -2.57091     -2.95256
H      -4.23631     -3.96897     -4.94805
H      -2.17263     -3.90172     -6.33764
H      -0.29389     -2.41515     -5.66602
H      -0.46296     -1.03975     -3.63981
H      -4.05265     -1.95839     -0.47196
108
Complex 3 - SI C-H activation Green Profile - adduct
C      -4.94524      0.82140     -1.99507
C      -4.61308      2.14280     -1.52784
C      -3.71039      2.73938     -2.49427
C      -3.43352      1.78483     -3.49273
C      -4.15536      0.56639     -3.17406
Ir     -2.79148      0.76982     -1.36467
Ta     -2.37894     -0.83972      0.28745
O      -0.54747     -0.92398      0.83315
Si      1.00064     -0.36615      0.77179
O       1.06222      1.14086      1.44296
Si      2.05856      2.09422      2.35067
O       1.12743      3.04816      3.30019
Si      1.24383      3.61282      4.88740
C      -5.28997      2.88296     -0.41388
C      -3.18751      4.14062     -2.42234
C      -2.56331      1.97115     -4.69669
C      -4.27096     -0.62666     -4.07380
C      -6.04093     -0.05350     -1.46396
C      -3.80048     -0.53513      1.86400
C      -3.49464     -0.93827      3.32375
C      -2.53080      0.08665      3.93975
C      -4.79907     -0.95554      4.13833
C      -2.85861     -2.33729      3.37411
O       1.54844     -0.33061     -0.78579
Si      2.54219      0.57694     -1.74841
O       1.94655      0.64743     -3.26988
Si      2.08901     -0.33384     -4.63726
O       1.92555     -1.41708      1.65901
Si      3.47356     -2.00374      1.69658
O       4.12096     -2.01708      0.17526
Si      5.01586     -1.05346     -0.83170
O       6.01761     -0.10425      0.08389
Si      6.07600      1.40703      0.75828
O       5.14360      2.43415     -0.14749
Si      3.60316      3.03366     -0.17493
O       2.64291      2.12042     -1.16705
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O	4.04608	-0.11854	-1.78388
O	5.88871	-1.98472	-1.87023
O	3.45620	-3.54068	2.26302
Si	2.24363	-4.60731	2.75610
O	4.41663	-1.08482	2.69456
Si	4.53343	0.45854	3.27435
O	5.56306	1.34390	2.32622
O	2.98467	3.03857	1.35876
O	3.03738	1.16142	3.30853
O	3.67390	4.56689	-0.74406
Si	2.62827	5.54939	-1.63539
O	5.10662	0.42239	4.80645
Si	6.62736	0.63704	5.51046
O	7.62433	1.95940	0.81629
C	-5.24667	-4.65308	-1.89575
C	-6.42632	-4.82495	-1.17011
C	-7.56620	-5.32781	-1.79747
C	-7.52743	-5.65975	-3.15163
C	-6.34891	-5.48948	-3.87793
C	-5.20922	-4.98658	-3.25041
H	-2.88754	-2.36376	-0.48568
H	7.96101	2.29895	-0.01822
H	6.42581	-2.66280	-1.44985
H	2.93111	-5.87971	3.11322
H	1.52738	-4.06176	3.94570
H	1.27669	-4.84251	1.64450
H	6.52000	0.11315	6.90117
H	7.66495	-0.12251	4.75432
H	6.97432	2.08708	5.53526
H	3.38876	-0.06314	-5.31663
H	2.00176	-1.77450	-4.25997
H	0.96010	0.02995	-5.53864
H	3.09910	6.94934	-1.43945
H	2.70080	5.18468	-3.07984
H	1.22755	5.40376	-1.14343
H	0.22019	4.68646	5.02505
H	0.95718	2.50630	5.84521
H	2.60506	4.16714	5.14556
H	-4.28030	0.45111	1.82464
H	-4.55058	-1.24452	1.43364
H	-4.60731	-1.22504	5.18418
H	-5.51031	-1.68273	3.72983
H	-5.28134	0.02828	4.12821
H	-2.67026	-2.64449	4.40952
H	-1.89389	-2.36434	2.85143
H	-3.51502	-3.08981	2.92031
H	-2.31180	-0.16200	4.98472
H	-1.58067	0.11899	3.39583
H	-2.96207	1.09386	3.91752
H	-5.83316	-1.11238	-1.63559
H	-6.99151	0.18122	-1.96121
H	-6.18886	0.09139	-0.39055
H	-5.00414	-0.44637	-4.87171
H	-3.31492	-0.86044	-4.54933
H	-4.58930	-1.51452	-3.52340
H	-3.16166	2.26389	-5.56945

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H      -2.03634      1.04935     -4.95534
H      -1.81015      2.74677     -4.53687
H      -3.92003      4.85243     -2.82475
H      -2.26542      4.25638     -2.99719
H      -2.97455      4.43640     -1.39156
H      -6.15488      3.44882     -0.78593
H      -5.65306      2.20210      0.36037
H      -4.61115      3.59407      0.06423
H      -1.80015      1.59957     -0.41753
H      -1.41019      0.13151     -1.86488
H      -4.28972     -4.85648     -3.81495
H      -6.31855     -5.74985     -4.93268
H      -8.41524     -6.05214     -3.64051
H      -8.48400     -5.46233     -1.23112
H      -6.45571     -4.57026     -0.11372
H      -4.35903     -4.25844     -1.40841
108
Complex 3 - SI C-H activation Green Profile - TS
C      -9.84158     -1.53840     -1.38350
C      -8.55631     -1.45342     -2.01186
C      -8.41094     -2.21701     -3.21656
C      -9.43210     -3.01983     -3.70398
C     -10.66391     -3.11089     -3.04357
C     -10.84961     -2.35397     -1.88403
Ir     -7.91845      0.84049     -2.36390
Ta     -6.53560     -0.58251     -0.74362
C      -7.50229     -1.22433      1.11571
C      -7.79134     -0.30320      2.32948
C      -7.92460     -1.16574      3.59740
C      -9.62632      2.28783     -2.66382
C      -8.34493      2.95612     -2.82778
C      -7.68465      2.35670     -3.95281
C      -8.53467      1.30430     -4.46739
C      -9.74827      1.30372     -3.69128
C     -10.68265      2.67290     -1.67599
C      -7.87136      4.14758     -2.05651
C      -6.38290      2.80032     -4.54229
C      -8.29265      0.48328     -5.69458
C     -10.93667      0.44449     -3.95985
O      -4.75810     -0.18008     -0.09344
Si     -3.17028      0.19459     -0.11794
O      -2.60213      0.18834     -1.67465
Si     -1.51266      0.98315     -2.62445
O      -0.07662      0.15751     -2.65024
Si      0.79867     -0.85237     -1.67981
O       1.59928     -1.86503     -2.70063
O      -2.33161     -0.92174      0.77758
Si     -0.84405     -1.64109      0.83849
O      -0.99845     -3.16286      1.42401
Si     -2.31622     -4.12622      1.86207
O      -2.95823      1.70031      0.53636
Si     -1.90124      2.57199      1.45264
O      -0.89824      3.43981      0.46245
Si     -0.25778      3.35532     -1.05890
O      -0.04406      4.86966     -1.64612
Si     -0.98067      5.93060     -2.56387
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O	0.16871	-0.79356	1.83179
Si	0.41515	0.73363	2.41139
O	0.96598	0.65282	3.94988
Si	2.49263	0.70615	4.67101
O	-0.18030	-1.73179	-0.67558
O	-1.00865	1.57363	2.42858
O	1.53132	1.51751	1.47103
Si	2.05638	1.52236	-0.09339
O	3.64755	1.93379	-0.02615
O	-2.75038	3.61251	2.38965
Si	-2.72111	4.00889	4.03094
C	-6.66395	0.71664	2.54594
C	-9.11274	0.44715	2.10977
O	-1.28051	2.52057	-2.05948
O	-2.09403	1.09046	-4.15317
Si	-1.75894	0.26043	-5.58605
O	1.22264	2.62485	-1.00749
O	1.86825	0.02135	-0.76649
H	-5.87729	-1.81222	-1.82482
H	4.03827	2.17239	-0.87194
H	1.97411	-2.64372	-2.27848
H	-1.74725	-5.44295	2.26462
H	-3.04391	-3.51166	3.01021
H	-3.23961	-4.29732	0.70375
H	2.31945	0.18123	6.05469
H	3.45776	-0.14472	3.91606
H	2.98206	2.11409	4.71590
H	-0.43291	0.68212	-6.12313
H	-1.77550	-1.21294	-5.35869
H	-2.83558	0.64227	-6.54438
H	-0.42963	7.29514	-2.33160
H	-0.87498	5.57785	-4.00966
H	-2.40964	5.87547	-2.13569
H	-3.69146	5.12647	4.20386
H	-3.13744	2.83729	4.85416
H	-1.35491	4.45315	4.43422
H	-8.37816	-1.86717	0.94787
H	-6.68294	-1.92477	1.39692
H	-8.16731	-0.55159	4.47388
H	-6.98986	-1.69750	3.81014
H	-8.71581	-1.91534	3.48162
H	-6.85589	1.32623	3.43735
H	-6.56983	1.40389	1.69585
H	-5.69643	0.22130	2.67989
H	-9.34068	1.09592	2.96414
H	-9.06999	1.07327	1.21172
H	-9.94800	-0.25322	1.99174
H	-10.64250	-0.56447	-4.25658
H	-11.53292	0.88053	-4.77180
H	-11.57671	0.35493	-3.08123
H	-8.78194	0.93580	-6.56662
H	-7.22615	0.40090	-5.91649
H	-8.68724	-0.52793	-5.57048
H	-6.55868	3.56729	-5.30697
H	-5.85278	1.97105	-5.01485
H	-5.72237	3.22597	-3.78398

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H      -8.24053      5.07407     -2.51507
H      -6.78067      4.19754     -2.02849
H      -8.22700      4.12253     -1.02405
H     -11.32492      3.46074     -2.08953
H     -11.31911      1.82362     -1.41926
H     -10.24619      3.05385     -0.74983
H      -7.91370      0.94181     -0.72053
H      -6.38592      0.33982     -2.59831
H      -7.45088     -2.19690     -3.72427
H      -9.26112     -3.59367     -4.61275
H     -11.45552     -3.74758     -3.42651
H     -11.80250     -2.39184     -1.35952
H     -10.02122     -0.96500     -0.47920
H      -7.65310     -1.94798     -1.17109
108
Complex 3 - SI C-H activation Green Profile - product
C      -5.51405     -2.09093     -0.74657
C      -4.46209     -1.64955     -1.57854
C      -4.10284     -2.49582     -2.65137
C      -4.76523     -3.69990     -2.88802
C      -5.80569     -4.10374     -2.05226
C      -6.17679     -3.29665     -0.97777
Ir     -3.76964      0.33035     -1.49026
Ta     -2.35871     -1.47061     -0.08122
C      -3.24064     -2.07105      1.88941
C      -3.63456     -1.04464      2.98802
C      -3.70721     -1.78024      4.33974
C      -5.46344      1.80044     -1.55357
C      -4.20334      2.52524     -1.44491
C      -3.42480      2.23515     -2.60314
C      -4.18481      1.31998     -3.44329
C      -5.45156      1.09437     -2.80054
C      -6.62281      1.92595     -0.61546
C      -3.85137      3.48812     -0.35372
C      -2.09824      2.83291     -2.95576
C      -3.79664      0.86537     -4.81578
C      -6.57877      0.28437     -3.35709
O      -0.63847     -0.98023      0.54951
Si      0.94444     -0.54733      0.55906
O       1.56275     -0.64252     -0.97004
Si      2.65374      0.10956     -1.95563
O       4.10712     -0.67850     -1.87311
Si      4.96811     -1.60103     -0.80802
O       5.81778     -2.66859     -1.72799
O       1.76465     -1.57597      1.56265
Si      3.26654     -2.25678      1.71412
O       3.12829     -3.73848      2.39377
Si      1.82276     -4.70478      2.86842
O       1.06716      1.00486      1.11460
Si      2.08740      1.96124      1.99271
O       3.10374      2.77216      0.97026
Si      3.79837      2.60989     -0.51996
O       3.98623      4.09355     -1.18847
Si      3.26711      4.91295     -2.47565
O       4.22696     -1.31791      2.67679
Si      4.41487      0.25379      3.14978
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O	4.91472	0.30370	4.70640
Si	6.41219	0.44878	5.47479
O	3.97308	-2.42524	0.22665
O	2.96822	1.04897	3.05779
O	5.54002	0.99702	2.18785
Si	6.12024	0.90419	0.64599
O	7.69756	1.36106	0.73984
O	1.18971	3.04762	2.82510
Si	1.18076	3.59811	4.42202
C	-2.60321	0.08732	3.11494
C	-5.01580	-0.43818	2.70434
O	2.83317	1.69086	-1.50478
O	2.10959	0.09996	-3.49958
Si	2.15895	-1.03039	-4.75563
O	5.29094	1.91746	-0.37012
O	5.99462	-0.64404	0.07184
H	-1.67171	-2.41049	-1.40138
H	8.12491	1.51495	-0.10787
H	6.18088	-3.41486	-1.24189
H	2.41933	-5.95908	3.40762
H	1.03524	-4.01464	3.93020
H	0.95439	-5.00812	1.69574
H	6.19908	0.02724	6.88784
H	7.42192	-0.43377	4.82149
H	6.86894	1.86755	5.42746
H	3.41341	-0.84143	-5.53979
H	2.09255	-2.41973	-4.21954
H	0.97673	-0.75330	-5.62044
H	3.81540	6.29790	-2.44811
H	3.61285	4.25113	-3.76701
H	1.78426	4.94852	-2.30893
H	0.18290	4.70360	4.47227
H	0.77668	2.49948	5.34529
H	2.52975	4.11107	4.80107
H	-4.05067	-2.80378	1.78371
H	-2.39657	-2.67062	2.27857
H	-4.01493	-1.10483	5.14895
H	-2.73190	-2.20224	4.60861
H	-4.42724	-2.60560	4.29749
H	-2.85625	0.75522	3.94799
H	-2.55536	0.70294	2.20832
H	-1.59933	-0.31094	3.29829
H	-5.30342	0.27042	3.49125
H	-5.02816	0.09722	1.74860
H	-5.78473	-1.21921	2.66455
H	-6.21375	-0.53873	-3.97469
H	-7.22375	0.91713	-3.97924
H	-7.19203	-0.14738	-2.56356
H	-4.11796	1.59254	-5.57285
H	-2.71410	0.74833	-4.90569
H	-4.25505	-0.09515	-5.06203
H	-2.23766	3.72936	-3.57326
H	-1.47975	2.13164	-3.52016
H	-1.53877	3.12318	-2.06414
H	-4.25998	4.48237	-0.57516
H	-2.76996	3.58816	-0.23914

