Reduction of CS_2 to an Ethanetetrathiolate by a Hydride-Bridged Uranium–Iridium Heterobimetallic Complex

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Experimental Procedures

General considerations: Unless otherwise noted, all reactions were performed using standard Schlenk line techniques under an atmosphere of nitrogen, or in an MBraun inert atmosphere glove box under an atmosphere of nitrogen. Glassware and Celite® were stored in an oven at ca. 150 °C for at least 3 h prior to use. Molecular sieves (4 Å) were activated by heating to 200 °C overnight under vacuum prior to storage in a glovebox. NMR spectra were recorded on Bruker AV-600 and AVB-400 spectrometers. ^{1}H and ^{13}C chemical shifts are given relative to residual solvent peaks and are recorded in units of parts per million (ppm). FT-IR samples were prepared as Nujol mulls pressed between KBr plates, with data collected with a Nicolet iS10 FT-IR spectrometer. Melting points were determined using sealed capillaries prepared under nitrogen on an OptiMelt automated melting point system. Elemental analyses were determined at the Microanalytical Facility at the College of Chemistry, University of California, Berkeley.

Materials: Tetrahydrofuran (THF) and *n*-hexane were purified by passage through columns of activated alumina and degassed by sparging with nitrogen. Deuterated solvents were degassed with three freeze-pump-thaw cycles and stored over molecular sieves. Hexamethyldisiloxane (HMDSO) was stirred over CaH_2, distilled, and sparged with nitrogen. Benzylpotassium,[1] Cp^*IrH_4,[2] and $(Cp^{iPr4})_2UI$[3] were synthesized according to literature procedures. CO_2 was sourced from Linde, research grade (4.8 RS, 99.998% purity). All other chemicals were purchased from commercial sources and used as received.

Synthesis of $(Cp^{iPr4})_2U(\mu\text{-}H)_3IrCp^*$ (1):

Cp^*IrH_4 (67.8 mg, 0.205 mmol, 1.05 equiv.) and benzyl potassium (27.1 mg, 0.208 mmol, 1.07 equiv.) were added to a 20 mL scintillation vial with THF (4 mL) to generate a solution of $K[Cp^*IrH_3]$. $(Cp^{iPr4})_2UI$ (162.4 mg, 0.195 mmol, 1.00 equiv) was dissolved in THF (4 mL) and added to the $K[Cp^*IrH_3]$ solution, forming a dark green slurry as KI salt crashed out of solution. After stirring at room temperature for 2 h, the solvent was removed *in vacuo*. The crude solid was then triturated with *n*-hexane (1 mL) and the product was extracted with HMDSO, filtered through Celite, and concentrated (1 mL). This solution was cooled to –40 °C, affording dark green crystals (110.9 mg, 51% yield). Mp ca. 197 °C; ^{1}H NMR (600 MHz, C_6D_6): δ 6.32 (s, 12H, broad), 4.41 (s, 15H, Cp*), 0.12 (s, 9 H, co-crystallized HMDSO), –6.55 (s, 12 H, broad), –31.04 (s, 1 H, broad); ^{13}C NMR (600 MHz, C_6D_6): δ 112.3, 39.1, 5.21, 1.69; IR (Nujol mull on KBr): 2033 (m), 1959 (s), 1253 (s), 1180 (m), 1146 (w), 1102 (w), 1058 (m), 1033 (w), 982 (w), 845 (s), 770 (m), 760 (m), 667 (w); Anal. Calcd (%) for $UIrC_{44}H_{76}\bullet 0.5C_6H_{18}OSi_2$: C, 50.56; H, 7.67. Found: C, 50.21; H, 7.62.

Synthesis of 2 from CS_2 and 1:

Compound **1** (29.7 mg, 0.027 mmol, 1.00 equiv.) was dissolved in 2 mL *n*-hexane in a 4 mL shell vial. From an *n*-hexane stock solution containing 20 μL CS_2/1 mL, CS_2 (1.61 μL, 0.027 mmol, 1.00 equiv.) was added to the shell vial containing the solution of **1**, which was sealed in a 20 mL

scintillation vial. The dark green solution immediately became red. This solution was cooled to –40 °C, affording X-ray quality, highly insoluble red crystals over several crops (10.4 mg, 34% yield). Mp 179-182 °C; ^{1}H NMR (700 MHz, d_8-THF): δ 30.3, 27.7, 25.3, 22.8, 20.7, 18.9, 16.7, 13.7, 6.17, 5.17, –7.33, –11.3, –12.1, –14.0, –21.2, –30.7, –37.3; No ^{13}C NMR spectrum was collected due to compound paramagnetism and insolubility; IR (Nujol mull on KBr): 2040 (s), 1958 (s), 1916 (s), 1309 (w), 1178 (m), 1145 (m), 1102 (m), 1074 (w), 1061 (w), 1030 (m), 979 (w), 924 (w), 775 (m), 700 (w), 662 (m), 535 (w), 508 (w). Anal. Calcd (%) for $U_2Ir_2C_{96}H_{166}S$: C, 49.93; H, 7.42; S, 5.55. Found: C, 50.28; H, 7.42; S, 5.43.

UV/Vis/NIR Spectra

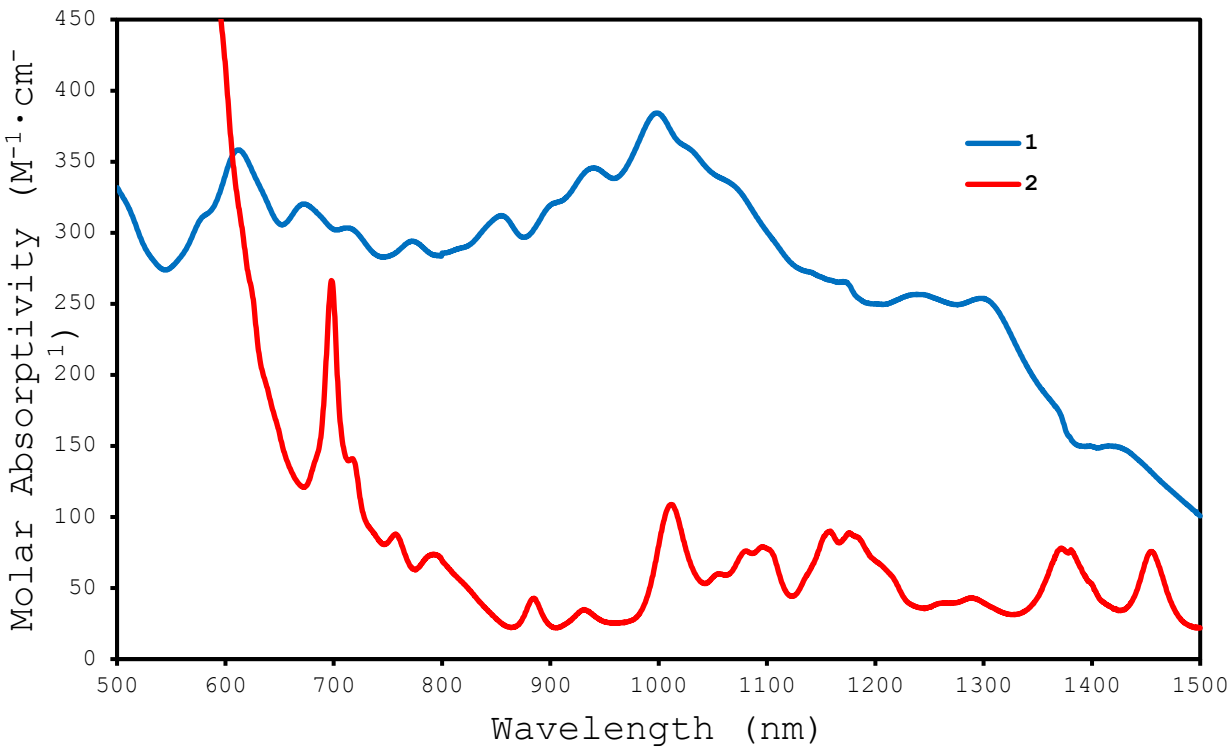


Figure S1. UV/Vis/NIR spectra of **1** and **2** in THF.

IR Spectra

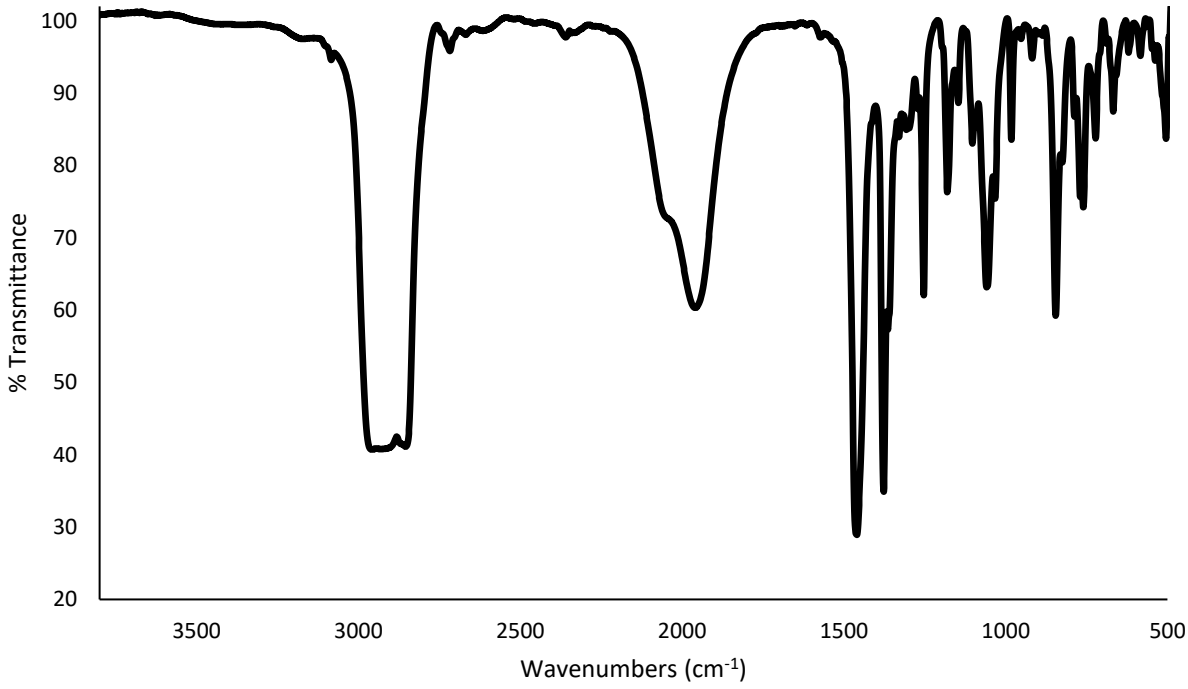


Figure S2. IR spectrum of **1** (Nujol mull).

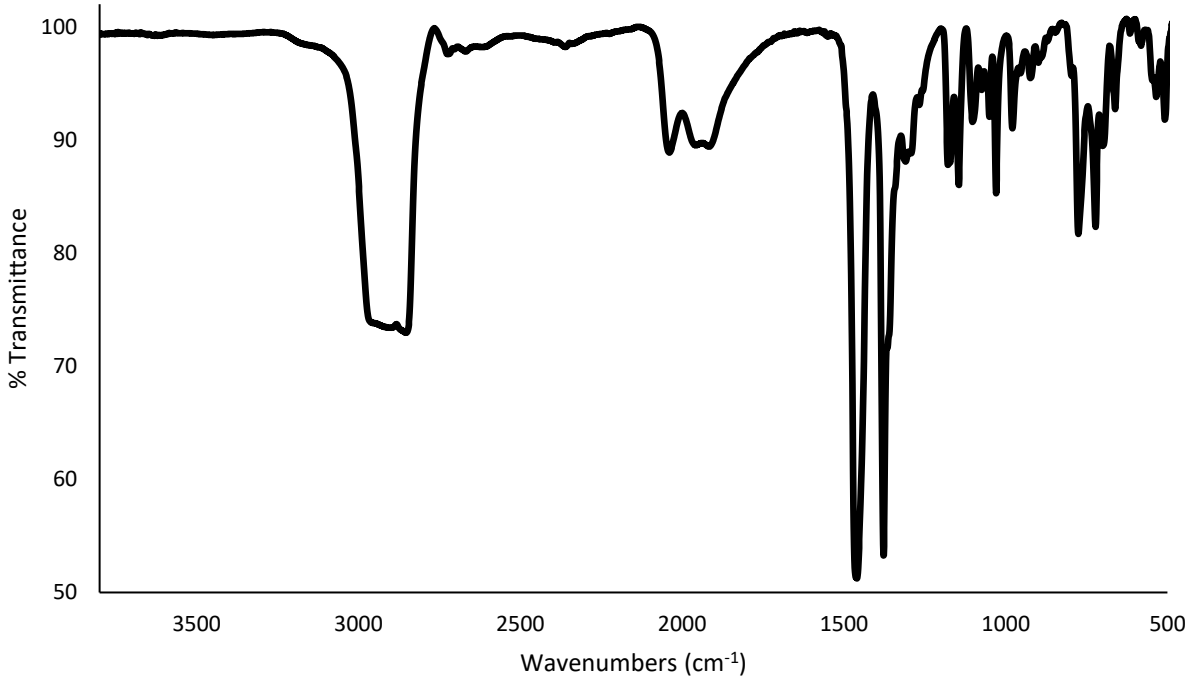


Figure S3. IR spectrum of **2** (Nujol mull).

