Uranyl-Cation Coordination Directed by Non-Covalent Interactions

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Electronic Supplementary Information

Experimental Procedures

General Methods. All reactions and manipulations were performed under an inert atmosphere (N_2) using standard Schlenk techniques or in a Vacuum Atmospheres, Inc. Nexus II drybox equipped with a molecular sieves 13X / Q5 Cu-0226S catalyst purifier system. Glassware was oven-dried overnight at 150 °C prior to use. ^{1}H NMR and ^{19}F NMR spectra were obtained on a Bruker DMX-300 Fourier transform NMR spectrometer at 300 MHz. Chemical shifts were recorded in units of parts per million downfield from residual proteo solvent peaks (^{1}H) or versus $CFCl_3$ (^{19}F). Elemental analyses were performed at the University of California, Berkeley Microanalytical Facility using a Perkin-Elmer Series II 2400 CHNS analyzer. UV-Vis data were collected on a Cary 5000 spectrometer in toluene in 1 mm path length air-free quartz cuvettes. The infrared spectra were obtained from 400–4000 cm^{-1} using a Perkin Elmer 1600 series infrared spectrometer.

Materials. Tetrahydrofuran, DME, Et_2O, CH_2Cl_2, hexanes, pentane, fluorobenzene, and toluene were purchased from Fisher Scientific. These solvents were sparged for 20 min with dry argon and dried using a commercial two-column solvent purification system comprising columns packed with Q5 reactant and neutral alumina respectively (for hexanes and pentane), or two columns of neutral alumina (for THF, Et_2O and CH_2Cl_2). All solvents were stored over 3 Å molecular sieves. Deuterated solvents were purchased from Cambridge Isotope Laboratories, Inc. and stored over potassium mirror overnight prior to use. Starting materials: $[UO_2Cl_2(THF)_2]_2$,[1] $KNPh^F_2$,[2] $KNPh^FPh$,[2] $KNAr^FPh(THF)_{0.5}$,[2] and $HNpyPh^F$,[3] prepared according to the reported procedures. 18-crown-6 was recrystallized from acetonitrile and dried under reduced pressure prior to use.

X-Ray Crystallography. X-ray intensity data were collected on a Bruker APEXII CCD area detector employing graphite-monochromated Mo-Kα radiation (λ=0.71073 Å) at a temperature of 143(1) K. In all cases, rotation frames were integrated using SAINT,[4] producing a listing of unaveraged F^2 and $\sigma(F^2)$ values which were then passed to the SHELXTL[5] program package for further processing and structure solution on a Dell Pentium 4 computer. The intensity data were corrected for Lorentz and polarization effects and for absorption using SADABS.[6] The structures were solved by direct methods (SHELXS-97).[7] Refinement was by full-matrix least squares based on F^2 using SHELXL-97.[7] All reflections were used during refinements. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using a riding model. The program SQUEEZE was used to correct the data in the structures of **2**, **3**, and **4-crown** for the presence of disordered solvent. In the structure of **2**, SQUEEZE estimated a total of 321 electrons in the cell due to disordered solvent; in structure **3**, a total of 260 electrons in the cell were due to disordered solvent and in structure **4-crown**, 241 electrons per cell were estimated. For compound **3**, there were many asymmetric anisotropic thermal parameters, especially in the THF molecules coordinated to the potassium cations and in the un-coordinated THF molecules. Modeling disorder did not improve the situation, presumably due to the poor quality of the data. Therefore thermal parameter restraints (DELU and SIMU) were applied to all the atoms in the structure. For compound **4-tol**, restraints were similarly applied on all the $–CF_3$ groups in order to produce a more visually acceptable model.

Electrochemistry. Voltammetry experiments (CV) were performed using a CH Instruments 620D Electrochemical Analyzer/Workstation and the data were processed using CHI software v9.24. All experiments were performed in an N_2 atmosphere drybox using electrochemical cells that consisted of a 4 mL vial, glassy carbon working electrode, a platinum

wire counter electrode, and a silver wire plated with AgCl as a quasi-reference electrode. The working electrode surfaces were polished prior to each set of experiments. Potentials were reported versus ferrocene, which was added as an internal standard for calibration at the end of each run. Solutions employed during these studies were ~3 mM in analyte and 100 mM in [^{n}Bu$_4$N][PF$_6$] in 2 mL of CH_2Cl_2. All data were collected in a positive-feedback IR compensation mode.

Synthetic Details and Characterization.

Synthesis of [K(THF)$_5$][UO$_2$(NPh$^F_2$)$_3$(THF)] (1). To a THF solution of [$UO_2Cl_2(THF)_2$]$_2$ (49 mg, 0.05 mmol, 1.0 equiv), KNPh$^F_2$(Et$_2$O) (138 mg, 0.3 mmol, 6.0 equiv) was added, causing and immediate color change to orange. After stirring 1 h, the mixture was filtered through Celite packed in a pipette. Volatiles were removed under vacuum, leaving an orange residue. This residue was dissolved in 1 ml THF and layered with 6 mL of hexanes. Storage at –21 °C gave orange crystals of **1** overnight, which were collected by filtration over a medium porosity fritted filter and washed with hexanes. Yield: 135 mg, 0.086 mmol, 86%. Single crystal suitable for X-ray analysis was grown in the same manner without drying. ^{1}H NMR (C_6D_6): 3.87 (s, THF), 1.50 (s, THF). ^{1}F NMR (C_6D_6): –150.53 (d, 6F, J = 23 Hz, *o*-F), –163.05 (t, 3F, J = 23 Hz, *p*-F), –164.98 (t, 6F, J = 23 Hz, m-F). Elemental analysis found (calculated) for $C_{40}H_8F_{30}N_3UO_3K{\cdot}2C_4H_8O$: C, 36.86 (36.73), H, 1.79 (1.54), N, 2.55 (2.68).