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H      -4.25785      3.16864      0.60856
H      -7.24856      2.78681     -0.88456
H      -7.25602      1.03593     -0.63861
H      -6.29043      2.06816      0.41551
H      -3.59887      0.18068      0.13869
H      -2.26045     -0.24588     -1.78178
H      -3.28515     -2.20426     -3.30323
H      -4.46195     -4.32677     -3.72282
H      -6.31926     -5.04442     -2.23301
H      -6.98233     -3.60531     -0.31600
H      -5.81596     -1.47646      0.09627
H      -2.59387     -3.19855     -0.00756
108
Complex 3 - SI C-H activation Blue Profile - adduct
Ir     -2.46217     -2.60332      1.30713
H      -1.64514     -3.04053     -3.95323
Si      0.81111      0.35705     -0.57049
O       0.69647      1.48449      0.63524
O       1.89850     -0.81772     -0.15225
O       1.27634      1.07510     -1.98345
Si      2.10549      2.38754     -2.54999
O       1.41952      2.88445     -3.95036
Si      0.62967      4.29170     -4.45090
C      -2.29370     -4.85556      1.27531
C      -0.98461     -4.25274      1.27351
C      -0.82196     -3.55351      2.52420
C      -2.00254     -3.80990      3.32639
C      -2.89660     -4.59939      2.56817
C      -2.84140     -5.78636      0.23653
C       0.06886     -4.43236      0.22316
C       0.43638     -2.90293      3.01199
C      -2.21160     -3.32791      4.72801
C      -4.23053     -5.11354      3.01227
Ta     -2.41564     -0.97536     -0.42340
C      -3.34108     -1.83444     -2.15031
C      -3.00468     -1.37232     -3.58590
C      -4.08524     -1.89084     -4.55060
O      -0.66961     -0.31233     -0.80950
Si      3.50988     -1.13739     -0.34272
O       4.05195     -0.46111     -1.74997
Si      4.81633      0.89584     -2.31313
O       5.85978      0.51665     -3.52687
Si      1.62267      2.16793      1.82805
O       0.67271      2.58194      3.09212
Si     -0.99493      2.63687      3.37420
C      -1.64266     -1.94544     -4.00445
O       2.04676      3.62102     -1.44608
Si      2.91425      4.19590     -0.16047
O       2.71819      5.81980     -0.11398
Si      2.51852      6.96106      1.11531
O       3.67256      1.96155     -2.86143
O       4.51556      3.84018     -0.36545
Si      5.62301      2.69261      0.08246
O       7.09200      3.37414      0.36541
O       2.36549      3.53000      1.25148
O       5.17162      1.98895      1.50484
```

Si	4.33233	0.67163	2.05307
O	5.01790	0.11804	3.43040
Si	6.03193	0.78344	4.60762
O	5.74648	1.57198	-1.13041
O	2.76103	1.09168	2.34993
O	4.38004	-0.54704	0.93608
C	-2.96323	0.16235	-3.66588
O	3.68340	-2.76388	-0.41021
Si	4.87253	-3.84971	0.10367
C	-7.30655	-1.18826	-0.39583
C	-6.99239	0.17133	-0.42010
C	-7.50280	0.98657	-1.43111
C	-8.32476	0.44242	-2.41841
C	-8.63744	-0.91709	-2.39476
C	-8.12908	-1.73209	-1.38311
H	-3.44512	0.36525	0.12941
H	7.55413	3.67882	-0.42115
H	5.44730	0.15505	-4.31693
H	4.75572	-4.06961	1.57380
H	4.61821	-5.12345	-0.62594
H	6.23148	-3.33067	-0.22768
H	5.95584	-0.12618	5.78506
H	7.43054	0.84260	4.09443
H	5.56683	2.15040	4.98205
H	0.17336	4.03492	-5.84556
H	-0.54175	4.57055	-3.57042
H	1.57230	5.44736	-4.42508
H	3.50791	6.72955	2.20747
H	2.74576	8.29343	0.48899
H	1.13225	6.88132	1.66001
H	-1.56443	1.26149	3.34056
H	-1.16037	3.23658	4.72794
H	-1.65729	3.49589	2.34989
H	-3.42989	-2.92751	-2.10221
H	-4.35565	-1.45593	-1.86901
H	-2.77096	0.49426	-4.69305
H	-2.16565	0.57992	-3.03885
H	-3.91571	0.60133	-3.34661
H	-1.39940	-1.66036	-5.03482
H	-0.84003	-1.57726	-3.35665
H	-3.86928	-1.58716	-5.58254
H	-5.07344	-1.50082	-4.28328
H	-4.13882	-2.98527	-4.52697
H	1.01467	-2.48368	2.18602
H	1.07509	-3.62701	3.53559
H	0.22201	-2.08873	3.70907
H	0.73123	-3.56654	0.16321
H	0.68555	-5.31371	0.44502
H	-0.37441	-4.57938	-0.76501
H	-2.61754	-6.83164	0.48871
H	-2.41132	-5.58590	-0.74774
H	-3.92706	-5.69332	0.14623
H	-4.13923	-6.12046	3.44019
H	-4.93329	-5.17509	2.17730
H	-4.67732	-4.47009	3.77439
H	-1.77885	-4.03166	5.45092

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H      -1.73831     -2.35659      4.89196
H      -3.27366     -3.22265      4.96341
H      -2.59565     -1.14443      1.98952
H      -6.90789     -1.82076      0.39271
H      -6.34661      0.59126      0.34588
H      -7.26179      2.04628     -1.44741
H      -8.72374      1.07788     -3.20475
H      -9.27922     -1.34037     -3.16301
H      -8.37569     -2.79044     -1.36265
H      -3.94362     -2.29747      0.70261
108
Complex 3 - SI C-H activation Blue Profile - TS
Ir     -2.16500     -2.77740      1.09178
H      -2.64396     -4.54030     -3.22093
Si      0.67581      0.80264     -0.52049
O       0.46299      1.85310      0.74644
O       1.81973     -0.32696     -0.12019
O       1.17023      1.64187     -1.85897
Si      1.96230      3.02164     -2.29684
O       1.32568      3.59429     -3.69361
Si      0.25028      4.83954     -4.07292
C      -3.50003     -4.17245      2.23785
C      -2.92723     -4.87042      1.11573
C      -1.50171     -4.91498      1.31744
C      -1.21658     -4.32645      2.61388
C      -2.43272     -3.87850      3.17629
C      -4.96345     -4.00957      2.51311
C      -3.69290     -5.56189      0.03097
C      -0.50810     -5.67210      0.49118
C       0.14197     -4.24871      3.23644
C      -2.61296     -3.22889      4.51255
Ta     -2.28422     -1.09466     -0.63260
C      -2.58259     -1.83398     -2.66775
C      -1.57156     -2.66197     -3.49681
C      -1.94696     -2.56409     -4.98646
O      -0.74805      0.07477     -0.85602
Si      3.44602     -0.56460     -0.25890
O       4.02105      0.21855     -1.59790
Si      4.73056      1.64941     -2.03328
O       5.84932      1.40898     -3.21584
Si      1.30057      2.49253      2.02140
O       0.27016      2.78455      3.26022
Si     -1.35483      2.42479      3.55254
C      -1.63905     -4.13084     -3.06410
O       1.79917      4.17160     -1.11516
Si      2.57472      4.70745      0.24280
O       2.28911      6.31362      0.38568
Si      1.89431      7.32695      1.67794
O       3.55852      2.69002     -2.56989
O       4.20222      4.45530      0.09407
Si      5.34096      3.32587      0.50983
O       6.76534      4.04976      0.89907
O       2.00023      3.92800      1.58540
O       4.86582      2.50952      1.86266
Si      4.07044      1.11873      2.28115
O       4.71934      0.51315      3.65587
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Si	5.74095	1.12229	4.85544
O	5.56588	2.29443	-0.76527
O	2.46847	1.43988	2.52948
O	4.23638	-0.01634	1.09100
C	-0.13724	-2.14740	-3.31403
O	3.71328	-2.17315	-0.41929
Si	4.88231	-3.23952	0.16788
C	-4.74883	-0.63921	-0.50395
C	-5.60675	-0.61994	0.63579
C	-6.83552	0.01454	0.58674
C	-7.29565	0.61552	-0.59097
C	-6.50765	0.52689	-1.73678
C	-5.27717	-0.12305	-1.72240
H	-3.62134	-0.01218	-0.07461
H	7.24403	4.42271	0.15286
H	5.49293	1.07726	-4.04532
H	4.64253	-3.51525	1.61428
H	4.73427	-4.49632	-0.61919
H	6.25122	-2.67664	-0.02067
H	5.71413	0.12865	5.96570
H	7.12764	1.25871	4.32451
H	5.24729	2.44424	5.33920
H	-0.13276	4.63951	-5.49893
H	-0.96015	4.76680	-3.20295
H	0.91784	6.16233	-3.90359
H	2.80900	7.08441	2.83116
H	2.05723	8.72120	1.17851
H	0.48064	7.09588	2.09425
H	-1.58553	0.95558	3.45949
H	-1.64035	2.90564	4.93388
H	-2.22285	3.14234	2.57408
H	-3.58551	-2.26366	-2.80892
H	-2.63803	-0.82047	-3.13000
H	0.55577	-2.69945	-3.96012
H	0.20553	-2.27260	-2.28118
H	-0.05773	-1.08464	-3.56853
H	-0.93313	-4.74166	-3.63966
H	-1.39545	-4.22290	-2.00178
H	-1.27403	-3.17103	-5.60466
H	-1.88428	-1.52901	-5.34247
H	-2.97052	-2.91695	-5.15879
H	-0.86354	-5.81993	-0.53019
H	-0.32330	-6.66438	0.92394
H	0.45068	-5.15022	0.43590
H	-3.12167	-5.60971	-0.89784
H	-3.93498	-6.59032	0.33131
H	-4.63307	-5.04891	-0.18477
H	-5.35953	-4.88722	3.04130
H	-5.53632	-3.88991	1.59046
H	-5.15917	-3.13571	3.14002
H	-2.86951	-3.97362	5.27705
H	-3.41662	-2.48836	4.49315
H	-1.70254	-2.71978	4.83794
H	0.38718	-5.18742	3.74987
H	0.91547	-4.07226	2.48502
H	0.20452	-3.44265	3.97148

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H      -0.78771     -1.99866      0.70966
H      -4.11233     -1.84737     -0.55719
H      -5.25367     -1.08062      1.55270
H      -7.45374      0.03077      1.48107
H      -8.26011      1.11238     -0.61862
H      -6.86449      0.94466     -2.67513
H      -4.70888     -0.19926     -2.64262
H      -2.67674     -1.28267      1.52778
108
Complex 3 - SI C-H activation Blue Profile - product
Ir     -2.46217     -2.60332      1.30713
H      -1.64514     -3.04053     -3.95323
Si      0.81111      0.35705     -0.57049
O       0.69647      1.48449      0.63524
O       1.89850     -0.81772     -0.15225
O       1.27634      1.07510     -1.98345
Si      2.10549      2.38754     -2.54999
O       1.41952      2.88445     -3.95036
Si      0.62967      4.29170     -4.45090
C      -2.29370     -4.85556      1.27531
C      -0.98461     -4.25274      1.27351
C      -0.82196     -3.55351      2.52420
C      -2.00254     -3.80990      3.32639
C      -2.89660     -4.59939      2.56817
C      -2.84140     -5.78636      0.23653
C       0.06886     -4.43236      0.22316
C       0.43638     -2.90293      3.01199
C      -2.21160     -3.32791      4.72801
C      -4.23053     -5.11354      3.01227
Ta     -2.41564     -0.97536     -0.42340
C      -3.34108     -1.83444     -2.15031
C      -3.00468     -1.37232     -3.58590
C      -4.08524     -1.89084     -4.55060
O      -0.66961     -0.31233     -0.80950
Si      3.50988     -1.13739     -0.34272
O       4.05195     -0.46111     -1.74997
Si      4.81633      0.89584     -2.31313
O       5.85978      0.51665     -3.52687
Si      1.62267      2.16793      1.82805
O       0.67271      2.58194      3.09212
Si     -0.99493      2.63687      3.37420
C      -1.64266     -1.94544     -4.00445
O       2.04676      3.62102     -1.44608
Si      2.91425      4.19590     -0.16047
O       2.71819      5.81980     -0.11398
Si      2.51852      6.96106      1.11531
O       3.67256      1.96155     -2.86143
O       4.51556      3.84018     -0.36545
Si      5.62301      2.69261      0.08246
O       7.09200      3.37414      0.36541
O       2.36549      3.53000      1.25148
O       5.17162      1.98895      1.50484
Si      4.33233      0.67163      2.05307
O       5.01790      0.11804      3.43040
Si      6.03193      0.78344      4.60762
O       5.74648      1.57198     -1.13041
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O	2.76103	1.09168	2.34993
O	4.38004	-0.54704	0.93608
C	-2.96323	0.16235	-3.66588
O	3.68340	-2.76388	-0.41021
Si	4.87253	-3.84971	0.10367
C	-7.30655	-1.18826	-0.39583
C	-6.99239	0.17133	-0.42010
C	-7.50280	0.98657	-1.43111
C	-8.32476	0.44242	-2.41841
C	-8.63744	-0.91709	-2.39476
C	-8.12908	-1.73209	-1.38311
H	-3.44512	0.36525	0.12941
H	7.55413	3.67882	-0.42115
H	5.44730	0.15505	-4.31693
H	4.75572	-4.06961	1.57380
H	4.61821	-5.12345	-0.62594
H	6.23148	-3.33067	-0.22768
H	5.95584	-0.12618	5.78506
H	7.43054	0.84260	4.09443
H	5.56683	2.15040	4.98205
H	0.17336	4.03492	-5.84556
H	-0.54175	4.57055	-3.57042
H	1.57230	5.44736	-4.42508
H	3.50791	6.72955	2.20747
H	2.74576	8.29343	0.48899
H	1.13225	6.88132	1.66001
H	-1.56443	1.26149	3.34056
H	-1.16037	3.23658	4.72794
H	-1.65729	3.49589	2.34989
H	-3.42989	-2.92751	-2.10221
H	-4.35565	-1.45593	-1.86901
H	-2.77096	0.49426	-4.69305
H	-2.16565	0.57992	-3.03885
H	-3.91571	0.60133	-3.34661
H	-1.39940	-1.66036	-5.03482
H	-0.84003	-1.57726	-3.35665
H	-3.86928	-1.58716	-5.58254
H	-5.07344	-1.50082	-4.28328
H	-4.13882	-2.98527	-4.52697
H	1.01467	-2.48368	2.18602
H	1.07509	-3.62701	3.53559
H	0.22201	-2.08873	3.70907
H	0.73123	-3.56654	0.16321
H	0.68555	-5.31371	0.44502
H	-0.37441	-4.57938	-0.76501
H	-2.61754	-6.83164	0.48871
H	-2.41132	-5.58590	-0.74774
H	-3.92706	-5.69332	0.14623
H	-4.13923	-6.12046	3.44019
H	-4.93329	-5.17509	2.17730
H	-4.67732	-4.47009	3.77439
H	-1.77885	-4.03166	5.45092
H	-1.73831	-2.35659	4.89196
H	-3.27366	-3.22265	4.96341
H	-2.59565	-1.14443	1.98952
H	-6.90789	-1.82076	0.39271

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H      -6.34661      0.59126      0.34588
H      -7.26179      2.04628     -1.44741
H      -8.72374      1.07788     -3.20475
H      -9.27922     -1.34037     -3.16301
H      -8.37569     -2.79044     -1.36265
H      -3.94362     -2.29747      0.70261
102
Complex 4 Ben.
C      -5.90050      5.11499     -7.40756
C      -6.58597      3.86059     -7.31451
C      -6.45339      3.17206     -8.58322
C      -5.68304      4.01999     -9.45782
C      -5.32003      5.19755     -8.72513
Ir     -4.41128      3.34430     -7.68970
Ta     -2.78820      3.11145     -5.60016
C      -7.43560      3.41401     -6.16511
C      -7.15527      1.90789     -8.97652
C      -5.39540      3.75834    -10.90441
C      -4.59534      6.38423     -9.28114
C      -5.93561      6.21298     -6.39536
H      -5.04762      6.84541     -6.44561
H      -5.99624      5.82163     -5.37907
H      -6.81122      6.85478     -6.56198
H      -7.03582      3.76431     -5.21107
H      -8.45469      3.80836     -6.26811
H      -7.50722      2.32510     -6.11736
H      -8.15547      2.12453     -9.37328
H      -7.27347      1.23536     -8.12396
H      -6.60139      1.36628     -9.74699
H      -5.31253      2.68862    -11.10932
H      -4.46166      4.22915    -11.22006
H      -6.20060      4.15846    -11.53365
H      -5.30703      7.09025     -9.72774
H      -4.04444      6.91788     -8.50388
H      -3.88317      6.09516    -10.05740
H      -3.62263      2.30090     -8.56038
H      -2.89136      3.87144     -7.74286
H      -4.40712      2.00000     -6.83416
O      -2.03415      1.37401     -5.99796
O      -1.04749      3.85064     -5.93541
O      -3.70361      2.29719     -4.11234
O      -3.27078      4.82433     -4.84208
C      -1.32624      0.22522     -6.05141
C       0.29888      3.90428     -6.03105
C      -3.85637      1.35257     -3.15114
C      -3.31835      6.02707     -4.23764
C      -1.53183     -0.65706     -7.13274
C      -0.79657     -1.84413     -7.17272
C       0.12231     -2.16336     -6.17859
C       0.31214     -1.28012     -5.12080
C      -0.39953     -0.08206     -5.03394
C      -2.51257     -0.33262     -8.22312
H      -0.95568     -2.52533     -8.00568
H       0.68528     -3.09097     -6.22748
H       1.02784     -1.51685     -4.33702
C      -0.18715      0.85109     -3.87947
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C      -4.60662      0.19468     -3.44206
C      -4.79038     -0.74809     -2.43050
C      -4.25346     -0.56073     -1.15896
C      -3.52428      0.59085     -0.89016
C      -3.31196      1.56726     -1.86985
C      -5.19034     -0.01597     -4.80909
H      -5.36744     -1.64325     -2.65029
H      -4.40944     -1.30488     -0.38325
H      -3.10857      0.75106      0.10232
C      -2.50483      2.79429     -1.54037
C       0.92184      3.54878     -7.24288
C       2.31266      3.64345     -7.31888
C       3.07067      4.07682     -6.23399
C       2.43285      4.43031     -5.04919
C       1.04277      4.35785     -4.92340
C       0.10412      3.09202     -8.41676
H       2.80395      3.36842     -8.24930
H       4.15212      4.14039     -6.31317
H       3.01663      4.77516     -4.19884
C       0.35673      4.75573     -3.64658
C      -2.58355      7.11051     -4.77352
C      -2.64102      8.34026     -4.11451
C      -3.40819      8.51598     -2.96553
C      -4.16014      7.45215     -2.48086
C      -4.14492      6.20249     -3.10743
C      -1.78397      6.96622     -6.03948
H      -2.07553      9.17561     -4.52162
H      -3.43344      9.47999     -2.46543
H      -4.78811      7.58662     -1.60249
C      -5.04079      5.10136     -2.60366
H       0.09128      1.85223     -4.22269
H      -1.09266      0.93679     -3.26947
H       0.61591      0.48793     -3.23220
H      -2.58219     -1.16018     -8.93471
H      -3.51304     -0.13236     -7.82784
H      -2.21818      0.56636     -8.77601
H      -0.31746      5.60671     -3.78919
H      -0.25431      3.94146     -3.24269
H       1.09060      5.03097     -2.88426
H       0.74996      2.83167     -9.25967
H      -0.49952      2.21555     -8.16326
H      -0.59180      3.87096     -8.74789
H      -2.69655      3.61191     -2.23628
H      -2.73394      3.14838     -0.53032
H      -1.42916      2.57988     -1.56660
H      -5.82105     -0.90904     -4.82651
H      -5.79460      0.84163     -5.12146
H      -4.40301     -0.14132     -5.55945
H      -4.87328      4.16615     -3.13851
H      -4.88408      4.91718     -1.53551
H      -6.09525      5.38149     -2.72324
H      -1.59641      7.94806     -6.48428
H      -0.81431      6.48911     -5.86690
H      -2.30581      6.34249     -6.77049
102
Complex 4 Lin.
```