NMR Spectra

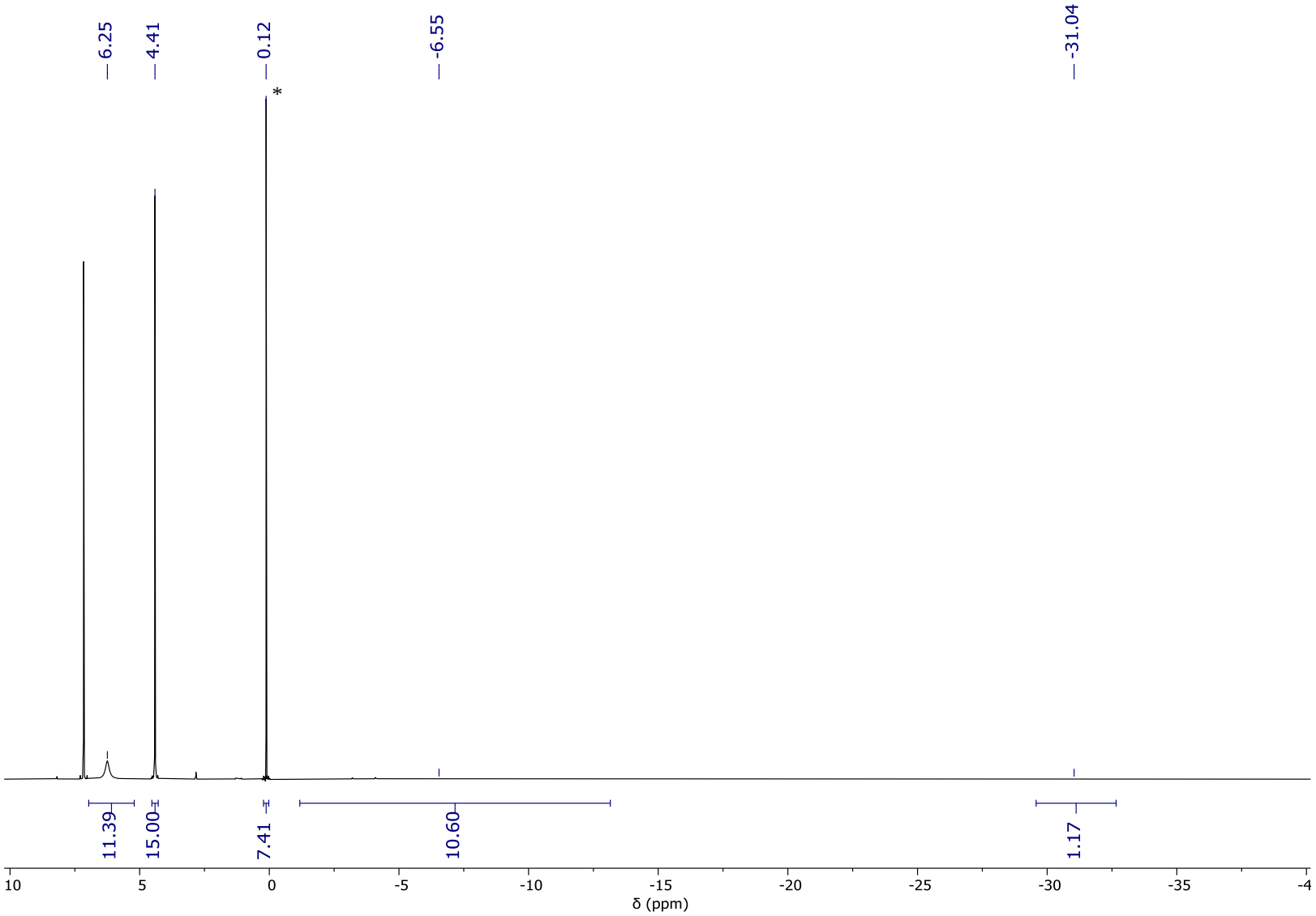


Figure S4. ^{1}H NMR spectrum of **1** at 298 K in C_6D_6. * = 0.5 equivalents of co-crystallized HMDSO.

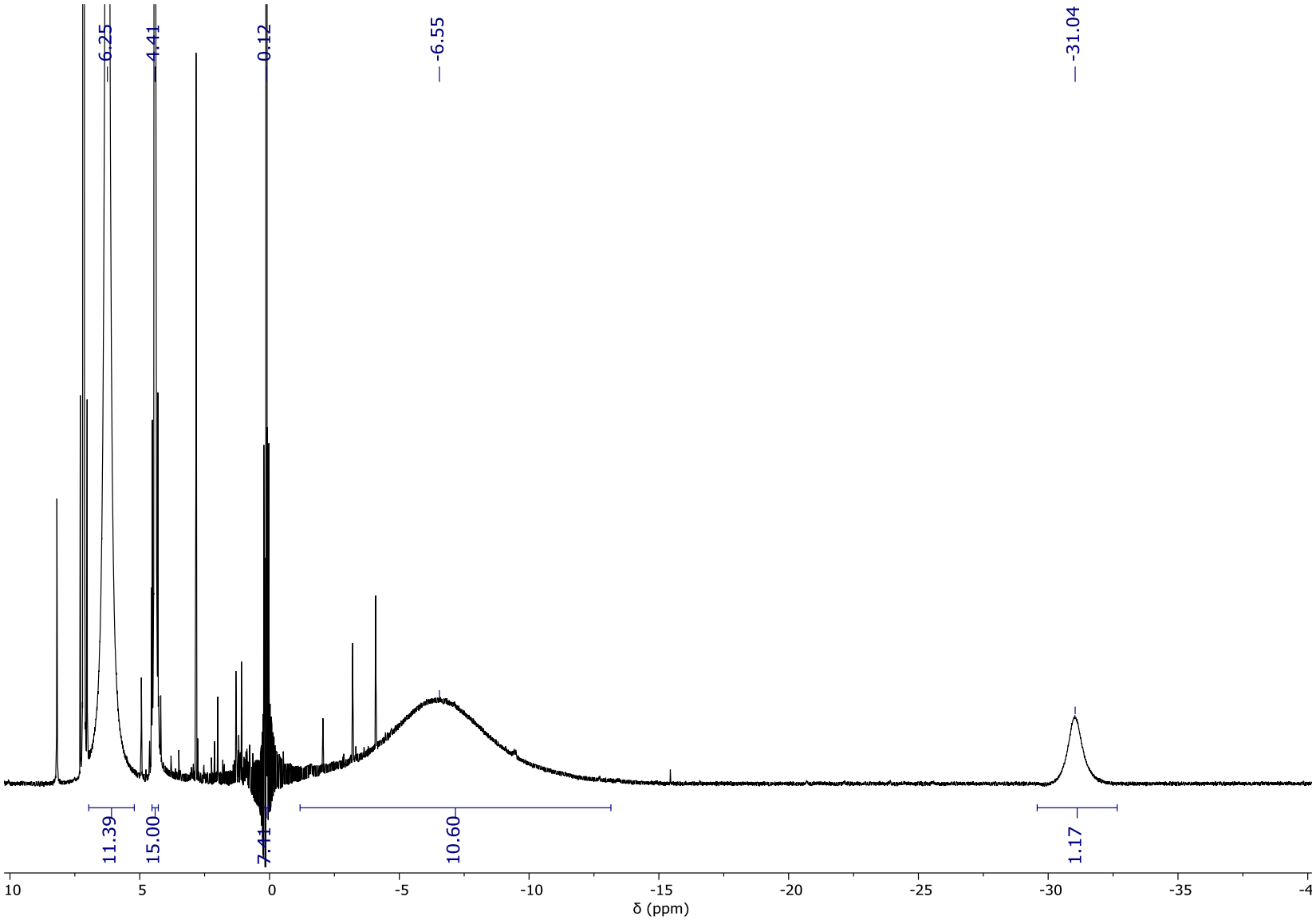


Figure S5. ^{1}H NMR spectrum of **1** at 298 K in C_6D_6, zoomed in to show broad peaks. Minor impurities appear as much sharper peaks and are thus visible despite low concentrations relative to **1**. * = 0.5 equivalents of co-crystallized HMDSO.

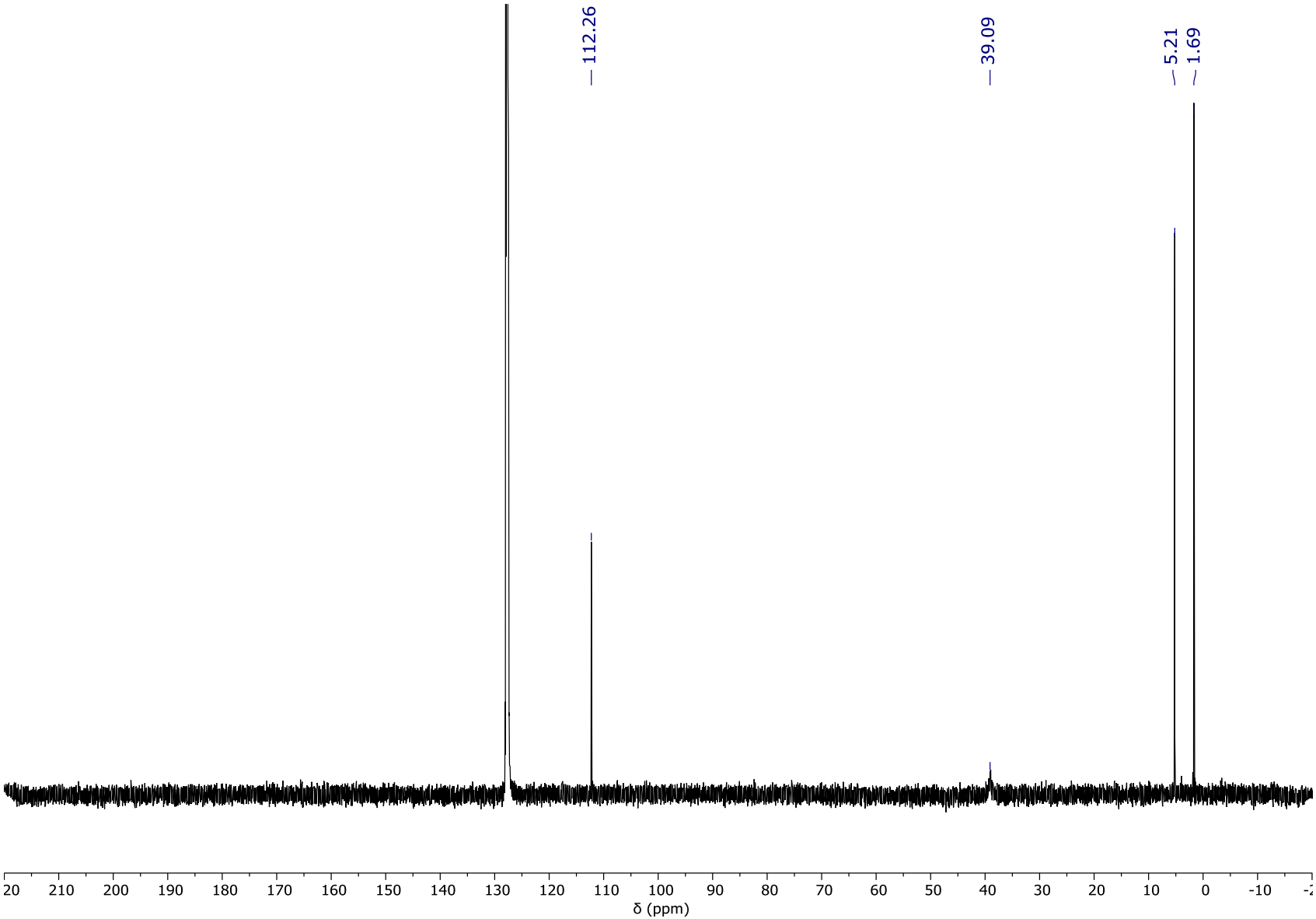


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of **1** at 298 K in C_6D_6.

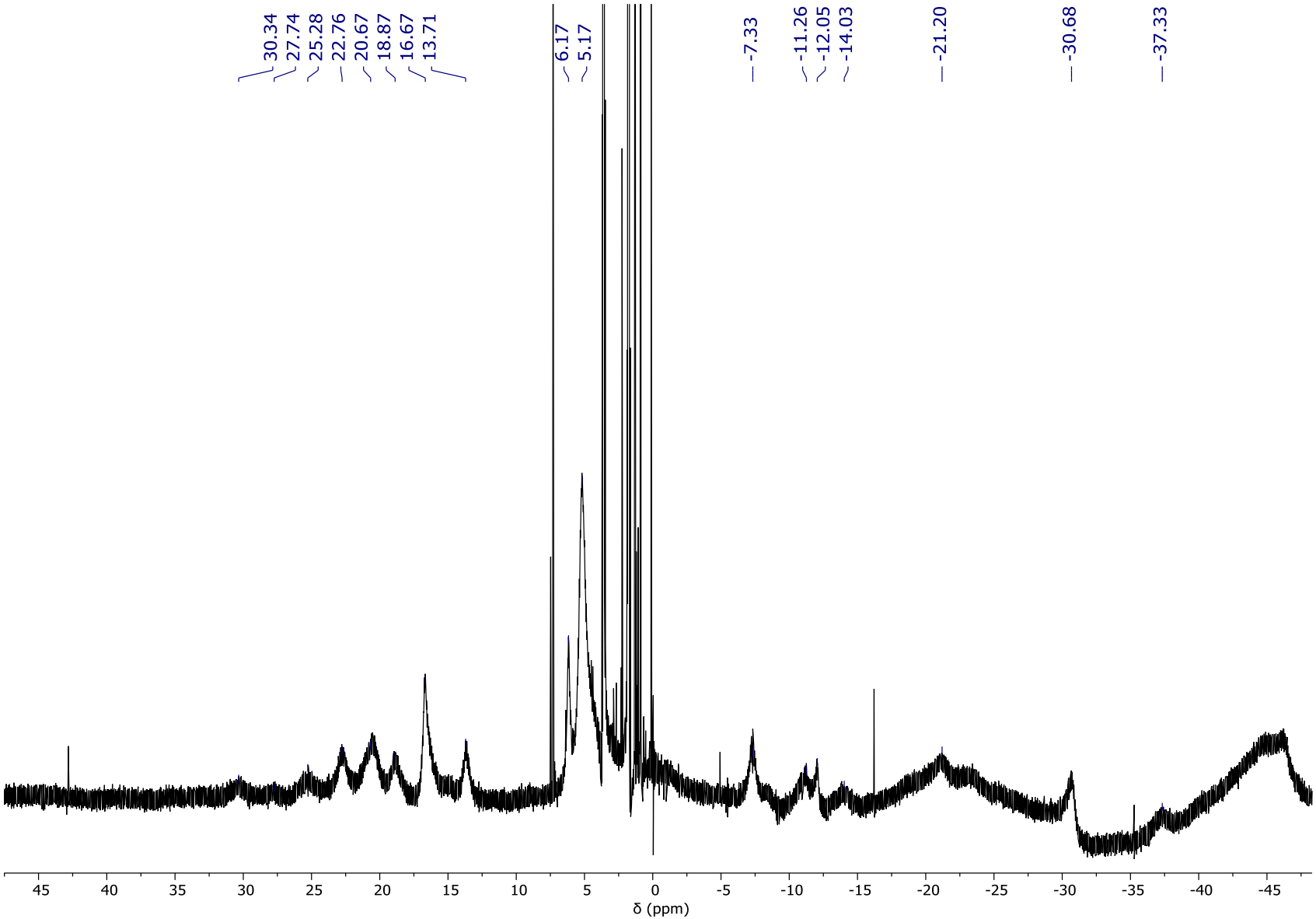


Figure S7. ^{1}H NMR spectrum of **2** at 298 K in d_8-THF.