Synthesis of [K(THF)$_4$]$_2$[UO$_2$(NPh^{F}Ph)$_4$] (2). To a THF solution of [$UO_2Cl_2(THF)_2$]$_2$ (120 mg, 0.12 mmol, 1.0 equiv), KNPhPh$^F_2$ (292 mg, 0.98 mmol, 8.0 equiv) was added, causing an immediate color change to dark red. After stirring 1 h, the mixture was filtered through Celite

packed in a pipette. Volatiles were removed under vacuum, leaving a dark red residue. This residue was dissolved in THF and layered with hexanes. Storage at –21 °C gave dark red crystals of **2** overnight, which were collected by filtration over a medium porosity fritted filter in 2 crops and washed with hexanes. Yield: 240 mg, 0.17 mmol, 72%. Single crystal suitable for X-ray analysis was grown in the same manner but without drying. No resonances were observed in the ^{1}H NMR spectrum of **2** collected in THF. ^{1}F NMR (thf-h_8): –145.90 (d, 8F, J = 23 Hz, *o*-F), –167.78 (t, 8F, J = 21 Hz, *m*-F), –169.54(t, 4F, J = 23 Hz, *p*-F). Elemental analysis found (calculated) for $C_{48}H_{20}F_{20}K_2N_4O_2U$: C, 41.49 (41.75), H, 1.51 (1.46), N, 3.61 (4.06).

Synthesis of KNPh^{F}py. To a vial containing HNpyPh^{F} (1.56 g, 6 mmol, 1 equiv) suspended in 5 mL Et_2O, a 10 mL Et_2O solution of $KNTMS_2$ (1.19 g, 6 mmol, 1 equiv) was added, resulting in a yellow mixture. The solution was stirred for 2 h, slowly becoming transparent. The solution was filtered through Celite on a coarse porosity fritted filter and evaporated under vacuum. The resulting yellow solids were collected by filtration on a medium porosity fritted filter, washed with 3 × 5 mL hexanes and dried for 5 h. The resulting yellow powder was identified by NMR spectroscopy as KNpyPh^{F} with negligible solvation by Et_2O. Yield: 1.71 g, 5.7 mmol, 96%. ^{1}H NMR (pyr-d_5): δ 8.15 (d, J = 6.0 Hz, 1H), 7.33 (m, 1H), 6.62 (d, J = 8.4 Hz, 1H), 6.35 (m, 1H). ^{19}F NMR (pyr-d_5): δ –152.88 (d, 2F, J = 17 Hz, *o*-F), –168.73 (t, 2F, J = 18 Hz, *m*-F), –179.56 (s, 1F, *p*-F). HRMS (MeCN) observed (calculated) for $[C_{11}H_4F_5N_2+2H]^{+}$: 261.0451 (261.0452).

Synthesis of [K(THF)$_3$][UO$_2$(NPh^{F}py)$_3$] (3). To a THF solution of $[UO_2Cl_2(THF)_2]_2$ (194 mg, 0.20 mmol, 1.0 equiv), KNpyPh^{F} (358 mg, 1.20 mmol, 6.0 equiv) was added, causing an immediate color change to red. After stirring 1.5 h, the mixture was filtered through Celite packed on a coarse porosity fritted filter and was washed with 2 × 2 mL of THF. The filtrate was

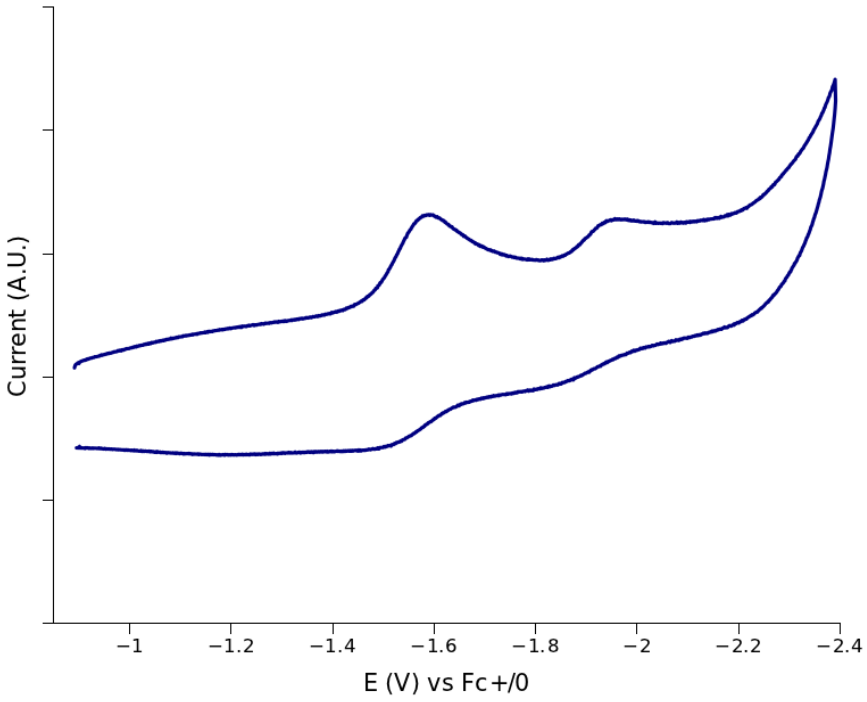
concentrated under vacuum and layered with hexanes. Storage at –21 °C produced red crystals of **3** overnight, which were collected by filtration on a medium porosity fritted filter and washed with pentane. Yield: 442 mg, 0.39 mmol, 98%. Single crystals suitable for X-ray analysis were grown in the same manner without drying. ^{1}H NMR (pyr-d_5): δ 8.96 (d, J = 6.0 Hz, 3H), 7.53 (m, 3H), 6.89 (d, J = 7.2 Hz, 3H), 6.50 (m, 3H), 3.67 (m, THF), 1.64 (m, THF). ^{19}F NMR (pyr-d_5): δ –145.90 (d, 2F, J = 20 Hz, *o*-F), –166.69 (m, 2F, J = 23 Hz, *m*-F), –168.75 (m, 1F, J = 20 Hz, *p*-F). Elemental analysis found (calculated) for $C_{33}H_{12}F_{15}N_6UO_2K{\cdot}0.5C_4H_8O$: C: 36.85 (37.45), H 1.75 (1.44), N 6.82 (7.49). (* Elemental analysis was attempted three times for this compound. High quality results were not obtainable due to persistent KCl adherence and variable solvation following multiple recrystallizations.)

