Chalcogen bonds provide supramolecular association of beta-octamolybdate and chalconium cations

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Supporting Information

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General information

(n-$Bu_4N)_4[\beta$-$Mo_8O_{26}]$[1] and the chalconium salts[2,3] were prepared according to the literature data. Other reagents were of commercial quality (Sigma–Aldrich) and were used without additional purification. Elemental analyses were carried out on a MICRO Cube CHN analyzer. IR spectra were recorded on a Bruker Vertex 60 FT-IR spectrometer. IR spectrum for **9** was recorded on a Shimadzu IRAffinity-1. Electrospray ionization (ESI) mass spectra (for **8**) were obtained on a Bruker maXis spectrometer equipped with an ESI source. The instrument was operated in positive ion mode using an m/z range of 50–1200. The nebulizer and drying gas flows were set to 1.0 bar and 4.0 L min^{-1}, respectively. For high resolution electrospray ionization (HRESI+), the studied compound was dissolved in MeOH. ^1H- and $^{13}C\{^1H\}$ NMR spectra were measured on a Bruker Avance 400 spectrometer in $(CD_3)_2SO$ at 298 K; the residual solvent signal was used as the internal standard.

Synthesis of $[S(bPh)Ph]_4[\beta$-$Mo_8O_{26}]$ (**1**): Solid [S(bPh)Ph](OTf) (0.038 g, $9.3\cdot10^{-5}$ mol) was added to the solution of $(Bu_4N)_4[\beta$-$Mo_8O_{26}]$ (0.050 g, $2.3\cdot10^{-5}$ mol) in 3 mL of DMF under gentle stirring. Formation of the crystalline product was found after several minutes after mixing. Crystals suitable for SCXRD were found after keeping of the mother liquor overnight. Crystalline product was washed with Et_2O (2 portions of 5 mL) and dryed in air overnight. Yield 0.048 g (92% based on initial octamolybdate) Calcd. for $C_{72}H_{52}Mo_8O_{26}S_4$ C, H, N, S(%): 38.8, 2.4, 5.8; found C, H, N(%): 38.5; 2.4; 0; 6.1. The use of N-methyl-2-pyrrolidone (NMP) istead of DMF gives 37 mg of the titled compound. IR (KBr, cm^{-1}): 3110(w), 3086(m), 3070(w), 3055(w), 3024(w), 3002(w), 2662(w), 2930(w), 2874(w), 1578(w), 1560(w), 1541(w), 1505(w), 1474(m), 14569w), 1447(s), 1422(m), 1402(w), 1301(w), 1290(w), 1274(w), 1261(w), 1222(w), 1180(w), 1163(w), 1126(w), 1060(w), 1049(w), 1033(w), 1022(w), 1000(m), 950(vs), 932(s), 918(vs), 905(vs), 884(s), 839(vs), 808(m), 786(m), 770(vs), 759(vs), 749(s), 739(vs), 718(vs), 703(vs), 680(s), 660(s), 612(s), 566(m), 550(s), 521(vs), 502(s), 486(s), 474(s), 457(s), 424(s), 413(s). IR spectra of the products isolated from DMF and NMP are identical.

Synthesis of $[S(bPh)Ph]_4[\alpha$-$Mo_8O_{26}]\cdot2DMSO$ (2): Solid [S(bPh)Ph](OTf) (0.038 g, $9.3\cdot10^{-5}$ mol) was added to the solution of $(Bu_4N)_4[\beta$-$Mo_8O_{26}]$ (0.050 g, $2.3\cdot10^{-5}$ mol) in 3 mL of DMSO under gentle stirring. The resulted solution was transferred into the i-PrOH atmosphere. After 2-3 days a crop of crystals has been analyzed with SCXRD. We found some crystals of **2** together with crystals of $[Na(DMSO)_6][S(bPh)Ph]_2[Na(\beta$-$Mo_8O_{26})]\cdot$xDMSO which is a major phase under such conditions.

Synthesis of $(Bu_4N)_2[S(bPh)Mes]_2[\alpha\text{-}Mo_8O_{26}]\cdot 2DMF$ (3): Solid [S(bPh)Mes](OTf) (0.013 g, $2.9\cdot10^{-5}$ mol) was added to the solution of $(Bu_4N)_4[\beta\text{-}Mo_8O_{26}]$ (0.015 g, $7\cdot10^{-6}$ mol) in 1 mL of DMF under gentle stirring. The resulted solution was transferred into the Et_2O atmosphere. Crystalline product was washed with Et_2O (2 portions of 1 mL) and dryed in air overnight. Yield 0.012 g (70% based on initial octamolybdate). Calcd. for $C_{80}H_{124}Mo_8N_4O_{28}S_2$ C, H, N, S(%): 39.7, 2.3, 5.2, 2.7; found C, H, N, S(%): 39.7, 2.6, 5.5, 2.8.

Synthesis of $[S(bPh)Mes]_4[\beta\text{-}Mo_8O_{26}]\cdot 4DMF\cdot 0.6H_2O$ (4): Solid [S(bPh)Mes](OTf) (0.042 g, $9.3\cdot10^{-5}$ mol) was added to the solution of $(Bu_4N)_4[\beta\text{-}Mo_8O_{26}]$ (0.050 g, $2.3\cdot10^{-5}$ mol) in 3 mL of DMF under gentle stirring. The resulted solution was transferred into the Et_2O atmosphere. Crystalline product was washed with Et_2O (2 portions of 5 mL) and dryed in air overnight. Yield 0.036 g (57% based on initial octamolybdate). Calcd. for $C_{80}H_{124}Mo_8N_4O_{28}S_2$ (without DMF and H_2O molecules) C, H, N, S(%): 39.7, 2.3, 5.2, 2.7; found C, H, N, S(%): 39.7, 2.6, 5.5, 2.8. IR (KBr, cm^{-1}): 3423(wide), 3087(w), 3080(m), 3047(w), 3000(w), 2971(w), 2927(w), 2878(w), 2852(w), 1665(m), 1595(m), 1567(m), 1508(w), 1478(w), 1468(m), 1446(s), 1420(m), 1406(m), 1375(w), 1299(m), 1279(w), 1249(w), 1227(w), 1162(w), 1132(w), 1058(w), 1051(w), 1030(w), 940(vs), 909(vs), 883(s), 837(vs), 786(m), 758(s), 718(vs), 704(vs), 672(s), 612(m), 576(w), 555(m), 516(m), 493(w), 472(m), 452(w).

Synthesis of $(Bu_4N)_2[S(bPh)PhBr]_2[\beta\text{-}Mo_8O_{26}]\cdot 2DMF$ (5): Solid [S(bPh)PhBr](OTf) (0.045 g, $9.2\cdot10^{-5}$ mol) was added to the solution of $(Bu_4N)_4[\beta\text{-}Mo_8O_{26}]$ (0.050 g, $2.3\cdot10^{-5}$ mol) in 3 mL of DMF under gentle stirring. The resulted soluting was transferred into the Et_2O atmosphere. Crystalline product was washed with Et_2O (2 portions of 5 mL) and dryed in air overnight. Yield 0.045 g of crystalline product. According to the analysis this is a mixture of 4:1 and 2:2:1 complexes. Calcd. for $Br_3C_{70}H_{72}Mo_8NO_{26}S_3$ (3:1, without solvate DMF) C, H, N, S(%): 34.4, 3.0, 0.6, 3.9; found C, H, N, S(%): 34.0; 2.5; 0.7; 4.4. The use of N-methylpirrolidone istead of DFM gives 30 mg (50% based on initial octamolybdate) of the titled compound. According to the elemental analysis this is 4:1 complex of $[S(bPh)PhBr]_2[\beta\text{-}Mo_8O_{26}]\cdot$formula. Calcd. for $Br_4C_{72}H_{48}Mo_8O_{26}S_4$ (without solvate NMP) C, H, N, S(%): 34.0, 1.9, 0, 5.0; found C, H, N, S(%): 33.7, 2.5, 0, 4.4. IR (KBr, cm^{-1}): 3074(m), 3057(m), 3004(w), 2960(w), 2932(w), 2871(w), 1679(m), 1664(w), 1623(w), 1565(m), 1478(sh), 1469(m), 1443(m), 1428(m), 1389(m), 1292(w), 1278(w), 1180(w), 1160(w), 1125(w0, 1115(w), 1090(w), 1066(m), 998(s), 941(vs), 923(s), 909(vs), 843(s), 808(m), 785(m), 765(s), 730(s), 704(vs), 688(s), 659(s), 623(m), 612(m), 565(sh), 554(m), 531(m), 504(m), 472(w), 451(w), 411(m).

Synthesis of $(Bu_4N)_2[S(bPh)PhF]_2[\beta\text{-}Mo_8O_{26}]\cdot 2DMF$ (6): Solid [S(bPh)PhF](OTf) (0.039 g, $9.2\cdot10^{-5}$ mol) was added to the solution of $(Bu_4N)_4[\beta\text{-}Mo_8O_{26}]$ (0.050 g, $2.3\cdot10^{-5}$ mol) in 3 mL of DMF under gentle stirring. The resulted soluting was transferred into the Et_2O atmosphere.

Crystalline product was washed with Et_2O (2 portions of 5 mL) and dryed in air overnight. Yield 0.043 g of crystalline product (78% based on initial octamolybdate). Calcd. for $C_{74}F_2H_{110}Mo_8N_4O_{28}S_2$ C, H, N, S(%): 37.5, 4.7, 2.4, 2.7; found C, H, N, S(%): 37.1; 4.2; 2.0; 2.2. IR (KBr, cm^{-1}): 3087(m), 3055(m), 3005(w), 2960(m), 2931(m), 2874(m), 1681(sh), 1673(s), 1593(sh), 1583(s), 1488(s), 1445(m), 1424(m), 1401(m), 1383(m), 1293(m), 1274(w), 1238(s), 1160(s), 1131(w0, 1096(m), 1063(m), 1032(w), 1013(w). 1009(m), 945(vs), 911(vs), 862(sh), 843(vs), 800(vs), 771(sh), 762(vs), 731(s), 710(s), 693(s), 663(vs), 625(m), 611(m), 558(m), 480(m), 450(w), 422(m), 409(m).

Synthesis of $(Bu_4N)_2[Se(bPh)Ph]_2[\beta\text{-}Mo_8O_{26}]$ (7): Solid [Se(bPh)Ph](OTf) (0.014 g, $2.9\cdot10^{-5}$ mol) was added to the solution of $(Bu_4N)_4[\beta\text{-}Mo_8O_{26}]$ (0.015 g, $7\cdot10^{-6}$ mol) in 3 mL of DMF under gentle stirring. The resulted soluting was transferred into the Et_2O atmosphere. Crystalline product was washed with Et_2O (2 portions of 1 mL) and dryed in air overnight. Yield – several crystals.

Synthesis of $[Te(bPh)Ph]_4[\beta\text{-}Mo_8O_{26}]$ (9): The solution of [Te(bPh)Ph](OTf) (14 mg, 0.027 mmol) in acetonitrile (1 mL) was added dropwise to the stirred solution of $(Bu_4N)_4[\beta\text{-}Mo_8O_{26}]$ (15 mg, 0.007 mmol) in acetonitrile (1 mL) and the resulting mixture was stirred at RT for 15 min. The precipitate which formed, was filtered off, washed with acetonitrile (2 x 0.5 mL), and dried at 50 °C in air. The product isolated as colorless crystalline solid. Yield: 76% (13 mg). M.p.: 335–340 °C (decomp.). ^{1}H NMR (400.13 MHz, $(CD_3)_2SO$): δ = 8.30 (d, $^3J_{HH}$ = 7.6 Hz, 2H, Ar), 8.20 (d, $^3J_{HH}$ = 7.2 Hz, 2H, Ar), 7.77 (t, $^3J_{HH}$ = 7.7 Hz, 2H, Ar), 7.62 (t, $^3J_{HH}$ = 7.2 Hz, 2H, Ar), 7.50 (d, $^3J_{HH}$ = 8.0 Hz, 2H, Ar), 7.42 – 7.36 (m, 3H, Ar). $^{13}C\{^1H\}$ NMR (101.61 MHz, $(CD_3)_2SO$): δ = 147.0, 135.6, 133.8, 133.2, 132.4, 131.3, 130.5, 130.0, 125.7 (Ar). HR-ESI(+) (ESI-TOF): *m/z* calcd for $C_{18}H_{13}Te^+$: 359.0074; found: 359.0071. The crystals of $[Te(bPh)Ph]_4[\beta\text{-}Mo_8O_{26}]\cdot2CH_3OH$ (**[9]·2CH$_3$OH**) were grown from the solution of crude product in MeOH : DMF mixture 1 : 1, v/v. Calcd. for $[Te(bPh)Ph]_4[\beta\text{-}Mo_8O_{26}]$ C, H(%): 33.2; 2.0; found C, H(%): 33.3; 1.7. IR (ATR, cm^{-1}): 3057(w), 1474(w), 1438(m), 995(m), 940(vs), 915(m), 890(vs), 877(vs), 835(s), 781(w), 743(vs), 701(vs), 684(s), 654(s), 612(m), 554(m), 520(m), 474(m), 451ms), 429(w), 412(s).