X-ray crystallography data

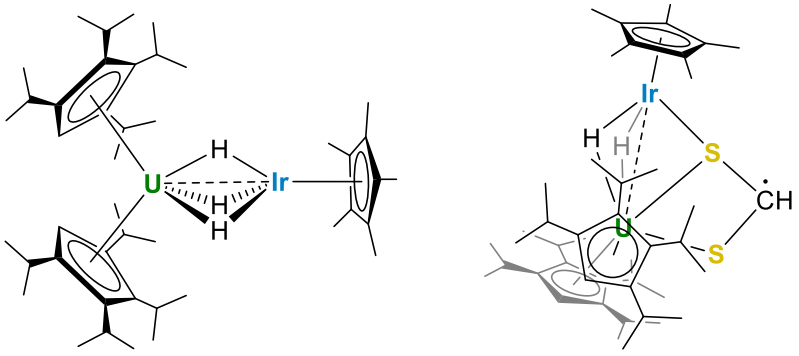
In a dry nitrogen glovebox, samples of single crystals were coated in Paratone-N oil for transport to the Advanced Light Source (ALS). Crystals were mounted on a MiTeGen 10 μm aperture Dual-Thickness MicroMount loop. X-ray diffraction data for **1** and **2** were collected at the ALS, Lawrence Berkeley National Lab, Berkeley, CA, station 12.2.1 using a silicon monochromated beam of 17 keV (λ = 0.7288 Å) synchrotron radiation. Data was collected at 100 K, with the crystals cooled by a stream of dry nitrogen. Bruker APEX3 software was used for the data collections, Bruker SAINT v8.37A or V8.38A software was used to conduct the cell refinement and data reduction procedures,[4] and absorption corrections were carried out by a multi-scan method utilizing the SADABS program.[4] CrysAlis Pro was used for the data collections and data processing, including a multi-scan absorption correction applied using the SCALE3 ABSPACK scaling algorithm within CrysAlis Pro. Initial structure solutions were found using direct methods (SHELXT),[5] and refinements were carried out using SHELXL-2014,[6] as implemented by Olex2.[7] Thermal parameters for all non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in calculated positions and refined isotropically. Thermal ellipsoid plots were made using Mercury.[8] The structures have been deposited to the Cambridge Crystallographic Data Centre (CCDC) with deposition numbers 2349727 (**1**) and 2349728 (**2**).

Compound	**1**	**2**
Empirical formula	$C_{47}H_{85}IrO_{0.5}SiU$	$C_{96}H_{166}Ir_2S_4U_2$
Formula weight	1116.46	2308.98
Temperature/K	100.0	100.0
Crystal system	triclinic	monoclinic
Space group	P-1	C2/c
a/Å	12.0803(12)	29.472(3)
b/Å	12.3459(12)	18.083(2)
c/Å	16.9963(17)	17.948(2)
α/°	105.679(4)	90
β/°	96.253(4)	99.352(4)
γ/°	96.290(4)	90
Volume/Å^3	2400.3(4)	9437.7(18)
Z	2	4
ρ_{calc}g/cm^3	1.545	1.625
μ/mm^{-1}	4.541	4.687
F(000)	1108.0	4576.0
Crystal size/mm^3	0.12 × 0.04 × 0.04	0.2 × 0.1 × 0.1
Radiation	synchrotron (λ = 0.7288)	synchrotron (λ = 0.7288)
2Θ range for data collection/°	4.62 to 61.044	4.62 to 54.194
Index ranges	$-16 \le h \le 16$, $-17 \le k \le 17$, $-23 \le l \le 23$	$-36 \le h \le 36$, $-22 \le k \le 22$, $-22 \le l \le 22$
Reflections collected	42447	61141
Independent reflections	13551 [R_{int} = 0.0666, R_{sigma} = 0.0693]	9655 [R_{int} = 0.0560, R_{sigma} = 0.0372]
Data/restraints/parameters	13551/15/535	9655/15/524
Goodness-of-fit on F^2	1.012	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0364, wR_2 = 0.0824	R_1 = 0.0336, wR_2 = 0.0800
Final R indexes [all data]	R_1 = 0.0461, wR_2 = 0.0878	R_1 = 0.0389, wR_2 = 0.0831
Largest diff. peak/hole / e Å^{-3}	0.95/–1.19	2.26/–1.32
CSD entry	2349727	2349728

Table S1. Crystal data for complexes **1** and **2**.

Computational details.

All DFT calculations were carried out with the Gaussian 09 suite of programs.[9] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional.[10,11] 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. Uranium atoms were treated with a small core effective core potential (60 MWB), associated with its adapted basis set.[12,13] Iridium atoms were treated with a small-core effective core potential (60 MWB), associated with its adapted basis set[14] augmented with a polarization function (ζ_f = 0.938).[15] For the other elements (S, H and C), Pople's triple-ζ basis set 6-311G(d,p) was used.[16–18] The electronic charges (at the DFT level) were computed using the natural population analysis (NPA) technique.[19] Dispersion corrections using the GD3-BJ approach as well as solvent effect within the SMD method were accounted for in the optimization process.



	1	Thioformate intermediate
Doublet	16.0 (16.2)	2.5 (3.1)
Quartet	0.0 (0.0)	0.0 (0.0)
Sextet	61.4 (59.1)	14.8 (0.9)

Table S2. Calculated energies (Δ_rH, Δ_rG in parentheses) for electronic ground states of **1** and the calculated thioformate intermediate. Energies are given in kcal/mol.

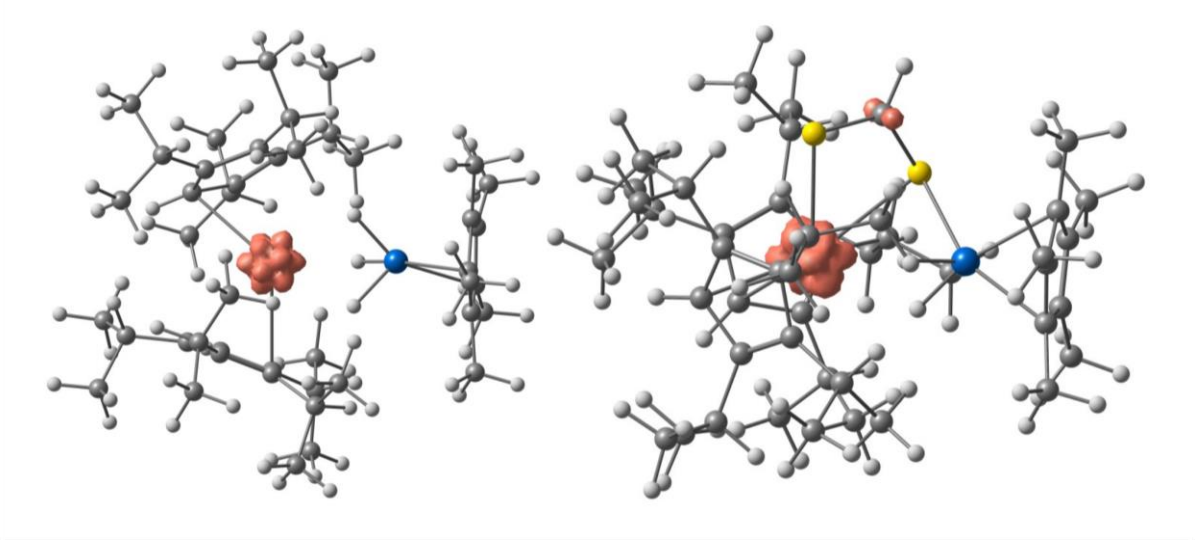
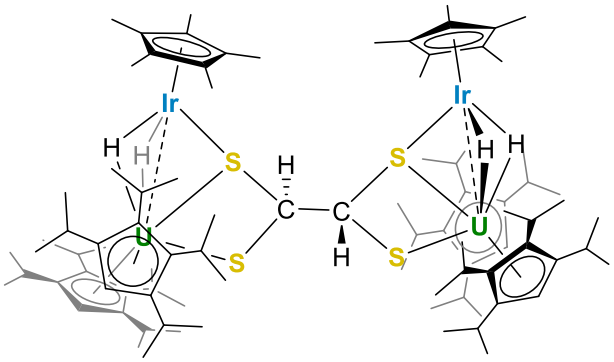


Figure S8. Unpaired spin density plot for **1** (left) and the calculated thioformate intermediate (right).



	2
Doublet	8.8 (8.8)
Quartet	0.0 (0.0)
Sextet	18.5 (12.8)

Table S3. Calculated energies ($\Delta_r H$, $\Delta_r G$ in parentheses) for electronic ground states of **2**. Energies are given in kcal/mol.

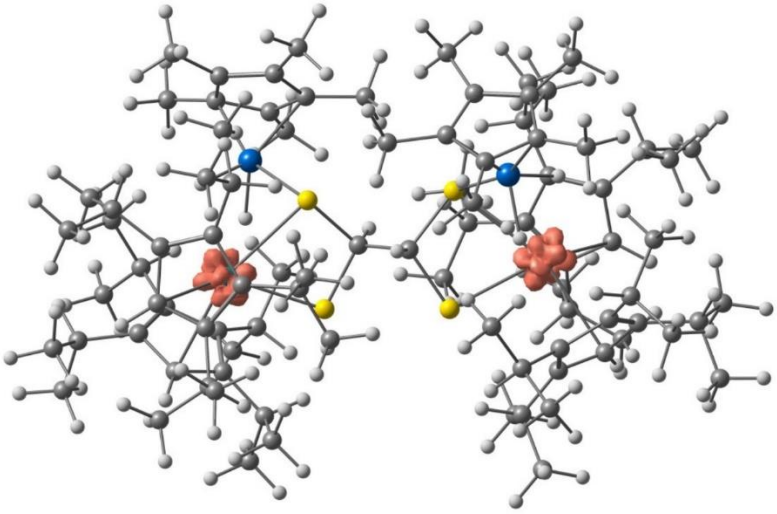


Figure S9. Unpaired spin density plot for **2**.

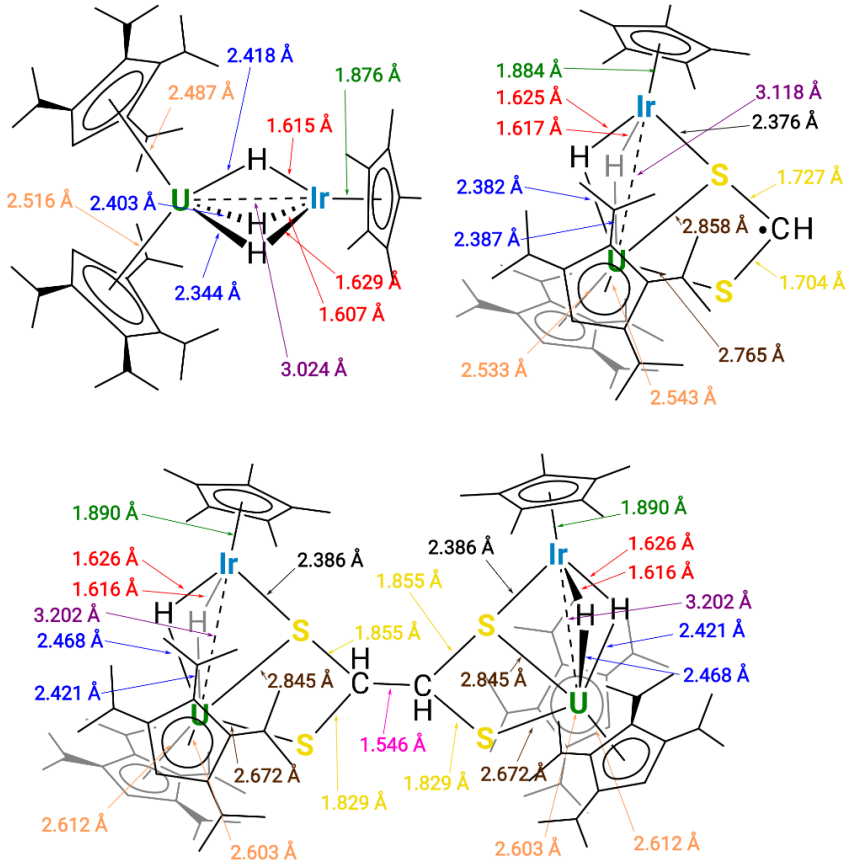


Figure S10. Calculated bond distances for **1** (top left), the thioformate intermediate (top right), and **2** (bottom).

Table S4 Computed coordinates for various spin states of **1**.