Ta	-2.59827	2.70398	-5.44724
O	-3.39470	1.96546	-3.87700
O	-0.74721	3.17427	-5.58529
C	-3.75711	1.06648	-2.93191
C	0.39502	3.88332	-5.73294
O	-1.98624	0.91402	-5.93856
C	-1.05816	-0.01479	-6.24166
O	-2.86819	4.50602	-4.72166
C	-3.52108	5.68453	-4.67963
C	-4.66137	5.82582	-3.86152
C	-5.31724	7.05993	-3.84038
C	-4.86658	8.13554	-4.60031
C	-3.73243	7.98060	-5.39363
C	-3.04031	6.76730	-5.44601
C	-0.13091	-0.43124	-5.26468
C	0.81477	-1.39661	-5.61686
C	0.84965	-1.94772	-6.89470
C	-0.08309	-1.53493	-7.84128
C	-1.04983	-0.57451	-7.53543
C	0.95115	4.55414	-4.62768
C	2.13906	5.26416	-4.82214
C	2.76334	5.30877	-6.06511
C	2.19936	4.62689	-7.13978
C	1.01460	3.90185	-6.99704
C	-3.21609	1.19383	-1.63855
C	-3.61739	0.27805	-0.66293
C	-4.52767	-0.73355	-0.95259
C	-5.05274	-0.83575	-2.23785
C	-4.68407	0.05515	-3.24830
Ir	-4.33499	3.09909	-7.43744
C	-6.40405	2.99937	-8.24840
C	-5.51327	2.49267	-9.26829
C	-4.61660	3.54129	-9.63732
C	-4.98082	4.73527	-8.88486
C	-6.08323	4.40072	-8.04781
C	-5.58631	1.13168	-9.88606
C	-3.58421	3.48371	-10.72018
C	-4.38876	6.09772	-9.06485
C	-6.83806	5.34824	-7.16929
C	-7.58759	2.27828	-7.68132
C	-2.07809	-0.15600	-8.54646
C	-0.16911	0.14397	-3.87829
C	-5.25828	-0.05871	-4.63136
C	-2.22149	2.27477	-1.32536
C	0.41262	3.15032	-8.14895
C	0.29307	4.49747	-3.27828
C	-1.80645	6.61794	-6.28781
C	-5.15273	4.68225	-3.02001
H	-5.93103	0.38357	-9.16875
H	-4.61590	0.80737	-10.26696
H	-6.29136	1.13736	-10.72699
H	-3.19763	2.47102	-10.85445
H	-4.01274	3.80851	-11.67707
H	-2.73604	4.13628	-10.50056
H	-4.91822	6.64637	-9.85492
H	-3.33586	6.04348	-9.35144

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H      -4.45190      6.68308     -8.14493
H      -6.19279      6.13193     -6.76726
H      -7.29551      4.83100     -6.32342
H      -7.64270      5.82799     -7.74119
H      -8.47253      2.41872     -8.31573
H      -7.40035      1.20472     -7.60352
H      -7.83528      2.64176     -6.68129
H      -0.07159     -1.96514     -8.84038
H       1.59501     -2.69594     -7.14866
H       1.53452     -1.71788     -4.86737
H      -5.76806     -1.62085     -2.47154
H      -4.83015     -1.43539     -0.18076
H      -3.20613      0.36994      0.33962
H       2.68514      4.64706     -8.11262
H       3.68561      5.86783     -6.19430
H       2.57518      5.79025     -3.97602
H      -3.36178      8.81782     -5.98129
H      -5.38801      9.08803     -4.56755
H      -6.19659      7.17155     -3.20975
H      -0.00215      1.22606     -3.89493
H      -1.13797     -0.03227     -3.39820
H       0.60548     -0.30660     -3.25158
H      -1.86218     -0.59761     -9.52395
H      -3.08246     -0.47461     -8.24324
H      -2.12364      0.93289     -8.65095
H      -0.77030      4.74455     -3.34001
H       0.36838      3.49433     -2.84215
H       0.77297      5.19411     -2.58544
H       1.03222      3.25261     -9.04409
H       0.31350      2.08376     -7.91967
H      -0.59271      3.51727     -8.38773
H      -2.52671      3.23920     -1.73991
H      -2.09449      2.38495     -0.24499
H      -1.23891      2.04391     -1.75296
H      -6.00279     -0.85856     -4.67336
H      -5.73609      0.87398     -4.94846
H      -4.47842     -0.27740     -5.36818
H      -5.35436      3.78959     -3.61963
H      -4.40966      4.38716     -2.27213
H      -6.07016      4.95751     -2.49227
H      -1.59721      7.54063     -6.83633
H      -0.92876      6.37907     -5.67926
H      -1.91370      5.80474     -7.01348
H      -4.01415      1.59601     -7.00993
H      -2.72987      3.44295     -7.40710
H      -4.61755      3.36880     -5.87383
19
ArOH
O      -0.88870      3.96572     -6.70475
C       0.39651      4.37079     -6.92993
C       1.26930      4.31405     -5.83222
C       2.58995      4.72000     -6.02547
C       3.03729      5.16955     -7.26674
C       2.15125      5.21547     -8.33830
C       0.81944      4.81869     -8.19093
C      -0.14989      4.86276     -9.34321
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C	0.76603	3.82605	-4.50317
H	2.48993	5.56406	-9.31129
H	4.06938	5.48126	-7.39676
H	3.27668	4.68069	-5.18301
H	-0.05939	4.44713	-4.13793
H	0.37726	2.80430	-4.57586
H	1.56312	3.83858	-3.75521
H	0.33963	5.22900	-10.24870
H	-0.55783	3.87029	-9.58111
H	-0.99900	5.53243	-9.14694
H	-1.39172	4.04475	-7.52254

83

(ArO)3TaH2IrCp*

Ta	-3.19495	2.49395	-5.07637
O	-3.64666	1.32092	-3.63679
C	-4.41091	0.30349	-3.14602
O	-1.55246	1.91456	-5.82757
C	-0.31384	1.36941	-5.93522
O	-2.85863	4.23337	-4.38410
C	-2.87031	5.58971	-4.50632
C	-3.87882	6.32214	-3.85878
C	-3.85646	7.71373	-3.98093
C	-2.86605	8.35883	-4.71703
C	-1.87272	7.60862	-5.33995
C	-1.85037	6.21448	-5.24441
C	0.49779	1.25903	-4.79209
C	1.76521	0.69133	-4.94567
C	2.21413	0.24982	-6.18725
C	1.39131	0.37632	-7.30311
C	0.11698	0.93828	-7.20080
C	-5.36933	0.59619	-2.16243
C	-6.11404	-0.46191	-1.63695
C	-5.91176	-1.76987	-2.06844
C	-4.94752	-2.03311	-3.03711
C	-4.17794	-1.00810	-3.59341
Ir	-4.95650	2.58504	-6.69552
C	-6.97689	3.23993	-7.77956
C	-6.40223	2.21770	-8.56661
C	-5.06927	2.63735	-8.95721
C	-4.85831	3.96615	-8.44230
C	-6.01445	4.32049	-7.65986
C	-7.04680	0.92744	-8.96788
C	-4.20612	1.92503	-9.95261
C	-3.72161	4.88156	-8.77996
C	-6.28132	5.66211	-7.04812
C	-8.34991	3.24076	-7.18246
C	-0.77980	1.09162	-8.39458
C	0.01367	1.73742	-3.45144
C	-3.13045	-1.29520	-4.63176
C	-5.57317	2.00903	-1.69652
C	-0.76646	5.40172	-5.89368
C	-4.94026	5.61781	-3.06453
H	-7.82221	0.62576	-8.25936
H	-6.31639	0.11605	-9.02253
H	-7.51621	1.01590	-9.95638
H	-4.24678	0.84095	-9.81673

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H      -4.53211      2.14227    -10.97890
H      -3.16095      2.22806     -9.86639
H      -3.97751      5.50909     -9.64443
H      -2.81770      4.32317     -9.03511
H      -3.48153      5.54595     -7.94612
H      -5.35823      6.13502     -6.70517
H      -6.94815      5.58203     -6.18560
H      -6.75772      6.33723     -7.77198
H      -9.06568      3.73683     -7.85087
H      -8.71232      2.22545     -7.00347
H      -8.37087      3.77181     -6.22745
H       1.73697      0.03551     -8.27616
H       3.20252     -0.18991     -6.28477
H       2.40523      0.59726     -4.07160
H      -4.77849     -3.05366     -3.37253
H      -6.49811     -2.58129     -1.64699
H      -6.85988     -0.24895     -0.87472
H      -1.09129      8.10631     -5.90930
H      -2.86567      9.44179     -4.80041
H      -4.63142      8.29424     -3.48592
H      -0.24435      2.80269     -3.46925
H      -0.88125      1.19709     -3.12290
H       0.78525      1.59556     -2.69008
H      -0.31639      0.66513     -9.28814
H      -1.74645      0.60360     -8.23541
H      -0.99463      2.14827     -8.59099
H      -5.92670      2.64989     -2.51174
H      -6.31094      2.04998     -0.89081
H      -4.63874      2.44648     -1.32766
H      -3.02883     -2.37211     -4.79000
H      -3.38471     -0.84073     -5.59707
H      -2.14954     -0.90401     -4.34051
H      -5.52026      4.93490     -3.69517
H      -4.50250      5.01606     -2.26088
H      -5.63000      6.33661     -2.61431
H      -0.10082      6.04125     -6.47925
H      -0.15787      4.87545     -5.14973
H      -1.17426      4.63535     -6.56178
H      -4.58861      1.04306     -6.35622
H      -5.50785      2.63031     -5.17206
102
Complex 4 formation Red Path. - adducT
C      -1.25221      2.92330      2.63825
C      -0.00311      2.81420      1.99144
C       0.90673      3.89067      1.98249
C       0.54582      5.07289      2.63272
C      -0.67901      5.20074      3.27974
C      -1.56432      4.12917      3.27363
O       0.33784      1.66049      1.36033
Ta      0.28221     -0.03724      0.47168
O      -0.64751     -0.94432      1.84998
C      -1.14401     -1.65326      2.88655
C      -2.01593     -2.72851      2.61712
C      -2.53727     -3.44279      3.69611
C      -2.21118     -3.11161      5.00932
C      -1.34043     -2.05588      5.25168
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C	-0.78360	-1.31158	4.20600
C	-2.35376	-3.09946	1.20228
C	0.19643	-0.20966	4.50872
C	2.24371	3.77839	1.30671
C	-2.23995	1.79157	2.66156
Ir	-1.22490	0.07789	-1.44270
C	-2.02823	1.73849	-2.79594
C	-2.73155	1.78346	-1.54310
C	-3.47279	0.55585	-1.40977
C	-3.27368	-0.21055	-2.62079
C	-2.39682	0.51015	-3.46804
C	-2.85601	3.00144	-0.68026
C	-4.48961	0.24273	-0.35500
C	-3.92921	-1.52087	-2.93181
C	-1.95975	0.11039	-4.84406
C	-1.31686	2.89654	-3.42685
O	1.55180	-1.44037	0.14030
C	2.34447	-2.53590	0.12971
C	2.65789	-3.13897	-1.10516
C	3.48238	-4.26562	-1.09983
C	3.99194	-4.78780	0.08577
C	3.66663	-4.18084	1.29374
C	2.83883	-3.05536	1.34292
C	2.11846	-2.58379	-2.39173
C	2.46065	-2.44425	2.66158
O	1.93203	1.19157	-0.91857
C	3.19909	1.02898	-1.46946
C	3.37955	1.22581	-2.84930
C	4.66634	1.08374	-3.37186
C	5.74613	0.77299	-2.55162
C	5.53968	0.61145	-1.18742
C	4.26882	0.73619	-0.61539
C	2.23030	1.61628	-3.73881
C	4.09718	0.53468	0.86394
H	-1.89856	3.50817	-0.53875
H	-3.24834	2.76005	0.30778
H	-3.54864	3.71839	-1.14197
H	-4.24333	0.71452	0.59808
H	-5.48462	0.59943	-0.65436
H	-4.56902	-0.83309	-0.17781
H	-4.91389	-1.36475	-3.39132
H	-4.07831	-2.11930	-2.02965
H	-3.33047	-2.11540	-3.62654
H	-1.94387	-0.97606	-4.96306
H	-0.95607	0.48046	-5.06905
H	-2.63829	0.51750	-5.60507
H	-2.02573	3.53851	-3.96800
H	-0.81816	3.51948	-2.67970
H	-0.56462	2.56751	-4.14771
H	0.12650	-0.34918	-2.16062
H	1.24393	1.23817	-1.61533
H	-1.08607	-1.44658	-0.98540
H	3.72543	-4.73659	-2.04953
H	4.63419	-5.66368	0.06783
H	4.05227	-4.58489	2.22703
H	-3.21195	-4.27178	3.49569

