Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

CF_3-Substituted Sulfonium Cations as Efficient Chalcogen Bond Donors towards Cyanometalates

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Experimental Section

2,8-Difluoro-S-(trifluoromethyl)dibenzothiophenium trifluoromethanesulfonate and potassium tetrakis-(pentafluorophenyl)borate were commercially obtained (Sigma Aldrich, ABCR GmBH) and used without further purification. 5-(Trifluormethyl)thianthrenium trifluoromethanesulfonate[1] was used from laboratory stock. Potassium pentacarbonylcyanomolybdate(0), tetraethylamonnium pentacarbonylcyanomolybdate(0) and 3-nitro-S-(trifluoromethyl)dibenzothiophenium hexafluoroantimonate were synthesized by modified procedures.[2,3] Also an old batch of tetraethylamonnium pentacarbonylcyanomolybdate(0) was used which later turned out to be contaminated with 18% of the analogous tungsten compound. All reactions were carried out in previously heated glassware under an atmosphere of argon using standard Schlenk techniques and an oil pump vacuum of 10^{-3} mbar. Solvents were dried over activated 3 Å molecular sieves and stored under argon. NMR spectra were measured on a JEOL ECX 400 (400 MHz).

Infrared (IR) spectroscopy

IR spectroscopy was measured on a FT (Fourier transformation) Nicolet iS10 or iS50 IR-spectrometer. The sample was directly measured by ATR (attenuated total reflection) technique. Characteristic absorptions are given in wavenumbers $\tilde{\nu}$ [cm^{-1}] and intensities are stated as vs (very strong), s (strong), m (medium) and w (weak).

Mass Spectrometry

Mass spectrometry was performed on an Agilent 6210 ESI TOF (electrospray ionization time-offlight spectrometer) of Agilent Technologies, Santa Clara, CA in negative mode. Flow rates were set to 10 $\mu L min^{-1}$. The evaluation of the resulting data occurred by using Mmass 5.5.0

Potassium pentacarbonylcyanomolybdate(0):

Molybdenum hexacarbonyl (2.00 g, 7.575 mmol, 1 equiv.) and potassium bis(trimethylsiyl)amide (1.51, 7.575 mmol, 1 equiv.) were suspended in 100 ml of benzene and heated to 80°C for 24 hours. The

reaction mixture was filtered and the residue extensively washed with benzene (300 mL) and diethylether (300 mL). The product was dried in vacuo resulting in an off-white solid (1.85 g). The obtained analytical data was in full agreement with the reported literature.[2]

Tetraethylammonium pentacarbonylcyanomolybdate(0):

Potassium pentacarbonylcyanomolybdate (1.17 g, 3.885 mmol, 1 equiv.) was dissolved in 5 ml of water. and slowly added to an aqueous solution of tetraethylammoniumbromide (0.98 g 4.663 mmol, 1.2 equiv.). The resulting suspension was filtered and the precipitate washed with water (200 mL). Recyrstallization in CH_2Cl_2/benzene resulted in a pink solid which was further dried in vacuo (1.52 g).

IR(ATR): $\tilde{\upsilon}_{max}$ = 2064 (m), 1994 (s), 1970 (vs), 1860 (vs),1812 (vs) cm^{-1}.

HRMS (ESI) calc. for MoC_6O_5N $[M]^-$: 263.8831; found: $[M]^-$ 263.8992, $[M\text{-}CO]^-$: 235.9224, $[M\text{-}2CO]^-$ 207.9088.

Elemental analysis for $C_{14}H_{20}MoO_5N$: calculated: C: 42.87%, 5.14%, N: 7.14%; found: C: 42.88, H: 5.22%, N: 7.17%,

2,8-Difluoro-S-(trifluoromethyl)dibenzothiophenium tetrakis(pentafluorophenyl)borate:

2,8-Difluoro-S-(trifluormethyl)thianthrenium trifluoromethanesulfonate (44.0 mg, 0.100 mmol, 1.0 equiv.) and $KB(C_6F_5)_4$ (70.0 mg, 0.100 mmol, 1 equiv.) were dissolved in 2 ml of *o*-difluorobenzene and stirred at room temperature for 1 h. The reaction mixture was filtered with a syringe filter and transferred to a fresh Schlenk flask and the solvent was evaporated *in vacuo*. This yielded the desired product as a colorless solid in quantitative yields (95.0 mg).