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122

Complex 1 - doublet

C       2.65404     -0.68846     -1.34896

C       3.19026      0.64556     -1.22805

C       3.46363      0.89289      0.15783

C       3.01516     -0.23671      0.88354

C       2.52864     -1.21713     -0.01893

C       3.42972      1.71770     -2.28451

C       2.11156      2.23698     -2.88295

C       4.37301      1.97658      0.71357

C       4.38128      2.04151      2.24170

C       2.08233     -2.60807      0.39600

C       3.24328     -3.61739      0.38116

C       2.55073     -1.60151     -2.56710

C       1.83117     -1.09672     -3.82270

C       1.42439     -2.62250      1.78087

C       4.45053      1.39300     -3.38415

C       5.81620      1.75401      0.22354

C       3.94394     -2.13277     -2.96013

U       0.64509      0.80135     -0.07891

C       0.10956      3.49584      0.59703

C       0.62915      2.86187      1.75581

C      -0.33233      1.95323      2.28156

C      -1.47253      1.99633      1.41222

C      -1.18682      2.93509      0.35910

C       0.64813      4.80539      0.04291

C       2.16776      4.86087     -0.11956

C      -2.16834      3.33322     -0.73826

C      -2.77471      4.73489     -0.53690

C      -2.83457      1.33107      1.57801

C      -3.90123      2.33706      2.05022

C      -0.22320      1.32541      3.66492

C      -0.96740      2.18827      4.69952

Ir     -1.45138     -1.10265     -1.22509

C      -3.43815     -1.35925     -2.25259
```

C	-3.47152	-2.11814	-1.03792
C	-2.43330	-3.12755	-1.12825
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C	-2.40139	-1.88661	-3.10179
C	-4.51706	-2.03770	0.02918
C	-2.18958	-4.20792	-0.12028
C	-0.76481	-3.92513	-2.96789
C	-2.15429	-1.50227	-4.52799
C	-4.39789	-0.27377	-2.63120
C	0.21353	5.96389	0.96220
C	-1.62199	3.22529	-2.17116
C	1.21611	1.11918	4.14159
C	-2.89704	0.09534	2.48119
H	1.32181	-2.94675	-0.31984
H	-0.69388	0.33807	3.65243
H	1.56032	3.12837	2.23903
H	-2.99680	2.61772	-0.68095
H	3.13127	-0.37553	1.95107
H	0.20336	4.98076	-0.94320
H	3.67910	-3.72703	-0.61443
H	2.90026	-4.60709	0.70563
H	4.04057	-3.29809	1.06179
H	2.12871	-2.32769	2.56656
H	1.07030	-3.63012	2.02444
H	0.55720	-1.95420	1.82414
H	-1.16477	-4.58237	-0.17484
H	-2.86545	-5.05700	-0.28739
H	-2.35493	-3.84755	0.89802
H	-3.65785	2.73824	3.03984
H	-4.88030	1.84818	2.12322
H	-4.00322	3.18392	1.36904
H	-3.10877	4.89493	0.49206
H	-3.63740	4.87400	-1.19899
H	-2.05277	5.52166	-0.77608
H	-3.12808	0.97996	0.57941
H	0.82231	-0.74299	-3.59321

H	1.74555	-1.91783	-4.54475
H	2.37723	-0.29698	-4.32871
H	2.67210	4.73234	0.84395
H	2.47491	5.83352	-0.51967
H	2.53783	4.08927	-0.79825
H	4.05181	2.95843	0.34756
H	3.38108	2.18724	2.65230
H	5.01345	2.86839	2.58223
H	4.78859	1.12048	2.67399
H	6.18678	0.77981	0.56127
H	6.48334	2.52759	0.62189
H	5.89017	1.77656	-0.86654
H	1.96837	-2.46541	-2.22437
H	-0.51645	3.18541	4.75472
H	-0.91410	1.73566	5.69686
H	-2.02165	2.31760	4.44290
H	-2.15590	-0.65556	2.19374
H	-3.88642	-0.36384	2.39010
H	-2.76444	0.34512	3.53724
H	-0.79216	3.91581	-2.35186
H	-2.40824	3.47446	-2.89403
H	-1.28612	2.20741	-2.39609
H	1.55632	1.45382	-3.40422
H	2.28609	3.05221	-3.59536
H	1.45581	2.66579	-2.10729
H	4.55311	-1.34996	-3.41986
H	3.85266	-2.95084	-3.68489
H	4.49508	-2.50424	-2.09284
H	5.37603	0.99435	-2.95838
H	4.70100	2.30186	-3.94355
H	4.07647	0.66248	-4.10472
H	1.79269	0.50679	3.44381
H	1.22114	0.61612	5.11457
H	1.73923	2.07299	4.26867
H	-0.09525	-3.40793	-3.65882
H	-1.24891	-4.73948	-3.52308

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H      -0.15220     -4.37792     -2.18449
H      -0.86546      5.96686      1.13132
H       0.49803      6.93201      0.53259
H       0.70048      5.87222      1.93927
H      -4.79303      0.23653     -1.74979
H      -5.24898     -0.68969     -3.18568
H      -3.92214      0.47771     -3.26560
H       3.86039      2.56398     -1.73571
H      -2.38705     -0.44882     -4.70349
H      -2.77724     -2.09732     -5.20983
H      -1.11143     -1.65979     -4.81357
H      -4.12535     -2.35295      0.99891
H      -5.36916     -2.68846     -0.21073
H      -4.90121     -1.02107      0.14312
H      -1.52368      0.51163     -1.13800
H      -0.91744     -1.01205      0.31567
H       0.10052     -0.93154     -1.62764
122
Complex 1 - quartet
C       2.58576     -0.65157     -1.34960
C       3.18343      0.64775     -1.22851
C       3.43071      0.89701      0.15259
C       2.93551     -0.20752      0.87947
C       2.41836     -1.16342     -0.02520
C       3.44777      1.71008     -2.27503
C       2.13013      2.27279     -2.81604
C       4.33727      1.97658      0.69598
C       4.31173      2.07179      2.21587
C       1.85411     -2.50821      0.36861
C       2.91135     -3.61456      0.30501
C       2.42286     -1.54975     -2.56009
C       1.72071     -0.99611     -3.79836
C       1.21543     -2.47788      1.75527
C       4.42398      1.34238     -3.39108
C       5.77610      1.72109      0.22680
C       3.78269     -2.14197     -2.95803
```

U	0.64350	0.91995	-0.19425
C	0.11002	3.52382	0.62527
C	0.64491	2.88776	1.76870
C	-0.28333	1.93946	2.26363
C	-1.42137	1.97027	1.40073
C	-1.16591	2.93854	0.37832
C	0.65088	4.81518	0.05593
C	2.17127	4.84690	-0.06469
C	-2.12021	3.29128	-0.74429
C	-2.74644	4.68167	-0.58594
C	-2.75444	1.26165	1.53692
C	-3.84384	2.23329	2.00871
C	-0.15310	1.25399	3.60692
C	-0.96435	2.01812	4.66081
Ir	-1.41234	-1.04405	-1.22396
C	-3.37402	-1.38623	-2.23581
C	-3.38744	-2.11245	-1.00428
C	-2.31873	-3.08650	-1.06433
C	-1.67993	-2.96876	-2.33348
C	-2.32454	-1.90371	-3.06875
C	-4.42608	-2.02533	0.06060
C	-2.01848	-4.10516	-0.01669
C	-0.60487	-3.85711	-2.86194
C	-2.07422	-1.53998	-4.49351
C	-4.34507	-0.32345	-2.62776
C	0.19411	5.98313	0.94188
C	-1.50629	3.16030	-2.14202
C	1.28775	1.12686	4.08809
C	-2.77883	0.01401	2.41509
H	1.05647	-2.75105	-0.34267
H	-0.55718	0.24192	3.53460
H	1.57548	3.15631	2.24546
H	-2.93248	2.55921	-0.70009
H	3.01908	-0.34076	1.94767
H	0.22962	4.96953	-0.94147
H	3.30979	-3.73499	-0.70395

H	2.48662	-4.57643	0.61306
H	3.75081	-3.38841	0.97065
H	1.94808	-2.24129	2.53274
H	0.78169	-3.45203	1.99950
H	0.40890	-1.74067	1.80624
H	-0.97841	-4.43127	-0.06723
H	-2.65365	-4.99090	-0.13931
H	-2.19148	-3.70541	0.98403
H	-3.61333	2.63524	2.99971
H	-4.81212	1.72402	2.07130
H	-3.95563	3.07976	1.32992
H	-3.11540	4.84692	0.42877
H	-3.58691	4.80549	-1.27739
H	-2.02277	5.47041	-0.80725
H	-3.02525	0.92185	0.53096
H	0.72758	-0.61230	-3.55711
H	1.59928	-1.79626	-4.53617
H	2.29275	-0.20750	-4.28803
H	2.64478	4.69656	0.90958
H	2.50962	5.81474	-0.44762
H	2.54573	4.07570	-0.73965
H	4.02970	2.94916	0.30065
H	3.30491	2.24230	2.59250
H	4.94722	2.89367	2.55879
H	4.68763	1.15200	2.67511
H	6.12474	0.74806	0.58729
H	6.45543	2.49051	0.60987
H	5.85392	1.71504	-0.86236
H	1.79964	-2.37913	-2.21205
H	-0.56283	3.02952	4.78190
H	-0.91940	1.51429	5.63263
H	-2.01341	2.11543	4.37748
H	-2.02603	-0.71162	2.10194
H	-3.75638	-0.46520	2.32826
H	-2.63491	0.24615	3.47148
H	-0.68945	3.86751	-2.30486

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H      -2.26037      3.35393     -2.91237
H      -1.13739      2.14498     -2.31942
H       1.51514      1.50827     -3.29477
H       2.28868      3.07400     -3.54527
H       1.54751      2.74122     -2.00774
H       4.41692     -1.39022     -3.43263
H       3.65441     -2.96745     -3.66716
H       4.32345     -2.51730     -2.08722
H       5.33505      0.90258     -2.97815
H       4.70690      2.23723     -3.95565
H       4.00519      0.62921     -4.10156
H       1.90692      0.59161      3.36849
H       1.32351      0.58100      5.03563
H       1.73862      2.10826      4.26142
H       0.02326     -3.33530     -3.58493
H      -1.03982     -4.72764     -3.36769
H       0.03956     -4.22606     -2.06243
H      -0.88627      5.97347      1.09388
H       0.47319      6.94660      0.50091
H       0.66482      5.91160      1.92737
H      -4.75462      0.18003     -1.75062
H      -5.18281     -0.75384     -3.18901
H      -3.87359      0.43350     -3.25695
H       3.92090      2.53470     -1.73294
H      -2.29073     -0.48589     -4.67931
H      -2.70367     -2.13451     -5.16778
H      -1.03456     -1.71640     -4.77331
H      -4.03061     -2.34201      1.02633
H      -5.27919     -2.67404     -0.17584
H      -4.80532     -1.00810      0.17139
H      -1.53780      0.56515     -1.17607
H      -0.87676     -0.87344      0.30463
H       0.13171     -0.85980     -1.63115
122
Complex 1 - sextet
C       2.72829     -0.68069     -1.47388
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C	2.58358	-1.29465	-0.11847
C	3.60714	1.70980	-2.30716
C	2.45452	2.37589	-3.07626
C	4.37695	1.83315	0.73589
C	4.26631	1.92606	2.25845
C	2.15945	-2.70857	0.20455
C	3.28386	-3.73113	-0.05390
C	2.57845	-1.54855	-2.70805
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C	1.67617	-2.85576	1.65156
C	4.72409	1.30711	-3.28558
C	5.84175	1.53632	0.34619
C	3.94299	-2.11560	-3.16025
U	0.42442	0.86294	0.17200
C	-0.01724	3.59858	0.65356
C	0.47307	3.00478	1.84625
C	-0.50218	2.11969	2.39298
C	-1.62567	2.14592	1.49716
C	-1.31231	3.04546	0.41514
C	0.59112	4.83811	0.02464
C	2.11326	4.77927	-0.12454
C	-2.27301	3.40824	-0.71098
C	-2.83983	4.83387	-0.58209
C	-2.99973	1.50528	1.66363
C	-4.04128	2.52355	2.16247
C	-0.40822	1.53246	3.79253
C	-1.08719	2.45411	4.82034
Ir	-1.44491	-1.17180	-1.13573
C	-3.42315	-1.47669	-2.16853
C	-3.42219	-2.25314	-0.95467
C	-2.35786	-3.22373	-1.06728
C	-1.72453	-3.05440	-2.34096
C	-2.38507	-1.96137	-3.02908

C	-4.45217	-2.20385	0.12845
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C	-0.67681	-3.94684	-2.92928
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C	-1.72221	3.20410	-2.13142
C	1.02889	1.24820	4.23558
C	-3.06841	0.24924	2.53820
H	1.31345	-2.95120	-0.45125
H	-0.92751	0.57113	3.80387
H	1.40251	3.27789	2.33241
H	-3.12438	2.72360	-0.61904
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H	0.16607	4.97027	-0.97658
H	3.56350	-3.79644	-1.10638
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H	1.26964	-3.86048	1.80589
H	0.89425	-2.12704	1.88831
H	-1.03046	-4.64048	-0.13573
H	-2.71077	-5.17974	-0.25446
H	-2.24749	-3.96712	0.94828
H	-3.78387	2.89545	3.15983
H	-5.03309	2.05893	2.22688
H	-4.11956	3.38813	1.49921
H	-3.19171	5.04393	0.43232
H	-3.68250	4.97430	-1.26951
H	-2.08665	5.58687	-0.83377
H	-3.31729	1.18469	0.66277
H	0.89417	-0.50882	-3.62271
H	1.66129	-1.73885	-4.64858
H	2.45104	-0.18779	-4.42040
H	2.60090	4.68408	0.85234
H	2.49374	5.69578	-0.58988

H	2.42140	3.93385	-0.74492
H	4.12045	2.81476	0.31795
H	3.23608	2.08485	2.58078
H	4.87291	2.75915	2.62726
H	4.63480	1.01451	2.74142
H	6.14651	0.55550	0.72615
H	6.50342	2.29093	0.78475
H	5.99214	1.54233	-0.73542
H	1.96998	-2.40070	-2.38493
H	-0.59409	3.43257	4.84233
H	-1.03689	2.02558	5.82874
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H	-2.30728	-0.48308	2.25272
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H	-2.95732	0.48209	3.60128
H	-0.88405	3.87382	-2.34781
H	-2.50515	3.41543	-2.87087
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H	1.99055	1.69638	-3.79259
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H	3.78827	-2.94605	-3.85828
H	4.54180	-2.48285	-2.32347
H	5.53365	0.76164	-2.79133
H	5.15283	2.20394	-3.74607
H	4.34603	0.68157	-4.09821
H	1.52765	0.57202	3.53161
H	1.03622	0.77266	5.22284
H	1.62079	2.16710	4.31530
H	-0.03608	-3.40464	-3.62906
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H      -0.77369     -1.20318      0.35668
H       0.02275     -0.72714     -1.65509
125
1 + CS2 - adduct
C       2.61085     -0.58106     -1.42659
C       3.17263      0.73771     -1.34112
C       3.48038      0.99594      0.02820
C       3.05014     -0.11803      0.78110
C       2.51886     -1.09202     -0.09492
C       3.42786      1.77901     -2.41346
C       2.13618      2.34401     -3.01826
C       4.38794      2.08923      0.54038
C       4.37329      2.21237      2.05920
C       2.00271     -2.44628      0.33258
C       3.08677     -3.52546      0.25688
C       2.40156     -1.49212     -2.61986
C       1.65536     -0.94767     -3.83499
C       1.40158     -2.41304      1.73603
C       4.41904      1.36944     -3.50363
C       5.82327      1.82959      0.06338
C       3.73970     -2.09937     -3.06707
S      -0.41434     -2.21299      4.90844
C      -1.79156     -2.77586      4.46009
S      -3.16894     -3.35336      4.02282
U       0.67964      0.92586     -0.15873
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C	0.09301	3.53408	0.62815
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C	-1.39286	1.96020	1.44437
C	-1.17335	2.92155	0.40776
C	0.61142	4.81333	0.01502
C	2.12584	4.83264	-0.16153
C	-2.15079	3.24198	-0.70472
C	-2.78681	4.62920	-0.56044
C	-2.71362	1.23954	1.61720
C	-3.79670	2.20926	2.10708
C	-0.06205	1.25997	3.61416
C	-0.82384	2.00934	4.71313
Ir	-1.36604	-1.07752	-1.12563
C	-3.34571	-1.45064	-2.09172
C	-3.32042	-2.17322	-0.85909
C	-2.23726	-3.12983	-0.93894
C	-1.63204	-3.00918	-2.22454
C	-2.30875	-1.95631	-2.94776
C	-4.33308	-2.09772	0.23071
C	-1.89578	-4.13418	0.10982
C	-0.55886	-3.88600	-2.77553
C	-2.09900	-1.59082	-4.37867
C	-4.33987	-0.40292	-2.46622
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C	-2.70906	0.00159	2.50782
H	1.19199	-2.72143	-0.35144
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H	0.58181	-1.69199	1.80216
H	-0.86026	-4.46604	0.01938
H	-2.53965	-5.01861	0.03119
H	-2.02158	-3.71712	1.11013
H	-3.54257	2.61817	3.08958
H	-4.76112	1.69671	2.19667
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H	1.47735	-1.76036	-4.54718
H	2.22722	-0.18791	-4.36913
H	2.63321	4.72412	0.80107
H	2.45572	5.77838	-0.60257
H	2.46869	4.02619	-0.81165
H	4.07400	3.05209	0.12810
H	3.36383	2.35448	2.44205
H	4.98392	3.06092	2.38180
H	4.78416	1.31455	2.53180
H	6.17665	0.86218	0.43424
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H	5.89111	1.80963	-1.02627
H	1.78855	-2.31417	-2.23847
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H       3.57330     -2.94932     -3.73836
H       4.32608     -2.44536     -2.21407
H       5.31020      0.91011     -3.06948
H       4.73534      2.24673     -4.07799
H       3.98934      0.65751     -4.20972
H       1.96820      0.55645      3.27391
H       1.46855      0.55378      4.97024
H       1.87816      2.07235      4.17976
H       0.04870     -3.35877     -3.51212
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125
1 + CS2 - TS
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C	10.89432	7.24447	7.51762
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C	9.01169	4.48653	2.11906
C	8.29740	5.35488	1.08289
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C	11.41827	7.16727	1.96759
C	12.53625	7.20739	5.63281
C	10.22237	3.79354	1.46510
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C	6.26391	3.97696	7.31877
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C	4.87681	8.68677	3.91888
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C	2.80821	8.41755	6.59291
C	6.19217	7.74640	8.86487
C	5.27851	8.82704	9.47308
Ir	5.31373	4.39737	4.13731
C	3.20997	4.25173	3.32470
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H	9.68689	9.65884	4.47349
H	10.74885	8.38658	5.72921
H	9.85164	7.34688	7.82759
H	11.47362	8.02331	8.02500
H	11.26176	6.27910	7.88257
H	12.88478	6.20136	5.89127
H	13.15131	7.93039	6.18124
H	12.71520	7.35669	4.56497
H	8.29818	3.68986	2.36008
H	5.69074	9.82481	9.28546
H	5.19771	8.69346	10.55810
H	4.26943	8.80311	9.05806
H	4.29463	5.46493	7.63938
H	2.58509	5.86783	7.52838
H	3.61710	6.77177	8.62445
H	6.38046	8.95898	2.34813
H	4.81345	8.40753	1.76845
H	5.88548	7.26984	2.59226
H	8.80873	7.85374	1.36669
H	9.66899	9.31839	1.83250
H	8.41720	8.64944	2.88764
H	10.99870	4.51036	1.18602
H	9.90965	3.27064	0.55325
H	10.67842	3.05723	2.13044
H	12.18789	6.56018	2.45320
H	11.89979	8.06136	1.55488
H	11.02388	6.59485	1.12405
H	8.24729	7.06517	9.23586
H	7.38467	7.62721	10.66437
H	7.99920	8.80035	9.50003
H	6.42963	2.71732	1.17410
H	5.35039	1.31733	1.14821
H	6.58132	1.46618	2.41084
H	5.86562	11.46712	5.44852