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H      -2.63325     -3.67455      5.83687
H      -1.07677     -1.79328      6.27381
H       4.81501      1.23006     -4.43873
H       6.74182      0.66802     -2.97198
H       6.37842      0.38185     -0.53472
H       1.24556      5.90548      2.62295
H      -0.94389      6.12949      3.77685
H      -2.52890      4.21920      3.76816
H       3.08985     -2.83939      3.46415
H       2.56806     -1.35488      2.65427
H       1.41788     -2.65994      2.91874
H       2.34668     -3.25403     -3.22528
H       1.03539     -2.43928     -2.34415
H       2.56009     -1.60609     -2.61641
H       3.21237      1.04265      1.25076
H       4.00966     -0.53128      1.09631
H       4.96737      0.91953      1.40455
H       2.55628      1.67399     -4.78008
H       1.40114      0.89930     -3.69337
H       1.82855      2.60041     -3.46673
H      -0.05411      0.28207      5.45354
H       1.21319     -0.60781      4.61196
H       0.22281      0.55032      3.72728
H      -3.10925     -3.88971      1.18031
H      -2.72454     -2.23884      0.63895
H      -1.46982     -3.46059      0.66372
H      -2.23915      1.23184      1.72241
H      -2.02146      1.07090      3.45637
H      -3.24997      2.17276      2.84052
H       2.67470      4.76965      1.14044
H       2.95322      3.21405      1.92392
H       2.17060      3.26095      0.34796
102
Complex 4 formation Red Path. - TS
C      -5.64514      4.93503     -7.40222
C      -6.42145      3.73476     -7.23383
C      -6.28799      2.95150     -8.44114
C      -5.43174      3.65537     -9.33570
C      -5.01611      4.87836     -8.69505
Ir     -4.20729      3.16047     -7.39156
Ta     -2.76708      3.08866     -5.35282
C      -7.39682      3.45396     -6.13244
C      -7.00736      1.66951     -8.72995
C      -5.08728      3.24575    -10.73493
C      -4.31281      6.02181     -9.35801
C      -5.65143      6.13885     -6.51234
H      -4.66944      6.61504     -6.47199
H      -5.93438      5.88775     -5.48971
H      -6.36993      6.88189     -6.88376
H      -7.11842      3.95888     -5.20597
H      -8.40052      3.80245     -6.41044
H      -7.47076      2.38492     -5.91727
H      -7.99214      1.86729     -9.17291
H      -7.16592      1.08506     -7.82054
H      -6.44903      1.04379     -9.43071
H      -5.10925      2.15981    -10.85470
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H	-4.09070	3.59018	-11.02204
H	-5.80297	3.67292	-11.44912
H	-5.04445	6.71915	-9.78828
H	-3.69966	6.58553	-8.65070
H	-3.66596	5.68598	-10.17126
H	-3.03801	2.45392	-8.19007
H	-2.39073	3.90482	-7.32979
H	-4.14175	1.66988	-6.83306
O	-1.57547	1.60534	-5.58837
O	-1.38312	4.18270	-6.68687
O	-3.76530	2.18431	-4.00494
O	-2.93691	4.78056	-4.47599
C	-0.77976	0.51145	-5.54273
C	-0.11789	4.00637	-7.20168
C	-4.23553	1.43421	-2.98536
C	-3.18821	5.91018	-3.76762
C	-0.44349	-0.13250	-6.75152
C	0.38114	-1.25709	-6.69461
C	0.86994	-1.73975	-5.48380
C	0.52281	-1.09355	-4.30328
C	-0.30727	0.03185	-4.30480
C	-0.96136	0.37487	-8.06574
H	0.64248	-1.75716	-7.62425
H	1.51437	-2.61391	-5.46165
H	0.89267	-1.46535	-3.35046
C	-0.70724	0.67602	-3.00922
C	-5.06049	0.32924	-3.28485
C	-5.56435	-0.42757	-2.22714
C	-5.26436	-0.11206	-0.90374
C	-4.43973	0.97253	-0.63087
C	-3.90510	1.76237	-1.65475
C	-5.36894	-0.02720	-4.71039
H	-6.20288	-1.27863	-2.45208
H	-5.67063	-0.70950	-0.09267
H	-4.19600	1.22325	0.39925
C	-2.97704	2.89775	-1.31463
C	0.09433	4.19289	-8.58351
C	1.38308	4.02517	-9.09246
C	2.45451	3.70789	-8.26336
C	2.23516	3.58155	-6.89864
C	0.96025	3.73255	-6.34094
C	-1.02297	4.61875	-9.49299
H	1.54238	4.16206	-10.15943
H	3.45146	3.58155	-8.67521
H	3.06745	3.36387	-6.23299
C	0.80918	3.60395	-4.85038
C	-2.26228	6.97265	-3.82373
C	-2.53913	8.13261	-3.09761
C	-3.69821	8.25417	-2.33688
C	-4.60496	7.20175	-2.30725
C	-4.37555	6.01671	-3.01374
C	-1.00264	6.86944	-4.63679
H	-1.82876	8.95503	-3.14122
H	-3.89766	9.16662	-1.78225
H	-5.52197	7.29095	-1.72888
C	-5.39227	4.91028	-2.95084

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H      -0.05390      0.34484     -2.19695
H      -0.65449      1.76758     -3.05935
H      -1.73598      0.41800     -2.73502
H      -0.64801     -0.28254     -8.88148
H      -2.05381      0.43493     -8.06887
H      -0.58673      1.38182     -8.27827
H      -0.11066      4.06555     -4.48368
H       0.81537      2.55296     -4.54592
H       1.64323      4.09670     -4.33974
H      -0.65762      4.74076    -10.51635
H      -1.84645      3.89792     -9.50636
H      -1.44410      5.57619     -9.16820
H      -3.30855      3.41228     -0.40732
H      -1.96261      2.52857     -1.12142
H      -2.91247      3.63443     -2.11564
H      -6.09330     -0.84506     -4.75601
H      -5.76876      0.82831     -5.26206
H      -4.46623     -0.34411     -5.24539
H      -5.33164      4.24855     -3.81603
H      -5.25231      4.28061     -2.06554
H      -6.40401      5.32462     -2.89209
H      -0.62113      7.86499     -4.88110
H      -0.21387      6.34834     -4.08091
H      -1.16277      6.31356     -5.56293
102
Complex 4 formation Black Path. - adduct
C       2.39236     -3.30722     -0.09559
C       2.57994     -2.11804      0.63529
C       3.74631     -1.89242      1.39050
C       4.73316     -2.87995      1.39113
C       4.57610     -4.05999      0.66963
C       3.41113     -4.26420     -0.06292
O       1.61942     -1.16400      0.62632
Ta      0.14645      0.04287      0.62466
O       1.76911      1.28881     -0.91419
C       3.14423      1.29514     -1.12177
C       3.85814      2.31474     -0.46764
C       5.24223      2.35869     -0.63821
C       5.90089      1.43080     -1.44222
C       5.16838      0.44236     -2.08460
C       3.77871      0.34779     -1.93553
C       3.14698      3.34372      0.36491
C       3.03876     -0.75148     -2.64959
C       3.91359     -0.62535      2.17789
C       1.13366     -3.55168     -0.87770
Ir     -1.26885     -0.02463     -1.40220
C      -2.16800      1.29701     -2.98667
C      -3.18265      0.29633     -2.71693
C      -2.64221     -0.97252     -3.03889
C      -1.28950     -0.78548     -3.52655
C      -1.01935      0.63017     -3.53718
C      -4.56663      0.57443     -2.21867
C      -3.34742     -2.28953     -2.94132
C      -0.45892     -1.85078     -4.17360
C       0.13945      1.30918     -4.20075
C      -2.37606      2.77934     -2.93999
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O	0.31531	1.74541	1.47861
C	-0.04700	2.74664	2.32144
C	0.21603	2.61594	3.69749
C	-0.15316	3.66855	4.53867
C	-0.75809	4.81757	4.03713
C	-0.99786	4.92675	2.67038
C	-0.64715	3.90153	1.78868
C	0.88563	1.38425	4.23807
C	-0.89989	4.01472	0.31356
O	-0.86333	-0.76505	2.03404
C	-1.88119	-1.48351	2.57184
C	-1.59688	-2.77907	3.04405
C	-2.63667	-3.52144	3.60725
C	-3.91858	-2.99173	3.72457
C	-4.16393	-1.69244	3.29172
C	-3.15849	-0.91002	2.71574
C	-0.19896	-3.32466	2.97699
C	-3.43796	0.50454	2.29270
H	-0.55956	-2.80986	-3.65899
H	0.60185	-1.59074	-4.18079
H	-0.76739	-2.00296	-5.21688
H	1.03113	0.67801	-4.21564
H	-0.10541	1.54560	-5.24526
H	0.39648	2.24982	-3.70661
H	-2.78957	3.14441	-3.88967
H	-1.43877	3.31003	-2.75804
H	-3.07367	3.06322	-2.14810
H	-4.58723	1.44211	-1.55420
H	-4.97151	-0.27532	-1.66326
H	-5.24904	0.78227	-3.05316
H	-3.83886	-2.53854	-3.89082
H	-2.65143	-3.09890	-2.70792
H	-4.11350	-2.27934	-2.16224
H	3.27749	-5.18532	-0.62559
H	5.35554	-4.81642	0.68045
H	5.63813	-2.71253	1.97028
H	-5.15547	-1.26062	3.40743
H	-4.71644	-3.58094	4.16763
H	-2.42635	-4.52592	3.96745
H	5.67361	-0.28794	-2.71236
H	6.97865	1.48177	-1.56692
H	5.80515	3.14257	-0.13754
H	-1.46409	5.82380	2.26945
H	-1.03799	5.62482	4.70791
H	0.04204	3.57777	5.60467
H	3.86514	0.25775	1.53226
H	3.12785	-0.52172	2.93415
H	4.87822	-0.61466	2.69207
H	1.23464	-4.44911	-1.49456
H	0.26797	-3.69611	-0.22035
H	0.88317	-2.70622	-1.52375
H	2.51204	2.88444	1.12588
H	3.86561	4.00205	0.85985
H	2.49031	3.96503	-0.25442
H	3.12121	-0.63650	-3.73703
H	3.46166	-1.72676	-2.38969