^{1}H NMR (400 MHz, Aceton-d_6): δ (ppm) = 8.86 (dd, $^2J_{HH}$ = 9.0 Hz, $^3J_{HH}$ = 4.5 Hz, 2H), 8.51 (dd, $^2J_{HH}$ = 8.5 Hz, 2H, $^4J_{HH}$ = 2.7), 7.84 (dt, $^3J_{HH}$ = 8.8 Hz, $^4J_{HH}$ = 2.7 Hz, 2H).

^{13}C{^{1}H} NMR (101 MHz, Aceton-d_6): δ (ppm) = 170.0, 167.5, 150.2, 148.0, 145.3 (d, J = 9.1 Hz), 140.3, 138.3, 135.9, 133.7 (d, J = 10.5 Hz), 126.0, 121.3 (d, J = 25 Hz), 120.6, 114.7 (d, J = 26.7 Hz).

^{19}F NMR (377 MHz, Aceton-d_6): δ (ppm) = −52.4 (s, 3F), −93.4 (s, 2F), −133.1 (s, 8F), −163.4 (t, $^3J_{FF}$ 21.0 Hz, 4F), −167.39 (t, $^3J_{FF}$ = 22.0 Hz, 8F).

2,8-Difluoro-S-(trifluoromethyl)dibenzothiophenium pentacarbonylcyanomolybdate(0):

2,8-Difluoro-S-(trifluormethyl)thianthrenium trifluoromethanesulfonate (25.0 mg, 57.0 µmol, 1.0 eq.) and $KB(C_6F_5)_4$ (40.0 mg, 57.0 µmol, 1.0 equiv.) were dissolved in 2 ml of *o*-difluorobenzene and stirred at room temperature for one hour. The reaction mixture was filtered with a syringe filter and transferred to a fresh Schlenk flask loaded with $[NEt_4][Mo(CO)_5(CN)]$ (22.0 mg, 57.0 µmol, 1.0 equiv.). The reaction mixture was stirred for 12 h at room temperature. All volatiles were removed and the mixture dissolved in a minimum amount of CH_2Cl_2, followed by layering with *n*-pentane and placing it in a −78

°C freezer. After a few days yellow crystals of the desired product could be obtained which where suitable for X-ray diffraction analysis. Removal of $[NEt_4][B(C_6F_5)_4]$ from the bulk was not possible.

5-(Trifluoromethyl)thianthrenium pentacarbonylcyanomolybdate(0):

5-(Trifluormethyl)thianthrenium trifluoromethanesulfonate (44.0 mg, 0.100 mmol, 1.0 equiv.) and $[NEt_4][Mo(CO)_5(CN)]$ (40.0 mg, 0.100 mmol, 1.0 equiv.) were dissolved in 2 ml of CH_2Cl_2 and stirred at room temperature for 12 h. The reaction mixture was layered with *n*-pentane and placed in a −78 °C freezer. After a few days yellow crystals could be obtained suitable for x-ray diffraction analysis. Removal of $[NEt_4][CF_3SO_3]$ from the bulk was not possible.

3-Nitro-S-(Trifluoromethyl)dibenzothiophenium pentacarbonylcyanomolybdate(0):

3-Nitro-S-(trifluoromethyl)dibenzothiophenium hexafluoroantimonate (41.0 mg, 76.0 µmol, 1.0 equiv.) and $NEt_4[Mo_{0.822}W_{0.178}(CO)_5(CN)]$ (30 mg, 0.076 mmol, 1 equiv refering to 100% Mo.) were dissolved in CH_2Cl_2 and stirred at room temperature for 12 h. The reaction mixture was layered with *n*-pentane and placed in a −78 °C freezer. After a few days red crystals could be obtained suitable for x-ray diffraction analysis. However, removal of $[NEt_4][SbF_6]$ from the bulk was not possible.

