Commensurate $(C_6H_{14}N_2)_2[Mo_8O_{26}]$ $4H_2O$ and incommensurate $(C_6H_{14}N_2)_2[Mo_8O_{26}]$ $4.66H_2O$: a structural versatility linked to solvent content.

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Supplementary material

Table 1 - Fractional atomic coordinates, equivalent isotropic displacement parameters ($Å^2$), and s.u.'s for $(C_6H_{14}N_2)_2[Mo_8O_{26}]\cdot 4H_2O$

Atom	x	y	z	U_{eq}
Mo1	0.25888(4)	0.37951(3)	-0.02610(3)	0.01868(14)
Mo2	0.47524(3)	0.44973(3)	0.17692(3)	0.01540(13)
Mo3	0.78573(4)	0.39209(3)	0.20671(3)	0.01813(14)
Mo4	0.57152(4)	0.35669(3)	0.02056(3)	0.01616(13)
Mo5	0.19472(4)	0.28345(3)	0.12704(3)	0.01999(14)
Mo6	0.40766(4)	0.30695(3)	0.31313(3)	0.01689(13)
Mo7	0.73264(4)	0.29683(3)	0.36259(3)	0.01807(13)
Mo8	0.50910(3)	0.21841(3)	0.16045(3)	0.01450(12)
Mo9	0.25284(4)	0.03970(3)	0.30053(3)	0.01699(13)
Mo10	0.47035(3)	0.11159(3)	0.50438(3)	0.01507(13)
Mo11	0.79453(4)	0.07729(3)	0.55027(3)	0.01802(14)
Mo12	0.58281(3)	0.03153(3)	0.35728(3)	0.01555(13)
O1	0.1439(3)	0.4283(3)	-0.0297(3)	0.0288(15)
O2	0.3126(3)	0.4319(2)	0.1275(2)	0.0197(12)
O3	0.2422(4)	0.3269(3)	-0.1334(3)	0.0329(16)
O4	0.2041(3)	0.2636(2)	0.0066(2)	0.0239(13)
O5	0.4323(3)	0.3823(2)	0.0356(2)	0.0190(12)
O6	0.6392(3)	0.4761(3)	0.0140(2)	0.0248(14)
O7	0.5415(3)	0.5700(2)	0.1852(2)	0.0244(13)
O8	0.4883(3)	0.4512(2)	0.2886(2)	0.0216(12)
O9	0.3831(3)	0.2770(2)	0.1667(2)	0.0172(11)
O10	0.5968(3)	0.3900(2)	0.1659(2)	0.0168(11)
O11	0.7750(3)	0.4135(2)	0.3246(2)	0.0207(12)
O12	0.6717(3)	0.2411(2)	0.2095(2)	0.0178(11)
O13	0.9058(3)	0.3505(3)	0.2219(3)	0.0279(14)
O14	0.8396(3)	0.5127(3)	0.2103(3)	0.0300(15)
O15	0.7127(3)	0.3312(2)	0.0753(2)	0.0200(12)
O16	0.5255(3)	0.2839(3)	-0.0866(2)	0.0278(14)
O17	0.4933(3)	0.2145(2)	0.0475(2)	0.0204(12)
O18	0.0803(3)	0.3319(3)	0.1124(3)	0.0320(16)
O19	0.2666(3)	0.3344(2)	0.2581(2)	0.0220(13)