Synthesis of [K(Toluene)]$_2$[UO$_2$(NAr^{F}Ph)$_4$] (4-tol). To a solution of $[UO_2Cl_2(THF)_2]_2$ (246 mg, 0.025 mmol, 1.0 equiv), KNAr^{F}Ph(THF)$_{0.5}$ (770 mg, 2.03 mmol, 8.0 equiv) was added, causing an immediate color change to dark red. After stirring 1.5 h, volatiles were removed in vacuum, leaving a green-black residue. This residue was dissolved in toluene, and the resulting green solution was filtered through Celite on a coarse porosity fritted filter. The filtrate was concentrated to a volume of 15 mL, and layered with 20 mL of pentane. Storage at –21 °C produced green-black crystals of **4-tol** overnight, which were collected by filtration over a medium porosity fritted filter and washed with pentane. Yield: 627 mg, 0.36 mmol, 71%. ^{1}H NMR (C_6D_6): δ 7.54 (8H), 7.32 (8H), 7.20 (4H), 7.02 (2H, tol), 6.82 (8H), 6.26 (4H), 2.12 (6H, tol-CH_3); peak multiplicity could not be assigned for this compound due to signal broadening. ^{19}F NMR (C_6D_6): δ –62.5 (24F). IR (KBr): 3060 (w), 2979 (w), 1605 (m), 1586 (m), 1479 (m), 1466 (m), 1368 (s), 1171 (s), 1125 (s), 1125 (s), 1024 (w), 994 (m), 953 (s), 858 (s), 826 (m), 778 (w), 774 (w), 731 (w), 708 (m), 700 (m), 682 (m), 604 (w), 505 (m), 460 (w). Elemental

analysis found (calculated) for $C_{56}H_{32}F_{24}K_2N_4O_2U{\cdot}2C_7H_8$: C, 47.92 (48.06); H, 3.02 (2.77); N, 3.13 (3.20).

Synthesis of $[K(18\text{-c-}6)]_2[UO_2(NAr^FPh)_4]$ (4-crown). To a solution of $KNAr^FPh(THF)_{0.5}$ (150 mg, 0.40 mmol, 8.0 equiv) in 4 mL THF, added $[UO_2Cl_2(THF)_2]_2$ (48 mg, 0.05 mmol, 1.0 equiv), resulting in an immediate color change to dark red. After stirring 45 minutes, volatiles were removed under reduced pressure to yield a black residue. This residue was extracted with toluene and filtered to produce a dark green solution. To this solution, 18-crown-6 (52 mg, 0.20 mmol, 2.0 equiv) was added, causing a color change to red with immediate formation of red precipitate. The red solid was collected by filtration over a medium frit and washed with toluene and then hexanes. Recrystallization from a DME solution layered with hexanes at –21 °C produced **4-crown** as a red crystalline solid. Yield: 151 mg, 0.07 mmol, 73%. Alternatively, **4-crown** could be prepared as a THF solvate by recrystallization from a THF solution layered with hexanes at –21 °C, but the solid produced from this route was multi-crystalline. ^{1}H NMR (pyr-d_5): δ 8.26 (s, 8H), 7.89 (d, J = 8 Hz, 8H), 7.29 (t, J = 8Hz, 8H), 7.10 (s, 4H), 6.80 (t, J = 7 Hz, 4H), 3.68 (m, 16H), 3.43 (s, 48H, 18-c-6), 1.64 (m, 16H). ^{19}F NMR (pyr-d_5): δ –61.1 (24F). IR (KBr): 3056 (w), 2913 (m), 1599 (m), 1587 (m), 1487 (m), 1474 (m), 1465 (m), 1368 (s), 1276 (s), 1168 (s), 1108 (s), 1028 (w), 993 (m), 982 (m), 962 (m), 951 (m), 910 (w), 855 (m), 837 (w), 770 (w), 728 (w), 699 (m), 681 (m), 604 (w), 504 (m), 465 (w). Elemental analysis found (calculated) for $C_{80}H_{80}F_{24}K_2N_4O_{14}U$: C, 45.75 (45.89); H, 4.08 (3.85); N, 2.49 (2.68).

Electrochemical Data



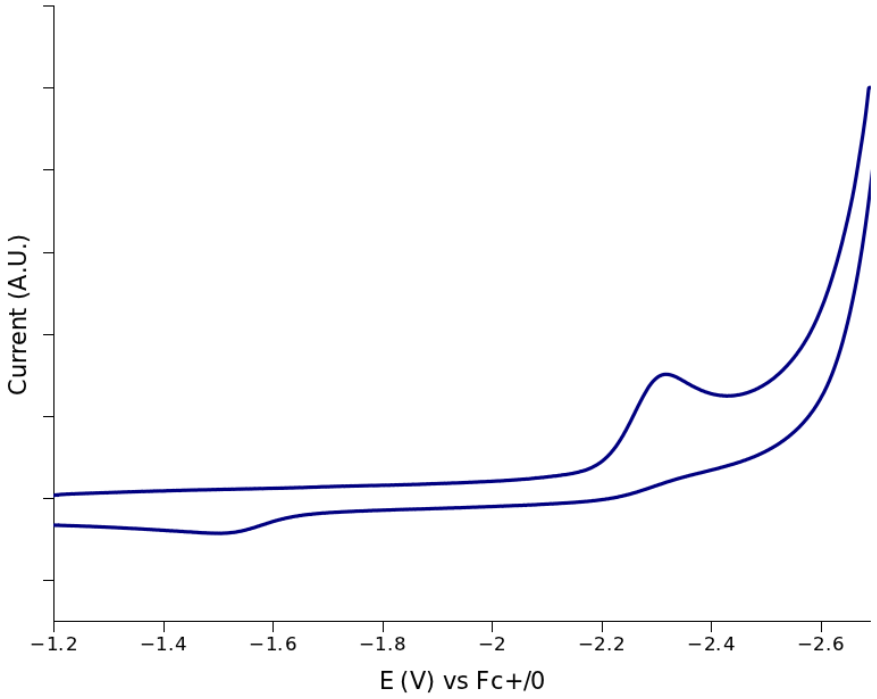


Figure S1. Cyclic voltammograms of **4-tol** (top) and **4-crown** (bottom) performed in CH_2Cl_2, referenced to an internal ferrocene/ferrocenium reference.