Crystallographic Details

X-Ray data were collected on a BRUKER D8 Venture system. Data were collected at 105(2) K using graphite-monochromated Mo Kα radiation (λα = 0.71073 Å). The strategy for the data collection was evaluated by using the Smart software. The data were collected by the standard "ψ-ω scan techniques" and were scaled and reduced using Saint+software. The structures were solved by using Olex2,[4] the structure was solved with the XT[5] structure solution program using Intrinsic Phasing and refined with the XL[6] refinement package using Least Squares minimization. If it is noted, bond length and angles were measured with Diamond Crystal and Molecular Structure Visualization Version 3.1.[7] Drawings were generated with Mercury.[8]

Identification code	**Ritter · $[Mo(CO)_5(CN)]$**	**$UmeF_2$ · $[Mo(CO)_5(CN)]\cdot CH_2Cl_2$**	**$UmeNO_2$ · $[Mo0_{.822}W_{0.178}(CO)_5(CN)]\cdot CH_2Cl_2$**
CCDC Number	2298717	2298718	2298719
Empirical formula	$C_{19}H_8F_3MoNO_5S_2$	$C_{20}H_8Cl_2F_5MoNO_5S$	$C_{20}H_9Cl_2F_3Mo_{0.822}W_{0.178}N_2O_7S$
Formula weight	547.32	636.17	645.19
Temperature/K	100.00	100.00	105.00
Crystal system	triclinic	monoclinic	triclinic
Space group	P-1	C2/c	P-1
a/Å	9.5818(4)	18.1737(7)	10.1988(4)
b/Å	10.4568(5)	10.1525(3)	10.2849(4)

c/Å	11.5348(5)	25.8418(7)	13.3894(5)
α/°	114.713(2)	90	73.1800(10)
β/°	94.029(2)	90.060(2)	85.274(2)
γ/°	96.506(2)	90	62.991(2)
Volume/Å^3	1034.22(8)	4768.0(3)	1195.77(8)
Z	2	8	2
ρ_{calc}g/cm^3	1.758	1.772	1.792
μ/mm^{-1}	0.894	0.933	0.927
F(000)	540.0	2496.0	636.0
Crystal size/mm^3	0.931 × 0.495 × 0.458	0.714 × 0.61 × 0.527	0.203 × 0.103 × 0.087
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.342 to 60.948	4.482 to 56.692	4.49 to 50.716
Index ranges	-13 ≤ h ≤ 13, -14 ≤ k ≤ 14, -16 ≤ l ≤ 16	-24 ≤ h ≤ 20, -13 ≤ k ≤ 13, -34 ≤ l ≤ 34	-12 ≤ h ≤ 12, -12 ≤ k ≤ 12, -16 ≤ l ≤ 16
Reflections collected	33264	29494	17918
Independent reflections	6242 [R_{int} = 0.0341, R_{sigma} =0.0228]	5912 [R_{int} = 0.0439, R_{sigma} =0.0339]	4343 [R_{int} = 0.0334, R_{sigma} = 0.0276]
Data/restraints/parameters	6242/0/280	5912/0/316	4343/0/325
Goodness-of-fit on F^2	1.076	1.185	1.109
Final R indexes [I>=2σ (I)]	R_1 = 0.0216, wR_2 = 0.0541	R_1 = 0.0462, wR_2 = 0.0929	R_1 = 0.0520, wR_2 = 0.1380
Final R indexes [all data]	R_1 = 0.0243, wR_2 = 0.0558	R_1 = 0.0550, wR_2 = 0.0966	R_1 = 0.0603, wR_2 = 0.1480
Largest diff. peak/hole / e Å^{-3}	0.48/-0.69	1.31/-0.74	1.25/-0.99

