Table A1: Crystal Data and Structure Refinement for C1

Empirical formula	C_{10} H_{12} Cl Mo N_3 O_4 S_2
Formula weight	433.76
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	7.3148(3)
b (Å)	7.5035(3)
c (Å)	14.9713(6)
α (^{o})	85.005(2)
β (^{o})	85.616(2)
γ (^{o})	66.987(2)
Volume (Å^3)	752.65(5)
Z,	2
Calculated density (Mgm^{-3})	1.914
Absorption coefficient (mm^{-1})	1.343
F(000)	432
Crystal size (mm)	0.50 x 0.30 x 0.20
Theta range for data collection (^{o})	1.37 to 26.00
Limiting indices	-9<=h<=8,
	-9<=k<=9,
	-17<=l<=18
Reflections collected / unique	5963 / 2925 [R(int) = 0.0154]
Data / restraints / parameters	2925 / 0 / 197
Goodness-of-fit on F^2	1.186
Final R indices [I>2sigma(I)]	R1 = 0.0269, *w*R2 = 0.0659
R indices (all data)	R1 = 0.0281, *w*R2 = 0.0665
Largest diff. peak and hole (e.A^{-3})	0.843 and -0.902

Table A2: Crystal Data and Structure Refinement for C2

Empirical formula	C_{12} H_{17} Cl Mo N_3 O_4 S_2
Formula weight	461.81
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	8.23390(10)
b (Å)	10.17390(10)
c (Å)	10.40170(10)
α (^{o})	78.4860(10)
β (^{o})	89.3120(10)
γ (^{o})	81.7320(10)
Volume (Å^3)	844.825(15)
Z,	2
Calculated density (Mgm^{-3})	1.815
Absorption coefficient (mm^{-1})	1.202
F(000)	464
Crystal size (mm)	0.10 x 0.10 x 0.10
Theta range for data collection (^{o})	2.06 to 26.00
Limiting indices	-10<=h<=10,
	-12<=k<=12,
	-12<=l<=12
Reflections collected / unique	7256 / 3305 [R(int) = 0.0144]
Data / restraints / parameters	3305 / 0 / 211
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0213, *w*R2 = 0.0591
R indices (all data)	R1 = 0.0233, wR2 = 0.0602
Largest diff. peak and hole (e.A^{-3})	0.623 and -0.465

Table A3: Crystal Data and Structure Refinement for C3

Empirical formula	$C_{16}\ H_{16}\ Cl\ Mo\ N_3\ O_4\ S_2$
Formula weight	510
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	7.05910(10)
b (Å)	9.56030(10)
c (Å)	14.5762(2)
α (^{o})	76.2800(10)
β (^{o})	81.3510(10)
γ (^{o})	81.9850(10)
Volume (Å^3)	939.24(2)
Z,	2
Calculated density (Mgm^{-3})	1.803
Absorption coefficient (mm^{-1})	1.116
F(000)	584
Crystal size (mm)	0.40 x 0.30 x 0.20
Theta range for data collection (^{o})	2.21 to 27.49
Limiting indices	-9<=h<=9,
	-12<=k<=12,
	-18<=l<=18
Reflections collected / unique	8953 / 4298 [R(int) = 0.0134]
Data / restraints / parameters	4298 / 0 / 246
Goodness-of-fit on F^2	1.116
Final R indices [I>2sigma(I)]	R1 = 0.0201, *w*R2 = 0.0602
R indices (all data)	R1 = 0.0206, *w*R2 = 0.0607
Largest diff. peak and hole (e.A^{-3})	0.360 and -0.729

Table A4: Crystal Data and Structure Refinement for C4

Empirical formula	$C_{28}\ H_{20}\ Mo\ N_2\ O_7$
Formula weight	552
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	
a (Å)	18.8765(2)
b (Å)	7.60060(10)
c (Å)	27.1933(4)
α (^{o})	90
β (^{o})	90
γ (^{o})	90
Volume (Å^3)	3901.50(9)
Z,	8
Calculated density (Mgm^{-3})	1.581
Absorption coefficient (mm^{-1})	0.695
F(000)	1936
Crystal size (mm)	0.15 x 0.10 x 0.10
Theta range for data collection (^{o})	1.50 to 27.50
Limiting indices	-24<=h<=24,
	-9<=k<=9,
	-35<=l<=35
Reflections collected / unique	34843 / 4482 [R(int) = 0.0375]
Data / restraints / parameters	4482 / 0 / 256
Goodness-of-fit on F^2	0.878
Final R indices [I>2sigma(I)]	R1 = 0.0620, *w*R2 = 0.1920
R indices (all data)	R1 = 0.0695, *w*R2 = 0.2024
Largest diff. peak and hole (e.A^{-3})	2.466 and -1.356