IR Spectra

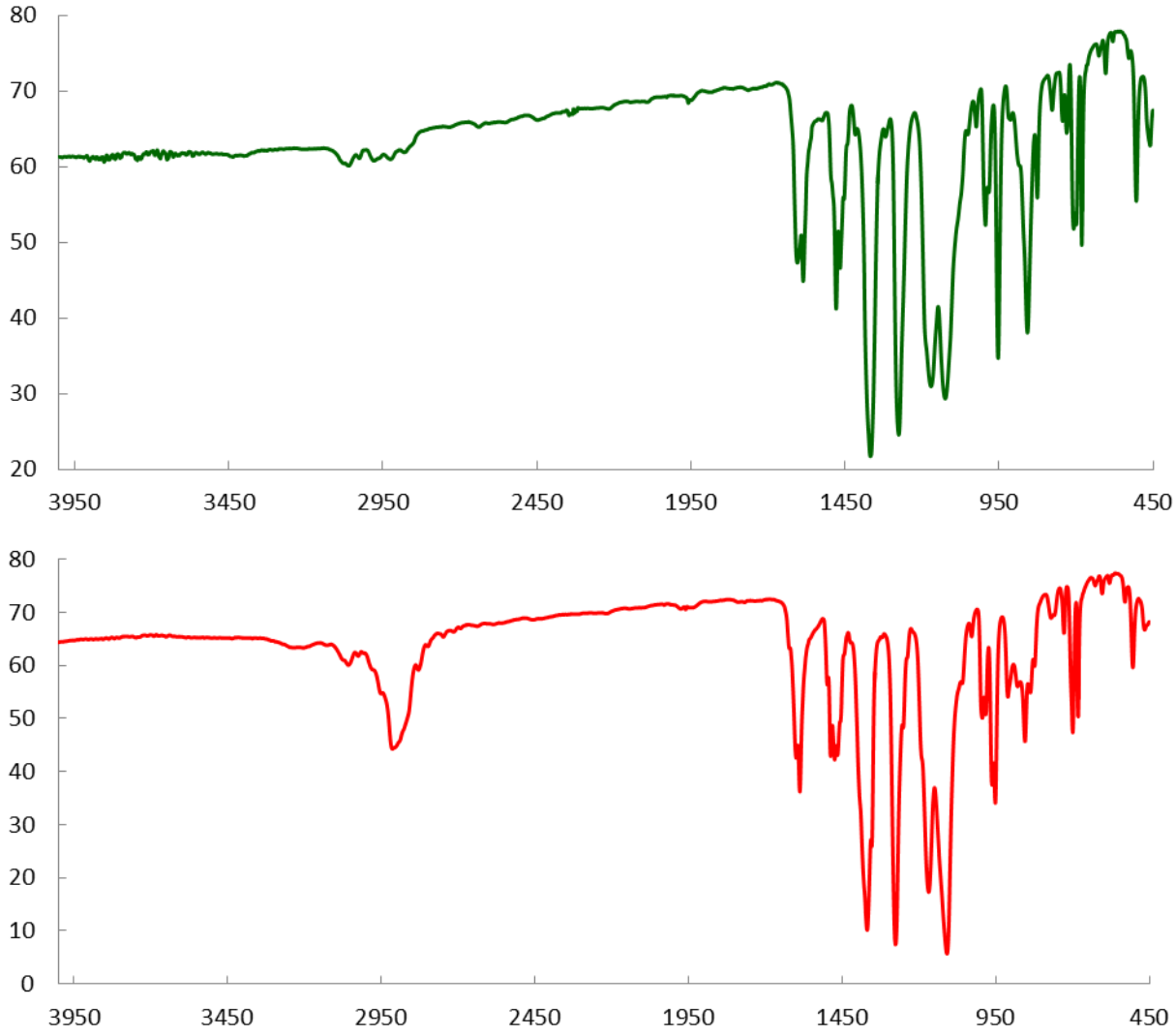


Figure S2. IR spectra of **4-tol** (top) and **4-crown** (bottom).