O20	0.1304(3)	0.1619(3)	0.1169(3)	0.0302(15)
O21	0.4502(3)	0.3767(3)	0.4206(2)	0.0269(14)
O22	0.3380(3)	0.1833(2)	0.3152(2)	0.0225(13)
O23	0.5473(3)	0.2849(2)	0.2999(2)	0.0183(11)
O24	0.7375(4)	0.3517(3)	0.4661(2)	0.0318(15)
O25	0.6430(3)	0.1530(3)	0.3514(2)	0.0244(13)
O26	0.8596(3)	0.2659(3)	0.3768(3)	0.0326(16)
O27	0.4466(3)	0.0978(2)	0.1529(2)	0.0236(13)
O28	0.2440(3)	-0.0133(3)	0.1952(2)	0.0284(14)
O29	0.1203(3)	0.0610(3)	0.2882(3)	0.0287(15)
O30	0.3059(3)	0.0801(2)	0.4507(2)	0.0181(11)
O31	0.4383(3)	0.0457(2)	0.3650(2)	0.0185(11)
O32	0.7852(3)	0.0859(2)	0.6684(2)	0.0212(12)
O33	0.5254(3)	0.2329(3)	0.5108(2)	0.0255(13)
O34	0.4806(3)	0.1136(2)	0.6158(2)	0.0200(12)
O35	0.6030(3)	0.0628(2)	0.5022(2)	0.0166(11)
O36	0.9235(3)	0.0487(3)	0.5637(3)	0.0313(16)
O37	0.8354(3)	0.2015(3)	0.5621(3)	0.0301(15)
O38	0.7321(3)	0.0195(2)	0.4192(2)	0.0199(12)
O39	0.5488(3)	-0.0410(3)	0.2517(2)	0.0273(14)
O1w	0.6356(5)	0.1282(3)	-0.0883(3)	0.049(2)
O2w	0.3364(6)	0.2032(4)	0.7346(4)	0.072(3)
O3w	0.9070(4)	0.0220(4)	0.3469(3)	0.058(3)
O4w	0.3259(5)	0.5541(4)	0.3805(4)	0.062(3)
O5w	0.0931(6)	0.4624(5)	0.3786(5)	0.095(3)
O6w	0.0438(9)	0.1717(8)	0.7667(7)	0.155(6)
N1	0.8624(4)	0.0250(4)	0.1750(3)	0.040(2)
N2	0.7548(4)	0.0513(3)	0.0324(3)	0.0333(19)
N3	0.1441(4)	0.3577(4)	0.4954(3)	0.038(2)
N4	0.2270(5)	0.2680(4)	0.6006(4)	0.041(2)
N5	0.1652(4)	0.7345(3)	0.2214(3)	0.0314(18)
N6	0.1766(4)	0.5803(4)	0.1333(3)	0.039(2)
C1	0.8958(6)	-0.0270(4)	0.1009(4)	0.046(3)
C2	0.8160(6)	-0.0218(5)	0.0127(4)	0.045(3)
C3	0.7329(7)	-0.0151(7)	0.1538(6)	0.076(4)
C4	0.6688(6)	0.0134(5)	0.0734(5)	0.047(3)
C5	0.8963(5)	0.1333(4)	0.1830(4)	0.036(2)
C6	0.8431(6)	0.1467(4)	0.0923(4)	0.042(2)
C7	0.2757(6)	0.4069(5)	0.5393(5)	0.045(3)
C8	0.3254(6)	0.3368(5)	0.5856(5)	0.043(3)
C9	0.0873(6)	0.3610(4)	0.5656(4)	0.037(2)
C10	0.1576(7)	0.3253(5)	0.6393(5)	0.050(3)
C11	0.1189(6)	0.2522(5)	0.4454(5)	0.052(3)
C12	0.1450(6)	0.1953(5)	0.5127(5)	0.048(3)
C13	0.2889(6)	0.7334(5)	0.2532(5)	0.050(3)
C14	0.2968(6)	0.6371(5)	0.2002(5)	0.046(3)
C15	0.0833(6)	0.6484(4)	0.2338(5)	0.045(3)
C16	0.0915(6)	0.5531(4)	0.1800(4)	0.040(3)
C17	0.1283(6)	0.7324(5)	0.1261(4)	0.043(3)
C18	0.1367(6)	0.6377(5)	0.0712(5)	0.047(3)

Table 2 – Anisotropic displacement parameters U^{ij} ($Å^2$) and their s.u.'s for $(C_6H_{14}N_2)_2[Mo_8O_{26}]\cdot 4H_2O$