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H       7.26216     12.44198      4.95689
H       7.26536     11.59433      6.51302
H       1.85442      5.63059      4.27242
H       1.30001      5.00605      2.71359
H       2.57146      6.23311      2.77703
H      10.77880      8.27125      3.64660
H       3.98638      5.70949      1.03782
H       3.58471      4.18700      0.23400
H       5.27367      4.60847      0.54826
H       3.06581      2.82163      6.42024
H       1.74454      2.27964      5.37117
H       1.91316      3.99493      5.76869
H       5.28214      5.99764      4.34617
H       5.85434      4.29191      5.84324
H       6.87512      4.50831      3.75450
125
1+ CS2 - product
C       2.53198     -0.62330     -1.44148
C       3.07043      0.65825     -1.10402
C       3.43585      0.61806      0.28238
C       3.13766     -0.67033      0.77486
C       2.60325     -1.44628     -0.27189
C       3.50419      1.80458     -1.99442
C       2.39913      2.62691     -2.65445
C       4.24381      1.64325      1.03948
C       4.02240      1.57108      2.54655
C       2.51109     -2.95532     -0.25707
C       3.94335     -3.51280     -0.23298
C       2.06498     -1.23008     -2.74988
C       1.35722     -0.32240     -3.74441
C       1.71370     -3.57381      0.88285
C       4.54986      1.36686     -3.02352
C       5.73182      1.46679      0.71459
C       3.18769     -1.99923     -3.45653
S       0.52007     -0.98677      2.74563
C      -0.73568     -2.12170      2.52328
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S	-1.28083	-3.24313	3.59899
U	0.72469	0.52146	0.39873
C	0.25651	3.33019	0.41902
C	0.58710	2.92712	1.73555
C	-0.47245	2.17710	2.29352
C	-1.45252	2.01564	1.26737
C	-0.99055	2.72313	0.09993
C	0.85981	4.56977	-0.20500
C	2.36775	4.69827	-0.02225
C	-1.83895	2.94000	-1.13893
C	-2.50891	4.32265	-1.14911
C	-2.82674	1.37622	1.35866
C	-3.95275	2.41963	1.35776
C	-0.60185	1.92935	3.78050
C	-1.52232	2.99981	4.38062
Ir	-1.33823	-1.14600	-0.85637
C	-3.45525	-1.29251	-1.57284
C	-3.25467	-2.29349	-0.55701
C	-2.22853	-3.18700	-0.99147
C	-1.78587	-2.74945	-2.29252
C	-2.54967	-1.57945	-2.64778
C	-4.04534	-2.45574	0.69219
C	-1.79776	-4.42395	-0.28054
C	-0.82696	-3.47417	-3.16927
C	-2.48332	-0.85250	-3.94536
C	-4.51514	-0.24344	-1.58068
C	0.19783	5.79914	0.44083
C	-1.14102	2.74230	-2.48379
C	0.73248	1.94782	4.51853
C	-3.04984	0.43482	2.53655
H	2.04077	-3.27058	-1.19319
H	-1.04579	0.94850	3.95113
H	1.45540	3.26707	2.28155
H	-2.62741	2.18330	-1.09079
H	3.33780	-1.02924	1.77372
H	0.63605	4.59068	-1.27478

H	4.58541	-3.03285	-0.97501
H	3.94274	-4.59140	-0.42119
H	4.39669	-3.34513	0.74894
H	2.07281	-3.24196	1.85960
H	1.79844	-4.66465	0.84771
H	0.65923	-3.31467	0.81733
H	-0.76994	-4.69078	-0.52903
H	-2.43858	-5.26859	-0.56096
H	-1.85913	-4.30878	0.80375
H	-3.81023	3.15415	2.15591
H	-4.91637	1.92906	1.53079
H	-4.02690	2.96161	0.41645
H	-2.90090	4.60457	-0.17097
H	-3.33645	4.33803	-1.86622
H	-1.79894	5.09372	-1.45864
H	-2.93520	0.76918	0.45047
H	0.56194	0.25231	-3.26798
H	0.89855	-0.93639	-4.52586
H	2.04332	0.35978	-4.24718
H	2.63211	4.73757	1.03835
H	2.72953	5.62344	-0.48063
H	2.90842	3.87087	-0.47418
H	3.94659	2.64269	0.71415
H	2.96825	1.68282	2.80578
H	4.57390	2.36788	3.05406
H	4.36748	0.61916	2.96008
H	6.07536	0.47756	1.03243
H	6.33514	2.22011	1.23160
H	5.92414	1.55538	-0.35723
H	1.31248	-1.96422	-2.44990
H	-1.08137	3.99460	4.25829
H	-1.67400	2.82364	5.45053
H	-2.50151	3.01431	3.89887
H	-2.27239	-0.32042	2.62196
H	-4.00288	-0.08336	2.41152
H	-3.11009	0.97241	3.48406

H	-0.36682	3.49120	-2.65987
H	-1.86978	2.84026	-3.29516
H	-0.69048	1.75311	-2.56623
H	1.95952	2.12590	-3.51355
H	2.79610	3.58605	-3.00195
H	1.59665	2.83854	-1.95017
H	3.99616	-1.33467	-3.76892
H	2.79884	-2.49694	-4.35146
H	3.62173	-2.76520	-2.81383
H	5.34227	0.77456	-2.55942
H	5.00990	2.24230	-3.49349
H	4.10409	0.76569	-3.81819
H	1.40548	1.16914	4.15712
H	0.56824	1.75883	5.58300
H	1.23367	2.91695	4.43258
H	-0.36157	-2.80580	-3.89445
H	-1.34584	-4.26335	-3.72725
H	-0.03607	-3.94857	-2.58582
H	-0.88991	5.74372	0.41548
H	0.50819	6.71768	-0.06870
H	0.49863	5.87640	1.49008
H	-4.79237	0.05698	-0.56928
H	-5.42143	-0.61228	-2.07582
H	-4.18815	0.65134	-2.11383
H	4.02465	2.48929	-1.31928
H	-2.76819	0.19390	-3.82654
H	-3.16851	-1.30573	-4.67158
H	-1.47912	-0.87985	-4.36921
H	-3.42025	-2.73754	1.54295
H	-4.78787	-3.25137	0.55603
H	-4.58380	-1.54414	0.94758
H	-0.85915	0.37622	-1.22550
H	-1.19416	-2.06809	1.52779
H	0.16819	-1.55038	-0.36601

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Radical intermediate - doublet

C	6.62521	6.69792	15.98269
C	7.32425	7.60170	15.13893
C	8.66143	7.73510	15.57412
C	8.83824	6.83854	16.67841
C	7.57767	6.18420	16.92310
C	9.60044	8.85029	15.15032
C	9.40491	10.07835	16.05751
C	10.06691	6.93499	17.58016
C	9.72883	7.64216	18.90752
C	7.27779	5.30650	18.13262
C	6.55944	6.06598	19.26605
C	5.11916	6.79486	16.20179
C	4.83920	8.08406	17.00548
C	9.44528	9.27080	13.68895
C	10.86440	5.66577	17.88338
C	6.50142	4.02016	17.82922
C	4.23855	6.83123	14.95197
U	8.44879	5.20334	14.31802
S	11.03887	6.11705	14.21198
C	11.59749	4.54328	13.79668
S	10.40436	3.29182	13.61304
Ir	9.50516	2.53798	15.68950
C	10.50365	1.61271	17.49583
C	11.24591	1.25477	16.32987
C	10.38051	0.45006	15.48314
C	9.10917	0.35157	16.11784
C	9.16578	1.08630	17.36661
C	12.69982	1.50927	16.08336
C	10.82232	-0.22864	14.22547
C	7.94370	-0.47191	15.66640
C	8.14194	1.01382	18.45419
C	11.06311	2.26764	18.71742
C	6.41586	5.58788	12.50135
C	7.50757	6.10730	11.75213
C	8.34794	4.99731	11.41767
C	7.68271	3.79520	11.87965

C	6.48397	4.16939	12.54688
C	7.48552	7.49045	11.10499
C	7.25129	7.35016	9.58864
C	9.65330	4.98301	10.61885
C	9.52245	4.46984	9.16966
C	8.03570	2.40828	11.36084
C	7.95756	1.22385	12.33146
C	5.32450	3.25921	12.92884
C	4.02953	3.70542	12.23142
C	6.38311	8.41475	11.63071
C	5.09753	3.07086	14.43308
C	7.17086	2.09119	10.12194
C	10.44069	6.30030	10.60391
H	8.03849	2.92504	15.08655
H	9.48841	4.07054	16.21641
H	12.65838	4.30593	13.77291
H	6.85574	8.22326	14.39113
H	10.63434	8.50702	15.27597
H	8.38242	10.46323	15.97273
H	10.09294	10.88074	15.76754
H	9.58770	9.84456	17.10897
H	9.61200	8.42793	13.01427
H	10.17783	10.04581	13.44018
H	8.45148	9.68575	13.48974
H	10.75840	7.59232	17.04256
H	10.64893	7.97568	19.40099
H	9.21711	6.96604	19.59910
H	9.08742	8.51594	18.76008
H	10.27435	4.93745	18.44410
H	11.73483	5.92692	18.49814
H	11.21683	5.18587	16.96922
H	8.25045	4.99406	18.52651
H	6.60294	5.47995	20.19169
H	5.50153	6.22146	19.03466
H	7.00708	7.04244	19.46607
H	5.51934	4.22386	17.39385

H	6.32837	3.46449	18.75781
H	7.06029	3.37919	17.14307
H	4.79306	5.94597	16.81128
H	3.79207	8.11858	17.32900
H	5.02623	8.96419	16.38041
H	5.47469	8.16745	17.88889
H	3.19739	7.01485	15.23893
H	4.26457	5.89427	14.39588
H	4.53363	7.64191	14.27693
H	5.57384	6.17570	12.83137
H	8.44502	7.99763	11.24809
H	8.04532	6.79428	9.09134
H	7.19281	8.33972	9.12058
H	6.30622	6.82965	9.39746
H	5.38966	8.00315	11.42098
H	6.44671	9.38498	11.12748
H	6.45112	8.59868	12.70203
H	5.55923	2.27012	12.52871
H	3.67699	4.67358	12.60190
H	3.22970	2.97659	12.40581
H	4.17635	3.79986	11.15107
H	5.97157	2.61966	14.91125
H	4.23773	2.41442	14.61277
H	4.89352	4.01989	14.93763
H	9.08063	2.45791	11.03599
H	8.45544	1.43737	13.27844
H	8.43944	0.35277	11.87217
H	6.92675	0.93401	12.55601
H	6.12797	1.91837	10.40815
H	7.53064	1.18172	9.62619
H	7.17770	2.90434	9.39255
H	10.29927	4.26055	11.13492
H	9.20795	3.42692	9.11893
H	10.49660	4.54036	8.67258
H	8.81123	5.05737	8.58179
H	9.98813	7.05160	9.95044

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H      11.44836      6.10977     10.21918
H      10.55012      6.71994     11.60605
H       6.99558      0.00262     15.93072
H       7.96680     -1.45935     16.14510
H       7.94804     -0.62485     14.58568
H       8.21739      1.86169     19.13813
H       8.27698      0.09758     19.04513
H       7.12547      1.00183     18.05412
H      10.29417      2.80264     19.27847
H      11.85617      2.97687     18.47331
H      11.48853      1.50490     19.38258
H      12.90837      1.60202     15.01487
H      13.31221      0.68517     16.47267
H      13.03211      2.43087     16.56686
H       9.98014     -0.66794     13.68780
H      11.52824     -1.03564     14.45789
H      11.32085      0.47089     13.54734
125
Radical intermediate - quartet
C       6.61824      6.65513     15.96146
C       7.30125      7.58215     15.13559
C       8.63682      7.69713     15.55769
C       8.82213      6.78848     16.64213
C       7.57148      6.13585     16.88755
C       9.58583      8.78381     15.12046
C       9.40566     10.01816     16.01091
C      10.05345      6.86325     17.52387
C       9.71659      7.54624     18.85718
C       7.28162      5.24075     18.07416
C       6.57279      5.99200     19.21082
C       5.12069      6.73083     16.17893
C       4.84215      8.00090     17.00256
C       9.42010      9.15950     13.65438
C      10.83048      5.58229     17.79651
C       6.49405      3.97347     17.74854
C       4.26149      6.78743     14.92168
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U	8.39373	5.20922	14.32012
S	11.01791	6.07650	14.25140
C	11.55633	4.53736	13.75675
S	10.37822	3.28567	13.59400
Ir	9.45236	2.60845	15.67578
C	10.47420	1.68969	17.45927
C	11.19585	1.34162	16.28400
C	10.32527	0.53212	15.45173
C	9.06627	0.43452	16.09856
C	9.13667	1.16962	17.34278
C	12.62889	1.63794	16.00198
C	10.75014	-0.13645	14.19066
C	7.88796	-0.36184	15.65164
C	8.12914	1.09510	18.43623
C	11.05140	2.32701	18.67337
C	6.40690	5.59886	12.48842
C	7.51695	6.10930	11.77081
C	8.36354	5.00475	11.47067
C	7.69623	3.81014	11.92990
C	6.48460	4.18650	12.55461
C	7.52844	7.48878	11.14067
C	7.33964	7.35526	9.62341
C	9.67673	4.98680	10.70743
C	9.56073	4.47142	9.26433
C	8.06289	2.42637	11.44170
C	7.97294	1.26779	12.43359
C	5.35323	3.28269	12.99087
C	4.03480	3.71696	12.34586
C	6.41944	8.40386	11.65277
C	5.22010	3.14386	14.50703
C	7.20982	2.10111	10.20488
C	10.45448	6.30308	10.71903
H	7.99188	2.98276	15.06768
H	9.42996	4.14198	16.18712
H	12.59794	4.34104	13.51959
H	6.83115	8.20701	14.39644