Synthesis of $(Bu_4N)_2[Te(bPh)Ph]_2[\beta\text{-}Mo_8O_{26}]$ (8): The crystals of titled compound were grown from the mixture of [Te(bPh)Ph](OTf) (5 mg, 0.01 mmol) and $(Bu_4N)_4[\beta\text{-}Mo_8O_{26}]$ (6 mg, 0.003 mmol) in in DMSO during hexane vapor diffusion. Yield – several crystals.

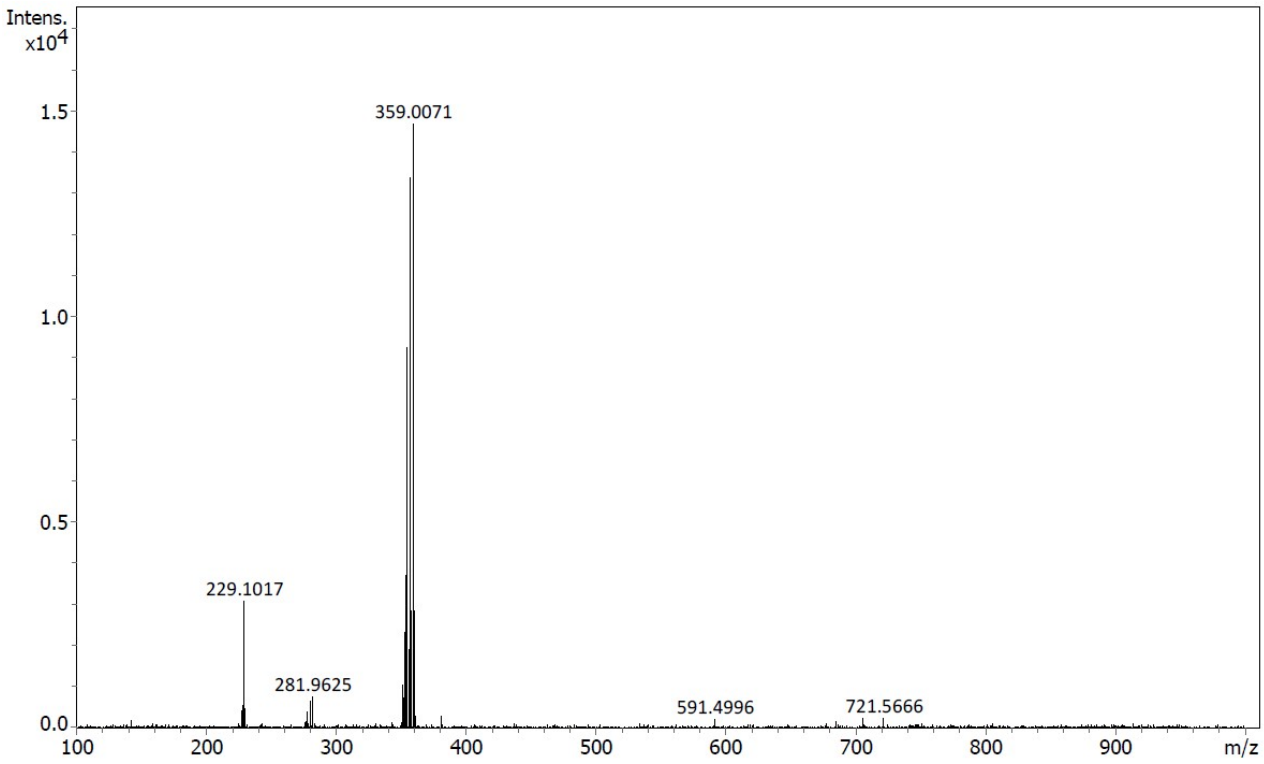


Figure S1. HR-ESI(+) data for the solution of $[Te(bpy)Ph]_4[\beta\text{-}Mo_8O_{26}]$ in MeOH.

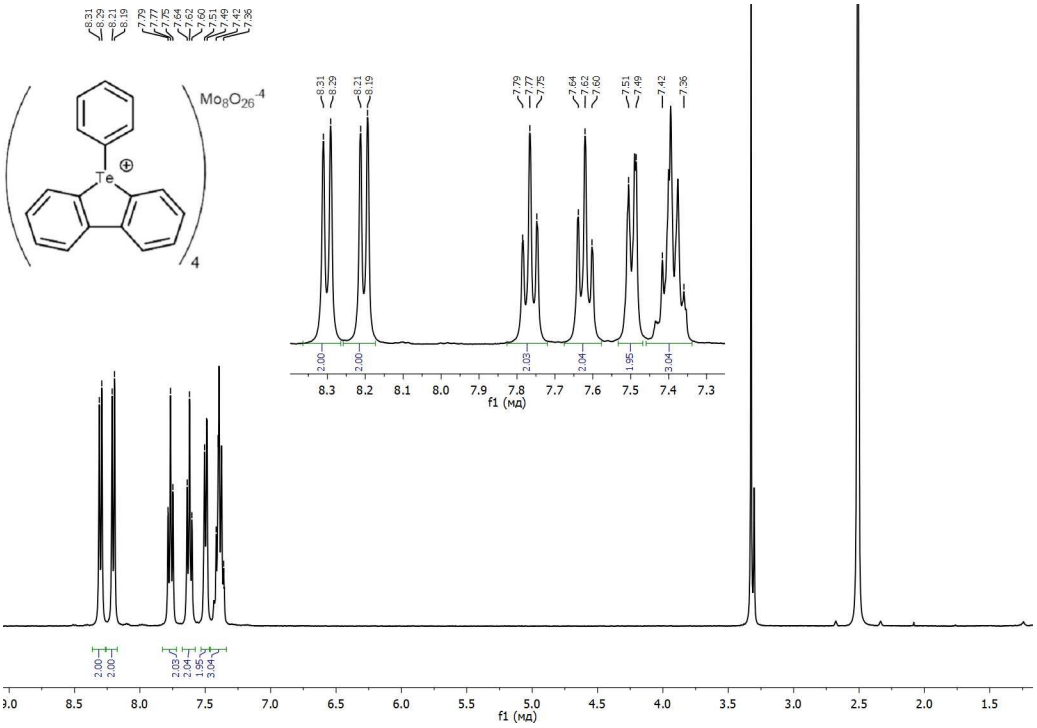
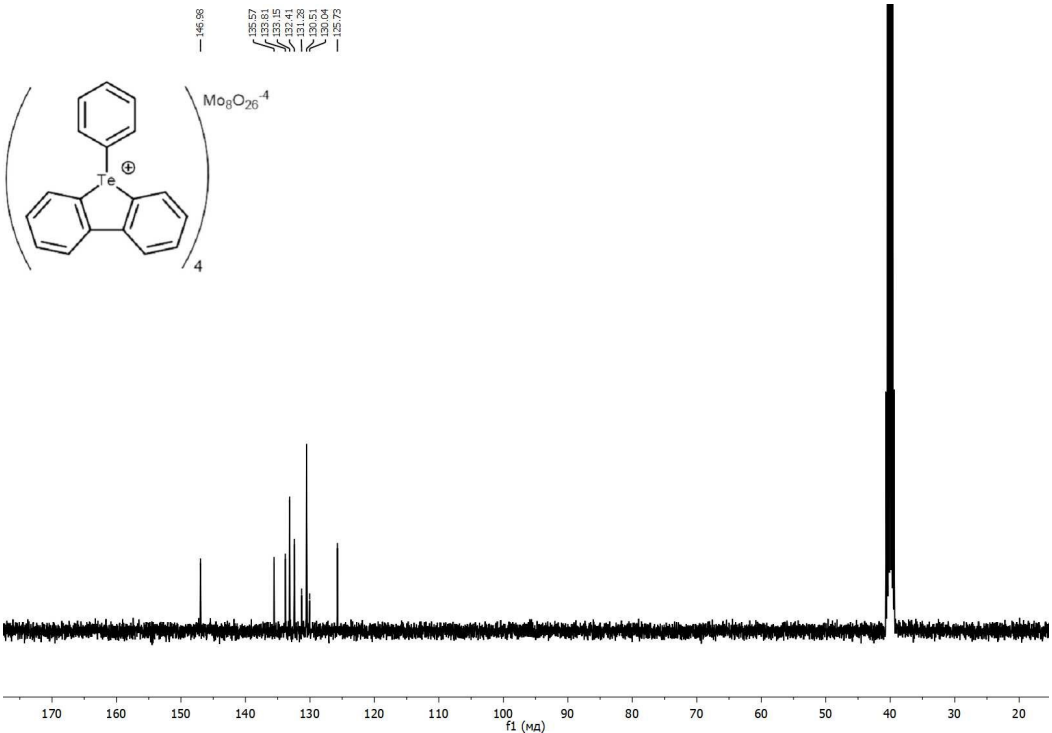


Figure S2. ^{1}H NMR spectrum of **8** in d^{6}-DMSO.

Figure S3. ^{13}C NMR spectrum of **8** in d^{6}-DMSO.



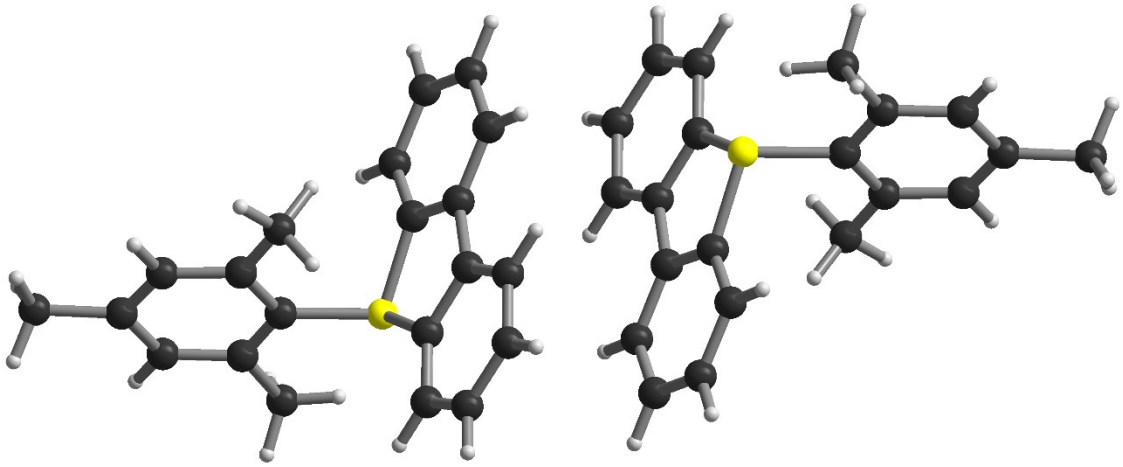


Figure S4. π-π stacked dimer of $[S(bPh)Mes]^+$ cations in the crystal structure of **3**.

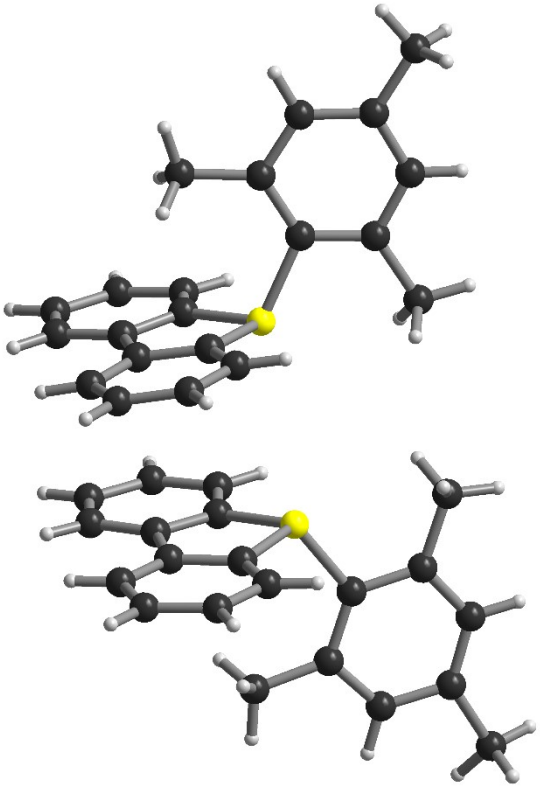


Figure S5. π-π stacked dimer of $[S(bPh)Mes]^+$ cations in the crystal structure of **4**.

X-ray single-crystal diffraction studies

The diffraction data for **1 - 7** were collected on a Bruker D8 Venture diffractometer with a CMOS PHOTON III detector and IμS 3.0 source (Mo Kα radiation, λ = 0.71073 Å) at 150 K. The φ- and ω-scan techniques were employed. Absorption correction was applied by SADABS (Bruker Apex3 software suite: Apex3, SADABS-2016/2 and SAINT, version 2018.7-2; Bruker AXS Inc.: Madison, WI, 2017). The structures were solved by SHELXT[4] and refined by full-matrix least-squares treatment against $|F|^2$ in anisotropic approximation with SHELX 2019/3[5] in ShelXle program[6].