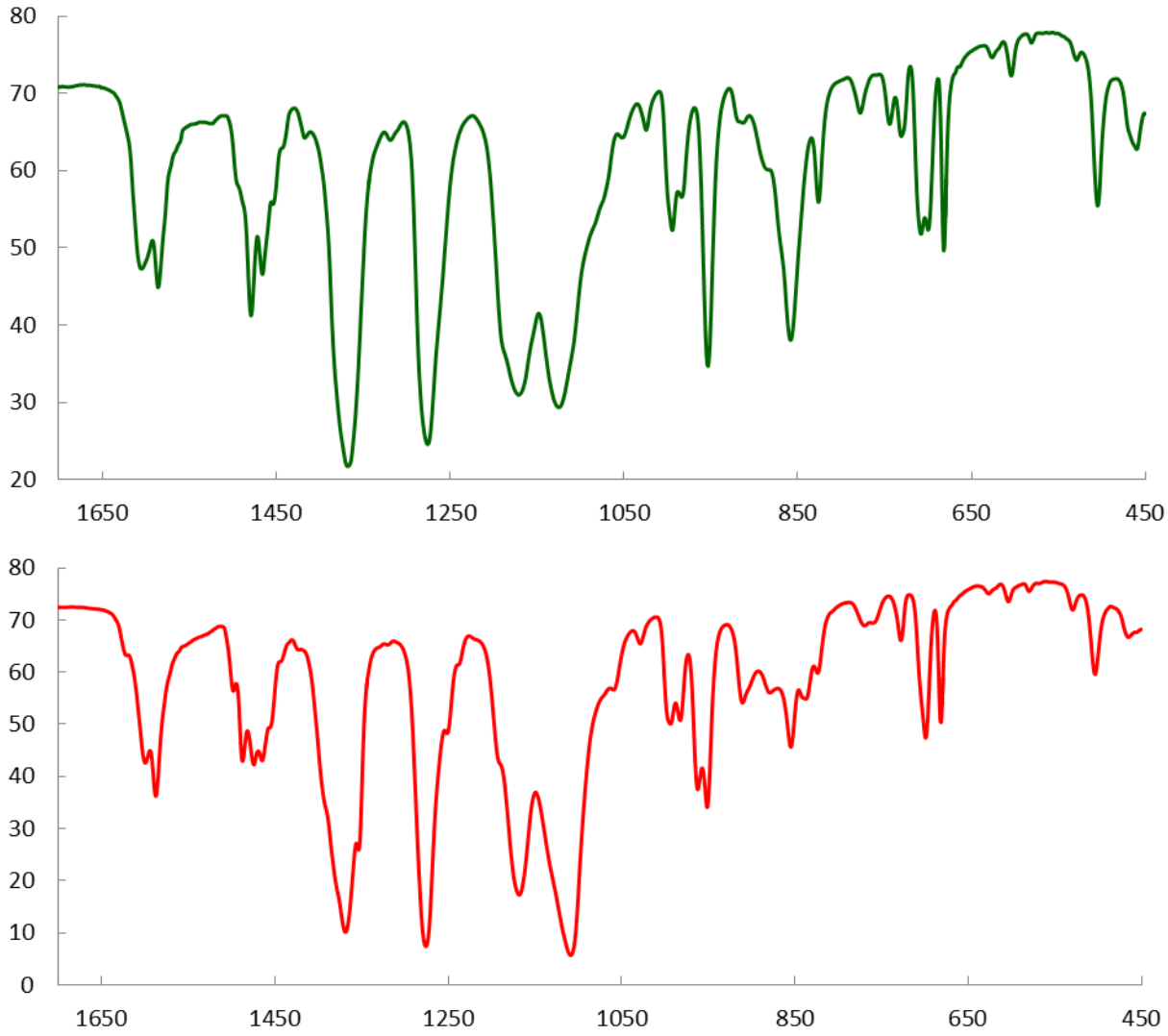


Figure S3. IR spectra of **4-tol** (top) and **4-crown** (bottom), highlighting the fingerprint region.

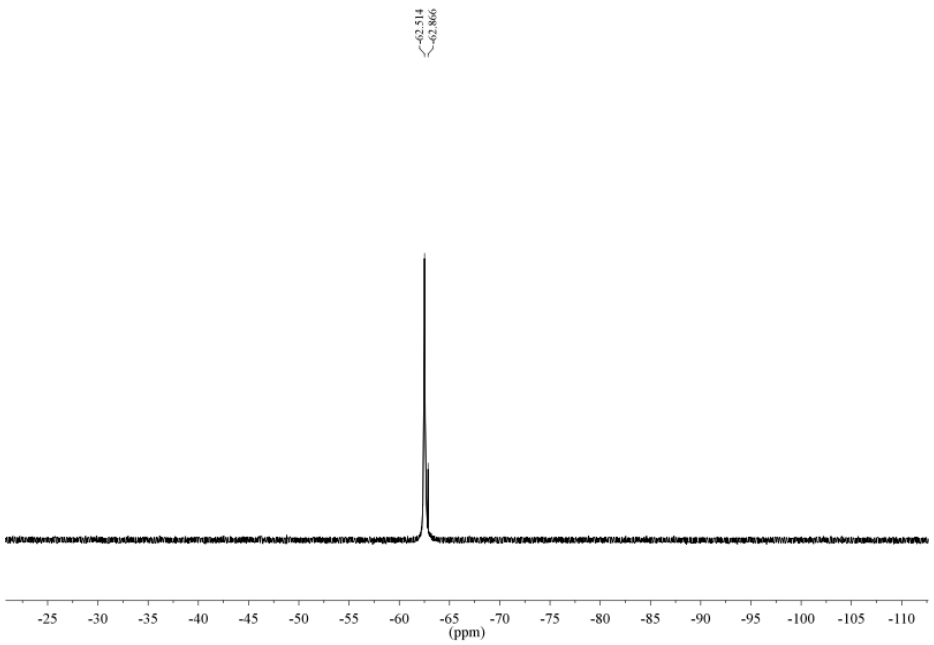


Figure S4. ^{19}F NMR spectrum of **4-tol** in benzene-d_6. The visible smaller resonance is due to a slight impurity of HNAr^{F}Ph.

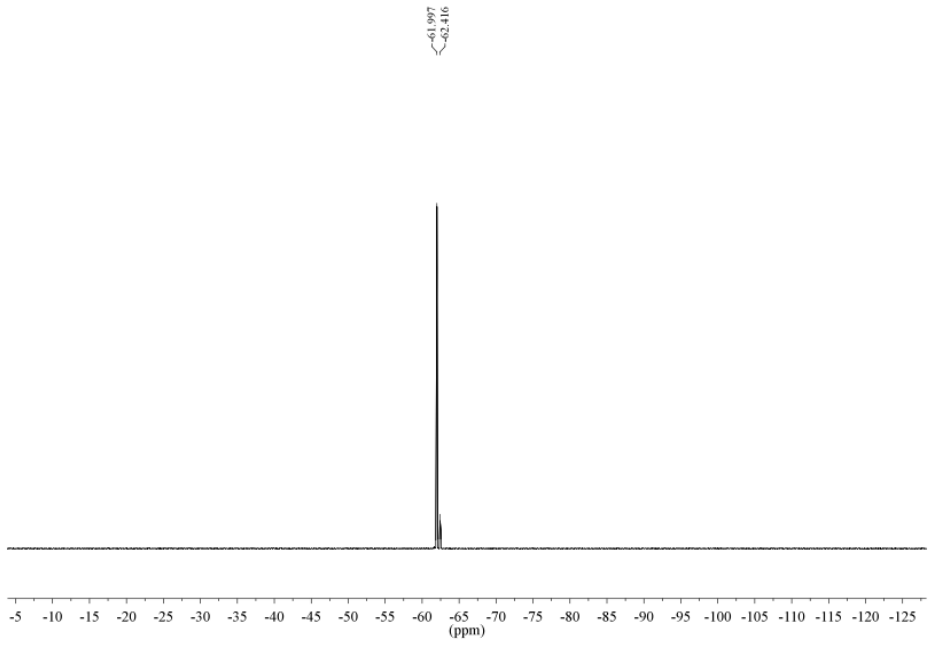


Figure S5. ^{19}F NMR spectrum of **4-crown** in pyridine-d_5. The visible smaller resonance is due to a slight impurity of HNAr^{F}Ph.