H	10.61239	8.42793	15.25014
H	8.38630	10.40862	15.92739
H	10.09966	10.81210	15.71566
H	9.58829	9.78554	17.06188
H	9.55250	8.28484	13.01638
H	10.16632	9.90301	13.35996
H	8.43277	9.58559	13.45606
H	10.74303	7.52503	16.99300
H	10.63359	7.87909	19.35420
H	9.20913	6.85617	19.53580
H	9.06996	8.41583	18.71801
H	10.21950	4.84304	18.31409
H	11.69100	5.80977	18.43569
H	11.19247	5.13184	16.87381
H	8.25393	4.91698	18.45395
H	6.62870	5.40915	20.13655
H	5.51375	6.14056	18.98617
H	7.01635	6.97004	19.40227
H	5.52076	4.19599	17.30765
H	6.30677	3.40664	18.66483
H	7.05111	3.33943	17.05911
H	4.80051	5.86945	16.76949
H	3.80328	8.02162	17.34919
H	5.00968	8.88879	16.38484
H	5.49724	8.07832	17.87034
H	3.21684	6.97079	15.19118
H	4.29504	5.85899	14.35633
H	4.57358	7.60375	14.26356
H	5.56567	6.18953	12.80559
H	8.48580	7.98323	11.31649
H	8.14857	6.80077	9.15266
H	7.29602	8.34470	9.15582
H	6.40326	6.83265	9.40346
H	5.43299	8.00117	11.40370
H	6.50080	9.38632	11.17954
H	6.45843	8.55572	12.72839

H	5.57239	2.28817	12.60164
H	3.70207	4.69313	12.70846
H	3.24128	2.99571	12.56769
H	4.13832	3.78850	11.25986
H	6.10830	2.67034	14.92851
H	4.35097	2.53406	14.77583
H	5.10137	4.11522	14.99229
H	9.10957	2.47625	11.13033
H	8.45607	1.50429	13.37944
H	8.46313	0.38809	12.00539
H	6.94092	0.98467	12.65110
H	6.16734	1.93034	10.48982
H	7.57275	1.19207	9.71309
H	7.21857	2.91333	9.47632
H	10.30930	4.26376	11.23366
H	9.26764	3.42281	9.22390
H	10.53244	4.55757	8.76701
H	8.83608	5.03910	8.67629
H	10.02952	7.04688	10.04152
H	11.48191	6.11890	10.39134
H	10.50725	6.72652	11.72201
H	6.95309	0.15388	15.87823
H	7.86804	-1.33074	16.16390
H	7.91179	-0.55067	14.57866
H	8.20401	1.94650	19.11309
H	8.28255	0.18432	19.02876
H	7.11147	1.06730	18.04433
H	10.29670	2.86531	19.24756
H	11.85254	3.02272	18.42464
H	11.47161	1.55081	19.32398
H	12.81825	1.66571	14.92793
H	13.28039	0.87091	16.43782
H	12.92125	2.60500	16.41456
H	9.91524	-0.63911	13.70309
H	11.51595	-0.88939	14.40614
H	11.17250	0.57954	13.48094

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Radical intermediate - sextet

C	6.66212	7.98244	18.30706
C	7.16294	8.74245	17.21863
C	8.44119	9.16114	17.52899
C	8.77848	8.63758	18.88194
C	7.69431	7.92056	19.34273
C	9.33262	10.03182	16.68928
C	9.30513	11.48779	17.19501
C	10.12044	8.88162	19.53661
C	10.02612	9.67106	20.85326
C	7.58779	7.18815	20.66266
C	6.50625	7.76654	21.59032
C	5.28075	7.38574	18.33305
C	4.20670	8.48735	18.31104
C	8.98701	9.97715	15.19926
C	10.94674	7.59473	19.70549
C	7.43899	5.66629	20.49698
C	5.07430	6.40259	17.16905
U	8.83861	3.91503	12.44543
S	11.07870	5.47547	12.38199
C	11.43878	4.09616	13.35924
S	11.08965	2.43056	12.87854
Ir	9.47615	1.72261	14.57118
C	9.82846	1.30847	16.73627
C	10.93453	0.76947	16.01811
C	10.42565	-0.24380	15.10237
C	9.01140	-0.33313	15.28411
C	8.61510	0.65420	16.26975
C	12.38134	1.09883	16.20911
C	11.27616	-1.11456	14.23153
C	8.09803	-1.32236	14.63101
C	7.25537	0.79344	16.88046
C	9.89253	2.31072	17.84626
C	6.72833	4.77052	11.06904
C	7.82333	5.14338	10.24025

C	8.37964	3.93255	9.71489
C	7.59792	2.82726	10.22164
C	6.56989	3.35936	11.05962
C	8.17958	6.58804	9.93288
C	7.47140	7.06855	8.65519
C	9.46620	3.73842	8.66242
C	8.84866	3.56987	7.26146
C	7.73149	1.39277	9.72584
C	8.05347	0.33899	10.79379
C	5.41098	2.64498	11.73004
C	4.09235	2.93292	10.99324
C	7.85203	7.53909	11.09057
C	5.27067	3.01370	13.21439
C	6.50306	0.96090	8.90571
C	10.58122	4.78812	8.60070
H	8.33811	1.70954	13.41849
H	9.01620	3.27231	14.80535
H	11.77520	4.23471	14.38425
H	6.62341	8.95953	16.30564
H	10.36502	9.66766	16.80072
H	8.29775	11.90528	17.09401
H	9.99410	12.11046	16.61346
H	9.59076	11.56057	18.24867
H	9.01222	8.95079	14.82141
H	9.70099	10.57044	14.61889
H	7.98859	10.38599	15.00851
H	10.69251	9.51498	18.84753
H	11.02761	9.93184	21.21441
H	9.52993	9.09932	21.64312
H	9.46254	10.59896	20.71524
H	10.48072	6.89912	20.41012
H	11.94884	7.82872	20.08309
H	11.05830	7.07391	18.74935
H	8.54048	7.33967	21.18014
H	6.53142	7.27067	22.56773
H	5.49806	7.63760	21.18451

H	6.66366	8.83781	21.74917
H	6.49553	5.38997	20.01597
H	7.46678	5.16804	21.47318
H	8.25299	5.26285	19.88640
H	5.15375	6.82438	19.26349
H	3.20423	8.04810	18.36619
H	4.26717	9.07634	17.39017
H	4.32567	9.17466	19.15408
H	4.07828	5.94884	17.22125
H	5.81793	5.59978	17.19170
H	5.16106	6.91198	16.20365
H	6.07724	5.46508	11.59026
H	9.25832	6.65610	9.76611
H	7.74029	6.45601	7.79030
H	7.73621	8.10795	8.42856
H	6.38346	7.01354	8.77463
H	6.77490	7.58974	11.28550
H	8.18679	8.55449	10.85375
H	8.35661	7.23868	12.01700
H	5.59455	1.56608	11.67857
H	3.84408	3.99846	11.04914
H	3.26283	2.37041	11.43776
H	4.15875	2.66568	9.93491
H	6.16724	2.74272	13.78682
H	4.42434	2.48706	13.67044
H	5.08728	4.08730	13.34165
H	8.58039	1.38255	9.03388
H	8.98553	0.57128	11.31689
H	8.16136	-0.64747	10.32617
H	7.26489	0.26258	11.54894
H	5.62326	0.81997	9.54127
H	6.69630	0.00861	8.39831
H	6.24721	1.70520	8.14551
H	9.96670	2.79170	8.90650
H	8.11662	2.75867	7.22762
H	9.62785	3.35268	6.52155

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H       8.33844      4.48677      6.94854
H      10.23344      5.73106      8.16706
H      11.38581      4.42057      7.95394
H      11.00820      4.99180      9.58634
H       7.08958     -0.91892     14.51594
H       8.02714     -2.23369     15.23827
H       8.45773     -1.60658     13.63991
H       7.08346      1.81152     17.23768
H       7.13671      0.11427     17.73523
H       6.46892      0.56108     16.15849
H       8.99799      2.93673     17.86976
H      10.75647      2.97087     17.74415
H       9.97094      1.80139     18.81510
H      12.90500      1.15864     15.25122
H      12.87751      0.32960     16.81479
H      12.50978      2.05611     16.71909
H      10.69857     -1.54545     13.41053
H      11.70508     -1.94230     14.81092
H      12.10391     -0.54994     13.79447
250
Coupling adduct - quintet
C      19.88154      6.78079     10.59366
C      19.20253      7.67498     11.46447
C      17.89002      7.90474     10.99389
C      17.70477      7.07922      9.83690
C      18.93727      6.37169      9.59642
C      16.99273      9.04475     11.44187
C      17.11980      9.39260     12.92453
C      16.51464      7.28721      8.90281
C      15.64268      6.08536      8.53391
C      19.22930      5.54130      8.35204
C      19.92257      4.19908      8.61395
C      21.39762      6.80853     10.42737
C      22.23466      6.73984     11.70583
C      17.27827     10.30046     10.59856
C      16.93570      8.01908      7.61352
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C	20.02659	6.31191	7.28084
C	21.77286	8.11670	9.69751
U	17.93090	5.30713	12.12513
S	15.87726	3.44828	12.66430
Ir	16.77082	2.80722	10.54510
C	17.32450	1.04411	9.28181
C	16.56550	1.96469	8.48042
C	15.24170	2.07408	9.06009
C	15.20266	1.20980	10.20265
C	16.48019	0.56262	10.34698
C	16.98348	2.51954	7.15602
C	14.07379	2.79698	8.46577
C	14.00235	0.95454	11.05768
C	16.79729	-0.56111	11.28167
C	18.69870	0.53742	8.97275
S	15.38990	6.33562	12.22386
C	14.74934	4.76629	12.52390
C	19.92094	5.51981	14.02245
C	18.82571	6.04334	14.76278
C	17.93319	4.95241	15.01524
C	18.56774	3.74964	14.51478
C	19.80103	4.10866	13.90427
C	18.88012	7.38768	15.48542
C	20.02849	8.29839	15.04060
C	16.60461	4.94889	15.77577
C	15.86935	6.29419	15.84728
C	18.13793	2.35191	14.93536
C	18.94493	1.91726	16.17762
C	20.93294	3.16816	13.51255
C	21.18431	3.02238	12.00732
C	19.06846	7.15379	16.99657
C	16.67450	4.34911	17.19568
C	18.19469	1.22887	13.89337
C	22.22962	3.53405	14.25212
C	9.12136	4.68919	13.77761
S	8.27163	3.17658	13.61286

Ir	7.93926	2.41043	15.82935
C	7.82581	0.99405	17.52471
C	9.13216	1.61154	17.54539
C	9.81796	1.26862	16.33688
C	8.94032	0.39586	15.57294
C	7.73449	0.20831	16.30622
C	9.71900	2.37104	18.69249
C	11.23808	1.59561	15.99523
C	9.31372	-0.26057	14.28090
C	6.62032	-0.73655	15.98388
C	6.86094	0.90732	18.66515
S	8.59860	6.03985	12.89502
U	6.58570	5.12738	14.59227
C	3.91678	5.20040	13.90640
C	4.46379	5.78109	12.73218
C	5.17980	4.73923	12.05166
C	4.96879	3.50883	12.78438
C	4.18675	3.80787	13.94012
C	3.96444	7.09906	12.14926
C	3.18733	7.97297	13.13795
C	5.96626	4.81615	10.73650
C	6.37857	6.22071	10.27448
C	5.22545	2.14556	12.15163
C	3.96634	1.68311	11.38573
C	3.47497	2.85368	14.88421
C	3.51705	3.29369	16.35112
C	3.01554	6.80841	10.97002
C	5.29628	4.12819	9.52713
C	5.67716	0.97810	13.03452
C	2.00607	2.67743	14.45783
C	5.88212	7.58205	15.72115
C	5.77738	6.74251	16.85920
C	7.11686	6.34646	17.20653
C	8.02428	6.97955	16.27929
C	7.23844	7.77565	15.37800
C	4.51186	6.68678	17.71431

C	3.25324	7.19471	17.00278
C	7.71533	8.92406	14.50765
C	6.95751	9.09087	13.18955
C	9.55458	7.02879	16.25413
C	10.32558	5.84498	16.85709
C	7.56935	5.57585	18.44297
C	6.54542	4.61201	19.04944
C	7.58519	10.24501	15.29554
C	10.13076	8.32704	16.85414
C	8.13170	6.49710	19.54176
C	4.66979	7.55343	18.97850
H	18.23397	3.06115	11.22270
H	16.86278	4.38378	10.17717
H	13.67853	4.57832	12.49014
H	19.67771	8.22175	12.26461
H	15.94798	8.75924	11.26965
H	18.31442	10.62970	10.73541
H	16.61952	11.12225	10.90173
H	17.12219	10.12236	9.53192
H	16.88744	8.53172	13.55536
H	16.41935	10.19316	13.18449
H	18.12595	9.74676	13.17280
H	15.84879	7.96758	9.44411
H	16.05199	8.42169	7.10543
H	17.43089	7.34018	6.91284
H	17.61937	8.84980	7.81206
H	16.20431	5.32612	7.98302
H	14.81977	6.42302	7.89206
H	15.21920	5.61490	9.42210
H	18.25473	5.30435	7.91339
H	19.98329	5.77313	6.32689
H	21.08264	6.39832	7.55285
H	19.63864	7.31949	7.11412
H	20.89678	4.32254	9.09449
H	20.10422	3.68267	7.66302
H	19.30380	3.55856	9.24677

H	21.70183	5.97265	9.78902
H	22.83236	8.11146	9.41533
H	21.60537	8.97562	10.35655
H	21.17795	8.27303	8.79607
H	23.29403	6.87673	11.46244
H	22.13720	5.78280	12.21751
H	21.96080	7.53538	12.40744
H	20.79267	6.09188	13.74684
H	17.94319	7.93635	15.34733
H	18.24545	6.59370	17.43903
H	19.14266	8.11233	17.52321
H	19.99231	6.59423	17.18105
H	21.00086	7.84057	15.25347
H	19.98457	9.24187	15.59434
H	19.99674	8.54277	13.97981
H	20.64977	2.17581	13.87153
H	22.62816	4.50057	13.92744
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H	22.06420	3.59189	15.33233
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H	22.01002	2.32510	11.82147
H	21.45406	3.97613	11.54418
H	17.08538	2.42970	15.22926
H	17.73052	1.51905	12.94955
H	17.66760	0.35078	14.28386
H	19.21874	0.91043	13.67520
H	19.98724	1.71055	15.91279
H	18.52692	0.99771	16.60466
H	18.95342	2.68317	16.95659
H	15.94550	4.28399	15.20169
H	16.94738	3.29331	17.19373
H	15.69046	4.43043	17.67165
H	17.39113	4.87338	17.83473
H	16.33279	6.98903	16.55358
H	14.84534	6.12271	16.19662
H	15.80117	6.77386	14.86883