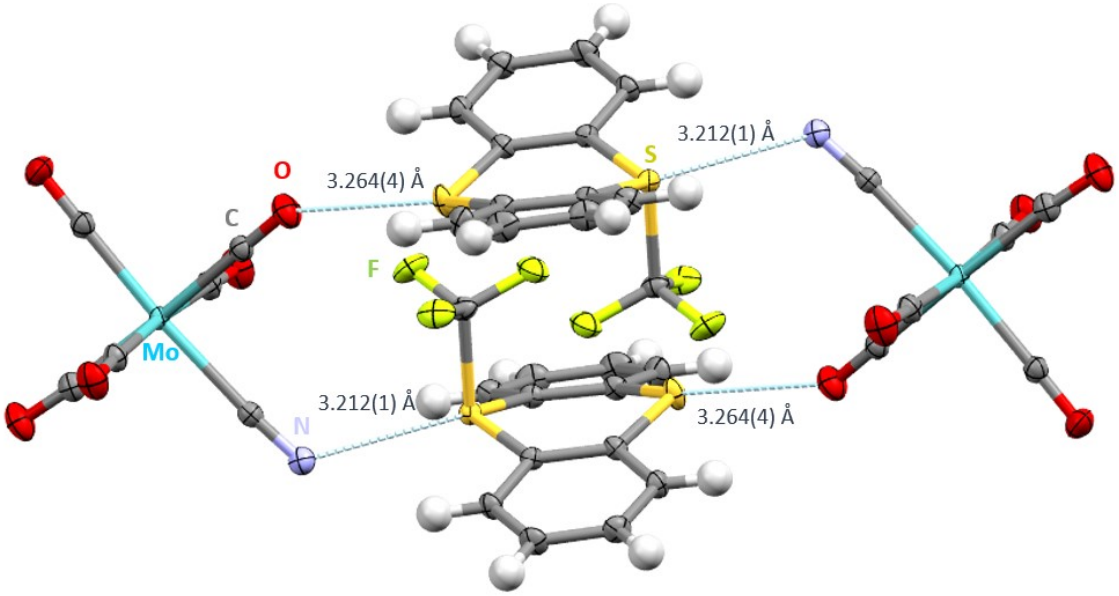

Fig. S1. Interchalcogen bonds in crystals of $[TT]^+[Mo(CO)_5CN]^-$. Thermal ellipsoids at the 50% probability level.

Computational Details

The energy calculations were carried out using the Turbomole 7.7 program[9] and the PBE0[10]-D3[11]/def2-TZVP[12] level of theory. For Mo, the def2-TZVP basis set used in this work includes effective core potentials (ECP),[13] and relativistic effects are used for the inner electrons.[12]The crystallographic coordinates have been used to evaluate the interactions in the solid state of the compounds, since we are interested to study the interactions as they stand in the solid state. The tetramers extracted from the solid-state structures were selected to study the chalcogen bonding interactions. The interaction energies were computed by subtracting the sum of the energies of the monomers to that of the assembly. The Bader's "Atoms in molecules" theory (QTAIM)[14] and noncovalent interaction plot (NCIPlot)[15] were used to study the interactions discussed herein using the Multiwfn program[16] and represented using the VMD visualization software.[17] The molecular electrostatic potential (MEP) surfaces were computed using the 0.001 a.u. isosurface as best estimation of the van der Waals surface at the same level of theory and represented using the GaussView program.[18] For the NCIplot representations, the following settings were used: RDG isosurface = 0.45, density cut-off = 0.04 a. u., color scale $-0.04 \leq (\text{sign}\lambda_2)\rho \leq 0.04$ a.u. Natural bond orbital (NBO)[19] calculations were performed using the NBO7.0 program.[20] The potential energy density (V) and the bond CP was used as energy predictor to estimate the HB and CH contributions. We have used the equation proposed by Espinosa et al. (E = 0.5 * V).[21]

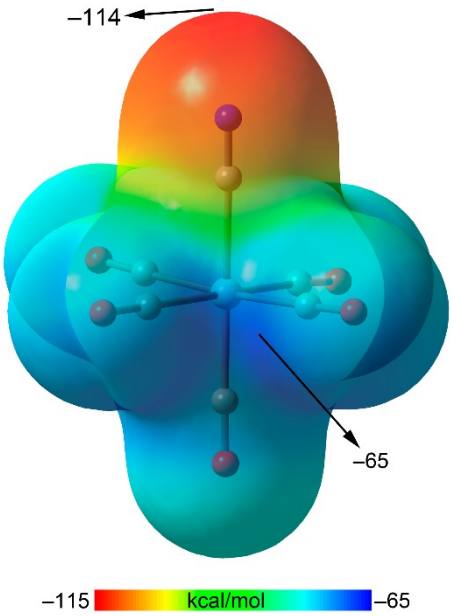

Fig. S2 MEP surface of $[Mo(CO)_5CN]^-$. Isovalue 0.001 a.u. Energies in kcal/mol