The diffraction data for **8 – [9]·2CH$_3$OH** were collected on a «SuperNova» (Agilent Technologies) diffractometer with monochromated CuKα radiation. Crystals were kept at 100(2) K during data collection. Structures have been solved by the Superflip[789], and the ShelXT[4] solution programs using Charge Flipping and Intrinsic Phasing and refined by means of the ShelXL[5] program incorporated in the OLEX2 program package[10]. H-atoms were refined in geometrically calculated positions.

CCDC 2381722 (**1**), 2381723 (**2**), 2381724 (**3**), 2381725 (**4**), 2381728 (**5**), 2381727 (**6**), 2381726 (**7**), 2358696 (**8**), 2358690 (**9**), contain the supplementary crystallographic data. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

Table S1. SCXRD Experimental details

	1	**2**	**3**	**4**
Chemical formula	$C_{72}H_{52}Mo_8O_{26}S_4$	$C_{76}H_{64}Mo_8O_{28}S_6$	$C_{80}H_{124}Mo_8N_4O_{28}S_2$	$C_{96}H_{104}Mo_8N_4O_{30.60}S_4$
M_r	2228.89	2385.15	2421.46	2699.19
Crystal system, space group	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
Temperature (K)	150	150	150	150
a, *b*, *c* (Å)	13.1211 (3), 16.1534 (4), 18.7995 (4)	12.1379 (10), 13.0829 (13), 14.3749 (14)	14.0874 (2), 22.1111 (3), 15.9464 (2)	18.3451 (5), 14.3426 (4), 20.4131 (6)
α, β, γ (°)	87.069 (1), 77.591 (1), 67.982 (1)	66.691 (3), 83.977 (3), 72.575 (3)	90, 107.361 (1), 90	90, 109.041 (1), 90
V (Å^3)	3605.75 (15)	2000.0 (3)	4740.83 (11)	5077.1 (2)
Z	2	1	2	2
Radiation type	Mo *K*a	Mo *K*a	Mo *K*a	Mo *K*a
μ (mm^{-1})	1.54	1.45	1.14	1.12
Crystal size (mm)	0.65 × 0.10 × 0.10	0.12 × 0.10 × 0.08	0.14 × 0.08 × 0.07	0.15 × 0.10 × 0.03
Diffractometer	Bruker D8 Venture diffractometer	Bruker D8 Venture diffractometer	Bruker D8 Venture diffractometer	Bruker D8 Venture diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.701, 0.747	0.600, 0.746	0.656, 0.746	0.642, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	76236, 24939, 18317	16045, 8881, 6518	55259, 14149, 9649	55494, 12600, 8357
R_{int}	0.039	0.046	0.082	0.090
θ values (°)	θ_{max} = 35.0, θ_{min} = 1.7	θ_{max} = 27.9, θ_{min} = 2.4	θ_{max} = 30.5, θ_{min} = 2.5	θ_{max} = 28.3, θ_{min} = 1.8
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.808	0.659	0.715	0.667
Range of *h*, *k*, *l*	$-17 \leq h \leq 21$, $-23 \leq k \leq 24$, $-27 \leq l \leq 25$	$-15 \leq h \leq 12$, $-17 \leq k \leq 16$, $-18 \leq l \leq 18$	$-17 \leq h \leq 20$, $-28 \leq k \leq 31$, $-22 \leq l \leq 19$	$-24 \leq h \leq 23$, $-19 \leq k \leq 18$, $-27 \leq l \leq 27$
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.084, 1.06	0.052, 0.134, 1.01	0.041, 0.076, 0.96	0.048, 0.102, 1.07
No. of reflections	24939	8881	14149	12600
No. of parameters	991	533	569	638
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2 + 0.4343P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0271P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 0.0242P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.68, -0.82	1.18, -1.32	0.69, -0.76	0.75, -0.78

	5	**6**	**7**	**8**
Chemical formula	$C_{74}H_{110}Br_2Mo_8N_4O_{28}S_2$	$C_{74}H_{110}F_2Mo_8N_4O_{28}S_2$	$C_{68}H_{98}Mo_8N_2O_{26}Se_2$	$C_{68}H_{98}Mo_8N_2O_{26}Te_2$
M_r	2495.11	2373.29	2284.92	2382.20
Crystal system, space group	Orthorhombic, *Pbcn*	Orthorhombic, *Pbcn*	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$
Temperature (K)	150	150	150	100
a, *b*, *c* (Å)	16.1172 (4), 19.3082 (5), 28.7181 (5)	16.0410 (4), 19.0021 (5), 28.9048 (7)	15.1096 (9), 15.4192 (8), 18.0328 (9)	14.3189 (2), 15.3993 (2), 18.8558 (3)
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 105.383 (2), 90	90, 105.413 (2), 90
V (Å^3)	8936.9 (4)	8810.5 (4)	4050.7 (4)	4008.19 (11)
Z	4	4	2	4
Radiation type	Mo *K*a	Mo *K*a	Mo *K*a	Cu *K*a
μ (mm^{-1})	2.10	1.23	2.17	16.18
Crystal size (mm)	0.13 × 0.05 × 0.04	0.11 × 0.04 × 0.04	0.20 × 0.12 × 0.05	0.18 × 0.1 × 0.06
Diffractometer	Bruker D8 Venture diffractometer	Bruker D8 Venture diffractometer	Bruker D8 Venture diffractometer	SuperNova, Single source at offset/far, HyPix3000
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan *CrysAlis PRO* 1.171.41.104a (Rigaku Oxford Diffraction, 2021) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.623, 0.746	0.581, 0.746	0.548, 0.746	0.570, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	82928, 10673, 7006	45051, 10939, 6397	36468, 11448, 7515	47163, 7227, 6689
R_{int}	0.113	0.082	0.085	0.040
θ values (°)	θ_{max} = 27.9, θ_{min} = 2.5	θ_{max} = 28.3, θ_{min} = 1.7	θ_{max} = 29.7, θ_{min} = 2.1	θ_{max} = 67.5, θ_{min} = 3.5
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.658	0.667	0.697	0.599
Range of *h*, *k*, *l*	-21≤ *h* ≤ 20, -23≤ *k* ≤ 25, -35≤ *l* ≤ 37	-21≤ *h* ≤ 15, -19≤ *k* ≤ 25, -36≤ *l* ≤ 38	-21≤ *h* ≤ 15, -15≤ *k* ≤ 21, -25≤ *l* ≤ 23	-17≤ *h* ≤ 17, -18≤ *k* ≤ 18, -22≤ *l* ≤ 22
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.088, 0.99	0.047, 0.103, 0.97	0.059, 0.155, 1.01	0.030, 0.078, 1.05
No. of reflections	10673	10939	11448	7227
No. of parameters	534	524	478	483
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0285P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.077P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 6.1521P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.79, -0.67	0.92, -0.65	4.21, -1.30	1.43, -0.95

	9
Chemical formula	$C_{74}H_{60}Mo_8O_{28}Te_4$
M_r	2675.14
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, *b*, *c* (Å)	11.6145 (3), 12.9674 (2), 14.5072 (4)
α, β, γ (°)	65.706 (2), 79.734 (2), 76.172 (2)
V (Å^3)	1925.83 (9)
Z	1
Radiation type	Cu *K*a
μ (mm^{-1})	22.74
Crystal size (mm)	0.23 × 0.2 × 0.13
Diffractometer	SuperNova, Single source at offset/far, HyPix3000
Absorption correction	Multi-scan *CrysAlis PRO* 1.171.41.104a (Rigaku Oxford Diffraction, 2021) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.306, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	40242, 7154, 6900
R_{int}	0.040
θ values (°)	θ_{max} = 69.1, θ_{min} = 3.4
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.606
Range of *h*, *k*, *l*	-14≤ *h* ≤ 14, -14≤ *k* ≤ 15, -17≤ *l* ≤ 17
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.024, 0.060, 1.02
No. of reflections, parameters	7154, 516
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0292P)^2 + 5.2951P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.80, -1.39

Computer programs: *APEX3* (Bruker-AXS, 2016), *CrysAlis PRO* 1.171.41.104a (Rigaku OD, 2021), *SAINT* (Bruker-AXS, 2016), *SHELXS2014*/5 (Sheldrick, 2014), *SHELXT* 2014/5 (Sheldrick, 2014), *SHELXL2019*/3 (Sheldrick, 2019).

Mass spectrometry

The high-resolution electrospray ionization mass spectrometric (HR-ESI-MS) measurements were performed at the Center of Collective Use «Mass spectrometric investigations» SB RAS. Spectra were obtained with a direct injection of liquid samples on an ESI quadrupole time-of-flight (ESI-Q-TOF) high-resolution mass spectrometer Maxis 4G (Bruker Daltonics, Germany). The spectra were recorded in the 300-3000 m/z range in negative mode.

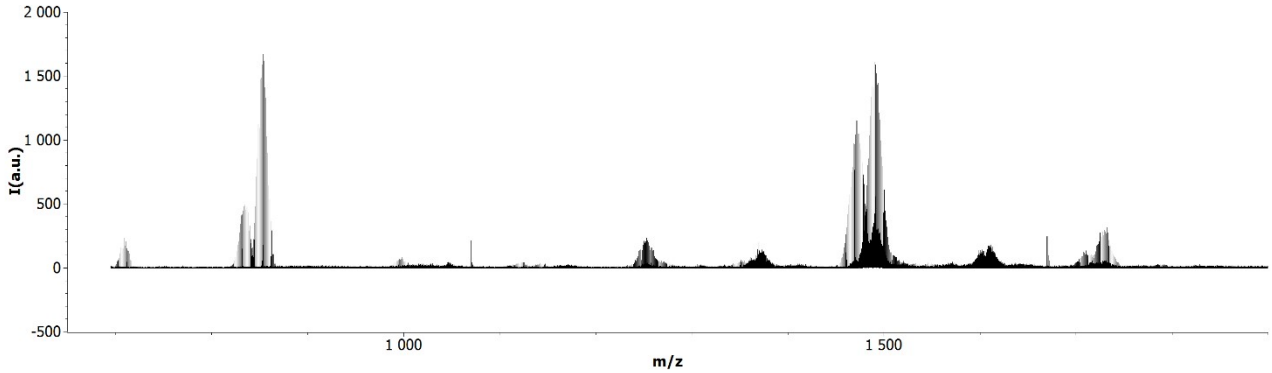


Figure S6. Full HR-ESI-MS(–) spectrum of **1** in CH_3CN.

Table S2. Molecular peaks assignment

Molecular peak	Exp	Calc
$\{[Mo_4O_{13}]^{3-} + (SC_{18}H_{13})^+ + H^+\}^-$	853.6344	853.6388
$\{[Mo_8O_{26}]^{4-} + 3Na^+\}^-$	1252.0861	1252.0833
$\{[Mo_8O_{26}]^{4-} + 2Na^+ + (SC_{18}H_{13})^+\}^-$	1491.1681	1491.1679
$\{[Mo_8O_{26}]^{4-} + Na^+ + 2(SC_{18}H_{13})^+\}^-$	1729.2519	1729.2522

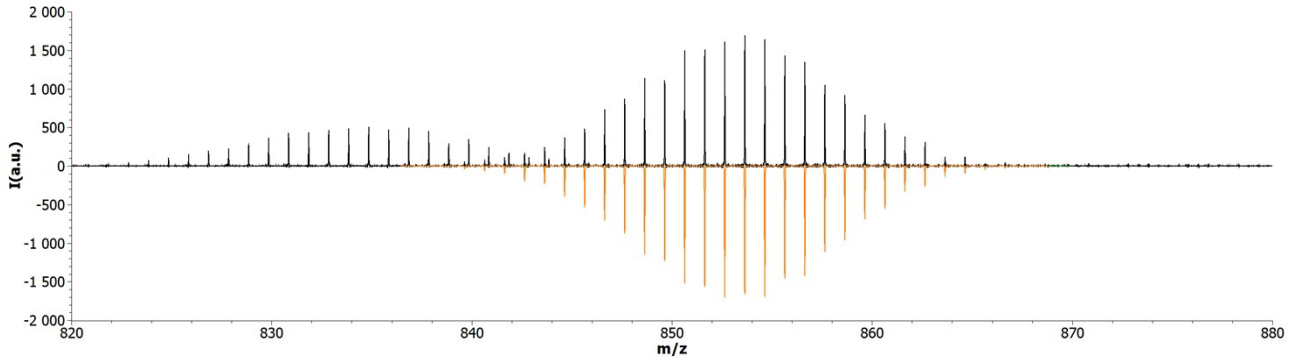


Figure S7. Zoomed area of HR-ESI-MS(–) spectrum of **1** between 820 – 880 m/z.