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H       1.97678     -0.79132     -2.39238
H       0.49434     -2.70928      3.56179
H      -0.16113     -4.34387      3.37051
H       0.19084     -3.34021      1.95562
H      -4.40844      0.83256      2.67577
H      -2.67533      1.19524      2.66730
H      -3.45190      0.60165      1.20232
H       0.32269      0.47890      3.99167
H       1.89085      1.26472      3.81773
H       0.98230      1.44268      5.32551
H      -1.30599      4.99887      0.06396
H       0.01997      3.85944     -0.25918
H      -1.60386      3.25042     -0.03077
H      -1.04343     -1.36836     -0.50800
H       1.26335      0.88093     -1.64500
H      -1.73649      0.78814     -0.07205
102
Complex 4 formation Black Path. - TS
C      -5.93143      3.51369     -9.10812
C      -5.49261      2.21892     -9.47672
C      -4.12541      2.32415     -9.95621
C      -3.75415      3.71388     -9.92895
C      -4.84603      4.44826     -9.34937
Ir     -4.06336      3.00888     -7.80694
Ta     -2.76837      2.90545     -5.63354
O      -2.73491      4.48005     -4.55516
C      -3.17774      5.39499     -3.65527
C      -2.94020      5.18063     -2.28509
C      -3.39274      6.14454     -1.38139
C      -4.05423      7.28976     -1.81562
C      -4.26635      7.48467     -3.17695
C      -3.83361      6.54946     -4.12058
C      -2.22125      3.95008     -1.81163
C      -4.06598      6.75983     -5.58876
C      -6.29710      0.95704     -9.43357
C      -3.35965      1.21584    -10.61099
C      -2.51948      4.31592    -10.52462
C      -4.94588      5.93934     -9.25320
C      -7.29226      3.88460     -8.60622
O      -3.91524      1.98276     -4.42112
C      -4.73255      1.43459     -3.49859
C      -4.23886      0.40907     -2.66824
C      -5.10406     -0.14480     -1.72113
C      -6.41618      0.29983     -1.59230
C      -6.87870      1.32039     -2.41900
C      -6.05522      1.90615     -3.38204
C      -2.82401     -0.07640     -2.80266
C      -6.55620      3.01528     -4.26234
O      -1.35940      4.05780     -6.92770
C      -0.02337      4.13166     -7.24622
C       0.68549      5.23458     -6.72579
C       2.04211      5.35924     -7.02665
C       2.68921      4.42689     -7.83480
C       1.96899      3.35654     -8.34824
C       0.60794      3.18163     -8.06633
C      -0.01576      6.26139     -5.88186
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C	-0.10885	1.98793	-8.63564
O	-1.34625	1.64800	-5.50104
C	-0.44822	0.64019	-5.41538
C	0.75319	0.86597	-4.71804
C	1.67181	-0.18245	-4.63604
C	1.41427	-1.41821	-5.22313
C	0.21721	-1.61757	-5.90403
C	-0.73568	-0.60106	-6.01539
C	1.03037	2.19905	-4.08507
C	-2.02339	-0.82636	-6.75595
H	-3.53601	0.25752	-10.11553
H	-2.28427	1.40423	-10.59488
H	-3.66146	1.10507	-11.66104
H	-1.67870	3.61980	-10.50889
H	-2.70067	4.59452	-11.57109
H	-2.21326	5.21825	-9.99005
H	-5.35679	6.36355	-10.17916
H	-3.96802	6.39582	-9.08381
H	-5.59858	6.24641	-8.43255
H	-7.24750	4.71966	-7.90264
H	-7.77656	3.04776	-8.09701
H	-7.94153	4.18895	-9.43730
H	-6.76641	0.76053	-10.40635
H	-5.67473	0.09311	-9.18734
H	-7.09272	1.01358	-8.68670
H	0.00713	-2.58066	-6.36345
H	2.14170	-2.22142	-5.14931
H	2.60419	-0.01794	-4.10127
H	-7.90115	1.67771	-2.32093
H	-7.07395	-0.14353	-0.85023
H	-4.73241	-0.93819	-1.07683
H	2.46377	2.62540	-8.98405
H	3.74485	4.53891	-8.06527
H	2.59211	6.20676	-6.62400
H	-4.77375	8.38113	-3.52580
H	-4.39679	8.02867	-1.09693
H	-3.21757	5.98714	-0.31977
H	1.03620	3.00330	-4.82832
H	0.26807	2.45190	-3.33976
H	2.00131	2.19390	-3.58299
H	-2.06961	-1.84840	-7.14196
H	-2.89758	-0.66863	-6.11440
H	-2.13017	-0.13545	-7.59853
H	-0.55933	5.80302	-5.05156
H	0.69869	6.98326	-5.47678
H	-0.75704	6.81450	-6.47004
H	0.14875	1.85364	-9.69228
H	0.18744	1.07155	-8.11274
H	-1.19451	2.07481	-8.55211
H	-2.10328	0.74491	-2.73672
H	-2.58741	-0.79884	-2.01706
H	-2.64970	-0.56281	-3.76758
H	-7.60889	3.22555	-4.05394
H	-5.99003	3.94006	-4.09942
H	-6.45370	2.76346	-5.32213
H	-2.78560	3.04142	-2.04517

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H      -1.23783      3.85687     -2.28503
H      -2.07210      3.98245     -0.72916
H      -4.39960      7.78274     -5.78429
H      -3.15952      6.56694     -6.16909
H      -4.82727      6.07296     -5.97478
H      -3.79366      1.60735     -7.01807
H      -2.25947      3.67467     -7.61289
H      -4.58807      3.69708     -6.42699
77
Complex 1 disp
C      11.56025      8.11273     13.79323
C      10.94234      8.13883     12.47970
C      11.49710      9.25156     11.75571
C      12.34647      9.97921     12.66213
C      12.40963      9.22957     13.90182
Ir     10.15372     10.08617     13.33350
Ta      8.61129     11.47973     12.23945
C       7.57819     10.12738     10.88434
C       6.92156     10.60470      9.57568
C       7.98968     10.74453      8.48639
C      10.10320      7.04335     11.90394
C      11.35018      9.49592     10.28779
C      13.23972     11.12289     12.30429
C      13.23164      9.62508     15.08463
C      11.29751      7.07082     14.83175
C       9.79530     12.94934     11.15581
C      10.15825     14.35233     11.68113
C      11.21746     14.97765     10.76196
C       7.14702     12.34944     13.57890
C       6.43533     11.80069     14.82665
C       5.80527     10.44062     14.50816
C      10.73073     14.25195     13.10010
C       8.91890     15.25318     11.68501
C       7.41933     11.65587     15.99029
C       5.32595     12.77990     15.23978
C       5.88042      9.57337      9.11773
C       6.21754     11.95103      9.78416
H      10.72612     12.41303     10.91332
H       9.25982     13.05578     10.19294
H       9.97477     13.91341     13.81725
H      11.55610     13.53427     13.14072
H      11.10255     15.22482     13.44398
H      11.47487     15.99578     11.07941
H      12.13899     14.38406     10.76661
H      10.85941     15.02886      9.72702
H       7.66268     13.29489     13.84089
H       6.37769     12.64689     12.83702
H       6.90160     11.31137     16.89350
H       7.89244     12.61757     16.22319
H       8.21254     10.94420     15.75205
H       4.79951     12.42848     16.13564
H       5.74039     13.77022     15.46265
H       4.58433     12.90043     14.44090
H       5.24034     10.05875     15.36686
H       6.57343      9.70147     14.25631
H       5.11091     10.51639     13.66212
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H       8.14786      9.20628     10.71017
H       6.78556      9.83225     11.60499
H       5.42015      9.86399      8.16495
H       5.07924      9.46829      9.85851
H       6.33897      8.58729      8.98215
H       5.70161     12.27562      8.87274
H       6.92836     12.74455     10.04928
H       5.46880     11.88695     10.58243
H       7.55236     11.10238      7.54683
H       8.77563     11.44859      8.77919
H       8.46741      9.77927      8.28393
H      11.55055      7.42680     15.83389
H      11.88785      6.16431     14.64435
H      10.24408      6.77723     14.84256
H      12.86553      9.15976     16.00316
H      14.27986      9.32576     14.95631
H      13.21663     10.70829     15.23360
H      14.23012     10.76892     11.98646
H      13.38681     11.79619     13.15293
H      12.82378     11.71197     11.48332
H      12.06450      8.88292      9.72237
H      11.54120     10.54007     10.02797
H      10.34825      9.24205      9.93504
H      10.72409      6.20410     11.56213
H       9.39579      6.65296     12.64065
H       9.52353      7.39298     11.04566
H       8.51424     15.36968     10.67262
H       9.16095     16.25324     12.06293
H       8.12257     14.84689     12.31830
H       8.83641      9.55275     14.08080
H      10.08289     11.24563     14.44682
12
Benzene disp
C       0.00525      0.00000      0.00161
C       0.00464     -0.00000      1.39622
C       1.21221      0.00000      2.09404
C       2.42030     -0.00000      1.39725
C       2.42095      0.00000      0.00251
C       1.21342      0.00000     -0.69529
H      -0.93670      0.00000      1.93932
H       1.21172     -0.00000      3.18082
H       3.36118      0.00000      1.94112
H       3.36237      0.00000     -0.54043
H       1.21373     -0.00000     -1.78206
H      -0.93531      0.00000     -0.54284
89
Complex 1 disp - C-H activation - adduct
C      -3.91210      0.39893      3.00029
C      -2.69110     -0.10092      3.45191
C      -1.84354      0.70713      4.21029
C      -2.22003      2.01404      4.51985
C      -3.44192      2.51304      4.06920
C      -4.28673      1.70698      3.30717
Ta     -0.14990      0.54758     -1.29670
C      -0.05923      0.92067     -3.44182
C      -0.44611      2.25611     -4.09603
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C	0.65377	3.28700	-3.81999
Ir	1.37240	-1.22422	-0.87878
C	1.62066	-1.66558	1.31480
C	2.85552	-1.08978	0.85116
C	3.49153	-2.06303	-0.01375
C	2.64936	-3.18804	-0.11920
C	1.46278	-2.94097	0.66985
C	3.49962	0.15556	1.37141
C	4.81646	-1.87362	-0.67763
C	2.90578	-4.43619	-0.89838
C	0.44269	-3.97780	1.01252
C	0.74266	-1.13878	2.40345
C	0.49823	2.03273	0.16300
C	-0.23500	3.28477	0.69294
C	-0.10782	4.45518	-0.28477
C	-2.19520	-0.00861	-0.83369
C	-2.92369	-1.32639	-1.14792
C	-2.72422	-1.71224	-2.61733
C	0.40835	3.69325	2.02716
C	-1.71689	2.99073	0.94037
C	-2.36452	-2.43431	-0.25793
C	-4.42481	-1.15639	-0.87865
C	-0.58000	2.07242	-5.61435
C	-1.78906	2.75492	-3.55012
H	0.61810	1.33398	1.01053
H	1.53436	2.29356	-0.11341
H	0.30397	2.89496	2.77026
H	1.47799	3.89795	1.90115
H	-0.06103	4.59535	2.43949
H	-0.56872	5.35949	0.13061
H	0.94269	4.68487	-0.49771
H	-0.60520	4.24440	-1.23551
H	-2.28721	0.21744	0.24412
H	-2.72652	0.82096	-1.34307
H	-2.85151	-3.39601	-0.45894
H	-2.51678	-2.19583	0.80162
H	-1.29049	-2.53830	-0.43396
H	-4.97211	-2.09027	-1.05761
H	-4.60480	-0.85481	0.15893
H	-4.85698	-0.38496	-1.52724
H	-3.29772	-2.61294	-2.86728
H	-1.66982	-1.92102	-2.82830
H	-3.05755	-0.91102	-3.28783
H	0.90529	0.57313	-3.83569
H	-0.78363	0.13619	-3.74354
H	-0.83652	3.01710	-6.11072
H	-1.36345	1.34417	-5.85373
H	0.35775	1.70833	-6.04872
H	-2.08265	3.70206	-4.01782
H	-1.75338	2.92758	-2.46792
H	-2.58540	2.02649	-3.74196
H	0.40259	4.26552	-4.24674
H	0.81815	3.42276	-2.74660
H	1.60447	2.96278	-4.25861
H	4.09829	0.64918	0.60081
H	4.16539	-0.06697	2.21622

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H       2.75605      0.87675      1.71932
H       4.97556     -0.82820     -0.95478
H       5.63798     -2.16619     -0.01099
H       4.89807     -2.47344     -1.58776
H       3.32868     -5.22293     -0.25969
H       3.60958     -4.26374     -1.71709
H       1.98260     -4.82908     -1.33342
H       0.09315     -4.51821      0.12872
H      -0.42938     -3.53876      1.50030
H       0.86859     -4.71748      1.70400
H       0.96892     -1.63193      3.35833
H       0.88129     -0.06569      2.54790
H      -0.31191     -1.30968      2.17862
H      -2.21395      3.84852      1.40701
H      -1.84770      2.13321      1.60673
H      -2.24806      2.77587      0.00625
H       2.08167     -0.38825     -2.04097
H      -2.40538     -1.12303      3.22168
H      -0.89461      0.31569      4.56541
H      -1.56147      2.64322      5.11179
H      -3.73355      3.53174      4.30880
H      -5.23779      2.09576      2.95419
H      -4.57429     -0.23366      2.41675
H       0.61950     -1.90100     -2.12771
89
Complex 1 disp - C-H activation - TS
C      11.63284      9.14777     14.48526
C      12.38256      8.78116     13.30998
C      11.64021      7.80567     12.58385
C      10.41508      7.54679     13.31360
C      10.42469      8.35691     14.49517
Ir     10.37831      9.71381     12.70945
Ta      8.82248     11.56787     11.96922
C       9.52552     13.57452     12.49752
C       8.57442     14.75973     12.84930
C       8.94480     15.33835     14.22005
C      13.72957      9.31310     12.94779
C      12.06956      7.10574     11.33733
C       9.41566      6.49447     12.96206
C       9.40270      8.35823     15.58128
C      12.10202     10.02947     15.59467
C       8.35938     11.56044     14.48983
C       9.26439     12.13699     15.39888
C       8.93446     12.37761     16.73110
C       7.67355     12.02043     17.21070
C       6.76821     11.40843     16.34555
C       7.11605     11.17189     15.01468
C       6.71352     11.04405     11.74069
C       6.14116      9.64712     11.41052
C       6.43483      8.65104     12.53695
C       9.15523     11.82137      9.81562
C       8.79169     12.84624      8.72334
C       8.85637     12.16556      7.34661
C       4.62032      9.76564     11.23102
C       6.73851      9.09761     10.11039
C       7.37926     13.40247      8.91864
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C	9.80714	13.99286	8.73179
C	7.09992	14.32934	12.89500
C	8.71126	15.87827	11.80916
H	10.23855	13.40946	13.31727
H	10.16351	13.83997	11.64075
H	8.82269	14.59127	15.00844
H	9.98668	15.67977	14.23272
H	8.30703	16.19610	14.46905
H	8.08313	16.73680	12.07820
H	9.74704	16.22997	11.73957
H	8.40015	15.54491	10.81505
H	6.17670	11.46194	12.60279
H	6.46162	11.72027	10.90420
H	6.12002	7.64021	12.25091
H	5.90100	8.91022	13.45700
H	7.50640	8.63186	12.75830
H	4.16605	8.79079	11.01309
H	4.14711	10.16119	12.13720
H	4.37367	10.44237	10.40441
H	6.24936	8.15677	9.83094
H	7.80916	8.89363	10.21554
H	6.60552	9.80079	9.28054
H	10.23369	11.59815	9.72741
H	8.68708	10.85295	9.54388
H	8.65066	12.87536	6.53490
H	8.12290	11.35389	7.27402
H	9.84845	11.73371	7.17056
H	7.12332	14.11887	8.12819
H	7.28264	13.91924	9.87800
H	6.63145	12.60166	8.89175
H	9.56035	14.74457	7.97208
H	9.84091	14.49648	9.69918
H	10.81539	13.61922	8.51696
H	12.71400	10.85435	15.22138
H	12.70919	9.46223	16.31241
H	11.25841	10.45795	16.13986
H	13.85201	10.34641	13.28072
H	14.51724	8.71444	13.42206
H	13.89466	9.28727	11.86822
H	12.62882	6.19105	11.57319
H	12.71317	7.74125	10.72396
H	11.20923	6.81950	10.72720
H	9.19447	6.49020	11.89185
H	8.47512	6.64218	13.49553
H	9.79699	5.50083	13.22923
H	9.71050	7.69225	16.39716
H	9.26441	9.35888	15.99755
H	8.43223	8.01610	15.21542
H	6.45238	15.18535	13.12374
H	6.93117	13.57124	13.66464
H	6.76492	13.92680	11.93260
H	11.07827	11.04076	12.09237
H	9.16725	10.65596	13.69678
H	10.26434	12.39107	15.05482
H	9.66091	12.83934	17.39563
H	7.40699	12.20259	18.24821