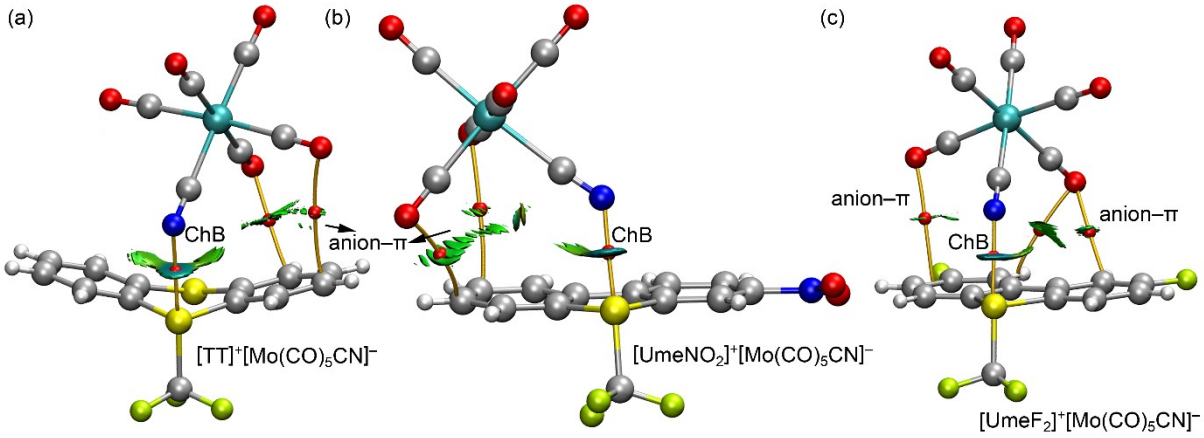

Fig. S3 QTAIM/NCIplot detailed analyses for the anion–π interactions in $[TT]^+[Mo(CO)_5CN]^-$ (a), $[UmeNO_2]^+[Mo(CO)_5CN]^-$ (b) and $[UmeF_2]^+[Mo(CO)_5CN]^-$ (c). Only intermolecular contacts are represented for clarity. NCIplot settings: RDG = 0.5, ρ cut-off = 0.04 a.u.; colour range $-0.035 \leq \text{sign}\lambda_2\rho \leq 0.035$ a.u.

Cartesian coordinates

Tetrameric assembly of [TT]+[Mo(CO)5CN]-

Mo	1.327399994	2.287599990	9.622499958
O	1.205699995	5.406899976	10.267399955
O	4.415099981	2.712799988	8.949499961
O	1.749699992	-0.829699996	9.100999960
O	-1.813099992	1.896399992	10.018299956
O	1.820499992	1.857899992	12.711299944
N	0.581699997	2.471099989	6.367599972
C	0.854799996	2.458299989	7.494599967
C	1.214799995	4.289299981	9.988199956
C	3.308099986	2.563699989	9.207899960
C	1.575399993	0.284199999	9.293999959
C	-0.688999997	2.030899991	9.888599957
C	1.663199993	2.015699991	11.573899949
S	-0.109500000	4.760399979	4.969599978
S	1.220499995	7.133899969	7.022699969
F	-1.962599991	6.253599973	3.899799983
F	-0.285099999	5.829199975	2.611999989
F	-0.113400000	7.327399968	4.150999982
C	-0.851799996	5.304899977	6.481699972
C	-2.046799991	4.651899980	6.800299970
H	-2.377799990	3.948799983	6.253799973
C	-2.734999988	5.053899978	7.934599965
H	-3.556499984	4.637299980	8.168999964
C	-2.214199990	6.072499973	8.726299962
H	-2.698399988	6.362099972	9.490599959
C	-1.008999996	6.669799971	8.422299963
H	-0.661099997	7.344899968	8.993499961
C	-0.296299999	6.292099972	7.284899968
C	2.133699991	6.083599973	5.951399974
C	3.520399985	6.270499973	5.953499974
H	3.908999983	6.941599970	6.502399972
C	4.329099981	5.474799976	5.153399977
H	5.268399977	5.617999975	5.150099977
C	3.787799983	4.472699980	4.357499981
H	4.355799981	3.924999983	3.827999983
C	2.429799989	4.277199981	4.340899981
H	2.050699991	3.585999984	3.809999983
C	1.608999993	5.104799978	5.110899978
C	-0.647599997	6.155599973	3.837599983
S	-1.888699992	0.673999997	5.407799976
S	-3.218699986	-1.699499993	3.354699985
F	-0.035600000	-0.819199996	6.477599972
F	-1.713099993	-0.394799998	7.765399966
F	-1.884799992	-1.892999992	6.226399973
C	-1.146399995	0.129499999	3.895699983