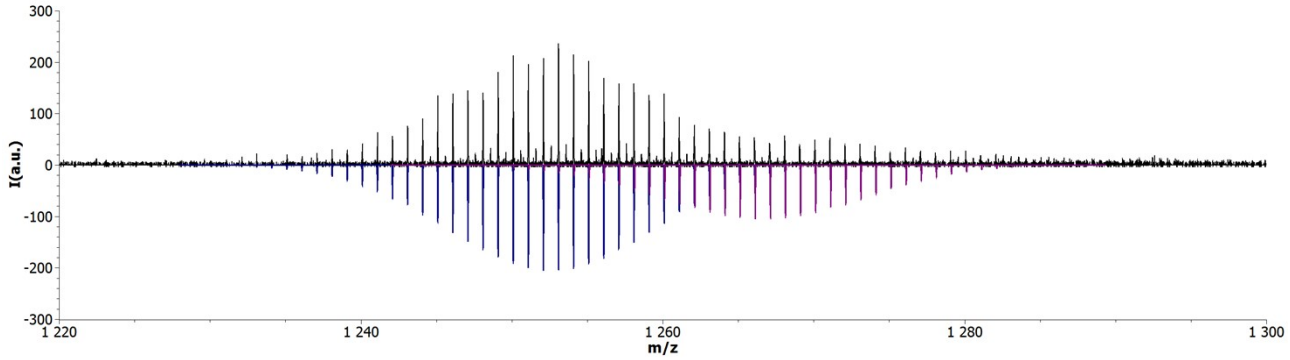


Figure S8. Zoomed area of HR-ESI-MS(–) spectrum of **1** between 1220 – 1300 m/z.

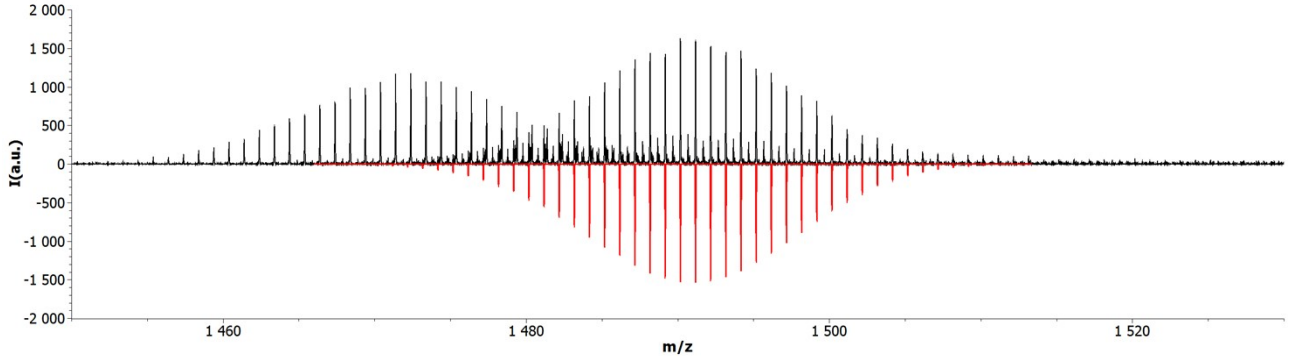


Figure S9. Zoomed area of HR-ESI-MS(–) spectrum of **1** between 1450 – 1530 m/z.

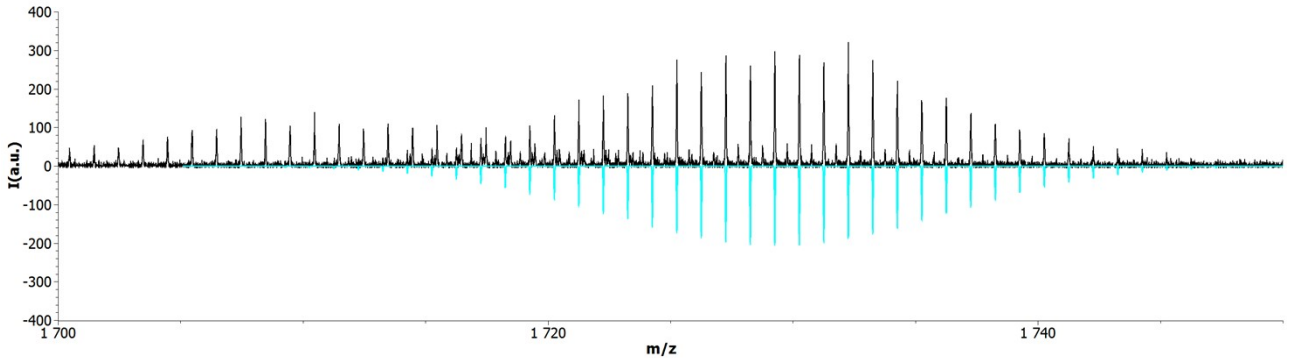


Figure S10. Zoomed area of HR-ESI-MS(–) spectrum of **1** between 1700 – 1750 m/z.

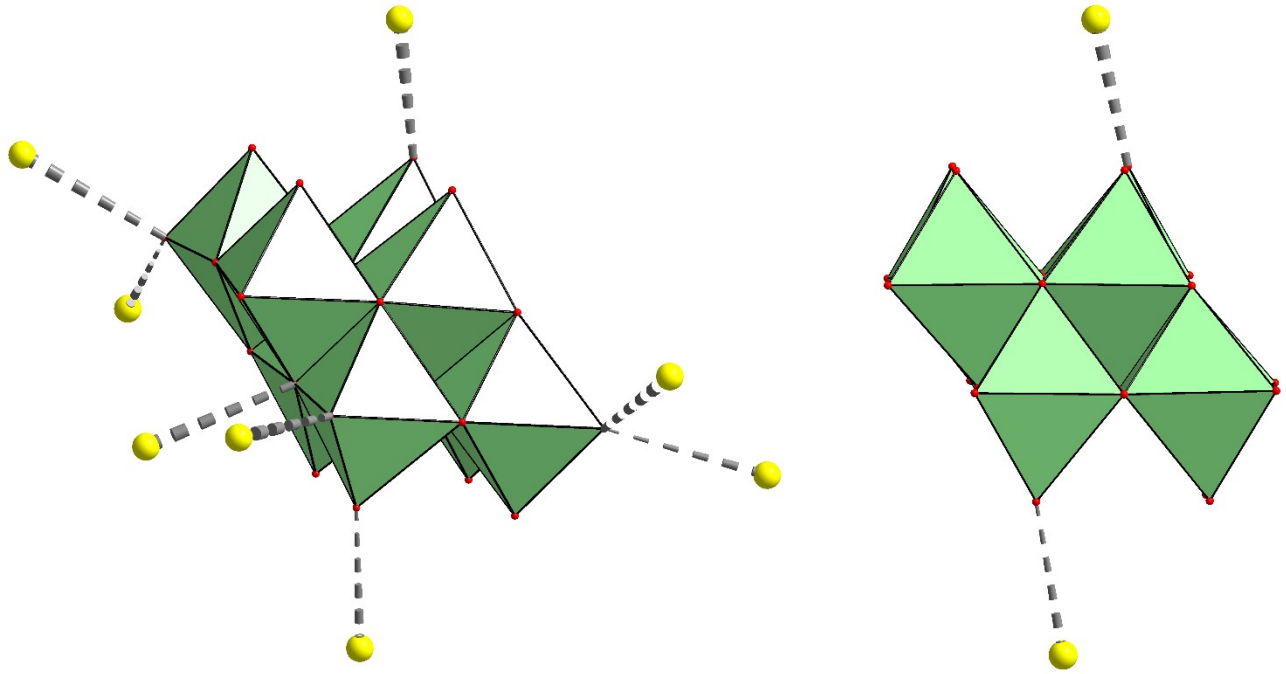


Figure S11. σ-(S^{IV})-hole···O=Mo interactions in the crystal structure of $(Me_3S)_4[Mo_8O_{26}]$ (CCDC 907956, DEPNUM)

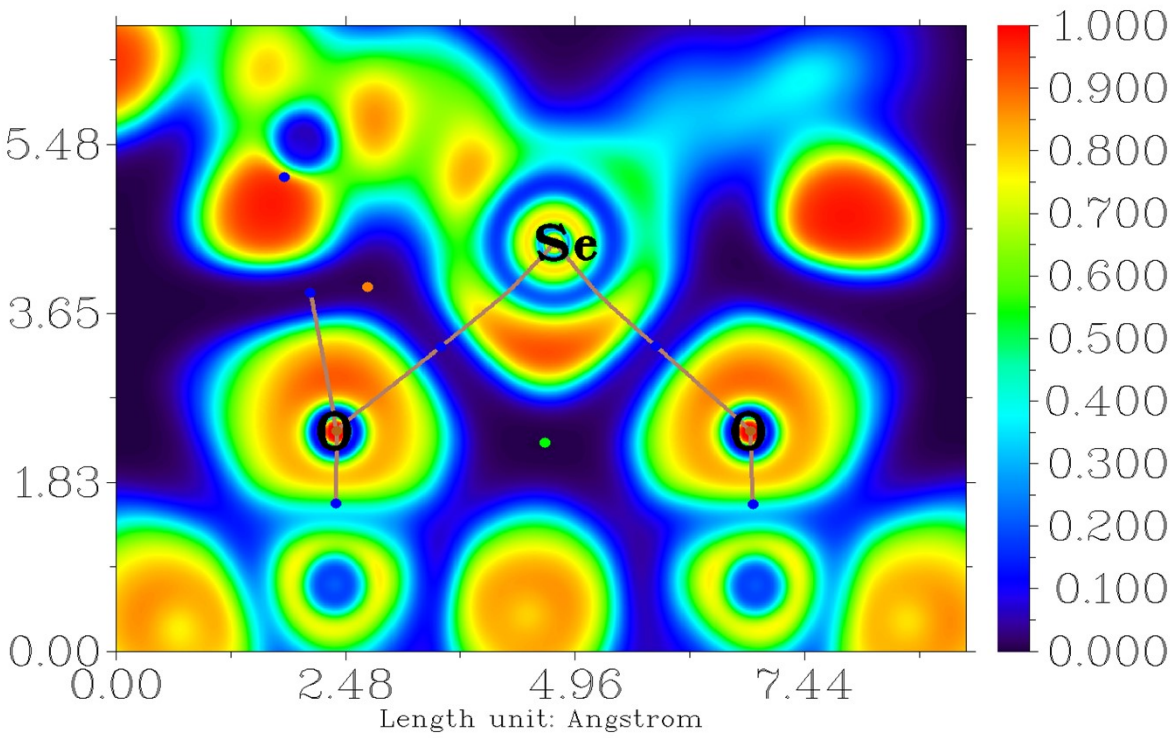


Figure S12. Visualization of electron localization function (ELF) distribution in the area of bifurcated intermolecular interactions Se···O in the X-ray structure **7**.

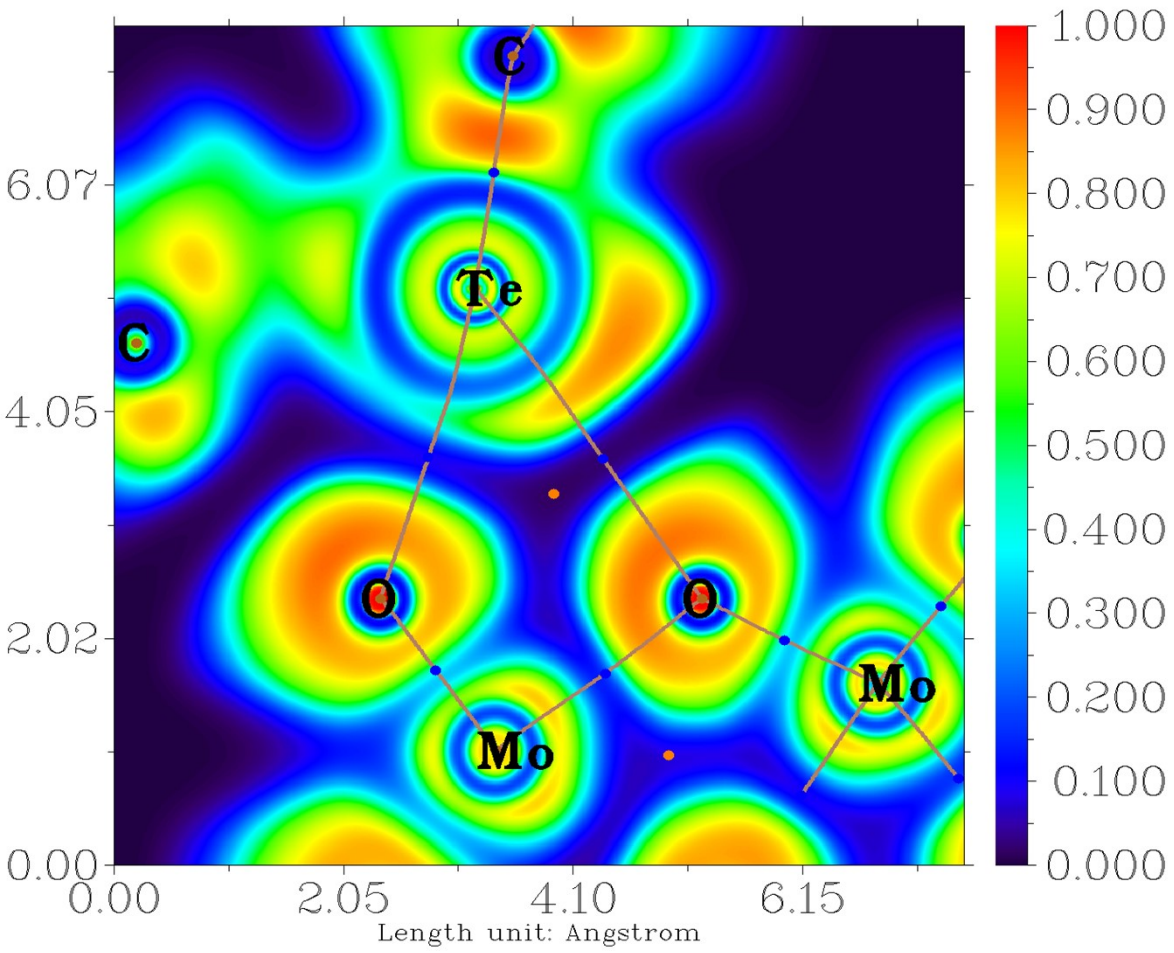


Figure S13. Visualization of electron localization function (ELF) distribution in the area of bifurcated intermolecular interactions Te···O in the X-ray structure **8**.