Table A5: Crystal Data and Structure Refinement for C6

Empirical formula	$C_{17}\ H_{17}\ Cl\ Mo\ N_2\ O_6\ S$
Formula weight	508.78
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	8.3916(8)
b (Å)	11.2114(10)
c (Å)	11.6265(11)
α (^{o})	67.5390(10)
β (^{o})	81.4410(10)
γ (^{o})	85.2190(10)
Volume (Å^3)	999.18(16)
Z,	2
Calculated density (Mgm^{-3})	1.691
Absorption coefficient (mm^{-1})	0.931
F(000)	512
Crystal size (mm)	0.30 x 0.20 x 0.20
Theta range for data collection (^{o})	1.91 to 24.99
Limiting indices	-9<=h<=9,
	-13<=k<=13,
	-13<=l<=13
Reflections collected / unique	10368 / 3487 [R(int) = 0.0202]
Data / restraints / parameters	3487 / 0 / 256
Goodness-of-fit on F^2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0274, *w*R2 = 0.1089
R indices (all data)	R1 = 0.0284, *w*R2 = 0.1118
Largest diff. peak and hole (e.A^{-3})	0.820 and -0.660

Table A6: Crystal data and structure refinement for C7

Empirical formula	$C_{14}\ H_{13}\ Cl\ Mo\ N_2\ O_6\ S$
Formula weight	468.71
Temperature	100 (1) K
Wavelength	0.71073 A
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a(Å)	8.28520(10)
b(Å)	10.0410(2)
c(Å)	10.4913(2)
α (^{o})	76.6300(10)
β (^{o})	86.4630(10)
γ (^{o})	87.7250(10)
Volume (Å^3)	847.23(3)
Z	2
Calculated density (Mgm^{-3})	2.135
Absorption coefficient (mm^{-1})	1.099
F(000)	532
Crystal size (mm)	0.30 x 0.20 x 0.20
Theta range for data collection (^{o})	2.00 to 27.50
Limiting indices	-10<=h<=10,
	-13<=k<=13,
	-13<=l<=13
Reflections collected / unique	7878 / 3864 [R(int) = 0.0136]
Data / restraints / parameters	3864 / 0 / 228
Goodness-of-fit on F^2	0.888
Final R indices [I>2sigma(I)]	R1 = 0.0269, *w*R2 = 0.0978
R indices (all data)	R1 = 0.0299, *w*R2 = 0.1024
Largest diff. peak and hole (e.A^{-3})	0.925 and -0.714

Table A7: Crystal Data and Structure Refinement for C8

Empirical formula	$C_{16}H_{15}ClMoN_2O_7S$
Formula weight	510.76
Temperature (K)	100 (1)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	P21/n
Unit cell dimensions	
a (Å)	10.4049(3)
b (Å)	14.0625(5)
c (Å)	12.6463(4)
α (^{o})	90
β (^{o})	100.837(2)
γ (^{o})	90
Volume (Å^3)	1817.39(10)
Z,	4
Calculated density (Mgm^{-3})	1.911
Absorption coefficient (mm^{-1})	1.030
F(000)	1048
Crystal size (mm)	0.40 x 0.30 x 0.20
Theta range for data collection (^{o})	2.19 to 25.50
Limiting indices	-12<=h<=12, -17<=k<=17, -15<=l<=15
Reflections collected / unique	13092 / 3357 [R(int) = 0.0417]
Data / restraints / parameters	3357 / 0 / 257
Goodness-of-fit on F^2	1.138
Final R indices [I>2sigma(I)]	R1 = 0.0396, *w*R2 = 0.0731
R indices (all data)	R1 = 0.0514, *w*R2 = 0.0775
Largest diff. peak and hole (e.A^{-3})	0.965 and -0.854