C	0.048600000	0.782499997	3.577099984
H	0.379599998	1.485599994	4.123599982
C	0.736799997	0.380499998	2.442799989
H	1.558299993	0.797099997	2.208399990
C	0.215999999	-0.638099997	1.650999993
H	0.700199997	-0.927699996	0.886799996
C	-0.989199996	-1.235399995	1.955099991
H	-1.337099994	-1.910499992	1.383899994
C	-1.701899993	-0.857699996	3.092499986
C	-4.131899982	-0.649199997	4.425999981
C	-5.518699976	-0.836099996	4.423899981
H	-5.907199974	-1.507199993	3.874999983
C	-6.327299972	-0.040400000	5.223999977
H	-7.266599968	-0.183599999	5.227299977
C	-5.785999975	0.961699996	6.019899974
H	-6.353999972	1.509399993	6.549399971
C	-4.427999981	1.157199995	6.036499974
H	-4.048999982	1.848399992	6.567399971
C	-3.607199984	0.329599999	5.266499977
C	-1.350599994	-0.721199997	6.539799971
Mo	-3.325599985	3.146799986	0.754899997
O	-3.203899986	0.027500000	0.110000000
O	-6.413299972	2.721599988	1.427899994
O	-3.747899984	6.264099973	1.276399994
O	-0.185099999	3.537999985	0.359099998
O	-3.818699983	3.576499984	-2.333899990
N	-2.579899989	2.963299987	4.009799982
C	-2.852999988	2.976099987	2.882799987
C	-3.212999986	1.145099995	0.389199998
C	-5.306299977	2.870699987	1.169499995
C	-3.573599984	5.150199977	1.083399995
C	-1.309199994	3.403499985	0.488799998
C	-3.661399984	3.418699985	-1.196499995

Tetrameric assembly of [UmeNO2]+[Mo(CO)5CN]-

Mo	6.614199971	9.387899959	2.283299990
O	6.005299974	11.359799950	4.707399979
O	5.714099975	11.623999949	0.249499999
O	9.647499958	10.407099955	2.271199990
O	3.602199984	8.423199963	2.521999989
O	7.218099968	7.493699967	-0.207299999
N	7.269099968	6.985299969	4.509099980
C	7.085499969	7.799799966	3.706799984
C	4.699999979	8.736699962	2.401699990
C	8.550799963	10.040699956	2.274999990
C	6.232599973	10.646299953	3.832199983
C	7.007199969	8.139899964	0.703699997
C	6.068599973	10.821599953	0.996799996
S	9.585699958	5.927999974	5.470299976
F	11.067899952	4.356899981	7.028499969
F	12.093899947	5.004399978	5.271699977
F	11.713399949	6.396799972	6.864699970
O	6.826499970	1.761299992	7.524999967
O	6.966399970	0.199099999	6.026599974
C	8.260899964	3.503599985	6.015099974
H	8.163499964	3.733399984	6.910799970
N	7.161799969	1.343199994	6.409199972
C	10.083199956	6.158199973	3.773399984
C	9.695999958	5.070199978	2.982599987
C	8.872599961	4.327099981	5.097699978
C	10.681099953	7.290699968	3.280699986
H	10.913299952	8.001099965	3.834399983
C	11.242799951	5.359399977	6.201899973
C	7.798499966	2.300299990	5.494299976
C	8.531699963	2.816799988	3.273099986
H	8.596499962	2.600199989	2.371399990
C	9.031399961	4.021499982	3.733699984
C	7.931399965	1.931799992	4.162299982
H	7.624099967	1.104999995	3.867999983
C	9.948099957	5.141399978	1.616099993
H	9.704399958	4.437999981	1.058299995
C	10.563499954	6.266199973	1.091399995
H	10.735299953	6.311899972	0.178799999
C	10.924399952	7.321899968	1.909099992
H	11.336599950	8.067399965	1.535599993
S	6.386999972	7.021599969	7.325099968
F	4.904699979	8.592699962	5.766899975

F	3.878799983	7.945199965	7.523699967
F	4.259299981	6.552799971	5.930699974
O	9.146099960	11.188299951	5.270399977
O	9.006199961	12.750499944	6.768799970
C	7.711699966	9.445999959	6.780299970
H	7.809199966	9.216199960	5.884599974
N	8.810899961	11.606399949	6.386199972
C	5.889399974	6.791399970	9.021999961
C	6.276599973	7.879399966	9.812799957
C	7.100099969	8.622499962	7.697699966
C	5.291499977	5.658899975	9.514699958
H	5.059299978	4.948499978	8.960999961
C	4.729899979	7.590199967	6.593499971
C	8.174099964	10.649299953	7.301099968
C	7.440899967	10.132799956	9.522299958
H	7.376199968	10.349399955	10.423999954
C	6.941299970	8.928099961	9.061699960
C	8.041299965	11.017799952	8.633099962
H	8.348599964	11.844599948	8.927399961
C	6.024499974	7.808199966	11.179299951
H	6.268299973	8.511599963	11.737099949