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H       5.78759     11.10776     16.70754
H       6.39089     10.67844     14.37821
H       9.47792      9.57076     11.36796
89
Complex 1 disp - C-H activation - product
C       2.24467     -2.16212      1.87089
C       3.21001     -1.81095      0.86806
C       2.92232     -2.55041     -0.33030
C       1.77823     -3.39728     -0.05399
C       1.36109     -3.15519      1.29119
Ir      1.16690     -1.25065      0.13752
Ta     -0.47783      0.70968     -0.50179
C       0.42894      2.69166     -0.22176
C       0.04775      4.14397      0.14997
C      -0.03629      4.30585      1.67268
C       4.34764     -0.86206      1.05308
C       3.73961     -2.56925     -1.57995
C       1.20199     -4.40344     -0.99352
C       0.25648     -3.84695      2.01870
C       2.22499     -1.70361      3.29131
C      -1.55879      1.33169      1.31915
C      -0.89235      1.12426      2.54525
C      -1.43875      1.52005      3.76577
C      -2.67632      2.16082      3.80296
C      -3.35731      2.39095      2.60727
C      -2.80929      1.97018      1.39646
C      -2.48452     -0.25983     -0.82848
C      -3.05162     -1.53392     -0.15056
C      -2.98549     -1.51800      1.37808
C      -0.49016      0.92150     -2.69217
C      -1.20077      1.89852     -3.65075
C      -1.35800      1.23822     -5.02866
C      -4.52802     -1.66133     -0.56310
C      -2.30244     -2.76627     -0.66806
C      -2.59302      2.27895     -3.13400
C      -0.34602      3.15862     -3.82205
C      -1.29214      4.58420     -0.44882
C       1.14854      5.08266     -0.37055
H       1.17885      2.35966      0.52312
H       1.00122      2.70114     -1.17062
H      -0.85361      3.72156      2.09679
H       0.89448      3.98676      2.15660
H      -0.20261      5.35842      1.93316
H       0.94383      6.12608     -0.09934
H       2.12556      4.81223      0.04758
H       1.22851      5.03199     -1.46297
H      -3.20686      0.55567     -0.68460
H      -2.51173     -0.47608     -1.90466
H      -3.44590     -2.42658      1.78675
H      -3.50898     -0.65347      1.79552
H      -1.95266     -1.47438      1.73295
H      -4.97640     -2.58380     -0.17175
H      -5.11412     -0.81675     -0.18216
H      -4.63269     -1.67505     -1.65462
H      -2.72654     -3.68836     -0.25133
H      -1.24450     -2.71462     -0.39899
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H      -2.36227     -2.83333     -1.76155
H       0.60415      0.99279     -2.85730
H      -0.73018     -0.11162     -2.98978
H      -1.81145      1.92590     -5.75400
H      -1.99567      0.34851     -4.96668
H      -0.38502      0.92562     -5.42562
H      -3.08706      2.97892     -3.81944
H      -2.53576      2.75983     -2.15320
H      -3.23357      1.39699     -3.03794
H      -0.85685      3.90522     -4.44201
H      -0.11502      3.62096     -2.86059
H       0.60675      2.91595     -4.30820
H       2.68574     -0.71887      3.39948
H       2.77597     -2.40172      3.93466
H       1.20359     -1.63681      3.67389
H       4.10129     -0.08006      1.77459
H       5.22970     -1.39737      1.42477
H       4.62094     -0.37766      0.11333
H       4.51440     -3.34509     -1.52973
H       4.23733     -1.61093     -1.74573
H       3.11885     -2.77471     -2.45534
H       1.23990     -4.05136     -2.02679
H       0.15992     -4.62481     -0.75524
H       1.76603     -5.34270     -0.93664
H       0.64996     -4.70680      2.57472
H      -0.22752     -3.17904      2.73482
H      -0.51082     -4.21216      1.33410
H      -1.52280      5.61525     -0.15241
H      -2.10430      3.94753     -0.09027
H      -1.28389      4.55428     -1.54092
H       1.61644      0.30256      0.00513
H      -0.25320     -0.86879      0.83341
H       0.08302      0.64167      2.55353
H      -0.89396      1.33351      4.68862
H      -3.10520      2.47746      4.74990
H      -4.32288      2.89142      2.61891
H      -3.38195      2.15428      0.49005
H       0.42438     -1.15652     -1.30683
111
Complex 2 disp
O       0.14971      0.23071      3.87657
Si      1.32907      1.02677      4.79957
Si     -0.28840      0.50785      2.32547
O      -1.93488      0.59576      2.23795
Si     -3.03932      1.48102      1.38936
O      -3.51211      0.63680      0.05963
Si     -2.99508     -0.60845     -0.89254
O      -4.26965     -1.54718     -1.27840
O       0.37687      1.94334      1.84451
Si      1.05119      2.59817      0.49262
O      -0.06927      3.49902     -0.32905
Si     -1.71191      3.53981     -0.45171
O      -2.20808      5.08567     -0.65380
Si     -3.18806      5.71706     -1.88637
O       0.26505     -0.72360      1.37417
Si     -0.23411     -1.55240      0.03959
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O	-1.88544	-1.51530	-0.07710
O	2.28512	3.54163	1.02475
O	1.61920	1.41372	-0.50956
Si	1.10395	0.53830	-1.80495
O	2.44420	0.28294	-2.72087
O	0.20849	-3.12501	0.16873
Si	-0.78587	-4.47810	-0.07512
O	0.44349	-0.89698	-1.31419
O	-2.38790	2.92829	0.92707
O	-4.36215	1.74933	2.31182
Si	-4.96255	3.16051	3.03034
O	-2.21491	2.66585	-1.76371
Si	-1.67935	1.44936	-2.73816
O	-2.16761	1.74115	-4.27286
Si	-2.91852	0.65988	-5.34648
O	-0.03033	1.37648	-2.67284
O	-2.31657	-0.00304	-2.26937
H	2.79031	3.97976	0.33081
H	2.30520	-0.26519	-3.50099
H	0.10452	-5.66396	0.05111
H	-1.85928	-4.51722	0.95680
H	-1.38761	-4.42443	-1.43799
H	1.46782	0.23338	6.05143
H	2.61933	1.06122	4.05561
H	0.87540	2.41179	5.10913
H	-3.20964	1.45166	-6.57321
H	-1.97353	-0.45035	-5.66572
H	-4.16464	0.11213	-4.75495
H	-3.42179	7.14223	-1.52533
H	-2.47877	5.62057	-3.19316
H	-4.47525	4.97328	-1.94223
H	-6.30039	2.80350	3.57425
H	-4.04791	3.58570	4.12818
H	-5.08022	4.24176	2.01403
Ta	-6.18921	-1.38751	-1.22984
Ir	-7.01584	-2.22054	-3.27195
C	-7.42384	-4.45661	-3.53643
C	-7.98705	-3.90307	-4.75185
C	-6.95554	-3.26547	-5.47171
C	-5.72476	-3.39785	-4.71692
C	-6.00929	-4.19296	-3.55167
C	-9.42310	-4.01418	-5.14897
C	-7.07848	-2.56317	-6.78438
C	-4.36163	-3.01437	-5.19530
C	-4.98547	-4.74941	-2.61372
C	-8.14531	-5.35967	-2.58910
C	-6.78321	0.63987	-0.75328
C	-6.76892	1.86651	-1.68538
C	-8.00549	1.85871	-2.58710
C	-6.73714	-2.85325	0.27316
C	-7.88531	-2.64357	1.27915
C	-9.19151	-2.35451	0.53051
C	-6.77053	3.14072	-0.82991
C	-5.49847	1.84954	-2.54171
C	-7.55878	-1.48741	2.23113
C	-8.06107	-3.92517	2.10586

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H      -6.91118     -3.78899     -0.27725
H      -5.79312     -3.00198      0.82874
H      -9.14957     -1.40141     -0.00906
H      -9.40181     -3.13624     -0.20694
H     -10.03959     -2.30021      1.22338
H      -8.85810     -3.81428      2.85151
H      -8.31988     -4.77404      1.46251
H      -7.13718     -4.17885      2.63846
H      -7.78916      0.52416     -0.30887
H      -6.10454      0.82784      0.09929
H      -7.99246      2.71493     -3.27199
H      -8.92469      1.92055     -1.99193
H      -8.05350      0.94345     -3.18352
H      -6.81789      4.04180     -1.45339
H      -7.62879      3.15971     -0.14802
H      -5.85973      3.20137     -0.22349
H      -5.44189      2.73066     -3.19146
H      -5.47800      0.96171     -3.18149
H      -4.60827      1.84844     -1.90861
H      -8.10953     -2.25931     -6.98207
H      -6.76069     -3.21237     -7.61063
H      -6.45792     -1.66327     -6.81616
H      -9.71980     -3.20377     -5.81968
H      -9.61653     -4.96232     -5.66726
H     -10.08029     -3.97739     -4.27590
H      -8.19340     -6.38486     -2.98040
H      -9.17141     -5.02326     -2.41901
H      -7.64621     -5.40490     -1.61802
H      -4.59261     -5.70322     -2.98980
H      -5.40210     -4.93432     -1.62061
H      -4.14454     -4.06302     -2.49501
H      -3.88368     -3.84109     -5.73825
H      -4.41058     -2.16035     -5.87489
H      -3.71102     -2.73799     -4.36232
H      -6.62666     -1.67754      2.77613
H      -8.35555     -1.34991      2.97148
H      -7.44203     -0.53797      1.69801
H      -6.79334     -0.72437     -3.79732
H      -8.37027     -1.57814     -2.67761
123
Complex 2 disp - C-H activation - adduct
C      -2.13954     -3.89550      1.09494
C      -0.71291     -3.82497      1.25086
C      -0.41415     -2.97552      2.37018
C      -1.65625     -2.49321      2.87829
C      -2.72768     -3.04696      2.09814
Ir     -1.48171     -1.75391      0.63786
Ta     -2.16295     -0.37633     -1.18843
O      -0.79290      0.92544     -1.57826
Si      0.69157      1.31214     -1.00715
O       0.54100      2.33048      0.28496
Si      1.27680      2.48687      1.75214
O       0.18633      2.95287      2.88066
Si     -0.90787      1.96657      3.72145
C       0.29413     -4.61859      0.48365
C       0.94655     -2.64760      2.89174
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C	-1.83824	-1.65848	4.10145
C	-4.17798	-2.94772	2.43999
C	-2.87031	-4.86290	0.22276
C	-5.49465	-2.66729	-1.06247
C	-5.61897	-3.51402	-2.16380
C	-6.87088	-3.72964	-2.73890
C	-7.99851	-3.10355	-2.20767
C	-7.87578	-2.26415	-1.10039
C	-6.62351	-2.04719	-0.52680
C	-3.97737	0.72214	-0.77240
C	-4.18637	1.62555	0.45857
C	-2.98192	2.55757	0.63006
C	-2.46083	-1.49085	-3.00962
C	-1.35520	-2.31432	-3.69997
C	-1.76227	-2.59780	-5.15187
C	-4.35059	0.76477	1.71401
C	-5.45212	2.47011	0.26161
C	-0.02729	-1.54658	-3.69072
C	-1.16956	-3.63839	-2.95743
O	1.52547	2.07377	-2.21928
Si	2.76199	3.17054	-2.27475
O	2.58250	4.03445	-3.65788
Si	1.17605	4.17083	-4.59419
O	1.53686	-0.01948	-0.55571
Si	2.95813	-0.82530	-0.55853
O	3.96328	-0.19029	-1.70994
Si	5.02865	1.07255	-1.80351
O	5.74461	1.30228	-0.33959
Si	5.55212	2.26281	0.99287
O	4.88258	3.69812	0.50912
Si	3.37519	4.36509	0.51086
O	2.67807	4.17887	-0.97293
O	4.23348	2.42867	-2.31461
O	6.24758	0.72011	-2.84930
O	2.70836	-2.40466	-0.90518
Si	3.13287	-3.34441	-2.24507
O	3.63030	-0.70541	0.94533
Si	3.45027	0.34614	2.20338
O	4.59463	1.53369	2.11512
O	2.43305	3.66002	1.67384
O	1.95026	1.04494	2.20706
O	3.49598	5.96192	0.85471
Si	2.48403	6.88572	1.85265
O	3.63341	-0.48915	3.60080
Si	3.08505	-0.05802	5.14399
O	7.00052	2.50941	1.72751
H	7.68406	2.87888	1.15749
H	5.98399	0.68344	-3.77537
H	2.11372	-4.42249	-2.34298
H	3.13768	-2.51495	-3.48099
H	4.48562	-3.92808	-2.01675
H	1.71502	-0.60547	5.34952
H	4.03359	-0.66211	6.11870
H	3.06131	1.42632	5.27989
H	0.93364	2.89759	-5.33052
H	0.00773	4.48882	-3.72509

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H       1.42937      5.28050     -5.55371
H       1.05597      6.59615      1.53919
H       2.76828      6.57839      3.28258
H       2.80452      8.30887      1.55489
H      -1.31057      0.83378      2.85411
H      -0.24488      1.46773      4.96132
H      -2.07111      2.82395      4.07883
H      -4.04075      1.34284     -1.68990
H      -4.80676      0.00112     -0.85395
H      -5.23028      0.11698      1.62762
H      -3.47571      0.12339      1.85751
H      -4.48313      1.39113      2.60418
H      -3.13019      3.24482      1.47111
H      -2.06512      1.99048      0.81695
H      -2.81411      3.16204     -0.26859
H      -3.36777     -2.10301     -2.89147
H      -2.75935     -0.65464     -3.67652
H       0.73125     -2.07599     -4.27812
H       0.35811     -1.43856     -2.67078
H      -0.13861     -0.54332     -4.11683
H      -0.36668     -4.23399     -3.40698
H      -0.92189     -3.44908     -1.90928
H      -2.08726     -4.23701     -2.98958
H      -1.01516     -3.21899     -5.66132
H      -1.86832     -1.66671     -5.72085
H      -2.72235     -3.12523     -5.19401
H      -0.10446     -4.95226     -0.47647
H       0.58880     -5.51244      1.04809
H       1.19388     -4.03213      0.28724
H      -2.36957     -5.00518     -0.73701
H      -2.93084     -5.84457      0.71195
H      -3.89272     -4.53748      0.02431
H      -4.44854     -3.69422      3.19949
H      -4.81370     -3.12405      1.57034
H      -4.42845     -1.96438      2.84529
H      -2.10366     -2.29482      4.95563
H      -2.64083     -0.92579      3.97930
H      -0.92149     -1.12579      4.36278
H       1.21844     -3.27375      3.75175
H       1.70935     -2.79501      2.12426
H       1.00307     -1.60443      3.20893
H      -5.64392      3.10951      1.13219
H      -6.33149      1.83267      0.11302
H      -5.35890      3.12035     -0.61614
H      -0.26176     -1.54620     -0.36207
H      -4.51782     -2.49547     -0.61622
H      -6.52444     -1.39741      0.33778
H      -8.75543     -1.78164     -0.68344
H      -8.97385     -3.27170     -2.65591
H      -6.96849     -4.38795     -3.59764
H      -4.74038     -4.00704     -2.56999
H      -1.32093     -0.18995      0.97851
123
Complex 2 disp - C-H activation - TS
C      -9.04323     -3.26290     -3.21830
C      -8.80971     -2.28407     -2.23769
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C	-9.87083	-2.01693	-1.34911
C	-11.11700	-2.62223	-1.48296
C	-11.33270	-3.55725	-2.49813
C	-10.28481	-3.88476	-3.35668
Ta	-6.82351	-0.78175	-2.18719
C	-8.32039	0.78450	-1.90872
C	-8.43635	1.78952	-0.74501
C	-8.97501	1.09419	0.51046
Ir	-6.20817	-2.33299	-0.31774
C	-5.25830	-4.32721	0.05578
C	-4.83705	-3.45957	1.13849
C	-6.00125	-3.07004	1.85955
C	-7.15350	-3.66188	1.22796
C	-6.68207	-4.47270	0.13094
C	-3.42999	-3.07190	1.45284
C	-6.02612	-2.24239	3.09924
C	-8.56371	-3.58099	1.70980
C	-7.53394	-5.33720	-0.73590
C	-4.33674	-5.04979	-0.86893
C	-6.58748	-1.37512	-4.28690
C	-5.42459	-2.22157	-4.84583
C	-4.07421	-1.60858	-4.46781
O	-5.40827	0.55197	-2.43998
Si	-3.90748	0.87853	-1.91193
O	-3.04824	1.58458	-3.14061
Si	-1.89350	2.75805	-3.25947
O	-0.39028	2.08799	-3.40019
Si	0.37038	0.70242	-2.91244
O	1.53286	0.29210	-4.00097
C	-5.47951	-3.64890	-4.29053
C	-5.53407	-2.27359	-6.37623
O	-3.09974	-0.47607	-1.42132
Si	-1.64190	-1.20609	-1.56861
O	-1.85323	-2.79076	-1.92656
Si	-1.19672	-3.78768	-3.12385
O	-3.95124	1.92175	-0.63066
Si	-3.17928	2.07779	0.81320
O	-2.04741	3.27275	0.71045
Si	-1.15867	3.96289	-0.50289
O	-0.99402	5.56461	-0.20713
Si	-2.20805	6.73355	-0.03520
O	-0.85329	-1.08811	-0.12078
Si	-0.97281	-0.06021	1.16338
O	-0.75621	-0.92305	2.54035
Si	-1.46028	-0.63832	4.05378
O	-0.74872	-0.50956	-2.77261
O	-2.46761	0.64423	1.24124
O	0.18080	1.11455	1.04896
Si	1.05294	1.86180	-0.13191
O	2.54585	2.11195	0.50534
O	-4.24781	2.49891	1.98159
Si	-5.40454	1.50141	2.71680
C	-9.41329	2.90401	-1.14682
C	-7.07877	2.41412	-0.42767
O	-1.93487	3.75360	-1.94678
O	-2.21836	3.62288	-4.61611