Table A8. Crystal Data and Structure Refinement for C9

Empirical formula	$C_{21}H_{30}O_7N_6ClPMo$
Formula weight	636.50
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	
a (Å)	9.5993(7)
b (Å)	21.8850(17)
c (Å)	13.8804(11)
α (^{o})	90
β (^{o})	106.5510(10)
γ (^{o})	90
Volume (Å^3)	2795.2(4)
Z,	6
Calculated density (Mgm^{-3})	1.652
Absorption coefficient (mm^{-1})	0.949
F(000)	1350
Crystal size (mm)	0.40 x 0.40 x 0.30
Theta range for data collection (^{o})	1.79 to 27.50
Limiting indices	-12<=h<=12
	-28<=k<=28
	-18<=l<=18
Reflections collected / unique	35132 / 6419 [R(int) = 0.0258]
Data / restraints / parameters	6419 / 0 / 341
Goodness-of-fit on F^2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0686, *w*R2 = 0.1997
R indices (all data)	R1 = 0.0739, *w*R2 = 0.2068
Largest diff. peak and hole (e.A^{-3})	3.147 and -1.115

Table A9: Crystal Data and Structure Refinement for C10

Empirical formula	$C_{19}\ H_{22}\ Mo\ N_2\ O_7\ S$
Formula weight	518.40
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	7.9629(7)
b (Å)	10.3906(10)
c (Å)	13.0994(12)
α (^{o})	81.380(3)
β (^{o})	72.455(4)
γ (^{o})	88.026(3)
Volume (Å^3)	1021.68(16)
Z,	2
Calculated density (Mgm^{-3})	1.685
Absorption coefficient (mm^{-1})	0.789
F(000)	528
Crystal size (mm)	0.30 x 0.30 x 0.20
Theta range for data collection (^{o})	2.20 to 25.49
Limiting indices	-9<=h<=9
	-12<=k<=12
	-15<=l<=15
Reflections collected / unique	14197 / 3324 [R(int) = 0.0331]
Data / restraints / parameters	3979 / 0 / 276
Goodness-of-fit on F^2	1.196
Final R indices [I>2sigma(I)]	R1 = 0.0429, *w*R2 = 0.1163
R indices (all data)	R1 = 0.0486, *w*R2 = 0.1631
Largest diff. peak and hole (e.A^{-3})	0.896 and -0.824

Table A10: Crystal Data and Structure Refinement for C12

Empirical formula	C_{20} H_{23} Mo N_3 O7
Formula weight	513.35
Temperature	100(1)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	8.1339(3)
b (Å)	10.5258(4)
c (Å)	12.9452(6)
α (^{o})	85.077(2)
β (^{o})	72.828(2)
γ (^{o})	88.216(2)
Volume (Å^3)	1054.98(7)
Z,	2
Calculated density (Mgm^{-3})	1.565
Absorption coefficient (mm^{-1})	0.669
F(000)	524
Crystal size (mm)	0.32 x 0.30 x 0.30
Theta range for data collection (^{o})	1.94 to 28.3
Limiting indices	-10<=h<=10,
	-14<=k<=14,
	-17<=l<=17
Reflections collected / unique	10571 / 5176 [R(int) = 0.0187]
Data / restraints / parameters	5176 / 0 / 284
Goodness-of-fit on F^2	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0255, *w*R2 = 0.0807
R indices (all data)	R1 = 0.0267, *w*R2 = 0.0820
Largest diff. peak and hole(e.A^{-3})	0.590 and -1.203

Table A11 Crystal Data and Structure Refinement for C13

Empirical formula	C_{21} H_{23} Mo N_4 O_7
Formula weight	539
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	8.82060(10)
b (Å)	9.6406(2)
c (Å)	12.9167(2)
α (^{o})	82.4180(10)
β (^{o})	84.6270(10)
γ (^{o})	71.9380(10)
Volume (Å^3)	1033.51(3)
Z,	2
Calculated density (Mgm^{-3})	1.684
Absorption coefficient (mm^{-1})	0.685
F(000)	533
Crystal size (mm)	0.35 x 0.30 x 0.20
Theta range for data collection (^{o})	1.59 to 26.00
Limiting indices	-10<=h<=10,
	-11<=k<=11,
	-15<=l<=15
Reflections collected / unique	8701 / 4020 [R(int) = 0.0170]
Data / restraints / parameters	4020 / 0 / 300
Goodness-of-fit on F^2	1.085
Final R indices [I>2sigma(I)]	R1 = 0.0255, *w*R2 = 0.0691
R indices (all data)	R1 = 0.0269, *w*R2 = 0.0701
Largest diff. peak and hole (e.A^{-3})	0.764 and -0.470