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.01580(18)	0.01817(18)	0.0225(2)	0.00485(14)	0.00681(16)	0.00696(15)
Mo2	0.01421(17)	0.01238(16)	0.02019(19)	0.00386(13)	0.00687(15)	0.00489(13)
Mo3	0.01457(18)	0.01746(18)	0.0230(2)	0.00302(14)	0.00833(16)	0.00697(15)
Mo4	0.01711(18)	0.01583(17)	0.01909(19)	0.00618(14)	0.00918(15)	0.00713(14)
Mo5	0.01552(18)	0.01765(18)	0.0279(2)	0.00319(14)	0.00980(17)	0.00805(15)
Mo6	0.01832(19)	0.01529(17)	0.02046(19)	0.00559(14)	0.01050(16)	0.00655(14)
Mo7	0.01560(18)	0.01834(18)	0.01871(19)	0.00269(14)	0.00569(15)	0.00551(14)
Mo8	0.01366(17)	0.01222(16)	0.01815(18)	0.00368(13)	0.00649(14)	0.00443(13)
Mo9	0.01405(17)	0.01775(18)	0.01901(19)	0.00330(13)	0.00595(15)	0.00667(14)
Mo10	0.01321(17)	0.01381(17)	0.01882(18)	0.00385(13)	0.00652(14)	0.00507(13)
Mo11	0.01324(17)	0.01954(18)	0.0219(2)	0.00333(13)	0.00701(15)	0.00811(15)
Mo12	0.01403(17)	0.01682(17)	0.01800(18)	0.00478(13)	0.00778(14)	0.00653(14)
O1	0.0243(19)	0.030(2)	0.038(2)	0.0123(15)	0.0139(17)	0.0144(17)
O2	0.0179(16)	0.0142(15)	0.0280(18)	0.0048(12)	0.0090(14)	0.0066(13)
O3	0.036(2)	0.033(2)	0.028(2)	0.0089(17)	0.0106(18)	0.0074(16)
O4	0.0244(18)	0.0191(16)	0.0239(18)	0.0027(13)	0.0079(15)	0.0026(13)
O5	0.0167(16)	0.0207(16)	0.0222(17)	0.0072(12)	0.0079(13)	0.0080(13)
O6	0.0213(18)	0.0234(18)	0.035(2)	0.0073(14)	0.0117(16)	0.0154(15)
O7	0.0240(18)	0.0168(16)	0.033(2)	0.0058(13)	0.0105(16)	0.0093(14)
O8	0.0248(18)	0.0181(16)	0.0225(17)	0.0048(13)	0.0105(15)	0.0061(13)
O9	0.0147(15)	0.0169(15)	0.0225(16)	0.0066(12)	0.0087(13)	0.0057(12)
O10	0.0139(15)	0.0181(15)	0.0210(16)	0.0064(12)	0.0078(13)	0.0073(12)
O11	0.0217(17)	0.0152(15)	0.0221(17)	0.0011(12)	0.0079(14)	0.0039(12)
O12	0.0140(15)	0.0163(15)	0.0251(17)	0.0061(12)	0.0088(13)	0.0060(12)
O13	0.0202(18)	0.034(2)	0.032(2)	0.0101(15)	0.0101(16)	0.0090(16)
O14	0.028(2)	0.0222(18)	0.040(2)	0.0017(15)	0.0152(18)	0.0124(16)
O15	0.0190(16)	0.0210(16)	0.0249(17)	0.0077(13)	0.0120(14)	0.0090(13)
O16	0.033(2)	0.0287(19)	0.0232(18)	0.0095(16)	0.0124(16)	0.0080(15)
O17	0.0220(17)	0.0180(16)	0.0225(17)	0.0057(13)	0.0102(14)	0.0054(13)
O18	0.0228(19)	0.033(2)	0.045(2)	0.0123(16)	0.0143(18)	0.0128(18)
O19	0.0218(17)	0.0228(17)	0.0286(18)	0.0104(14)	0.0155(15)	0.0089(14)
O20	0.030(2)	0.0213(18)	0.041(2)	0.0022(15)	0.0191(18)	0.0095(16)
O21	0.035(2)	0.0249(18)	0.0235(18)	0.0109(15)	0.0135(16)	0.0047(14)
O22	0.0206(17)	0.0202(16)	0.0308(19)	0.0060(13)	0.0119(15)	0.0125(14)
O23	0.0159(15)	0.0200(16)	0.0191(16)	0.0043(12)	0.0068(13)	0.0062(12)
O24	0.037(2)	0.030(2)	0.0228(19)	0.0029(17)	0.0115(17)	0.0024(15)
O25	0.0198(17)	0.0237(17)	0.035(2)	0.0066(14)	0.0119(15)	0.0169(15)
O26	0.0217(19)	0.039(2)	0.040(2)	0.0125(17)	0.0084(17)	0.0175(18)
O27	0.0228(18)	0.0166(15)	0.0284(19)	0.0018(13)	0.0087(15)	0.0056(13)
O28	0.033(2)	0.0264(18)	0.0224(18)	0.0041(15)	0.0107(16)	0.0048(14)
O29	0.0204(18)	0.034(2)	0.041(2)	0.0139(16)	0.0131(17)	0.0200(17)
O30	0.0163(15)	0.0228(16)	0.0178(16)	0.0084(13)	0.0073(13)	0.0068(12)
O31	0.0154(15)	0.0203(16)	0.0203(16)	0.0052(12)	0.0068(13)	0.0061(12)
O32	0.0226(17)	0.0164(15)	0.0239(17)	0.0029(13)	0.0097(14)	0.0062(13)
O33	0.0245(18)	0.0197(16)	0.032(2)	0.0037(14)	0.0108(16)	0.0102(14)
O34	0.0170(16)	0.0217(16)	0.0181(16)	0.0021(12)	0.0071(13)	0.0024(12)
O35	0.0151(15)	0.0177(15)	0.0163(15)	0.0040(11)	0.0056(12)	0.0043(12)
O36	0.0201(18)	0.047(2)	0.036(2)	0.0154(17)	0.0142(17)	0.0196(18)
O37	0.031(2)	0.0240(18)	0.032(2)	0.0004(15)	0.0105(17)	0.0108(15)
O38	0.0172(16)	0.0245(17)	0.0220(17)	0.0085(13)	0.0107(14)	0.0072(13)
O39	0.029(2)	0.0315(19)	0.0225(18)	0.0103(16)	0.0096(16)	0.0070(15)