Computational Details

Gaussian 09 Rev. D.01 was used for all electronic structure calculations.[8] The B3LYP hybrid DFT method was employed, with a 60-electron small core pseudopotential on uranium with published segmented natural orbital basis set incorporating quasi-relativistic effects,[9,10] and the 6-31G* basis set for all other atoms. Geometry optimization on **4-tol** and the anionic portion of **4-crown** was carried out starting from the coordinates of the X-ray crystal structures. Frequency calculations indicated that the optimized geometry were minima by absence of imaginary frequencies. Calculated metal-ligand bond lengths were in good agreement with the X-ray crystal structures. Molecular orbitals were rendered with the program Chemcraft v1.6.[11] Mayer bond orders were calculated with Gaussian with keyword IOp(6/80=1). TD-DFT calculations incorporated dichloromethane solvation using a PCM model.

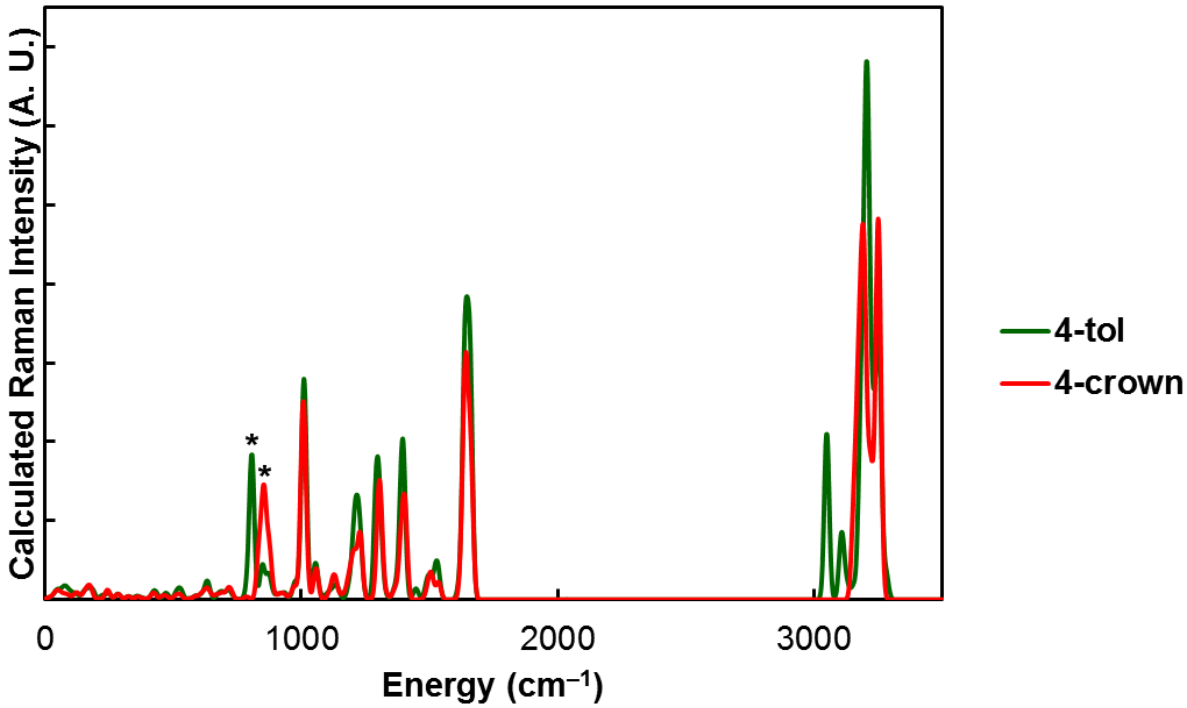


Figure S6. Calculated raman spectra for complexes **4-tol** and **4-crown**, with the predicted ν_1 O=U=O vibrational modes for each complex indicated (*), with underlying transition energies of 807 cm^{-1} for **4-tol** and 854 cm^{-1} for **4-crown**. The predicted spectral lines were slightly broadened.

Table S1. Optimized geometry of anion of **4-crown**.

U	-0.00002097	0.38614611	-0.00007017
F	-6.22552818	5.40882152	-0.47646329
F	-4.46809042	6.17863017	0.55293035
F	-4.36444395	5.69560337	-1.55973919
F	-7.01844446	0.68408933	-0.58172230
F	-5.68465363	-0.60972829	0.55307872
F	-5.33625391	-0.27971941	-1.56323172
F	-5.47682540	-4.50435283	2.81668640
F	-3.57173248	-5.46119409	3.21632490
F	-4.85926083	-6.21365001	1.63015197
F	-5.14833566	-3.76508280	-2.64666569
F	-3.06909622	-4.19352420	-3.10281308
F	-3.76407774	-2.13552183	-3.05616153
O	1.20554059	0.40712232	1.31277642
N	-1.38373937	2.11911599	1.13361149
N	-1.23814201	-1.37550515	1.24369764
C	-0.86780304	3.00856700	2.09892297
C	-1.62863174	3.40662158	3.22350249
H	-2.64405419	3.03432560	3.33034499
C	-1.09819159	4.25686516	4.19149118
H	-1.71209649	4.53751592	5.04619313
C	0.20899032	4.73978375	4.07980847
H	0.62074973	5.40362384	4.83671057
C	0.97540073	4.35366204	2.97727777
H	1.99102534	4.72370064	2.85294178
C	0.44637831	3.50836709	2.00374216
H	1.04656396	3.23283419	1.14641117
C	-2.69207726	2.35537418	0.71974380
C	-3.18889942	3.66365400	0.49244383
H	-2.54995594	4.51240922	0.71032457
C	-4.46040534	3.87546765	-0.03516881
C	-5.30887190	2.80675552	-0.33871338
H	-6.29848834	2.97624414	-0.74201170
C	-4.84469719	1.51407185	-0.08906106
C	-3.57283280	1.28621087	0.43385311
H	-3.24290359	0.27487506	0.63711533
C	-4.87782655	5.27569549	-0.37086107
C	-5.71345786	0.33091510	-0.41710406
C	-0.84985058	-1.45712086	2.61538124
C	-1.32363748	-0.51802795	3.54524642
H	-2.00291791	0.25520219	3.20225592
C	-0.90207409	-0.55312667	4.87574340
H	-1.26873528	0.19898020	5.57102922
C	-0.00542179	-1.53166847	5.30764876
H	0.33276561	-1.55025473	6.34151198