Table A12: Crystal Data and Structure Refinement for C14

Empirical formula	$C_{21}H_{24}MoN_2O_7S$
Formula weight	544.43
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	10.5921(4)
b (Å)	13.2852(5)
c (Å)	16.6410(6)
α (^{o})	70.8350(10)
β (^{o})	87.001(2)
γ (^{o})	81.736(2)
Volume (Å^3)	2188.91(14)
Z,	4
Calculated density (Mgm^{-3})	1.652
Absorption coefficient (mm^{-1})	0.741
F(000)	1112
Crystal size (mm)	0.40 x 0.30 x 0.20
Theta range for data collection (^{o})	1.30 to 26.00
Limiting indices	-13<=h<=12,
	-16<=k<=16,
	-20<=l<=20
Reflections collected / unique	16942 / 8499 [R(int) = 0.0230]
Data / restraints / parameters	8499 / 0 / 581
Goodness-of-fit on F^2	1.087
Final R indices [I>2sigma(I)]	R1 = 0.0234, *w*R2 = 0.0693
R indices (all data)	R1 = 0.0253, *w*R2 = 0.0709
Largest diff. peak and hole (e.A^{-3})	0.353 and -0.682

Table A13. Crystal Data and Structure Refinement for C15

Empirical formula	$C_{18} H_{20} Mo N_2 O_7 S$
Formula weight	504
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	
a (Å)	7.75270(10)
b (Å)	20.6173(4)
c (Å)	12.6506(2)
α (^{o})	90
β (^{o})	100.9310(10)
γ (^{o})	90
Volume (Å^3)	1985.38(6)
Z,	4
Calculated density (Mgm^{-3})	1.677
Absorption coefficient (mm^{-1})	0.810
F(000)	1024
Crystal size (mm)	0.37 x 0.30 x 0.30
Theta range for data collection (^{o})	1.98 to 27.50
Limiting indices	-10<=h<=10,
	-26<=k<=26,
	-16<=l<=16
Reflections collected / unique	18375 / 4556 [R(int) = 0.0169]
Data / restraints / parameters	4556 / 0 / 266
Goodness-of-fit on F^2	1.153
Final R indices [I>2sigma(I)]	R1 = 0.0242, *w*R2 = 0.1191
R indices (all data)	R1 = 0.0245, *w*R2 = 0.1200
Largest diff. peak and hole (e.A^{-3})	0.473 and -1.683

Table A14. Crystal Data and Structure Refinement for C16

Empirical formula	$[Mo(C_{14}H_9ClN_2O_4)O_2(CH_4O)]\cdot C_{10}H_8N_2$
Formula weight	620.85
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	P2(1)/n
Unit cell dimensions	
a (Å)	6.9575(3)
b (Å)	7.4541(4)
c (Å)	47.197(2)
α (^{o})	90
β (^{o})	92.0073(6)
γ (^{o})	90
Volume (Å^3)	2446.2(2)
Z,	4
Calculated density (Mgm^{-3})	1.686
Absorption coefficient (mm^{-1})	0.700
F(000)	1256
Crystal size (mm)	0.25 x 0.20 x 0.20
Theta range for data collection (^{o})	2.60 to 28.20
Limiting indices	-9<=h<=9
	-9<=k<=9
	-61<=l<=61
Reflections collected / unique	29717 / 5408 [R(int) = 0.032]
Data / restraints / parameters	5604 / 3 / 356
Goodness-of-fit on F^2	1.23
Final R indices [I>2sigma(I)]	R1 = 0.0490, *w*R2 = 0.1380
R indices (all data)	R1 = 0.0497, *w*R2 = 0.1203
Largest diff. peak and hole (e.A^{-3})	0.550 and -1.250

Table A15. Crystal Data and Structure Refinement for C17

Empirical formula	$[Mo(C_{14}H_{12}N_2O_4)O_2(H_2O)]\cdot 0.5C_{10}H_8N_2$
Formula weight	443.27
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	7.9237 (1)
b (Å)	10.1869(1)
c (Å)	13.3215(2)
α (^{o})	78.7841(5)
β (^{o})	78.4605(5)
γ (^{o})	69.5728(5)
Volume (Å^3)	978.15(2)
Z,	2
Calculated density (Mgm^{-3})	1.685
Absorption coefficient (mm^{-1})	0.720
F(000)	502
Crystal size (mm)	0.25 x 0.20 x 0.25
Theta range for data collection (^{o})	2.50 to 28.20
Limiting indices	-10<=h<=10
	-13<=k<=13
	-17<=l<=17
Reflections collected / unique	9175 / 4266 [R(int) = 0.019]
Data / restraints / parameters	4445 / 24 / 275
Goodness-of-fit on F^2	0.98
Final R indices [I>2sigma(I)]	R1 = 0.026, *w*R2 = 0.076
R indices (all data)	R1 = 0.0485, *w*R2 = 0.1367
Largest diff. peak and hole (e.A^{-3})	0.730 and -0.720