Computational details

The single point calculations based on the experimental X-ray geometries of structures **1-[9]·2CH$_3$OH** were carried out at the DFT level of theory using the dispersion-corrected hybrid functional ωB97XD[11] with the help of Gaussian-09[12] program package (X-ray structures **3** and **4** were not used for computational studies because they did not featuring any interesting noncovalent interactions involving chalcogen atoms, also X-ray structure **4** has disordering in the cationic moiety). The Douglas–Kroll–Hess 2nd order scalar relativistic calculations requested relativistic core Hamiltonian were carried out using the DZP-DKH basis sets[13–16] for all atoms. The topological analysis of the electron density distribution with the help of the atoms in molecules (QTAIM) method developed by Bader[17] has been performed by using the Multiwfn program (version 3.7)[18].

Note that electrostatic, charge-transfer and dispersion terms have been identified as significantly contributing to such type of noncovalent interactions[19,20], especially when using heavier chalcogens as σ-hole donors.[21] Indeed, results of cation-cluster intermolecular interaction energies analysis performed in CrystalExplorer program [https://crystalexplorer.net/] based on the X-ray structure of **8** reveal following electrostatic, dispersion, polarization and exchange-repulsion terms: 1.019, 0.651, 0.901, and 0.811 (CE-HF model) or 1.057, 0.740, 0.871, and 0.618 kJ/mol, respectively (CE-B3LYP model).

The Cartesian atomic coordinates for model supramolecular associates are presented in **Table S1**, Supporting Information.

Table S3. Values of the density of all electrons – $\rho(\mathbf{r})$, Laplacian of electron density – $\nabla^2\rho(\mathbf{r})$ and appropriate λ_2 eigenvalues, energy density – H_b, potential energy density – $V(\mathbf{r})$, Lagrangian kinetic energy – $G(\mathbf{r})$, and electron localization function – ELF (a.u.) at the bond critical points (3, –1), corresponding to intermolecular interactions Ch···O (Ch = S, Se, Te) in the obtained X-ray structures **1**, **2, 5**–**[9]·2CH$_3$OH**, and estimated strength for these interactions E_{int} (kcal/mol).

Contact*	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	λ_2	H_b	$V(\mathbf{r})$	$G(\mathbf{r})$	ELF	E_{int}**
6								
S···O 2.755 Å	0.020	0.071	-0.020	0.002	-0.013	0.015	0.071	4.1
S···O 2.765 Å	0.020	0.069	-0.020	0.002	-0.013	0.015	0.072	4.1
7								
Se···O 2.755 Å	0.021	0.075	-0.021	0.003	-0.014	0.017	0.071	4.4
Se···O 2.935 Å	0.015	0.054	-0.015	0.002	-0.009	0.011	0.055	2.8
Se···O 3.118 Å	0.011	0.036	-0.011	0.001	-0.006	0.007	0.037	1.9
Se···O 3.306 Å	0.008	0.025	-0.008	0.001	-0.004	0.005	0.030	1.3
2								
S···O 2.901 Å	0.015	0.053	-0.015	0.002	-0.009	0.011	0.048	2.8
S···O 3.296 Å	0.007	0.024	-0.007	0.001	-0.004	0.005	0.027	1.3
S···O 3.336 Å	0.007	0.026	-0.007	0.001	-0.004	0.005	0.022	1.3
S···O 3.565 Å	0.005	0.014	-0.005	0.001	-0.002	0.003	0.016	0.6
S···O 3.699 Å	0.003	0.011	-0.003	0.000	-0.002	0.002	0.010	0.6
5								
S···O 2.747 Å	0.021	0.072	-0.021	0.003	-0.013	0.016	0.075	4.1
S···O 2.766 Å	0.020	0.070	-0.020	0.002	-0.013	0.015	0.070	4.1
1								
S···O 2.731 Å	0.021	0.076	-0.021	0.002	-0.014	0.016	0.069	4.4
S···O 2.875 Å	0.017	0.060	-0.017	0.002	-0.011	0.013	0.059	3.5
S···O 2.912 Å	0.015	0.053	-0.015	0.002	-0.009	0.011	0.055	2.8
S···O 2.935 Å	0.014	0.050	-0.014	0.002	-0.008	0.010	0.049	2.5
S···O 3.102 Å	0.011	0.042	-0.011	0.002	-0.007	0.009	0.032	2.2
S···O 2.757 Å	0.019	0.071	-0.019	0.002	-0.013	0.015	0.065	4.1
S···O 2.801 Å	0.019	0.069	-0.019	0.003	-0.012	0.015	0.065	3.8
S···O 2.856 Å	0.017	0.060	-0.017	0.003	-0.010	0.013	0.060	3.1
S···O 2.964 Å	0.013	0.048	-0.013	0.002	-0.008	0.010	0.046	2.5
8								
Te···O 2.743 Å	0.027	0.073	-0.027	0.000	-0.020	0.020	0.119	6.3
Te···O 2.925 Å	0.020	0.063	-0.020	0.000	-0.015	0.015	0.077	4.7
Te···O 3.000 Å	0.017	0.053	-0.017	0.000	-0.012	0.012	0.064	3.8
Te···O 3.194 Å	0.012	0.042	-0.012	0.001	-0.008	0.009	0.040	2.5
[9]·2CH$_3$OH								
Te···O 2.900 Å	0.021	0.056	-0.021	0.000	-0.014	0.014	0.093	4.4
Te···O 2.912 Å	0.020	0.056	-0.020	0.001	-0.013	0.014	0.085	4.1
Te···O 3.028 Å	0.017	0.054	-0.017	0.001	-0.012	0.013	0.063	3.8
Te···O 3.070 Å	0.015	0.048	-0.015	0.001	-0.010	0.011	0.052	3.1
Te···O 3.241 Å	0.011	0.038	-0.011	0.001	-0.007	0.008	0.034	2.2
Te···O 3.435 Å	0.008	0.028	-0.008	0.001	-0.005	0.006	0.021	1.6

* The Bondi's (shortest) van der Waals radii for O, S, Se, and Te atoms are 1.52, 1.80, 1.90, and 2.00 Å, respectively.[22] ** $E_{int} \approx -V(\mathbf{r})/2$.[23]

Table S4. Values of the density of all electrons – $\rho(\mathbf{r})$, Laplacian of electron density – $\nabla^2\rho(\mathbf{r})$ and appropriate λ_2 eigenvalues, energy density – H_b, potential energy density – $V(\mathbf{r})$, Lagrangian kinetic energy – $G(\mathbf{r})$, and electron localization function – ELF (a.u.) at the bond critical points (3, –1), corresponding to intermolecular interactions C···C in the obtained X-ray structures **1–5** and **[9]·2CH$_3$OH**, and estimated strength for these interactions E_{int} (kcal/mol).

Contact*	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	λ_2	H_b	$V(\mathbf{r})$	$G(\mathbf{r})$	ELF	E_{int}**
2								
C···C 3.334 Å	0.007	0.021	-0.007	0.001	-0.003	0.004	0.026	0.9
4_dimer1								
C···C 3.283 Å	0.007	0.019	-0.007	0.001	-0.003	0.004	0.030	0.9
C···C 3.473 Å	0.005	0.016	-0.005	0.001	-0.002	0.003	0.022	0.6
C···C 3.460 Å	0.005	0.015	-0.005	0.001	-0.002	0.003	0.019	0.6
C···C 3.789 Å	0.003	0.009	-0.003	0.001	-0.001	0.002	0.013	0.3
C···C 3.531 Å	0.004	0.013	-0.004	0.000	-0.002	0.002	0.021	0.6
3_pp								
C···C 3.397 Å	0.006	0.017	-0.006	0.001	-0.002	0.003	0.024	0.6
C···C 3.441 Å	0.006	0.018	-0.006	0.001	-0.002	0.003	0.025	0.6
C···C 3.397 Å	0.006	0.017	-0.006	0.001	-0.002	0.003	0.024	0.6
C···C 3.441 Å	0.006	0.018	-0.006	0.001	-0.002	0.003	0.025	0.6
5								
C···C 3.554 Å	0.005	0.013	-0.005	0.001	-0.002	0.003	0.020	0.6
C···C 3.418 Å	0.005	0.016	-0.005	0.001	-0.002	0.003	0.021	0.6
C···C 3.554 Å	0.005	0.013	-0.005	0.001	-0.002	0.003	0.020	0.6
C···C 3.418 Å	0.005	0.016	-0.005	0.001	-0.002	0.003	0.021	0.6
1_pp								
C···C 3.574 Å	0.004	0.012	-0.004	0.001	-0.001	0.002	0.019	0.3
C···C 3.603 Å	0.004	0.013	-0.004	0.000	-0.002	0.002	0.019	0.6
C···C 3.621 Å	0.004	0.011	-0.004	0.001	-0.001	0.002	0.013	0.3
C···C 3.290 Å	0.007	0.021	-0.007	0.001	-0.003	0.004	0.026	0.9
C···C 3.414 Å	0.006	0.020	-0.006	0.002	-0.002	0.004	0.025	0.6
C···C 3.414 Å	0.006	0.020	-0.006	0.002	-0.002	0.004	0.025	0.6
[9]·2CH$_3$OH_pp								
C···C 3.432 Å	0.005	0.017	-0.005	0.001	-0.002	0.003	0.021	0.6
C···C 3.370 Å	0.006	0.018	-0.006	0.001	-0.002	0.003	0.026	0.6
C···C 3.477 Å	0.005	0.016	-0.005	0.001	-0.002	0.003	0.019	0.6
C···C 3.686 Å	0.003	0.010	-0.003	0.001	-0.001	0.002	0.013	0.3
C···C 3.596 Å	0.005	0.013	-0.005	0.000	-0.002	0.002	0.022	0.6
C···C 3.596 Å	0.005	0.013	-0.005	0.000	-0.002	0.002	0.022	0.6

* The Bondi's (shortest) van der Waals radii for O, S, Se, and Te atoms are 1.52, 1.80, 1.90, and 2.00 Å, respectively.[22] ** $E_{int} \approx -V(\mathbf{r})/2$.[23]

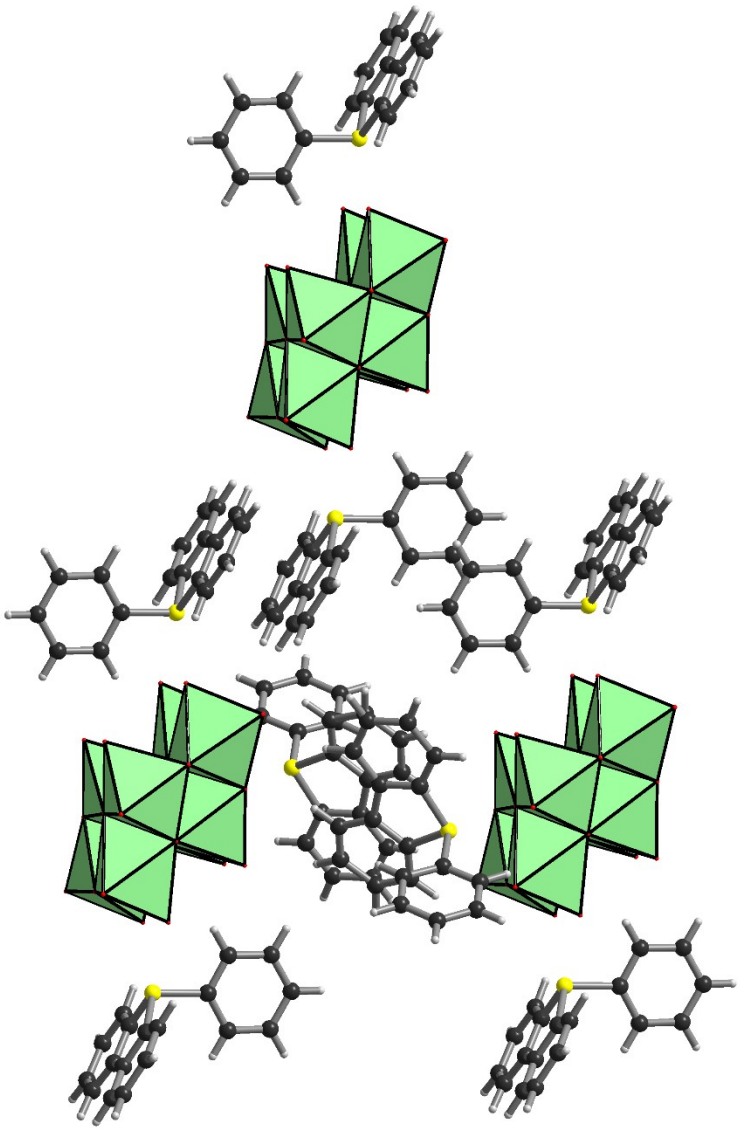


Figure S12. Model for calculations from the crystal structure of **1**.