H	17.86142	-0.59629	11.52633
H	16.52851	-1.52559	10.83001
H	16.24739	-0.47159	12.22105
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H	18.64044	-0.36526	8.35090
H	19.24312	0.27860	9.88404
H	18.05675	2.71310	7.11756
H	16.46355	3.45179	6.92560
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H	13.37960	3.14052	9.23638
H	13.51758	2.13958	7.78431
H	14.38993	3.67331	7.89715
H	14.28628	0.71234	12.08423
H	13.42512	0.11238	10.65560
H	13.34429	1.82585	11.09239
H	6.37450	2.76786	15.57271
H	7.96477	3.95040	16.30222
H	10.00071	4.72066	14.41501
H	5.05781	8.12228	15.28129
H	8.77163	8.76063	14.26387
H	6.52768	10.49920	15.43014
H	8.06080	11.06998	14.75228
H	8.03208	10.18631	16.29051
H	7.02374	8.19777	12.56643
H	7.36849	9.93036	12.61812
H	5.89812	9.30460	13.36560
H	9.81697	7.04923	15.18773
H	11.22608	8.29255	16.82611
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H	10.35343	5.88423	17.95049
H	11.36585	5.88853	16.51366
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H	8.39990	4.94245	18.12287
H	8.52962	5.89632	20.36875
H	7.36932	7.16219	19.95596

H	8.94111	7.12756	19.16942
H	5.70199	5.12040	19.52043
H	7.02937	4.02371	19.83800
H	6.16370	3.91633	18.29744
H	4.31435	5.65682	18.03038
H	3.73992	7.55300	19.55946
H	4.89205	8.58921	18.69900
H	5.46867	7.20923	19.63475
H	2.38478	7.07040	17.65807
H	3.04442	6.66797	16.07291
H	3.33274	8.26223	16.77025
H	3.25028	5.70615	14.58792
H	4.80197	7.69178	11.76937
H	3.49465	6.23025	10.17906
H	2.65132	7.74451	10.53029
H	2.14678	6.23824	11.31796
H	2.27423	7.47140	13.47742
H	2.88269	8.90317	12.64697
H	3.76812	8.24056	14.02016
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H	1.46057	3.62106	14.56957
H	1.50709	1.92575	15.08095
H	1.91633	2.36915	13.41331
H	4.54518	3.37447	16.71819
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H	3.02299	4.25997	16.49370
H	6.02813	2.29820	11.42131
H	6.48095	1.25181	13.71814
H	6.02600	0.15942	12.39317
H	4.85403	0.57826	13.63461
H	3.20957	1.32161	12.08885
H	4.20793	0.85172	10.71219
H	3.51304	2.48268	10.79648
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H       6.74964     -1.67591     16.53720
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H       6.95503      1.75880     19.34023
H       7.03982     -0.00472     19.25031
H       5.82683      0.87786     18.31300
H       8.94465      2.85165     19.29281
H      10.41109      3.14508     18.35398
H      10.27463      1.68827     19.34796
H      11.38201      1.68331     14.91557
H      11.91815      0.81214     16.35582
H      11.55242      2.53884     16.44826
H       8.43477     -0.61962     13.74188
H       9.96966     -1.12051     14.46553
H       9.84598      0.43097     13.62201
250
Coupling TS - quintet
 C     6.759558     6.776926    16.003524
 C     7.415019     7.669057    15.117458
 C     8.777433     7.790797    15.470392
 C     9.012629     6.893906    16.567871
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 C     9.672580     8.923442    14.999400
 C     9.528705    10.140811    15.930122
 C    10.297438     6.969603    17.389176
 C    10.077399     7.701366    18.727791
 C     7.515518     5.410538    18.130944
 C     6.869970     6.200871    19.286694
 C     5.268737     6.884193    16.310774
 C     5.034193     8.204511    17.076789
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C	6.707343	4.131708	17.886547
C	4.305519	6.858299	15.122319
U	8.529682	5.253052	14.223342
S	11.022676	6.274780	13.696193
C	11.487714	4.685616	14.071882
S	10.488518	3.336368	13.588593
Ir	9.557784	2.444851	15.602586
C	10.498354	1.490077	17.401512
C	11.236100	1.079859	16.252344
C	10.341405	0.315629	15.395622
C	9.060996	0.281219	16.011849
C	9.131385	1.032763	17.252643
C	12.703744	1.249039	16.016337
C	10.767080	-0.385075	14.143329
C	7.865628	-0.488475	15.544405
C	8.093373	1.012925	18.329319
C	11.062508	2.149651	18.619587
C	13.763662	4.566401	12.246063
S	14.344846	6.196303	12.226312
U	16.890082	5.240329	11.971563
Ir	15.952001	2.526188	10.571033
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C	14.402290	1.433554	9.351641
C	14.742970	0.611883	10.492444
C	16.130166	0.267848	10.413442
C	16.667013	0.891134	9.217608
C	13.027800	1.882090	8.963903
C	13.782834	0.145217	11.538932
C	16.872147	-0.720240	11.257416
C	18.036432	0.621449	8.676773
C	15.645702	2.185159	7.171365
S	14.943114	3.316777	12.590861
C	6.322098	5.497464	12.571233
C	7.315779	6.095840	11.755072
C	8.207252	5.046878	11.345628
C	7.665672	3.800809	11.839402

C	6.495310	4.087742	12.599933
C	7.148886	7.473475	11.118100
C	6.795976	7.314290	9.626118
C	9.454288	5.135846	10.458098
C	9.282920	4.570915	9.031539
C	8.071925	2.447523	11.270106
C	8.126603	1.234463	12.207730
C	5.413124	3.113243	13.044950
C	4.086954	3.430484	12.333121
C	6.034371	8.323470	11.735520
C	5.193051	3.027049	14.559585
C	7.151522	2.093131	10.082711
C	10.096409	6.524102	10.327789
C	18.945296	5.599338	13.734271
C	17.892065	6.153006	14.515073
C	17.024144	5.070651	14.867374
C	17.639600	3.847230	14.393030
C	18.832383	4.182887	13.694063
C	17.983102	7.522499	15.187659
C	18.302883	7.334750	16.683396
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H      10.19947      0.66156     14.75876
250
Coupling TS - septet
C       6.76351      6.82592     15.78789
C       7.40617      7.69578     14.86866
C       8.75756      7.87576     15.24136
C       8.99593      7.05105     16.39420
C       7.76264      6.39070     16.72124
C       9.63538      9.00161     14.72271
C       9.39501     10.28542     15.53708
C      10.24157      7.22979     17.25829
C       9.92891      8.01067     18.54970
C       7.51944      5.56645     17.97849
C       6.77660      6.34087     19.08485
C       5.26338      6.87460     16.05321
C       4.93164      8.21775     16.73697
C       9.43006      9.30094     13.23626
C      11.06264      5.98836     17.61637
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C	6.81014	4.22999	17.73091
C	4.34445	6.71867	14.84075
U	8.57049	5.23610	14.09404
S	11.27092	6.31276	13.87949
C	11.90273	4.73818	13.95246
S	10.82818	3.38664	13.54800
Ir	9.92550	2.55302	15.60762
C	10.93534	1.73306	17.43990
C	11.62889	1.22995	16.30212
C	10.70664	0.41042	15.53113
C	9.44674	0.43467	16.18947
C	9.56045	1.27856	17.36641
C	13.08805	1.37150	16.00905
C	11.08762	-0.39654	14.33196
C	8.22933	-0.35251	15.81748
C	8.55984	1.35349	18.47545
C	11.53860	2.48155	18.58553
C	13.50950	4.72050	12.35180
S	14.22406	6.29126	12.28277
U	16.74757	5.22387	12.10428
Ir	15.56415	2.64584	10.62218
C	14.49163	1.84830	8.80257
C	13.83366	1.34338	9.95963
C	14.77896	0.51636	10.69278
C	16.01773	0.53892	9.98994
C	15.86496	1.38537	8.82252
C	12.38426	1.48400	10.29455
C	14.42389	-0.32094	11.87893
C	17.24121	-0.25795	10.31818
C	16.81509	1.45437	7.66996
C	13.84419	2.58640	7.67591
S	14.66067	3.40908	12.69891
C	6.40069	5.34312	12.30832
C	7.42243	5.91391	11.50582
C	8.33745	4.85566	11.18599
C	7.79908	3.63135	11.72928

C	6.59625	3.94133	12.42638
C	7.28549	7.28186	10.84159
C	7.04377	7.13280	9.32757
C	9.60436	4.90084	10.33294
C	9.42772	4.36858	8.89589
C	8.24947	2.25431	11.26023
C	8.36432	1.13232	12.29778
C	5.54233	2.96661	12.93103
C	4.17017	3.26439	12.30670
C	6.11914	8.11199	11.38725
C	5.42956	2.87345	14.45719
C	7.34118	1.77287	10.10877
C	10.31844	6.25681	10.27618
C	18.87578	5.37614	13.84453
C	17.85784	5.94927	14.65499
C	16.94146	4.89593	14.97345
C	17.49244	3.66410	14.44302
C	18.69450	3.97118	13.74750
C	18.01242	7.30036	15.35251
C	18.24092	7.08704	16.86163
C	15.66788	4.95043	15.81845
C	15.81441	4.38229	17.24587
C	17.05568	2.29232	14.93921
C	16.99096	1.13189	13.94027
C	19.76757	2.99886	13.28063
C	21.09304	3.27118	14.01077
C	19.20150	8.13231	14.85952
C	19.98677	2.94920	11.76510
C	17.95349	1.87246	16.12248
C	14.97892	6.31866	15.90019
C	17.98758	7.59888	11.41822
C	16.65850	7.81953	10.99577
C	16.44081	6.99715	9.83904
C	17.67315	6.30951	9.54932
C	18.64821	6.72247	10.51530
C	15.78667	8.96471	11.48116

C	16.06525	10.22611	10.64421
C	15.21516	7.19069	8.94957
C	15.56974	7.96676	7.66572
C	17.93864	5.49871	8.28721
C	18.67972	6.29904	7.19743
C	20.15492	6.78567	10.27603
C	20.45832	8.12528	9.56888
C	15.96745	9.29218	12.96369
C	14.38141	5.96537	8.57103
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H	15.42763	11.05237	10.97797
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H	15.29207	10.10277	13.25552
H	16.98862	9.62262	13.18312
H	14.54421	7.83296	9.52977
H	14.65722	8.35408	7.19883
H	16.05952	7.31949	6.93198
H	16.23482	8.81316	7.85993
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H	13.51940	6.28631	7.97459
H	14.01277	5.44060	9.45344
H	16.95583	5.24411	7.87741
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H	19.74229	6.40972	7.43247
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H	18.08688	3.51362	9.16440

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H	19.12580	6.46236	17.02672
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H	19.16336	8.36502	13.79623
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H	21.51980	4.23778	13.72367
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H	20.95333	3.28136	15.09603
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H	20.80401	2.26233	11.51532
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H	16.03648	2.41331	15.32092
H	16.45310	1.40256	13.03117
H	16.47718	0.28502	14.40930
H	17.98374	0.77730	13.64658
H	18.96182	1.62508	15.77455
H	17.54755	0.98060	16.61437
H	18.05039	2.66227	16.87104
H	14.95854	4.28868	15.30234
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H	14.86920	4.51157	17.78508
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H	11.93250	2.33100	9.77436
H	15.30713	-0.76966	12.33664
H	13.75430	-1.13597	11.57697
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H	8.48273	2.86737	14.94213
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H	6.89659	8.27326	14.11114
H	10.68896	8.72481	14.85260
H	8.35272	10.61059	15.44427
H	10.03739	11.09859	15.17809
H	9.60404	10.13668	16.59949
H	9.62710	8.42200	12.61684
H	10.10783	10.09733	12.90969
H	8.40765	9.63701	13.03227
H	10.91202	7.86371	16.66636
H	10.85601	8.36741	19.01445
H	9.42093	7.37732	19.28363
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H	6.83617	5.79247	20.03297
H	5.71514	6.46086	18.84912

H	7.19754	7.33681	19.24483
H	5.82374	4.36664	17.27941
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H	7.40471	3.59135	17.07201
H	5.00516	6.07798	16.75850
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H	4.42966	5.73159	14.38504
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H	8.20127	7.86859	10.97679
H	7.88607	6.67725	8.80680
H	6.86424	8.11387	8.87136
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H	6.11854	9.10507	10.92548
H	6.16609	8.24506	12.46720
H	5.83126	1.97167	12.58022
H	3.77204	4.22608	12.64711
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H	4.23398	3.30251	11.21486
H	6.37266	2.54287	14.90344
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H	8.81599	0.24913	11.82859
H	7.38938	0.82348	12.68666
H	6.34357	1.51753	10.48156
H	7.75447	0.87317	9.63544
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H	10.37354	4.45695	8.34637

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H       8.22103     -1.31404     16.34694
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Complex 2 - triplet
C      18.73302      6.74247     10.48581
C      18.05385      7.60307     11.38975
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C      17.77840      6.35178      9.49084
C      15.84797      8.96463     11.43364
C      16.01830      9.27525     12.92106
C      15.33583      7.24242      8.85259
C      14.52449      6.01769      8.42666
C      18.07052      5.56587      8.21936
C      18.79998      4.23733      8.44091
C      20.24224      6.81748     10.26152
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C      16.11403     10.24077     10.61529
C      15.70761      8.05120      7.59396
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C	18.82841	6.38554	7.15563
C	20.54837	8.17946	9.60022
U	16.76834	5.21664	12.03316
S	14.68912	3.36134	12.56863
Ir	15.63097	2.66138	10.49267
C	16.01719	1.42610	8.68951
C	14.63844	1.86401	8.63332
C	13.95486	1.33090	9.76324
C	14.89138	0.50977	10.51305
C	16.14938	0.56628	9.84969
C	14.01516	2.61242	7.49946
C	12.49176	1.43074	10.04724
C	14.51706	-0.34180	11.68294
C	17.37822	-0.21186	10.20226
C	16.99924	1.52061	7.56554
S	14.31560	6.25061	12.14687
C	13.40204	4.67548	12.33567
C	12.37826	4.67762	13.49389
S	11.09276	3.36049	13.26073
Ir	10.15326	2.65082	15.33563
C	9.77228	1.41599	17.13969
C	11.15142	1.85422	17.19377
C	11.83338	1.32135	16.06311
C	10.89567	0.50224	15.31310
C	9.63832	0.55782	15.97894
C	11.77621	2.60248	18.32689
C	13.29584	1.42223	15.77658
C	11.26774	-0.34856	14.14188
C	8.40937	-0.22054	15.62700
C	8.79223	1.50960	18.26551
S	11.46552	6.25260	13.67374
U	9.00546	5.21631	13.80186
C	18.93481	5.32086	13.75721
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C	17.00701	4.83391	14.89223
C	17.55052	3.60730	14.35064