Table A16. Crystal Data and Structure Refinement for C18

Empirical formula	$C_{28}\ H_{36}\ Mo_2\ N_4\ O_{12}$
Formula weight	814.50
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	
a (Å)	8.8304(4)
b (Å)	12.5291(5)
c (Å)	14.4997(6)
α (^{o})	90
β (^{o})	99.696(2)
γ (^{o})	90
Volume (Å^3)	1581.29(12)
Z,	2
Calculated density (Mgm^{-3})	1.711
Absorption coefficient (mm^{-1})	0.862
F(000)	828
Crystal size (mm)	0.45 x 0.45 x 0.30
Theta range for data collection (^{o})	2.16 to 27.50
Limiting indices	-11<=h<=11
	-16<=k<=16
	-18<=l<=17
Reflections collected / unique	13584 / 3625 [R(int) = 0.0251]
Data / restraints / parameters	3625 / 0 / 214
Goodness-of-fit on F^2	1.133
Final R indices [I>2sigma(I)]	R1 = 0.0333, *w*R2 = 0.0866
R indices (all data)	R1 = 0.0372, *w*R2 = 0.0898
Largest diff. peak and hole (e.A^{-3})	0.589 and -0.805

Table A17. Crystal Data and Structure Refinement for C19

Empirical formula	$C_{24}H_{24}Cl_4Mo_2N_4O_{12}$
Formula weight	862.15
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	C 2/c
Unit cell dimensions	
a (Å)	20.5338(2)
b (Å)	14.64580(10)
c (Å)	13.24770(10)
α (^{o})	90
β (^{o})	129.51(2)
γ (^{o})	90
Volume (Å^3)	3073.74(4)
Z,	4
Calculated density (Mgm^{-3})	1.863
Absorption coefficient (mm^{-1})	1.224
F(000)	2216
Crystal size (mm)	0.40 x 0.30 x 0.20
Theta range for data collection (^{o})	2.07 to 27.50
Limiting indices	-26<=h<=26
	-19<=k<=19
	-17<=l<=17
Reflections collected / unique	14499 / 3536 [R(int) = 0.0182]
Data / restraints / parameters	3536 / 0 / 204
Goodness-of-fit on F^2	0.980
Final R indices [I>2sigma(I)]	R1 = 0.0193, *w*R2 = 0.0538
R indices (all data)	R1 = 0.0212, *w*R2 = 0.0553
Largest diff. peak and hole (e.A^{-3})	0.534 and -0.461

Table A18. Crystal Data and Structure Refinement for C20

Empirical formula	$C_{30}\ H_{28}\ C_{l2}\ Mo_2\ N_8\ O_6\ S_2$
Formula weight	923.52
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	P 21/n
Unit cell dimensions	
a (Å)	12.5483(2)
b (Å)	11.93150(10)
c (Å)	23.2930(3)
α (^{o})	90
β (^{o})	100.9000(10)
γ (^{o})	90
Volume (Å^3)	3424.51(8)
Z,	4
Calculated density (Mgm^{-3})	1.791
Absorption coefficient (mm^{-1})	1.067
F(000)	1848
Crystal size (mm)	0.40 x 0.30 x 0.30
Theta range for data collection (^{o})	1.93 to 28.30
Limiting indices	-16<=h<=16,
	-15<=k<=15
	-31<=l<=31
Reflections collected / unique	33860 / 8497 [R(int) = 0.0190]
Data / restraints / parameters	8484 / 0 / 453
Goodness-of-fit on F^2	1.081
Final R indices [I>2sigma(I)]	R1 = 0.0194, *w*R2 = 0.0502
R indices (all data)	R1 = 0.0216, *w*R2 = 0.0515
Largest diff. peak and hole (e.A^{-3})	0.454 and -0.419