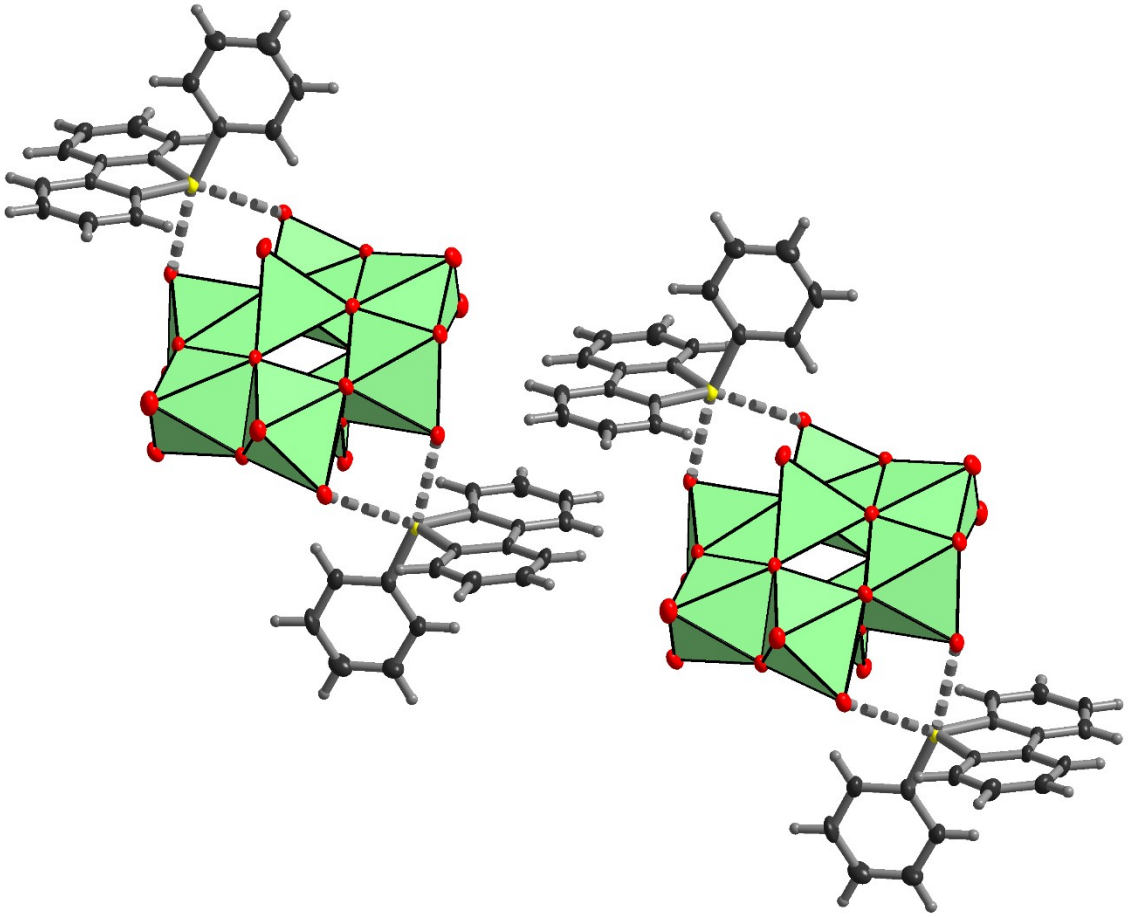


Figure S13. Model for calculations from the crystal structure of **2**.

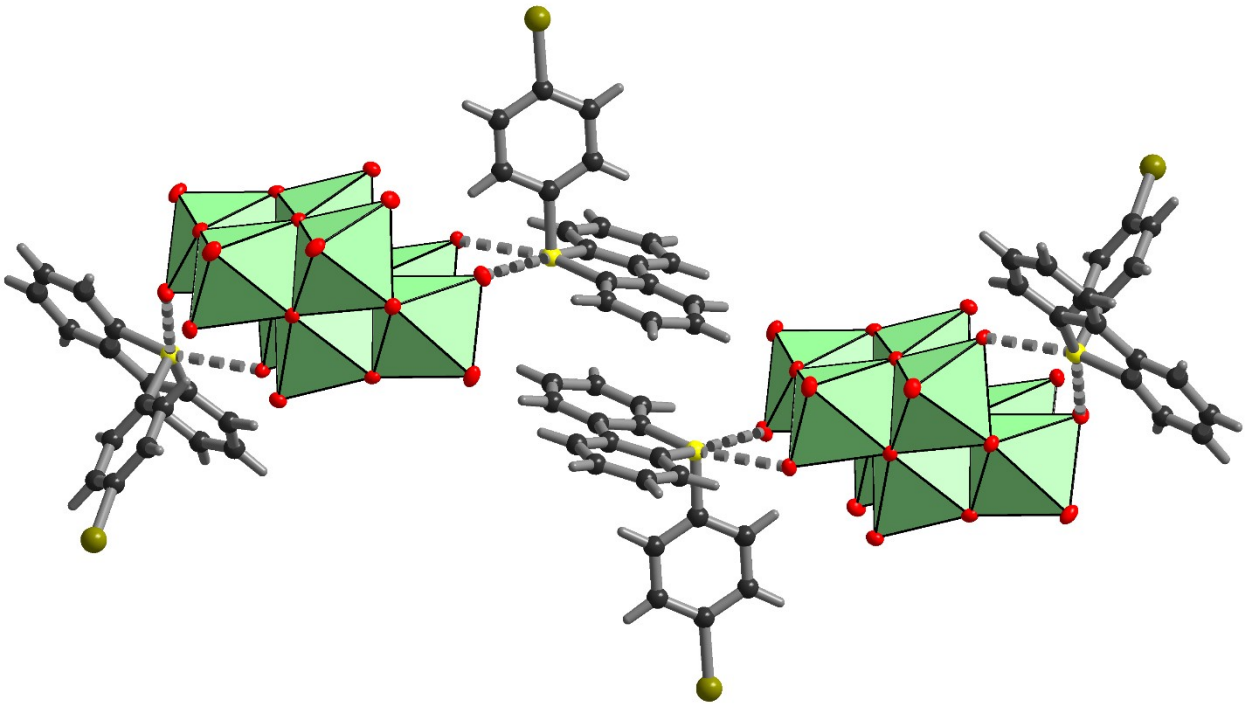


Figure S14. Model for calculations from the crystal structure of **5**.

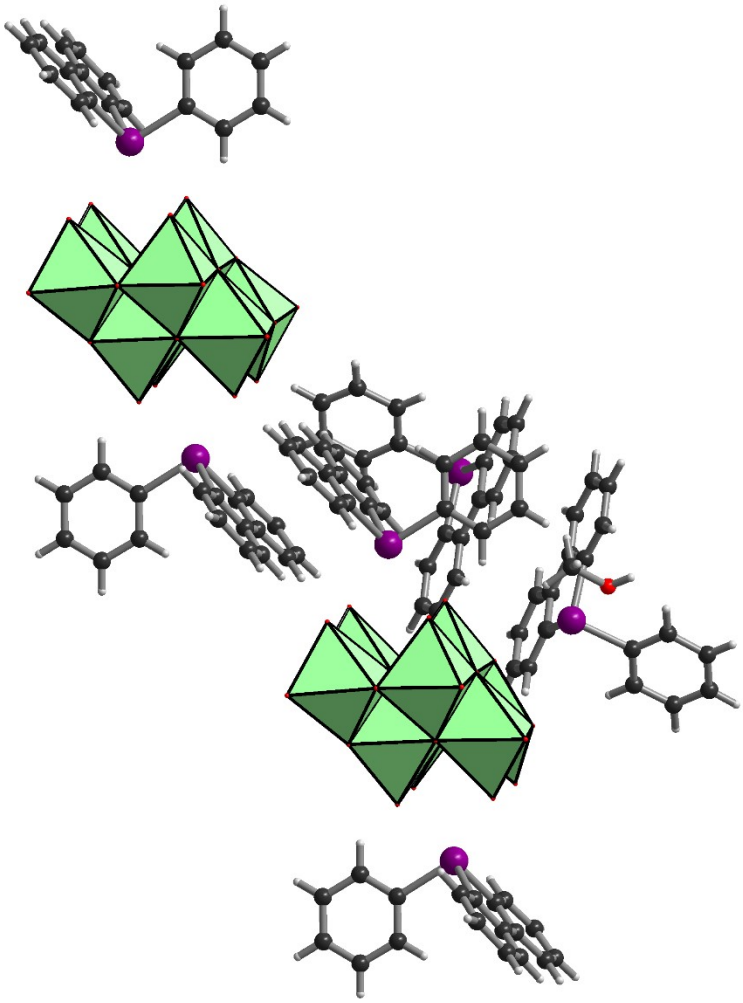


Figure S15. Model for calculations from the crystal structure of **9**.

Table S5. Cartesian atomic coordinates for model supramolecular associates.

Atom	X	Y	Z
6			
S	5.979924	10.708823	16.533257
F	0.965668	13.664410	16.978390
C	4.752948	8.311519	17.328139
H	4.676529	8.642877	18.215256
C	4.287759	7.068781	16.983882
H	3.858181	6.535753	17.642045
C	4.428920	6.574727	15.692127
H	4.106672	5.704905	15.483116
C	5.036874	7.338611	14.706184
H	5.138895	6.994559	13.826582
C	5.492438	8.611752	15.021536
C	5.343257	9.064002	16.323119
C	6.143703	9.603661	14.152657
C	6.509438	9.482048	12.813787
H	6.299108	8.693119	12.327724
C	7.187972	10.532864	12.196091
H	7.432260	10.456837	11.281370
C	7.512000	11.695793	12.898767
H	7.978056	12.399041	12.462767
C	7.155890	11.821206	14.237926
H	7.389255	12.597252	14.734569
C	6.454898	10.793193	14.821514
C	4.448169	11.652088	16.624307
C	3.432774	11.361356	15.755717
H	3.544387	10.705935	15.078160
C	2.228095	12.051132	15.888969
H	1.500860	11.877301	15.302519

C	2.120620	12.995536	16.889075
C	3.118370	13.267266	17.753328
H	2.997758	13.915181	18.439412
C	4.327862	12.590791	17.632217
H	5.049290	12.767872	18.223754
Mo	8.721171	13.017579	18.131403
Mo	7.446874	15.320253	20.059353
Mo	6.260000	13.005607	21.928627
Mo	7.489062	10.663218	20.082477
O	9.940608	12.986795	16.950353
O	8.697109	14.842350	18.712968
O	7.274594	13.038671	17.231597
O	8.663744	11.165444	18.684063
O	5.974791	10.693052	19.298579
O	7.866506	9.014976	20.216306
O	6.768981	11.108248	21.892206
O	4.823047	12.988125	21.045585
O	5.748613	12.995346	23.604238
O	6.745401	14.895746	21.872262
O	7.651076	13.005607	20.334527
O	5.979604	15.251085	19.215333
O	7.786783	16.978566	20.227290
Mo	7.319829	13.017579	25.225797
Mo	8.594126	15.320253	23.297847
Mo	9.781000	13.005607	21.428573
Mo	8.551938	10.663218	23.274723
O	6.100392	12.986795	26.406847
O	7.343891	14.842350	24.644232
O	8.766407	13.038671	26.125603
O	7.377256	11.165444	24.673137