C	18.74845	3.91854	13.65021
C	18.08515	7.23780	15.28073
C	19.30037	8.04682	14.81231
C	15.73906	4.88484	15.74214
C	15.04356	6.24975	15.81003
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C	19.81569	2.94776	13.16852
C	20.04084	2.92952	11.65350
C	18.28326	7.02579	16.79426
C	15.89716	4.32345	17.17084
C	17.03125	1.08969	13.81151
C	21.14031	3.19621	13.90915
C	6.84028	5.32465	12.06508
C	7.85347	5.89359	11.24649
C	8.76921	4.83782	10.93318
C	8.22685	3.61155	11.48079
C	7.02667	3.92275	12.17753
C	7.69400	7.24236	10.54456
C	6.48282	8.05440	11.01802
C	10.03666	4.88609	10.08252
C	10.73477	6.24952	10.01270
C	8.66679	2.23573	11.00081
C	7.76512	1.79108	9.82976
C	5.95901	2.95231	12.65913
C	5.73851	2.92925	14.17480
C	7.49410	7.03624	9.03045
C	9.87556	4.32406	8.65433
C	8.74532	1.09276	12.01855
C	4.63240	3.20397	11.92332
C	7.73270	7.60355	14.44760
C	7.05578	6.73992	15.35099
C	8.01340	6.34626	16.34210
C	9.24878	7.03165	16.06585
C	9.05293	7.83342	14.89233
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C	4.62786	6.68204	14.36218
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C	9.76423	9.27554	12.91149
C	10.45806	7.23337	16.97389
C	11.26832	6.00609	17.39403
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C	6.99503	4.22878	17.38854
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H	14.79900	8.68255	11.28375
H	17.15499	10.56393	10.72932
H	15.46735	11.05620	10.95932
H	15.92492	10.09140	9.54973
H	15.78891	8.40245	13.53666
H	15.33596	10.07831	13.21877
H	17.03627	9.60937	13.15121
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H	14.80095	8.44034	7.11633
H	16.21825	7.42497	6.85588
H	16.36096	8.89898	7.81953
H	15.10976	5.32730	7.81386
H	13.66751	6.34241	7.82431
H	14.15441	5.46808	9.29307
H	17.09693	5.31478	7.78594
H	18.79089	5.86645	6.19047
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H	18.47710	7.98569	17.28686
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H	15.03221	4.21624	15.23149
H	16.14006	3.25965	17.17959
H	14.95686	4.45314	17.71958
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H	14.04887	6.12876	16.24980
H	14.90405	6.67889	14.81592

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H	18.02985	1.44664	7.91760
H	14.74312	3.24441	6.98792
H	13.19624	3.25240	7.83327
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H	12.28968	1.58731	11.10976
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H	13.84114	-1.14599	11.36579
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H	12.89547	4.48451	14.43804
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H	11.63493	5.45870	16.52474
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H	7.00848	5.85315	19.64319
H	5.91185	6.49281	18.42212

H	7.39321	7.37101	18.81868
H	6.01602	4.36785	16.92333
H	6.82361	3.73015	18.34893
H	7.58690	3.56519	16.75381
H	5.26008	6.03113	16.28610
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H	5.39597	8.98883	15.52799
H	5.88766	8.36505	17.10351
H	3.59376	6.88492	14.66222
H	4.64719	5.68279	13.92604
H	4.88227	7.40638	13.58156
H	5.97289	5.86110	12.41420
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H	6.45372	9.01168	10.48763
H	6.49240	8.27466	12.08440
H	6.28667	1.94873	12.37733
H	4.20293	4.17518	12.19006
H	3.89565	2.43455	12.18189
H	4.77279	3.19275	10.83807
H	6.64035	2.60166	14.69926
H	4.92450	2.24314	14.43798
H	5.47252	3.91819	14.55915
H	9.68283	2.35723	10.61133
H	9.28240	1.38653	12.92099
H	9.26675	0.24203	11.56435
H	7.75620	0.73392	12.31973
H	6.75942	1.54630	10.18719
H	8.17103	0.89193	9.35041
H	7.66056	2.56782	9.06840
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H	9.63055	3.26075	8.64631
H	10.81537	4.45157	8.10428

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H      10.87973      6.67718     11.00668
H       7.50137      0.32606     15.89183
H       8.39577     -1.17360     16.17101
H       8.36389     -0.44278     14.55918
H       8.88970      2.45134     18.80929
H       8.96047      0.69274     18.98052
H       7.76099      1.43561     17.91522
H      11.04862      3.23346     18.84024
H      12.59378      3.24342     17.99165
H      12.18223      1.89656     19.06303
H      13.49573      1.58266     14.71424
H      13.80576      0.49836     16.08062
H      13.75198      2.24633     16.32870
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H      11.93924     -1.15685     14.45808
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Complex 2 - quintet
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C      18.05191      7.60624     11.38583
C      16.73186      7.83745     10.94132
C      16.53564      7.03750      9.76663
C      17.77065      6.35190      9.48947
C      15.84598      8.96666     11.43718
C      16.02141      9.27750     12.92398
C      15.32651      7.24114      8.85883
C      14.51532      6.01491      8.43739
C      18.05941      5.56431      8.21829
C      18.78792      4.23533      8.44045
C      20.23719      6.81760     10.25395
C      21.15693      6.68214     11.46901
C      16.10805     10.24251     10.61729
C      15.69444      8.04880      7.59830
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Ir	15.62888	2.65550	10.49225
C	16.00949	1.42292	8.68670
C	14.63044	1.86151	8.63338
C	13.94845	1.32728	9.76341
C	14.88614	0.50711	10.51230
C	16.14342	0.56329	9.84639
C	14.00570	2.61199	7.50169
C	12.48602	1.42798	10.05019
C	14.51422	-0.34483	11.68274
C	17.37225	-0.21579	10.19718
C	16.98940	1.51766	7.56084
S	14.31907	6.25577	12.15698
C	13.40485	4.68136	12.33594
C	12.37961	4.68056	13.49314
S	11.09553	3.36200	13.25990
Ir	10.15707	2.65167	15.33525
C	9.77761	1.41777	17.14023
C	11.15653	1.85678	17.19341
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C	9.64360	0.55883	15.98006
C	11.78136	2.60632	18.32566
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C	11.27265	-0.34773	14.14276
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C	8.79812	1.51156	18.26654
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U	9.00594	5.21540	13.80139
C	18.94488	5.32491	13.76465
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C	18.75782	3.92322	13.65102
C	18.09264	7.24185	15.28684
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C	15.74865	4.88633	15.74736
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C	18.29130	7.03460	16.80096
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C	17.03813	1.09404	13.80763
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C	7.85165	5.89125	11.24658
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C	8.22798	3.60968	11.48075
C	7.02759	3.91937	12.17784
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C	6.47700	8.04928	11.01833
C	10.03595	4.88661	10.08226
C	10.73271	6.25077	10.01336
C	8.66957	2.23441	11.00078
C	7.76832	1.78839	9.82992
C	5.96101	2.94759	12.65923
C	5.74100	2.92272	14.17495
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C	9.87492	4.32540	8.65377
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C	4.63387	3.19864	11.92415
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H	16.34765	8.89742	7.82115
H	15.09939	5.32345	7.82478
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H	14.14785	5.46730	9.30617
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H	6.28942	1.94455	12.37639
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Complex 2 - septet
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C       9.22017      7.04696     16.05840
C       5.53477      6.94074     15.40009
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C       7.57482      5.64240     17.55467
C       6.80879      6.50263     18.58071
C      10.39556      7.23208     17.01516
C       9.99469      8.06096     18.25169
C      10.05431      8.92519     14.39403
C       9.79721     10.21784     15.18919
C       4.67370      6.82308     14.13885
C       9.96584      9.23181     12.89682
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C	11.16376	5.99350	17.48305
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C	12.34858	4.54908	13.68078
S	11.03040	3.27485	13.39529
Ir	10.01094	2.62264	15.45001
C	9.43165	0.55292	16.11265
C	9.54677	1.42969	17.26211
C	10.93210	1.84016	17.35365
C	11.63923	1.27120	16.25735
C	10.70829	0.46016	15.48909
C	8.53117	1.56704	18.35126
C	11.53761	2.59666	18.49261
C	13.11211	1.33585	16.01771
C	11.09996	-0.41209	14.33967
C	8.19821	-0.20595	15.73372
C	13.44110	4.49933	12.58808
S	14.48514	6.02418	12.60542
U	16.73997	4.53017	12.76820
Ir	15.67237	2.36703	10.80406
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C	16.20931	1.25379	9.00687
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C	14.04221	1.12203	9.85402
C	14.89214	0.24327	10.64636
C	17.34120	1.46104	8.04871
C	14.35105	2.57240	7.71006
C	12.56405	1.25470	10.03303
C	14.40670	-0.63645	11.75420
C	17.38597	-0.51202	10.53823
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C	6.94518	5.34273	11.96645
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C	8.91951	4.76306	10.95934
C	8.29478	3.56695	11.48682

C	7.07034	3.93586	12.11186
C	7.96628	7.20463	10.47542
C	7.86537	6.98770	8.95307
C	10.24500	4.74737	10.19732
C	10.15786	4.18425	8.76319
C	8.71231	2.16841	11.05547
C	8.67942	1.03769	12.09185
C	5.94362	3.01146	12.55662
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C	11.01433	6.07519	10.17812
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C	18.93006	3.41985	14.10519
C	18.20248	6.88442	15.41955
C	18.68095	6.94292	16.88251
C	16.11358	4.43839	16.42357
C	16.50106	4.03441	17.85918
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C	19.15838	7.76275	14.60237
C	15.33272	5.75861	16.45509
C	18.35022	1.15579	16.38837
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C	17.89353	8.00908	10.71683
C	18.58292	7.54122	9.58163
C	17.61342	7.43959	8.47051
C	16.40231	7.90122	8.93446
C	16.58667	8.32692	10.33900
C	20.07715	7.37594	9.50108

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C	14.96061	8.69005	6.96743
C	17.89178	6.82278	7.11828
C	18.87537	7.63233	6.25686
C	15.99219	9.32800	12.59450
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H	14.63254	8.61595	11.10738
H	16.34349	11.08929	10.49084
H	14.64807	11.09497	11.01377
H	15.08631	10.44622	9.42562
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H	15.20576	9.87209	13.12682
H	16.91875	9.90708	12.68589
H	14.34309	8.34875	8.97025
H	13.92236	8.74164	6.61915
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H	15.31831	9.71425	7.11628
H	15.19817	5.86856	7.41182
H	13.53825	6.44058	7.61969
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H	17.57928	4.78457	7.81499

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H	19.89365	5.35982	13.60034
H	17.20842	7.34595	15.37319
H	18.01962	6.39575	17.55500
H	18.73247	7.98050	17.23275
H	19.68128	6.50430	16.97034
H	20.17315	7.35109	14.60231
H	19.21806	8.75231	15.06919
H	18.86111	7.93770	13.56350
H	19.62178	1.43724	13.75066
H	21.73159	3.63229	14.03103
H	22.03653	1.89209	13.90607
H	21.20817	2.55488	15.32982
H	19.19707	2.31032	11.50724
H	20.91403	1.88484	11.65925
H	20.42129	3.57931	11.72371
H	16.40184	1.91138	15.93869
H	16.29800	1.10601	13.57826
H	16.59176	-0.17967	14.76588
H	17.90886	0.40894	13.75220
H	19.28460	0.88182	15.88700
H	17.94653	0.24663	16.85120
H	18.60178	1.86221	17.18510
H	15.39818	3.68083	16.07301
H	16.90945	3.02248	17.90781
H	15.62045	4.07042	18.51161
H	17.25114	4.70941	18.28249
H	15.89609	6.56319	16.93663
H	14.41432	5.62434	17.03664
H	15.04019	6.08746	15.45280

H	18.32342	0.03237	10.40496
H	17.44439	-1.42863	9.93677
H	17.31500	-0.80300	11.58843
H	17.26302	2.42198	7.53583
H	17.35218	0.67362	7.28256
H	18.30576	1.44057	8.56215
H	15.13691	3.23559	7.34318
H	13.50989	3.19692	8.01780
H	14.01962	1.94844	6.86969
H	12.29799	1.40038	11.08447
H	12.05365	0.35078	9.67489
H	12.16894	2.10253	9.46957
H	15.23794	-1.07694	12.30889
H	13.79535	-1.45724	11.35747
H	13.79396	-0.07298	12.46325
H	8.60263	2.96140	14.70785
H	9.94328	4.18020	15.87505
H	12.80986	4.34778	14.65323
H	7.37710	8.18047	13.52627
H	11.08558	8.60748	14.59430
H	8.77409	10.57694	15.02290
H	10.48950	11.00743	14.87024
H	9.93023	10.07083	16.26463
H	10.21010	8.35367	12.29477
H	10.68000	10.02072	12.63263
H	8.96784	9.58718	12.61219
H	11.12301	7.82864	16.45339
H	10.89170	8.43588	18.75926
H	9.44347	7.45273	18.97632
H	9.36803	8.92008	17.99320
H	10.54214	5.31670	18.07540
H	12.00120	6.30857	18.11807
H	11.56113	5.43605	16.63376
H	8.52139	5.35687	18.02959
H	6.78802	5.99194	19.55308
H	5.76755	6.65884	18.27727

H	7.26753	7.48459	18.72612
H	5.83616	4.51850	16.82200
H	6.57525	3.85745	18.27683
H	7.37767	3.64951	16.70439
H	5.18665	6.17459	16.10147
H	4.18289	8.39784	16.31441
H	5.46222	9.11857	15.31838
H	5.84790	8.49682	16.92651
H	3.63009	7.05623	14.38266
H	4.68907	5.81933	13.71281
H	4.98896	7.53390	13.36579
H	6.08256	5.92032	12.25800
H	8.87168	7.78959	10.66937
H	8.74399	6.49519	8.53797
H	7.75231	7.95077	8.44041
H	6.98939	6.37377	8.71440
H	5.81879	7.57126	10.57293
H	6.79787	9.01821	10.31385
H	6.69750	8.29968	11.91796
H	6.24558	1.99327	12.29898
H	4.25689	4.29593	11.99239
H	3.88469	2.56724	11.98683
H	4.85351	3.27816	10.67842
H	6.51437	2.65362	14.63032
H	4.80376	2.34230	14.28756
H	5.38951	4.00268	14.42817
H	9.75736	2.24507	10.73495
H	9.16349	1.32402	13.02702
H	9.20053	0.16276	11.68475
H	7.65930	0.71760	12.32693
H	6.83784	1.54093	10.12158
H	8.27685	0.81839	9.39275
H	7.85439	2.50883	9.05409
H	10.88134	4.04751	10.75737
H	9.87397	3.12986	8.74463
H	11.13690	4.27105	8.27543

H	9.43788	4.72625	8.14370
H	10.54679	6.82638	9.53488
H	12.02328	5.90387	9.78645
H	11.12498	6.48681	11.18382
H	7.29441	0.36635	15.95515
H	8.14382	-1.14697	16.29637
H	8.18454	-0.44997	14.66949
H	8.62525	2.52103	18.87435
H	8.66013	0.76566	19.09194
H	7.51189	1.50025	17.96600
H	10.80579	3.24467	18.97813
H	12.37249	3.22233	18.17072
H	11.91379	1.89533	19.24911
H	13.34998	1.46950	14.95954
H	13.59244	0.40886	16.35903
H	13.56767	2.16378	16.56558
H	10.22927	-0.86285	13.85919
H	11.75026	-1.22619	14.68457
H	11.64584	0.15579	13.58098

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