Table A19. Crystal Data and Structure Refinement for C21

Empirical formula	$C_{30}H_{26}C_{l4}Mo_2N_8O_8S_2$
Formula weight	1024.41
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	9.0527(2)
b (Å)	9.2002(2)
c (Å)	12.3846(2)
α (^{o})	71.9720(10)
β (^{o})	72.5420(10)
γ (^{o})	89.1080(10)
Volume (Å^3)	932.25(3)
Z,	1
Calculated density (Mgm^{-3})	1.825
Absorption coefficient (mm^{-1})	1.132
F(000)	510
Crystal size (mm)	0.25 x 0.20 x 0.10
Theta range for data collection (^{o})	2.34 to 26.00
Limiting indices	-11<=h<=11,
	-11<=k<=11
	-15<=l<=15
Reflections collected / unique	7899 / 3614 [R(int) = 0.0190]
Data / restraints / parameters	3614 / 0 / 249
Goodness-of-fit on F^2	0.982
Final R indices [I>2sigma(I)]	R1 = 0.0263, *w*R2 = 0.0886
R indices (all data)	R1 = 0.0295, *w*R2 = 0.0919
Largest diff. peak and hole (e.A^{-3})	0.866 and -0.524

Table A20. Crystal Data and Structure Refinement for C22

Empirical formula	$C_{36} H_{62} Mo_2 N_{10} O_{12} P_2$
Formula weight	1080
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	
a (Å)	8.2462(4)
b (Å)	8.3898(4)
c (Å)	18.9782(10)
α (^{o})	86.238(2)
β (^{o})	83.245(2)
γ (^{o})	68.532(2)
Volume (Å^3)	1213.05(10)
Z,	1
Calculated density (Mgm^{-3})	1.480
Absorption coefficient (mm^{-1})	0.648
F(000)	558
Crystal size (mm)	0.40 x 0.20 x 0.08
Theta range for data collection (^{o})	1.08 to 26.00
Limiting indices	-10<=h<=10
	-10<=k<=10
	-23<=l<=21
Reflections collected / unique	10168 / 4715 [R(int) = 0.0193]
Data / restraints / parameters	4715 / 0 / 287
Goodness-of-fit on F^2	1.167
Final R indices [I>2sigma(I)]	R1 = 0.0321, *w*R2 = 0.0969
R indices (all data)	R1 = 0.0335, *w*R2 = 0.0977
Largest diff. peak and hole (e.A^{-3})	1.369 and -0.732

Table A21. Crystal Data and Structure Refinement for C23

Empirical formula	$C_{28}\ H_{36}\ Mo_2\ N_4\ O_{12}$
Formula weight	868.56
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	8.36030(10)
b (Å)	10.18100(10)
c (Å)	11.94300(10)
α (^{o})	94.2080(10)
β (^{o})	107.7120(10)
γ (^{o})	112.4400(10)
Volume (Å^3)	874.054(15)
Z,	1
Calculated density (Mgm^{-3})	1.650
Absorption coefficient (mm^{-1})	0.787
F(000)	442
Crystal size (mm)	0.27 x 0.14 x 0.10
Theta range for data collection (^{o})	1.83 to 27.50
Limiting indices	-10<=h<=10
	-12<=k<=13
	-15<=l<=15
Reflections collected / unique	8361 / 3984 [R(int) = 0.0133]
Data / restraints / parameters	3984 / 0 / 229
Goodness-of-fit on F^2	1.160
Final R indices [I>2sigma(I)]	R1 = 0.0207, *w*R2 = 0.0602
R indices (all data)	R1 = 0.0214, *w*R2 = 0.0606
Largest diff. peak and hole (e.A^{-3})	0.463 and -0.452

Table A22. Crystal Data and Structure Refinement for C24

Empirical formula	$C_{15}\ H_{13}\ Mo\ N_3\ O_5$
Formula weight	443.27
Temperature (K)	100(1)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	
a (Å)	10.04650(10)
b (Å)	14.5139(2)
c (Å)	12.6256(2)
α (^{o})	90
β (^{o})	113.0800(10)
γ (^{o})	90
Volume (Å^3)	1693.63(4)
Z,	4
Calculated density (Mgm^{-3})	1.738
Absorption coefficient (mm^{-1})	0.814
F(000)	896
Crystal size (mm)	0.40 x 0.30 x 0.20
Theta range for data collection (^{o})	2.20 to 25.99
Limiting indices	-12<=h<=12
	-17<=k<=17
	-15<=l<=15
Reflections collected / unique	14197 / 3324 [R(int) = 0.0331]
Data / restraints / parameters	3324 / 0 / 238
Goodness-of-fit on F^2	1.121
Final R indices [I>2sigma(I)]	R1 = 0.0429, *w*R2 = 0.1163
R indices (all data)	R1 = 0.0497, *w*R2 = 0.1203
Largest diff. peak and hole (e.A^{-3})	0.896 and -0.824