C	0.46831464	-2.47682128	4.39329134
H	1.19040309	-3.22840655	4.70064599
C	0.04623144	-2.44415063	3.06478774
H	0.42876981	-3.17028174	2.35395329
C	-2.17285770	-2.29943468	0.82729677
C	-2.79248128	-3.24034919	1.69787517
H	-2.52202143	-3.25225952	2.74582656
C	-3.73516659	-4.15569913	1.23285066
C	-4.12655230	-4.19233009	-0.10537724
H	-4.85802438	-4.90675250	-0.46010166
C	-3.53924694	-3.26281450	-0.97083794
C	-2.59471787	-2.34331070	-0.53199009
H	-2.17744883	-1.63152708	-1.23241971
C	-4.39904153	-5.07559020	2.21465513
C	-3.88093243	-3.32113223	-2.43191870
F	6.22440421	5.40975139	0.47684750
F	4.46689443	6.17927666	-0.55263643
F	4.36314768	5.69604734	1.55997639
F	7.01827444	0.68514788	0.58170727
F	5.68479995	-0.60884623	-0.55326429
F	5.33619972	-0.27904618	1.56304285
F	5.47752921	-4.50409909	-2.81610289
F	3.57247710	-5.46103893	-3.21571565
F	4.85991184	-6.21320608	-1.62933091
F	5.14943605	-3.76298069	2.64674912
F	3.07051078	-4.19255403	3.10319626
F	3.76430974	-2.13415772	3.05622841
O	-1.20559272	0.40682930	-1.31290704
N	1.38342435	2.11918677	-1.13395099
N	1.23825986	-1.37540502	-1.24369955
C	0.86738364	3.00843306	-2.09940347
C	1.62811555	3.40631208	-3.22410696
H	2.64357069	3.03409610	-3.33092710
C	1.09753808	4.25629129	-4.19225521
H	1.71136907	4.53681540	-5.04705221
C	-0.20968664	4.73909713	-4.08061386
H	-0.62154903	5.40272874	-4.83764235
C	-0.97601316	4.35312908	-2.97797013
H	-1.99167250	4.72308331	-2.85367054
C	-0.44685143	3.50809702	-2.00428352
H	-1.04694793	3.23265412	-1.14686513
C	2.69167847	2.35569303	-0.71998434
C	3.18823492	3.66405347	-0.49251547
H	2.54913549	4.51270041	-0.71035529
C	4.45963832	3.87607087	0.03525557
C	5.30829515	2.80750442	0.33878719

H	6.29784348	2.97715361	0.74218314
C	4.84439913	1.51475423	0.08896117
C	3.57262927	1.28668511	-0.43409031
H	3.24296699	0.27529372	-0.63751198
C	4.87673952	5.27635419	0.37111384
C	5.71336467	0.33173980	0.41697980
C	0.85007439	-1.45717554	-2.61542309
C	1.32395662	-0.51820459	-3.54535016
H	2.00322581	0.25505832	-3.20240222
C	0.90249151	-0.55345303	-4.87587767
H	1.26922851	0.19855579	-5.57122988
C	0.00583564	-1.53201363	-5.30773248
H	-0.33226100	-1.55071006	-6.34162337
C	-0.46800463	-2.47703951	-4.39329819
H	-1.19008570	-3.22864961	-4.70060944
C	-0.04601803	-2.44421652	-3.06476604
H	-0.42861603	-3.17025511	-2.35387654
C	2.17320168	-2.29909454	-0.82720773
C	2.79290596	-3.24010851	-1.69761742
H	2.52239541	-3.25230102	-2.74554858
C	3.73575590	-4.15521454	-1.23244207
C	4.12724596	-4.19147578	0.10576403
H	4.85884266	-4.90572211	0.46059589
C	3.53987755	-3.26184158	0.97105475
C	2.59517849	-2.34258633	0.53205585
H	2.17784541	-1.63072172	1.23236434
C	4.39970530	-5.07525299	-2.21405968
C	3.88176009	-3.31977238	2.43210754

Table S2. Optimized coordinates of **4-tol**.

U	0.00662906	0.16751801	-0.03412401
N	-0.68434896	1.79452615	-1.69394014
N	-0.36919901	-1.64191412	-1.64461014
N	0.47306806	-1.46774712	1.74163912
N	0.60721314	1.94973814	1.55255811
O	1.72169619	0.18870998	-0.60020106
O	-1.69765407	0.17104505	0.56728203
C	0.18650412	2.67540720	-2.37691419
C	1.31344622	3.22690822	-1.73790615
H	1.47697323	3.01159420	-0.69025906
C	2.19070530	4.07228527	-2.41800820
H	3.02439337	4.51174428	-1.87526816
C	1.97392129	4.39150529	-3.76119630
H	2.64512036	5.06713933	-4.28486834
C	0.86118520	3.84975228	-4.41239135
H	0.67127919	4.08903030	-5.45622543