Tetrameric assembly of [UmeF2]+[Mo(CO)5CN]-

Mo	10.787299953	1.453599994	11.022799952
O	12.648399945	-0.029400000	8.932699961
N	9.583399958	3.281299986	8.500699963
O	8.677699962	-0.889399996	10.599499954
O	13.305099942	3.390899985	11.307099951
O	11.861499948	-0.407099998	13.329499942
O	8.924199961	3.140199986	12.998699943
C	9.981199956	2.668099988	9.387299959
C	9.384499959	-0.007100000	10.747599953
C	12.371799946	2.758399988	11.240699951
C	11.485399950	0.289299999	12.500699945
C	11.964499948	0.485299998	9.687599958
C	9.580999958	2.528999989	12.304299946
S	7.283399968	3.841099983	7.162799969
F	4.645999980	3.504599985	6.869499970
F	6.294699972	-1.677999993	8.658299962
F	5.399199976	5.475199976	6.417299972
F	5.725999975	3.849799983	5.048699978
F	5.819899975	4.754399979	12.683699945
C	7.307799968	1.088299995	6.587299971
H	7.650799967	1.270699994	5.720299975
C	7.030099969	2.105599991	7.479099967
C	7.064999969	-0.211199999	7.009599969
H	7.250899968	-0.949999996	6.442199972
C	6.535199971	1.897499992	8.769699962
C	6.281599973	0.596999997	9.177999960
H	5.939899974	0.406899998	10.043599956
C	6.421899972	3.140199986	9.537699958
C	6.812599970	5.551399976	9.319599959
H	7.064799969	6.292999972	8.782899962
C	6.769699970	4.265099981	8.808899961
C	6.545999971	-0.404099998	8.275299964
C	5.634099975	4.182799982	6.317799972
C	6.123499973	4.584899980	11.381499950
C	6.073199973	3.300599986	10.874199952
H	5.812199975	2.562299989	11.412499950
C	6.465999972	5.700599975	10.651999953
H	6.466699972	6.560199971	11.056599952
S	10.876699952	3.841099983	5.758099975
F	13.514199941	3.504599985	6.051399974
F	11.865499948	-1.677999993	4.262599981
F	12.760899944	5.475199976	6.503599972
F	12.434199946	3.849799983	7.872199966
F	12.340199946	4.754399979	0.237199999
C	10.852299953	1.088299995	6.333599972
H	10.509299954	1.270699994	7.200599969
C	11.130099951	2.105599991	5.441799976
C	11.095199952	-0.211199999	5.911299974
H	10.909299952	-0.949999996	6.478699972
C	11.624999949	1.897499992	4.151199982
C	11.878599948	0.596999997	3.742899984
H	12.220299947	0.406899998	2.877299987
C	11.738299949	3.140199986	3.383199985
C	11.347499950	5.551399976	3.601299984
H	11.095399952	6.292999972	4.137999982

C	11.390399950	4.265099981	4.111899982
C	11.614099949	-0.404099998	4.645599980
C	12.525999945	4.182799982	6.603099971
C	12.036599947	4.584899980	1.539399993
C	12.086999947	3.300599986	2.046699991
H	12.347999946	2.562299989	1.508399993
C	11.694199949	5.700599975	2.268899990
H	11.693499949	6.560199971	1.864299992
Mo	7.372899968	1.453599994	1.898099992
O	5.511699976	-0.029400000	3.988199983
N	8.576799963	3.281299986	4.420199981
O	9.482399959	-0.889399996	2.321399990
O	4.854999979	3.390899985	1.613799993
O	6.298699972	-0.407099998	-0.408599998
O	9.235999960	3.140199986	-0.077800000
C	8.178999964	2.668099988	3.533599985
C	8.775599962	-0.007100000	2.173299991
C	5.788399975	2.758399988	1.680199993
C	6.674799971	0.289299999	0.420199998
C	6.195699973	0.485299998	3.233299986
C	8.579199963	2.528999989	0.616599997

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