Si	-3.63944	3.53251	-5.53830
O	0.34768	3.29790	-0.55788
O	1.15441	0.90917	-1.48020
H	3.17255	2.53774	-0.09019
H	1.22794	0.24176	-4.91363
H	-2.20515	-4.85032	-3.38150
H	-0.92768	-3.01081	-4.36391
H	0.06762	-4.38750	-2.60991
H	-2.87777	-1.09704	4.03972
H	-0.67281	-1.43177	5.03606
H	-1.40574	0.81449	4.38182
H	-3.71160	2.21505	-6.23153
H	-4.83342	3.71946	-4.66685
H	-3.54563	4.63389	-6.53571
H	-3.54403	6.11053	-0.25838
H	-2.11923	7.29335	1.34204
H	-1.95777	7.80067	-1.04376
H	-5.74690	0.37636	1.80795
H	-4.83334	0.97884	3.99209
H	-6.59622	2.34533	3.00176
H	-8.04948	1.34734	-2.82701
H	-9.31050	0.35835	-2.11177
H	-9.98190	0.69551	0.34149
H	-8.32775	0.26447	0.81442
H	-9.03761	1.80033	1.34700
H	-7.16815	3.17571	0.35581
H	-6.36896	1.65762	-0.08858
H	-6.64130	2.89025	-1.31049
H	-7.53745	-1.78401	-4.65240
H	-6.51758	-0.36435	-4.73257
H	-3.25651	-2.12898	-4.97971
H	-3.90160	-1.69181	-3.39282
H	-4.02036	-0.55033	-4.74203
H	-4.62066	-4.23566	-4.63784
H	-5.46455	-3.63684	-3.19580
H	-6.38478	-4.17384	-4.61498
H	-4.73798	-2.89019	-6.81262
H	-5.45578	-1.26994	-6.81018
H	-6.49587	-2.69723	-6.68792
H	-4.84431	-5.35466	-1.78602
H	-3.94221	-5.95364	-0.38745
H	-3.49165	-4.41830	-1.14698
H	-7.08082	-5.48408	-1.71903
H	-7.67279	-6.32434	-0.27720
H	-8.52188	-4.89725	-0.89038
H	-8.78735	-4.39075	2.41652
H	-9.27039	-3.65828	0.87972
H	-8.75322	-2.63204	2.21795
H	-6.05601	-2.89178	3.98320
H	-6.90615	-1.59522	3.13588
H	-5.13467	-1.61752	3.17908
H	-3.00916	-3.69840	2.24913
H	-2.78813	-3.17880	0.57709
H	-3.37564	-2.03246	1.78047
H	-9.54706	3.62879	-0.33393
H	-10.39855	2.49459	-1.39842

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H      -9.04390      3.44919     -2.02321
H      -5.10740     -1.79489     -1.38056
H      -7.64819     -2.42719     -1.47915
H      -9.70531     -1.32725     -0.52630
H     -11.91748     -2.37525     -0.78972
H     -12.30109     -4.03838     -2.60457
H     -10.43165     -4.62924     -4.13546
H      -8.24043     -3.55562     -3.88636
H      -6.58595     -0.79223      0.05497
123
Complex 2 disp - C-H activation - product
C      -5.06319     -1.53004     -3.04695
C      -4.51275     -1.50636     -1.75274
C      -5.37374     -1.95658     -0.72289
C      -6.67534     -2.39213     -0.96359
C      -7.17884     -2.40449     -2.26440
C      -6.36326     -1.96859     -3.30597
Ta     -2.56085     -0.56436     -1.09265
C      -3.94239      1.14480     -0.86313
C      -4.07714      2.04534      0.38158
C      -4.69783      1.24317      1.53241
Ir     -1.88081     -2.20123      0.80880
C      -0.69357     -4.03696      1.25290
C      -0.39730     -3.04320      2.26968
C      -1.60960     -2.78152      2.98459
C      -2.66729     -3.56328      2.40511
C      -2.08654     -4.35216      1.34379
C       0.95090     -2.48549      2.58429
C      -1.74740     -1.93250      4.20230
C      -4.07143     -3.65241      2.90270
C      -2.82145     -5.35574      0.51900
C       0.30300     -4.67601      0.34552
C      -1.83407     -1.09830     -3.10306
C      -1.24078     -2.46853     -3.49785
C       0.14162     -2.62690     -2.85834
O      -1.14329      0.81218     -1.17644
Si      0.38482      1.12095     -0.75249
O       1.19417      1.82762     -2.01632
Si      2.26885      3.06733     -2.19567
O       3.79844      2.47482     -2.40490
Si      4.61237      1.11255     -1.93622
O       5.74499      0.72035     -3.06218
C      -2.12933     -3.64183     -3.07369
C      -1.07568     -2.50448     -5.02479
O       1.20935     -0.25691     -0.33312
Si      2.72796     -0.85289     -0.49645
O       2.65856     -2.46304     -0.79664
Si      3.56103     -3.40088     -1.87802
O       0.41542      2.17056      0.52241
Si      1.20724      2.40684      1.93863
O       2.27715      3.64990      1.78247
Si      3.08018      4.34202      0.50879
O       3.20090      5.95349      0.76768
Si      1.97026      7.06722      1.10840
O       3.56860     -0.64097      0.91012
Si      3.49681      0.36102      2.21298
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O	3.81293	-0.50979	3.56494
Si	3.20536	-0.24805	5.12411
O	3.52775	-0.12476	-1.74783
O	1.98601	1.01231	2.38048
O	4.60278	1.57346	2.04258
Si	5.38233	2.32530	0.79999
O	6.89781	2.63691	1.35097
O	0.14158	2.78302	3.12841
Si	-0.91830	1.65721	3.82620
C	-5.01503	3.21298	0.04003
C	-2.73175	2.61281	0.82844
O	2.24074	4.07047	-0.88750
O	1.83107	3.90418	-3.53766
Si	0.36191	3.74507	-4.37254
O	4.60434	3.72787	0.39107
O	5.44214	1.35045	-0.53441
H	7.47806	3.06976	0.71486
H	5.40942	0.65536	-3.96313
H	3.01680	-4.78122	-1.76156
H	3.40325	-2.89191	-3.26739
H	4.99783	-3.37119	-1.48152
H	1.84333	-0.84350	5.23419
H	4.13998	-0.93200	6.05865
H	3.14122	1.21218	5.41455
H	0.29825	2.41355	-5.03871
H	-0.78477	3.90537	-3.43471
H	0.35779	4.83158	-5.39060
H	0.64500	6.38573	1.06886
H	2.22193	7.63468	2.46233
H	2.03218	8.14119	0.07842
H	-1.16431	0.55542	2.85875
H	-0.28837	1.11487	5.06552
H	-2.17755	2.37177	4.16467
H	-3.56523	1.75303	-1.70972
H	-4.94999	0.83034	-1.15085
H	-5.66309	0.81571	1.23790
H	-4.04515	0.41728	1.83616
H	-4.86408	1.87988	2.41005
H	-2.85774	3.28956	1.68181
H	-2.04637	1.81561	1.12010
H	-2.24438	3.17173	0.02438
H	-2.67910	-0.86795	-3.76771
H	-1.07777	-0.33631	-3.33369
H	0.60777	-3.56936	-3.17076
H	0.08048	-2.62287	-1.76830
H	0.80521	-1.80802	-3.15844
H	-1.69636	-4.59255	-3.40997
H	-2.23545	-3.68306	-1.98555
H	-3.13502	-3.55941	-3.49626
H	-0.60493	-3.44015	-5.35239
H	-0.44906	-1.67443	-5.37182
H	-2.04618	-2.42406	-5.52809
H	-0.15706	-4.99753	-0.59144
H	0.74403	-5.55860	0.82568
H	1.11024	-3.98504	0.09998
H	-2.31089	-5.54691	-0.42658

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H      -2.89555     -6.30658      1.06065
H      -3.83498     -5.01863      0.28965
H      -4.16423     -4.42178      3.68012
H      -4.76199     -3.91190      2.09663
H      -4.39998     -2.70278      3.33240
H      -1.83536     -2.57529      5.08665
H      -2.63973     -1.30254      4.16258
H      -0.87383     -1.29563      4.34383
H       1.40976     -3.02095      3.42406
H       1.62173     -2.58167      1.72984
H       0.89005     -1.42741      2.84441
H      -5.16082      3.87266      0.90488
H      -5.99945      2.84843     -0.27536
H      -4.60463      3.81818     -0.77666
H      -0.82608     -1.58349     -0.25308
H      -2.98884     -2.40746     -0.35756
H      -5.02066     -1.96074      0.30712
H      -7.29498     -2.72874     -0.13523
H      -8.19037     -2.74902     -2.46226
H      -6.73809     -1.96948     -4.32701
H      -4.47432     -1.19356     -3.89590
H      -2.40009     -0.68160      1.10200
96
Complex 3 disp
C       0.97388     -1.04469     -0.48062
C       2.05496     -2.07618     -0.42038
C       3.31772     -1.94441      0.25981
C       4.16284     -3.03978     -0.16692
C       3.42660     -3.85942     -1.04321
C       2.09027     -3.30616     -1.16761
Ir      2.18848     -3.74541      1.06831
Ta      0.45996     -3.54441      2.63677
C       0.43714     -1.46774      3.17285
C       0.02514     -1.03513      4.59261
C      -0.28067      0.46852      4.59543
C       3.78218     -0.77132      1.06084
C       5.56697     -3.25685      0.29037
C       3.92974     -5.09075     -1.72163
C       1.03656     -3.79047     -2.11158
H      -1.04133     -3.88862      1.69519
O       0.84610     -4.66126      4.16853
Si      2.29628     -5.25303      4.66715
O       2.80761     -6.47418      3.69554
Si      4.14464     -6.91175      2.83842
O       4.80009     -8.21471      3.62863
Si      4.68619     -8.82979      5.15041
O       4.66175    -10.46552      4.97580
O       2.13096     -5.88595      6.19000
Si      2.81451     -7.16822      6.98506
O       1.66853     -7.79400      7.97746
Si      0.01442     -7.42217      7.98499
O       3.37546     -4.00635      4.73568
Si      4.70107     -3.52792      5.57434
O       6.06204     -4.01976      4.78510
Si      6.52620     -5.19193      3.71072
O       7.66737     -4.53883      2.73252
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Si	8.46057	-3.05277	2.90106
O	4.10055	-6.67597	7.89746
Si	5.23124	-5.48022	7.89202
O	5.56594	-5.08424	9.44475
Si	6.96257	-4.36201	10.07446
O	3.31095	-8.33664	5.93110
O	4.65032	-4.14550	7.10870
O	6.62419	-5.96885	7.14855
Si	7.07983	-7.11509	6.05484
O	8.56068	-7.62996	6.55005
O	4.72239	-1.89373	5.69409
Si	4.64858	-0.97271	7.11442
C	-1.22290	-1.80318	5.04433
C	1.17787	-1.31410	5.56245
O	5.25947	-5.69615	2.79000
O	3.75914	-7.34744	1.31275
Si	2.28457	-7.86932	0.66005
O	7.17011	-6.46858	4.53517
O	5.99745	-8.36282	6.04989
H	8.97870	-8.27129	5.96460
H	4.45405	-10.94893	5.78309
H	-0.61080	-8.37530	8.94288
H	-0.19148	-6.01858	8.44121
H	-0.55796	-7.60704	6.62106
H	6.54819	-3.66048	11.32056
H	7.97162	-5.41440	10.37901
H	7.51671	-3.38735	9.09093
H	2.44981	-9.31739	0.33382
H	1.18269	-7.70020	1.64511
H	2.01502	-7.10608	-0.58352
H	9.21121	-3.02110	4.18899
H	9.39979	-2.95877	1.75013
H	7.47775	-1.93432	2.85987
H	4.54215	0.44523	6.67377
H	3.46074	-1.35812	7.92452
H	5.89505	-1.17550	7.90716
H	1.35261	-0.95065	2.86311
H	-0.35072	-1.16468	2.44504
H	-0.56193	0.81419	5.59771
H	-1.10708	0.70484	3.91504
H	0.59316	1.04691	4.27449
H	-1.56070	-1.46507	6.03091
H	-1.02493	-2.87980	5.12780
H	-2.05451	-1.66084	4.34327
H	0.93110	-0.96577	6.57163
H	1.40046	-2.38265	5.62115
H	2.09056	-0.80471	5.23722
H	-0.01420	-1.50110	-0.58560
H	1.12562	-0.38245	-1.34288
H	0.96375	-0.41919	0.41486
H	1.23276	-3.44407	-3.13503
H	0.99270	-4.88247	-2.13254
H	0.04704	-3.43043	-1.81956
H	4.55306	-4.83305	-2.58742
H	3.10741	-5.70935	-2.08694
H	4.53497	-5.70360	-1.04810