C	-0.01874589	3.00682123	-3.73601230
H	-0.88095596	2.59886622	-4.25623234
C	-2.05398607	1.99361519	-1.92937316
C	-2.92702915	0.90274413	-2.10915317
H	-2.51428714	-0.09628496	-2.17236418
C	-4.30704825	1.09453817	-2.20196518
C	-4.86458327	2.37010028	-2.14925417
H	-5.93389236	2.51521432	-2.23513318
C	-4.00596319	3.46147835	-1.98373916
C	-2.62889808	3.28649230	-1.89204115
H	-1.98381802	4.14758036	-1.75632614
C	-5.20879235	-0.10698790	-2.26103218
C	-4.60641720	4.81925447	-1.75501214
C	0.58652606	-1.78329515	-2.68384821
C	0.85237210	-0.71874507	-3.56714729
H	0.26320908	0.18662801	-3.48249328
C	1.85779618	-0.81690310	-4.53356036
H	2.02951521	0.02060896	-5.20587141
C	2.62130621	-1.98456721	-4.65123337
H	3.39214227	-2.06706923	-5.41312543
C	2.35457617	-3.05874728	-3.79219630
H	2.93530319	-3.97428637	-3.86384131
C	1.34980609	-2.96219526	-2.82836423
H	1.15764006	-3.79983532	-2.16540218
C	-1.44897511	-2.52345916	-1.66678814
C	-2.26464818	-2.68024816	-0.52397205
H	-1.99726014	-2.16217312	0.38469902
C	-3.42522428	-3.44797419	-0.55400505
C	-3.80716333	-4.14828424	-1.69842014
H	-4.71215440	-4.74111126	-1.72098214
C	-2.98936326	-4.03750524	-2.82490723
C	-1.84460916	-3.24406621	-2.82201123
H	-1.26688811	-3.15494421	-3.73384729
C	-4.25003535	-3.52862918	0.69742204
C	-3.32951530	-4.82351830	-4.06373032
C	-0.40759001	-1.44809610	2.86243821
C	-0.39219399	-0.39486202	3.79670828
H	0.32477608	0.40687302	3.66741227
C	-1.28465605	-0.37416400	4.87484736
H	-1.24021503	0.44528606	5.58837343
C	-2.21851015	-1.40378506	5.04223238
H	-2.90352520	-1.39350305	5.88595943
C	-2.24207217	-2.45930714	4.12163730
H	-2.96034224	-3.26743519	4.22862231
C	-1.34115210	-2.48590716	3.05487722
H	-1.36200312	-3.31091523	2.35109117

C	1.57136912	-2.30927421	1.87918013
C	2.06378615	-2.72743625	3.14391323
H	1.55181212	-2.41627922	4.04590430
C	3.20345822	-3.51509234	3.25649524
C	3.90994027	-3.94162738	2.13025415
H	4.79371232	-4.55824745	2.22648916
C	3.42651124	-3.55871634	0.87949405
C	2.28010017	-2.77257426	0.74540904
H	1.89675214	-2.52982623	-0.23835803
C	3.74222526	-3.84038437	4.62463934
C	4.12821328	-4.03402639	-0.35889904
C	-0.32712192	2.78007122	2.19835416
C	-1.52926900	3.15346727	1.55746711
H	-1.67461202	2.88106526	0.52035303
C	-2.50816806	3.89913435	2.21817716
H	-3.39667112	4.20134439	1.66731212
C	-2.31995603	4.30614038	3.54350626
H	-3.07057308	4.90451144	4.05233930
C	-1.12390695	3.96907632	4.18569331
H	-0.94812293	4.29125935	5.20952339
C	-0.14523389	3.22332925	3.53069226
H	0.77486717	2.97282821	4.05153130
C	1.96378325	2.23079713	1.75834312
C	2.48206631	3.54543022	1.66805511
H	1.79747328	4.37736229	1.54410311
C	3.85449143	3.77598721	1.66915211
C	4.76962747	2.72403911	1.79082012
H	5.83594858	2.91259610	1.78948613
C	4.26667341	1.43146702	1.92003813
C	2.89284130	1.18585403	1.93025513
H	2.52665425	0.17322496	2.04009114
C	4.38335849	5.15212030	1.37663909
C	5.19566645	0.25307791	1.96297814
F	-4.70404233	-1.10173499	-3.01249124
F	-5.40618040	-0.62482294	-1.00964209
F	-6.43688644	0.19224215	-2.73990922
F	-5.73117630	5.01318050	-2.47561220
F	-3.75788711	5.82495254	-2.03720317
F	-4.96640022	4.96968848	-0.44161705
F	-3.67590132	-4.30946025	1.64922711
F	-4.41062933	-2.29913208	1.28369509
F	-5.48661047	-4.01561419	0.48473703
F	-4.65779541	-5.05023129	-4.17188233
F	-2.93370626	-4.19348626	-5.19216641
F	-2.72600328	-6.03686940	-4.06380332
F	2.76731818	-3.89652536	5.55867240

F	4.63053534	-2.90659432	5.04054337
F	4.38849028	-5.02817247	4.64267034
F	5.25863635	-4.71225747	-0.10381702
F	3.35043320	-4.82090044	-1.13458710
F	4.49796634	-2.97689832	-1.17052310
F	3.50643445	6.12681641	1.68118412
F	5.53276256	5.40958629	2.03700614
F	4.67108552	5.28328431	0.04667399
F	4.90943841	-0.60936915	2.95093122
F	5.11331543	-0.47218814	0.79282005
F	6.49235057	0.61081291	2.08306115
K	3.86977934	-0.44475011	-1.89108216
C	5.86769551	1.10495596	-4.21070833
C	5.43272451	2.14244005	-3.36842227
H	4.75294947	2.89724512	-3.75580730
C	5.85440353	2.21748305	-2.03618117
H	5.50896054	3.03340912	-1.40660312
C	6.71679560	1.24421096	-1.51738513
H	7.03711463	1.28907595	-0.48150805
C	7.14562560	0.19658687	-2.34003119
H	7.81307962	-0.56547620	-1.94593016
C	6.72281054	0.12903587	-3.67230629
H	7.07441760	-0.68243920	-4.30590534
C	5.45620448	1.06558997	-5.66482742
H	6.13019055	1.67968500	-6.27624548
H	4.44359342	1.45773902	-5.80717044
H	5.48976749	0.04755689	-6.06680348
K	-3.36044820	0.47465711	2.53464618
C	-6.64756842	1.34629024	2.10773015
C	-6.33575041	2.06203029	3.27775524
H	-6.33264138	3.14941137	3.25264823
C	-6.04744739	1.39681423	4.47272133
H	-5.82396737	1.97025827	5.36872941
C	-6.05940140	-0.00259087	4.51982634
H	-5.85453043	-0.51969692	5.45317139
C	-6.34714645	-0.72743392	3.36112625
H	-6.34473345	-1.81338900	3.37768925
C	-6.63309246	-0.05760887	2.16599615
H	-6.84063948	-0.63036890	1.26678309
C	-7.02250246	2.06502730	0.83254005
H	-6.40699539	2.95503836	0.66269504
H	-8.06865254	2.39608735	0.87119106
H	-6.91540847	1.40602825	-0.03264701

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