O	10.066209	10.693052	24.058621
O	8.174494	9.014976	23.140894
O	9.272019	11.108248	21.464994
O	11.217953	12.988125	22.311615
O	10.292387	12.995346	19.752962
O	9.295599	14.895746	21.484938
O	8.389924	13.005607	23.022673
O	10.061396	15.251085	24.141867
O	8.254217	16.978566	23.129910
7			
Mo	11.503700	7.297445	11.261057
Mo	9.174459	8.330840	9.218982
Mo	10.783156	6.971329	6.714767
Mo	13.038271	5.966614	8.771446
O	10.737129	5.797619	11.405714
O	11.905121	7.734271	12.860986
O	8.378595	6.844583	9.472307
O	10.043139	8.460515	10.924101
O	7.951662	9.525982	9.310610
O	9.462089	8.173718	7.335474
O	11.402644	7.327204	8.926362
O	10.663478	7.200766	5.028251
O	12.654819	6.312620	6.890373
O	10.031094	5.452229	6.980784
O	13.248191	6.621004	10.598969
O	12.179763	4.531703	9.028944
O	14.704596	5.475358	8.545592
Mo	13.931938	8.121755	6.125703
Mo	16.261180	7.088360	8.167778
Mo	14.652482	8.447871	10.671993

Mo	12.397367	9.452586	8.615313
O	14.698509	9.621581	5.981045
O	13.530517	7.684929	4.525774
O	17.057043	8.574617	7.914453
O	15.392500	6.958685	6.462659
O	17.483976	5.893218	8.076150
O	15.973549	7.245482	10.051286
O	14.032994	8.091996	8.460397
O	14.772160	8.218434	12.358509
O	12.780819	9.106580	10.496387
O	15.404545	9.966971	10.405976
O	12.187447	8.798196	6.787791
O	13.255875	10.887497	8.357815
O	10.731042	9.943842	8.841167
Se	9.106390	4.020094	9.144566
C	7.510129	3.905683	8.076150
C	6.399405	4.709024	8.203073
H	6.369925	5.407128	8.845462
C	5.328004	4.465400	7.363293
H	4.541658	4.993832	7.439290
C	5.389740	3.456985	6.413976
H	4.643552	3.314110	5.843151
C	6.506279	2.655186	6.271404
H	6.542538	1.974783	5.609264
C	7.591256	2.881848	7.144220
C	8.829643	2.084676	7.206812
C	9.165173	1.008416	6.382679
H	8.611969	0.771515	5.648680
C	10.307351	0.300674	6.652174
H	10.529639	-0.443795	6.106300

C	11.143056	0.644523	7.700596
H	11.925968	0.130847	7.863127
C	10.850790	1.734660	8.521251
H	11.421762	1.980319	9.239880
C	9.693905	2.445485	8.244801
C	8.350348	3.262703	10.750234
C	8.084663	4.214067	11.770836
H	8.327120	5.126822	11.660969
C	7.466832	3.780788	12.923578
H	7.291935	4.398188	13.622978
C	7.099326	2.459362	13.073105
H	6.660521	2.166444	13.862585
C	7.386339	1.548088	12.029899
H	7.179676	0.627654	12.137627
C	7.957733	1.982909	10.870202
H	8.078055	1.380404	10.145592
2			
Mo	8.851810	4.450685	12.398326
Mo	8.629871	8.120581	11.426270
Mo	6.280272	6.118857	10.188365
Mo	5.268019	3.380520	11.900154
O	10.029260	3.536469	11.571207
O	9.520890	5.137802	13.882545
O	8.340320	5.800721	11.342846
O	10.061281	7.616686	12.594215
O	9.484293	8.046814	9.944955
O	8.466634	9.781424	11.736209
O	6.804668	7.811940	10.911202
O	7.064181	6.149067	8.683026
O	4.654214	6.430714	9.828794

O	6.253625	4.233476	10.512559
O	7.467342	3.418085	12.847657
O	5.399403	1.751198	11.477487
O	3.674994	3.814108	11.485407
Mo	6.302740	6.525667	14.001874
Mo	6.524679	2.855770	14.973929
Mo	8.874278	4.857494	16.211834
Mo	9.886530	7.595832	14.500045
O	5.125290	7.439882	14.828992
O	5.633660	5.838549	12.517655
O	6.814230	5.175631	15.057354
O	5.093269	3.359666	13.805984
O	5.670257	2.929538	16.455244
O	6.687915	1.194928	14.663991
O	8.349882	3.164412	15.488997
O	8.090368	4.827285	17.717174
O	10.500336	4.545638	16.571405
O	8.900925	6.742876	15.887640
O	7.687208	7.558267	13.552542
O	9.755146	9.225153	14.922713
O	11.479555	7.162244	14.914793
S	9.772898	5.148836	8.401995
C	9.168918	3.592183	7.772219
C	9.131384	2.418803	8.483704
H	9.415757	2.381321	9.389772
C	8.660214	1.289739	7.827659
H	8.623816	0.456349	8.283208
C	8.244887	1.375583	6.508969
H	7.926770	0.592693	6.076375
C	8.276448	2.561144	5.802764

H	7.986559	2.593590	4.899085
C	8.743336	3.718422	6.445609
C	8.830806	5.073630	5.949285
C	9.455938	5.951669	6.848212
C	9.649439	7.285186	6.578930
H	10.054248	7.859007	7.217722
C	9.237616	7.765898	5.351320
H	9.413103	8.670355	5.121401
C	8.568090	6.943235	4.444474
H	8.241718	7.308398	3.630674
C	8.372221	5.583450	4.725636
H	7.937552	5.018204	4.097918
C	11.547167	4.957220	8.416384
C	12.242801	4.486377	7.304935
H	11.792488	4.269797	6.498171
C	13.626760	4.346187	7.421096
H	14.136052	4.024374	6.686405
C	14.255938	4.675903	8.610425
H	15.196452	4.564526	8.682432
C	13.563342	5.153900	9.673033
H	14.024319	5.391134	10.468946
C	12.190553	5.297470	9.607033
H	11.697248	5.620333	10.352297
S	4.040100	9.694675	9.330490
C	2.591582	9.975967	8.337183
C	2.602949	10.550309	7.076573
H	3.406511	10.861520	6.677534
C	1.387016	10.645329	6.428449
H	1.345755	11.037815	5.564687
C	0.204377	10.168806	7.035653

H	-0.624506	10.259732	6.581596
C	0.235471	9.573900	8.273822
H	-0.558973	9.231645	8.666169
C	1.447244	9.482119	8.941748
C	1.719050	8.932766	10.289478
C	0.827806	8.346959	11.171244
H	-0.095467	8.287931	10.955053
C	1.307068	7.844532	12.385654
H	0.707264	7.432413	12.996237
C	2.645860	7.941997	12.701136
H	2.943212	7.606012	13.538431
C	3.575831	8.513265	11.844449
H	4.499713	8.561964	12.058911
C	3.056734	9.013143	10.641920
C	5.921923	11.473818	10.099396
H	6.510735	10.728622	10.065406
C	4.552770	11.331804	9.820874
C	3.691376	12.388999	9.898755
H	2.766342	12.273100	9.716580
C	4.191645	13.641485	10.251197
H	3.607883	14.389677	10.305635
C	5.537107	13.792688	10.521799
H	5.872184	14.643575	10.777842
C	6.385462	12.743337	10.426759
H	7.312211	12.875146	10.585833
5			
C	6.451715	10.828039	14.730662
C	7.128638	11.864889	14.110064
H	7.353231	12.663843	14.571507
C	7.457428	11.671807	12.777257

H	7.918622	12.356302	12.307687
C	7.130249	10.501730	12.118177
H	7.358533	10.404938	11.200863
C	6.475891	9.464880	12.768067
H	6.263611	8.662624	12.307343
C	6.135818	9.627069	14.115233
C	5.523364	8.642350	15.026171
C	5.109152	7.344839	14.766273
H	5.209015	6.968735	13.899302
C	4.549886	6.607266	15.794668
H	4.241999	5.724881	15.623479
C	4.430618	7.138242	17.076069
H	4.031057	6.614256	17.760853
C	4.877065	8.400998	17.370143
H	4.827472	8.753546	18.251272
C	5.400874	9.134709	16.332845
C	4.445124	11.708492	16.524108
C	3.432964	11.376391	15.647057
H	3.576084	10.723929	14.972124
C	2.206445	12.009700	15.764801
H	1.494725	11.801616	15.171485
C	2.040438	12.944217	16.754714
C	3.059045	13.293696	17.632339
H	2.915456	13.949344	18.304142
C	4.287175	12.666179	17.510574
H	5.005519	12.888185	18.091053
S	6.005269	10.807379	16.462364
Br	0.345392	13.770994	16.958325
O	9.860664	13.179198	16.766201
O	8.665413	15.026607	18.557636

O	7.800241	17.166341	20.083429
O	6.793561	15.084724	21.758268
O	5.832976	13.182287	23.507201
O	4.849988	13.169737	20.967659
O	6.808066	11.288539	21.771766
O	5.964492	10.866848	19.208388
O	7.870351	9.192634	20.071367
O	7.202616	13.215691	17.106511
O	8.636240	11.356504	18.535236
O	5.957401	15.439030	19.121373
O	7.655831	13.190397	20.201173
Mo	8.675244	13.206423	17.978392
Mo	7.456461	15.515876	19.936679
Mo	6.306822	13.194452	21.823459
Mo	7.500139	10.849857	19.957356
O	6.256536	13.179198	26.310949
O	7.451787	15.026607	24.519514
O	8.316959	17.166341	22.993721
O	9.323639	15.084724	21.318882
O	10.284224	13.182287	19.569949
O	11.267212	13.169737	22.109491
O	9.309134	11.288539	21.305384
O	10.152708	10.866848	23.868762
O	8.246849	9.192634	23.005783
O	8.914584	13.215691	25.970639
O	7.480960	11.356504	24.541914
O	10.159799	15.439030	23.955777
O	8.461369	13.190397	22.875977
Mo	7.441956	13.206423	25.098758
Mo	8.660739	15.515876	23.140471

Mo	9.810378	13.194452	21.253691
Mo	8.617061	10.849857	23.119794
1_part1			
C	16.875085	14.764581	-0.474730
C	16.592049	14.592596	-1.817261
H	16.116568	13.830848	-2.127148
C	17.028839	15.576621	-2.696806
H	16.840579	15.501627	-3.624779
C	17.748364	16.679651	-2.216387
H	18.048999	17.341270	-2.828289
C	18.028554	16.826046	-0.869819
H	18.513818	17.581117	-0.559969
C	17.592373	15.851878	0.028994
C	17.796355	15.774694	1.481445
C	18.455412	16.662298	2.323555
H	18.849697	17.455434	1.979536
C	18.525385	16.364960	3.684437
H	18.962917	16.973064	4.268739
C	17.979943	15.217511	4.201557
H	18.030468	15.054687	5.136301
C	17.349855	14.284414	3.376880
H	17.002713	13.467594	3.717009
C	17.259558	14.614047	2.036001
C	14.800796	13.595169	1.086173
C	14.167469	14.797377	1.371892
H	14.655829	15.611440	1.395124
C	12.807693	14.778772	1.621644
H	12.353868	15.586752	1.830566
C	12.106657	13.588465	1.568611
H	11.170143	13.587028	1.729784

C	12.750239	12.410134	1.285461
H	12.257269	11.598567	1.258669
C	14.128142	12.395799	1.035525
H	14.582489	11.585603	0.837632
S	16.570387	13.547277	0.785957
C	10.626671	6.031816	1.894885
C	10.763373	4.970267	1.013872
H	11.534732	4.416300	1.015780
C	9.704801	4.756741	0.119830
H	9.742900	4.032519	-0.494384
C	8.598611	5.601030	0.129555
H	7.888167	5.440541	-0.480162
C	8.506822	6.665903	1.000476
H	7.745259	7.232847	0.988199
C	9.544543	6.900269	1.898371
C	9.725923	8.029117	2.828197
C	8.886205	9.109972	3.069507
H	8.045424	9.176078	2.633240
C	9.298551	10.093369	3.959145
H	8.724913	10.828230	4.139844
C	10.540036	10.023327	4.593343
H	10.804877	10.718096	5.184875
C	11.393363	8.952346	4.370750
H	12.243742	8.899072	4.790483
C	10.949106	7.966454	3.511757
C	12.723280	4.924560	5.090277
H	13.597195	5.153055	4.793181
C	11.597421	5.420085	4.450391
C	10.300224	5.128518	4.850985
H	9.550747	5.497105	4.398753