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H       6.27200     -2.66162     -0.30453
H       5.86048     -4.30481      0.20970
H       5.68379     -2.95992      1.33434
H       4.35837     -0.07192      0.44054
H       2.94177     -0.21563      1.48320
H       4.42170     -1.08468      1.89020
H       3.04938     -4.12449      2.34852
H       1.68535     -5.26465      1.18842
108
Complex 3 disp - C-H activation - adduct
C      -4.41842      0.92300     -0.13384
C      -4.35464     -0.04985     -1.13249
C      -4.59893      0.29083     -2.46189
C      -4.90877      1.61150     -2.79476
C      -4.97114      2.58525     -1.79586
C      -4.72820      2.24024     -0.46524
Ta     -1.35333     -1.44210     -0.44850
C      -1.80020     -1.93124     -2.50026
C      -0.82689     -2.69901     -3.41630
C      -0.48996     -4.05487     -2.78741
Ir     -2.56972     -2.79150      1.07041
C      -4.73365     -3.49306      1.13232
C      -4.00003     -4.26924      0.17388
C      -2.99676     -5.01701      0.89172
C      -3.19284     -4.77119      2.30393
C      -4.24046     -3.83847      2.45248
C      -4.33552     -4.41642     -1.27382
C      -2.10151     -6.06647      0.31634
C      -2.39037     -5.40042      3.39487
C      -4.77550     -3.28331      3.73214
C      -5.96426     -2.68812      0.86494
O       0.54834     -1.58568     -0.14982
Si      1.53718     -0.27264     -0.14118
O       3.11932     -0.74137     -0.05648
Si      4.52108      0.03794     -0.46153
O       5.02139      1.04426      0.74680
Si      4.60792      1.94787      2.06504
O       5.79811      1.82943      3.18118
Si      7.46257      2.07505      2.98598
O       1.14985      0.66084      1.15443
Si      1.62197      1.63968      2.39179
O       3.21606      1.39069      2.75102
O       1.29264      0.57506     -1.54265
Si      1.08299      2.15896     -1.96291
O       2.50035      2.79162     -2.52189
Si      4.10778      2.50216     -2.25587
O       4.98184      2.85533     -3.60268
O       0.71070      1.28394      3.70269
Si     -0.62476      0.22329      3.70803
O       1.39509      3.21215      1.94235
Si      1.13805      4.01376      0.52304
O      -0.01799      5.15999      0.73843
Si     -1.66943      4.86898      0.45731
C      -1.49857     -2.92519     -4.77772
C       0.46267     -1.90112     -3.62956
O      -0.01418      2.28552     -3.16767
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Si	-1.71237	2.18346	-3.08241
O	0.55931	2.98101	-0.63045
O	4.29203	0.91025	-1.84159
O	5.69180	-1.08344	-0.69741
Si	7.12288	-1.26845	0.19312
O	4.69093	3.49338	-1.07963
Si	4.15825	4.36696	0.21897
O	5.02085	5.75651	0.37265
O	2.54645	4.71203	0.02435
O	4.41818	3.52349	1.60784
H	-1.64202	0.23712	0.03432
H	4.88327	6.39845	-0.33275
H	4.76853	2.31684	-4.37297
H	6.80408	-1.47569	1.63374
H	7.80331	-2.46550	-0.37178
H	7.97963	-0.05899	0.03372
H	8.14346	0.75204	3.05886
H	7.72800	2.71550	1.66623
H	7.91859	2.95388	4.09746
H	-2.11394	1.21280	-4.13669
H	-2.08280	1.71834	-1.72366
H	-2.26268	3.53378	-3.38237
H	-2.40571	5.96259	1.14949
H	-1.94673	4.90656	-1.00604
H	-2.05187	3.54185	1.01360
H	-0.15930	-1.15371	3.40227
H	-1.18742	0.30110	5.08564
H	-1.62019	0.68667	2.70509
H	-2.77530	-2.44223	-2.48905
H	-1.99430	-0.92798	-2.92727
H	1.10824	-2.40113	-4.36081
H	1.03163	-1.79952	-2.70276
H	0.24948	-0.89332	-4.00169
H	0.19067	-4.62884	-3.42716
H	-0.00570	-3.93587	-1.81106
H	-1.39476	-4.65497	-2.64409
H	-0.84147	-3.48133	-5.45735
H	-1.74382	-1.96988	-5.25652
H	-2.42907	-3.49440	-4.66907
H	-1.87445	-5.86697	-0.73309
H	-2.57127	-7.05762	0.37346
H	-1.15076	-6.11934	0.85304
H	-3.44955	-4.64276	-1.87054
H	-5.05188	-5.23537	-1.42105
H	-4.79037	-3.50861	-1.67919
H	-6.86564	-3.29492	1.02373
H	-5.99381	-2.31933	-0.16271
H	-6.03045	-1.82146	1.52771
H	-5.65339	-3.84696	4.07319
H	-5.08121	-2.24031	3.61398
H	-4.02787	-3.32037	4.52862
H	-2.78739	-6.39134	3.64998
H	-1.34707	-5.53069	3.09564
H	-2.40155	-4.79473	4.30453
H	-1.08868	-2.66390	1.67009
H	-4.12180	-1.07776	-0.85057

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H      -4.20705      0.64514      0.89421
H      -4.77972      2.99805      0.31117
H      -5.20852      3.61275     -2.05648
H      -5.10667      1.87973     -3.82882
H      -4.54280     -0.46619     -3.23868
H      -2.71587     -1.31761      1.69557
108
Complex 3 disp - C-H activation - TS
C      -8.69180     -4.31251     -0.75370
C      -7.82102     -5.42996     -0.55367
C      -7.37692     -5.41737      0.82750
C      -7.95630     -4.28003      1.46037
C      -8.74508     -3.56777      0.48787
Ir     -6.65576     -3.52355     -0.27137
Ta     -5.21943     -1.93851     -1.55276
O      -3.29381     -2.07123     -1.18157
Si     -2.28296     -0.79243     -1.28802
O      -2.39478      0.24311     -0.02210
Si     -2.50674      1.27470      1.24073
O      -3.56684      0.77514      2.37716
Si     -4.48634     -0.64063      2.52808
C      -7.52036     -6.51358     -1.53606
C      -6.52839     -6.46127      1.47299
C      -7.78658     -3.88619      2.89024
C      -9.58245     -2.35710      0.73592
C      -9.46904     -3.99324     -1.98620
C      -7.30424     -0.77814     -1.90813
C      -8.01636     -0.93029     -3.11243
C      -8.90990      0.04200     -3.55433
C      -9.15102      1.17446     -2.77485
C      -8.51647      1.30717     -1.53779
C      -7.61669      0.33757     -1.10596
H      -5.10776     -0.39318     -0.68789
C      -5.05205     -2.01556     -3.72486
C      -4.86488     -3.36772     -4.44423
C      -4.50945     -3.10902     -5.91406
C      -3.73585     -4.17648     -3.79499
C      -6.16764     -4.17172     -4.37204
O      -2.58900      0.02370     -2.70127
Si     -2.84025      1.58631     -3.16114
O      -3.84891      1.62290     -4.45064
Si     -5.54776      1.64545     -4.46942
O      -0.69925     -1.29717     -1.32634
Si      0.60030     -0.27860     -1.42383
O       0.51909      0.55919     -2.84650
Si      0.19851      2.12022     -3.28888
O       0.65887      3.18147     -2.11685
Si     -0.02637      4.06535     -0.89936
O      -1.64979      4.22416     -1.18872
Si     -3.07147      3.51191     -0.76224
O      -3.52878      2.40669     -1.90327
O      -1.41666      2.28350     -3.61425
O       1.08394      2.52389     -4.61565
O       1.97314     -1.17432     -1.37881
Si      3.19726     -1.10848     -0.20944
O       0.62742      0.80392     -0.18411
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Si	0.38238	1.79244	1.10571
O	0.25054	3.34956	0.55720
O	-2.94791	2.77510	0.70871
O	-0.99301	1.37628	1.91841
O	-4.24258	4.66072	-0.68867
Si	-5.90154	4.37006	-0.88547
O	1.64435	1.68779	2.14326
Si	3.11500	2.52766	2.08300
O	0.68382	5.54400	-0.79578
H	0.61144	6.08234	-1.59168
H	0.98288	1.92275	-5.36206
H	2.63676	-1.40941	1.13743
H	4.19745	-2.13768	-0.60414
H	3.82203	0.24520	-0.20652
H	4.14914	1.61099	2.63765
H	3.44146	2.88494	0.67347
H	3.00865	3.75751	2.91663
H	-5.98082	0.70727	-5.54021
H	-6.05886	1.23671	-3.14016
H	-5.98787	3.03065	-4.80537
H	-6.60376	5.56486	-0.34108
H	-6.21704	4.19873	-2.33085
H	-6.28986	3.14593	-0.13109
H	-3.83698	-1.74472	1.77664
H	-4.53401	-0.95092	3.98622
H	-5.86040	-0.37443	2.02427
H	-5.84980	-1.45343	-4.22119
H	-4.13706	-1.41209	-3.85697
H	-3.56036	-5.11022	-4.34253
H	-3.97327	-4.44562	-2.75861
H	-2.79793	-3.61103	-3.78113
H	-6.06003	-5.14611	-4.86382
H	-6.45625	-4.34353	-3.32887
H	-6.98711	-3.63834	-4.86845
H	-4.38600	-4.04755	-6.46891
H	-3.57298	-2.54532	-5.99513
H	-5.29304	-2.52445	-6.41003
H	-7.71641	-6.19205	-2.56067
H	-8.14280	-7.39532	-1.33854
H	-6.47445	-6.82527	-1.47952
H	-8.99039	-4.40425	-2.87806
H	-10.48097	-4.41312	-1.92356
H	-9.56784	-2.91380	-2.12560
H	-10.59121	-2.63619	1.06620
H	-9.68319	-1.75360	-0.16994
H	-9.14112	-1.71984	1.50633
H	-8.56342	-4.34964	3.51075
H	-7.86392	-2.80382	3.01490
H	-6.81523	-4.20064	3.27898
H	-7.14252	-7.29246	1.84295
H	-5.80268	-6.87427	0.76818
H	-5.97285	-6.05495	2.32171
H	-5.22505	-4.00454	-0.91432
H	-7.16251	-1.94742	-1.23508
H	-7.12252	0.45251	-0.14583
H	-8.72091	2.17257	-0.91323

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H      -9.84318      1.93764     -3.11933
H      -9.42196     -0.08480     -4.50465
H      -7.85417     -1.81412     -3.72096
H      -5.78502     -2.52844      0.65839
108
Complex 3 disp - C-H activation - product
C      -4.88668     -4.17561      1.05132
C      -3.87433     -5.12637      0.70543
C      -2.81853     -5.05264      1.68592
C      -3.21078     -4.06252      2.66524
C      -4.47234     -3.51397      2.27545
Ir     -2.97334     -3.06503      0.68133
Ta     -1.80835     -1.12808     -0.59493
O       0.12547     -1.27440     -0.31191
Si      1.31245     -0.16935     -0.42020
O       1.18619      1.09175      0.61955
Si      0.83615      2.05407      1.89471
O      -0.46688      1.61350      2.77057
Si     -1.05952      0.09658      3.24098
C      -3.91222     -6.06694     -0.45297
C      -1.61977     -5.93826      1.76726
C      -2.44384     -3.71286      3.89715
C      -5.27252     -2.50128      3.02502
C      -6.18797     -3.95973      0.35247
C      -3.40817      0.33745     -1.05663
C      -4.48629     -0.09940     -1.85878
C      -5.50876      0.75708     -2.25712
C      -5.48968      2.09592     -1.85723
C      -4.45142      2.55435     -1.05068
C      -3.43378      1.68426     -0.65208
H      -1.51623      0.30737      0.40045
C      -1.53692     -1.16534     -2.76418
C      -1.05655     -2.39242     -3.56662
C      -0.55230     -1.91362     -4.93621
C       0.07695     -3.14013     -2.85828
C      -2.23778     -3.34617     -3.78049
O       1.32810      0.49613     -1.94053
Si      1.29313      2.06406     -2.45844
O       0.50725      2.12046     -3.89535
Si     -1.14657      2.36236     -4.19529
O       2.78444     -0.87518     -0.11274
Si      4.19007     -0.00465     -0.02082
O       4.40925      0.76657     -1.46393
Si      4.34437      2.30467     -2.06480
O       4.73868      3.38859     -0.88972
Si      3.94252      4.38618      0.16043
O       2.41721      4.64857     -0.41874
Si      0.85493      4.16233     -0.23986
O       0.48100      3.02559     -1.38289
O       2.83595      2.60848     -2.67726
O       5.47302      2.50539     -3.24508
O       5.43010     -1.04296      0.25542
Si      6.50758     -1.00682      1.56178
O       4.16186      1.08925      1.21128
Si      3.74546      2.22203      2.32962
O       3.91585      3.72975      1.66928
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O	0.58207	3.57035	1.28248
O	2.19012	2.03584	2.85920
O	-0.10757	5.47088	-0.47030
Si	-1.77040	5.52943	-0.77429
O	4.73101	2.08404	3.63004
Si	6.31370	2.65382	3.82358
O	4.74999	5.80799	0.32917
H	4.79820	6.33853	-0.47378
H	5.35997	1.92701	-4.00761
H	5.76876	-1.19780	2.84161
H	7.46132	-2.12760	1.33792
H	7.23373	0.29470	1.58805
H	7.07356	1.58709	4.53314
H	6.92717	2.92695	2.49303
H	6.28039	3.89733	4.64311
H	-1.50858	1.47203	-5.33206
H	-1.94720	2.03844	-2.98786
H	-1.34329	3.78914	-4.58490
H	-2.14835	6.96910	-0.74437
H	-2.06267	4.94052	-2.11027
H	-2.50033	4.77754	0.28543
H	-0.26934	-0.98571	2.59688
H	-0.90274	0.01684	4.72483
H	-2.49902	0.01768	2.88568
H	-2.40797	-0.73740	-3.26993
H	-0.75874	-0.37859	-2.79956
H	0.42919	-3.97758	-3.47269
H	-0.24864	-3.54702	-1.89463
H	0.92918	-2.48132	-2.66675
H	-1.93882	-4.21797	-4.37463
H	-2.63193	-3.70954	-2.82477
H	-3.05656	-2.84500	-4.31052
H	-0.22935	-2.75664	-5.56011
H	0.29938	-1.23443	-4.82180
H	-1.33874	-1.37665	-5.47873
H	-4.52643	-5.67514	-1.26625
H	-4.33774	-7.02913	-0.14313
H	-2.91168	-6.25549	-0.84771
H	-6.13121	-4.25613	-0.69724
H	-6.98360	-4.54889	0.82554
H	-6.48596	-2.90908	0.38502
H	-5.97620	-2.99369	3.70754
H	-5.84964	-1.87078	2.34487
H	-4.63069	-1.84636	3.61817
H	-2.67935	-4.41937	4.70239
H	-2.69711	-2.71153	4.25270
H	-1.36668	-3.75240	3.72224
H	-1.84490	-6.85055	2.33435
H	-1.27631	-6.23739	0.77444
H	-0.78888	-5.43223	2.26442
H	-2.36046	-3.27966	-0.81187
H	-3.64562	-1.63659	0.24747
H	-2.63922	2.05999	-0.01320
H	-4.43585	3.59056	-0.72328
H	-6.28378	2.77065	-2.16613
H	-6.32055	0.38517	-2.87790

H	-4.52638	-1.13774	-2.18763
H	-1.61349	-2.33275	1.17319

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