C	10.139794	4.275451	5.940094
H	9.266247	4.048670	6.237429
C	11.249324	3.754002	6.594294
H	11.127191	3.166722	7.330942
C	12.533581	4.080299	6.184891
H	13.283373	3.728983	6.649878
S	11.878180	6.520919	3.055010
O	18.287571	10.304795	-2.339703
O	16.149308	11.262567	-1.007449
O	15.919241	8.667024	-1.927549
O	13.656445	9.512401	-0.473079
O	18.366182	10.287700	0.396373
O	16.751792	11.336751	2.380075
O	19.134800	10.324144	3.130064
O	16.733673	8.769958	3.288247
O	14.124571	9.528587	2.556608
O	14.521939	7.238462	3.927582
O	14.159986	7.201948	1.067088
O	16.227186	8.723102	0.644474
O	13.675151	7.036589	-1.635040
Mo	17.213352	9.926383	-1.064519
Mo	17.760409	9.967146	2.204092
Mo	15.095487	8.130805	2.583950
Mo	14.603521	8.111192	-0.598230
O	14.010504	4.670475	2.339703
O	16.148767	3.712703	1.007449
O	16.378834	6.308246	1.927549
O	18.641630	5.462869	0.473079
O	13.931893	4.687570	-0.396373
O	15.546283	3.638518	-2.380075

O	13.163275	4.651126	-3.130064
O	15.564402	6.205312	-3.288247
O	18.173504	5.446683	-2.556608
O	17.776136	7.736808	-3.927582
O	18.138089	7.773322	-1.067088
O	16.070889	6.252168	-0.644474
O	18.622924	7.938681	1.635040
Mo	15.084723	5.048887	1.064519
Mo	14.537666	5.008124	-2.204092
Mo	17.202588	6.844465	-2.583950
Mo	17.694554	6.864078	0.598230
1_part2			
C	15.995025	7.092982	8.820223
C	15.741662	7.011057	7.471270
H	15.273539	6.270374	7.103542
C	16.194449	8.054297	6.658888
H	16.030335	8.030775	5.723484
C	16.886087	9.127841	7.217114
H	17.192884	9.827680	6.652997
C	17.135940	9.192827	8.580381
H	17.607364	9.932629	8.947136
C	16.688929	8.162630	9.406159
C	16.860269	7.997217	10.854756
C	16.336864	6.795935	11.323431
C	16.406872	6.375401	12.650547
H	16.054232	5.540670	12.934486
C	17.024674	7.254186	13.533579
H	17.072530	7.030111	14.455514
C	17.576385	8.455975	13.095366
H	18.012422	9.021968	13.720663

C	17.500622	8.845390	11.758157
H	17.876771	9.668468	11.469649
C	13.887916	5.863755	10.254140
C	13.198309	4.679884	10.081461
H	13.650037	3.878521	9.843142
C	11.809457	4.702185	10.270656
H	11.302643	3.907341	10.148679
C	11.174242	5.868982	10.632163
H	10.233328	5.874461	10.759333
C	11.899842	7.040179	10.812366
H	11.452885	7.838463	11.068486
C	13.259808	7.047876	10.621703
H	13.760767	7.846662	10.738523
S	15.663984	5.808705	10.003655
C	9.299805	-1.784230	11.026701
C	9.396461	-2.867509	10.169177
H	10.126924	-3.472774	10.211365
C	8.366367	-3.025978	9.239902
H	8.381997	-3.763912	8.642571
C	7.327327	-2.120994	9.179161
H	6.640158	-2.251849	8.535899
C	7.253320	-1.024064	10.031364
H	6.531710	-0.409733	9.971027
C	8.268015	-0.846760	10.980091
C	8.460013	0.270149	11.908632
C	7.655175	1.379881	12.136914
H	6.826555	1.477221	11.681928
C	8.081189	2.346322	13.041415
H	7.522075	3.092630	13.220095
C	9.305276	2.244361	13.690110

H	9.577236	2.931551	14.287220
C	10.139831	1.147623	13.476692
H	10.984950	1.072791	13.903601
C	9.671712	0.172489	12.609258
C	10.363796	-2.357038	13.582575
C	9.105248	-2.632133	14.075289
H	8.330769	-2.265555	13.665483
C	9.000919	-3.460500	15.187703
H	8.143328	-3.673434	15.537246
C	10.137734	-3.975791	15.790705
H	10.053259	-4.533364	16.555558
C	11.394060	-3.686860	15.286980
H	12.167309	-4.042554	15.707907
C	11.526063	-2.870044	14.161354
H	12.381416	-2.670396	13.799938
S	10.577966	-1.287446	12.157833
O	17.619643	2.443309	7.051958
O	15.413510	3.459015	8.214470
O	17.455009	2.365547	9.793173
O	15.671104	3.527209	11.551345
O	17.900979	2.422528	12.595312
O	15.434060	0.978044	12.506862
O	12.927603	1.819769	11.536298
O	13.143198	-0.473684	12.935899
O	15.211248	0.923500	9.837031
O	13.037001	-0.502420	10.043475
O	15.164894	0.891840	7.237116
O	12.821234	1.835214	8.491747
O	12.841207	-0.636290	7.294003
Mo	16.426108	2.086095	8.223278

Mo	16.626166	2.107226	11.519966
Mo	13.853596	0.394645	11.644567
Mo	13.703399	0.389452	8.428805
O	12.662358	-3.040065	11.298658
O	14.868491	-4.055771	10.136146
O	12.826992	-2.962303	8.557443
O	14.610897	-4.123965	6.799270
O	12.381022	-3.019284	5.755304
O	14.847940	-1.574800	5.843754
O	17.354398	-2.416525	6.814318
O	17.138803	-0.123072	5.414716
O	15.070753	-1.520256	8.513585
O	17.245000	-0.094336	8.307140
O	15.117107	-1.488596	11.113500
O	17.460767	-2.431971	9.858868
O	17.440794	0.039533	11.056613
Mo	13.855893	-2.682851	10.127338
Mo	13.655835	-2.703982	6.830650
Mo	16.428405	-0.991401	6.706049
Mo	16.578602	-0.986208	9.921811
[9]·2CH$_3$OH			
Te	0.931835	3.994886	8.736180
C	0.258788	2.291416	9.781395
C	1.148863	1.923373	10.806615
C	2.612317	3.718931	10.001345
C	0.779374	0.868521	11.648240
H	1.341686	0.620592	12.371711
C	2.419165	2.668699	10.899321
C	1.760379	2.916627	7.087467
C	-0.931044	1.624626	9.557810

H	-1.520490	1.898734	8.865242
C	-1.240967	0.543595	10.370351
H	-2.032088	0.044658	10.206752
C	3.448848	2.369952	11.797297
H	3.349554	1.656965	12.417155
C	-0.402797	0.186332	11.422837
H	-0.646068	-0.532816	11.993616
C	4.611328	3.118358	11.777302
H	5.309238	2.912008	12.388071
C	3.772004	4.482736	9.975896
H	3.874592	5.198804	9.359674
C	4.778634	4.165511	10.884779
H	5.586148	4.667528	10.890232
C	2.026410	3.638855	5.945910
H	1.828308	4.567432	5.911373
C	2.874077	1.655425	4.891607
H	3.268124	1.224244	4.142687
C	2.014683	1.563029	7.131093
H	1.801126	1.062552	7.910915
C	2.586338	3.001324	4.849798
H	2.773763	3.498721	4.060888
C	2.582701	0.939357	6.036799
H	2.773644	0.009240	6.071336
Mo	-2.850650	5.965535	8.929409
Mo	-0.746353	6.876865	11.193435
Mo	-1.099076	7.354706	6.604850
Mo	1.081376	8.274044	8.859607
O	-2.617995	6.240412	10.841880
O	-2.912802	6.680370	7.110553
O	0.637849	8.064459	10.728088

O	0.354571	8.477007	7.096738
O	-1.178976	7.289721	8.941042
O	-1.381299	7.855799	4.999945
O	-2.026121	4.495826	8.689282
O	-4.540129	5.514335	8.994303
O	-0.769637	7.043024	12.888502
O	1.866150	6.764758	8.641111
O	-0.330403	5.833871	6.449431
O	-0.007566	5.347715	10.929314
O	2.335655	9.422678	8.922138
Mo	-2.160747	9.433765	9.248245
Mo	-4.265044	8.522435	6.984218
Mo	-3.912322	8.044594	11.572803
Mo	-6.092774	7.125256	9.318047
O	-2.393402	9.158888	7.335774
O	-2.098596	8.718930	11.067101
O	-5.649247	7.334841	7.449566
O	-5.365968	6.922293	11.080916
O	-3.832422	8.109579	9.236611
O	-3.630099	7.543501	13.177708
O	-2.985277	10.903474	9.488372
O	-0.471268	9.884965	9.183351
O	-4.241761	8.356276	5.289152
O	-6.877547	8.634542	9.536542
O	-4.680994	9.565429	11.728222
O	-5.003832	10.051585	7.248339
O	-7.347053	5.976622	9.255516
8			
Te	9.205726	5.183270	4.720929
C	9.058875	3.164461	5.263473

C	8.759391	4.215947	7.457355
C	11.336055	5.244614	4.788088
C	8.933636	5.427340	6.801561
C	8.836112	2.993764	6.636954
C	11.997903	5.930113	3.787278
H	11.511701	6.333199	3.077492
C	12.025512	4.631758	5.827087
H	11.557757	4.158784	6.505268
C	13.389373	6.021879	3.832051
H	13.856277	6.496112	3.153870
C	9.134315	2.092662	4.381180
H	9.275969	2.241138	3.454113
C	8.689958	1.681066	7.101804
H	8.538107	1.525192	8.026237
C	14.088716	5.418151	4.865783
H	15.035444	5.479538	4.892120
C	9.001620	0.809006	4.876318
H	9.072161	0.062654	4.290317
C	8.491339	4.237744	8.833470
H	8.365997	3.425562	9.308855
C	8.859424	6.643917	7.452088
H	8.982494	7.456806	6.975386
C	13.418941	4.727536	5.857375
H	13.906946	4.315398	6.560576
C	8.763569	0.610999	6.232679
H	8.650488	-0.272026	6.565844
C	8.413568	5.454243	9.495848
H	8.228374	5.466624	10.428182
C	8.600273	6.651468	8.824252
H	8.552169	7.475797	9.295686

Te	2.588313	10.096175	2.025456
C	1.371184	11.579182	1.140397
C	3.682441	11.785144	2.637662
C	1.881748	12.868977	1.355045
C	1.511308	9.875060	3.850487
C	0.182490	9.404401	6.210293
H	-0.271190	9.229233	7.025426
C	3.099629	12.985542	2.187298
C	0.247812	11.324430	0.366086
H	-0.062248	10.438047	0.227816
C	1.207479	13.928333	0.757192
H	1.524427	14.815659	0.879660
C	-0.408221	12.407636	-0.198845
H	-1.192491	12.267181	-0.715053
C	1.457314	9.915858	6.237947
H	1.866865	10.112301	7.071516
C	3.697172	14.175646	2.563918
H	3.326139	15.002802	2.280794
C	2.153520	10.147253	5.060677
H	3.043251	10.481246	5.076480
C	-0.445910	9.142361	5.009320
H	-1.331072	8.800341	5.001419
C	4.839242	14.159130	3.357983
H	5.235996	14.982727	3.620037
C	5.405503	12.976749	3.770159
H	6.190737	12.991447	4.304802
C	0.223113	9.382331	3.804397
H	-0.201197	9.210362	2.972144
C	4.837666	11.754067	3.411974
H	5.226222	10.931317	3.684563

C	0.078074	13.704195	-0.013169
H	-0.369354	14.437294	-0.418760
Mo	8.786130	5.331057	0.461690
Mo	5.928320	4.507992	1.716917
Mo	8.505385	8.321871	1.654366
Mo	5.661432	7.496800	2.981230
O	7.309596	4.065251	0.335667
O	6.872194	8.878828	2.429599
O	9.472882	7.160453	0.306037
O	7.183311	6.447999	1.359785
O	4.822253	5.854541	2.466208
O	9.575183	4.773093	1.861771
O	4.363518	8.426835	3.597255
O	9.263079	9.812271	1.368345
O	9.325904	7.676421	3.007567
O	4.824681	3.229515	1.513067
O	9.730152	4.652122	-0.837652
O	6.877286	4.063283	3.063270
O	6.505830	6.939084	4.353921
Mo	5.927682	7.260517	-0.461690
Mo	8.785493	8.083581	-1.716917
Mo	6.208428	4.269703	-1.654366
Mo	9.052380	5.094774	-2.981230
O	7.404216	8.526323	-0.335667
O	7.841618	3.712746	-2.429599
O	5.240930	5.431120	-0.306037
O	7.530502	6.143575	-1.359785
O	9.891559	6.737033	-2.466208
O	5.138629	7.818481	-1.861771
O	10.350294	4.164738	-3.597255

O	5.450733	2.779302	-1.368345
O	5.387909	4.915152	-3.007567
O	9.889132	9.362058	-1.513067
O	4.983661	7.939451	0.837652
O	7.836527	8.528290	-3.063270
O	8.207982	5.652489	-4.353921

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