O1w	0.059(3)	0.035(2)	0.042(3)	0.024(2)	-0.003(2)	0.001(2)
O2w	0.084(4)	0.047(3)	0.062(4)	0.032(3)	-0.006(3)	-0.001(3)
O3w	0.045(3)	0.110(4)	0.041(3)	0.044(3)	0.022(2)	0.032(3)
O4w	0.071(4)	0.048(3)	0.063(4)	0.018(3)	0.027(3)	0.003(3)
O5w	0.070(4)	0.085(5)	0.088(5)	-0.011(3)	-0.018(4)	0.045(4)
O6w	0.127(8)	0.147(9)	0.149(9)	0.028(7)	0.018(7)	0.010(7)
N1	0.036(3)	0.051(3)	0.029(3)	0.007(2)	0.006(2)	0.021(2)
N2	0.028(2)	0.035(3)	0.033(3)	0.014(2)	0.003(2)	0.008(2)
N3	0.031(3)	0.045(3)	0.038(3)	0.013(2)	0.011(2)	0.009(2)
N4	0.040(3)	0.037(3)	0.051(3)	0.015(2)	0.017(3)	0.015(2)
N5	0.033(3)	0.018(2)	0.037(3)	0.0040(17)	0.012(2)	-0.0021(18)
N6	0.039(3)	0.028(2)	0.047(3)	0.006(2)	0.024(3)	-0.005(2)
C1	0.043(4)	0.030(3)	0.049(4)	0.019(3)	-0.003(3)	-0.003(3)
C2	0.047(4)	0.051(4)	0.036(3)	0.026(3)	0.015(3)	-0.004(3)
C3	0.041(5)	0.111(8)	0.061(5)	-0.011(5)	0.021(4)	0.030(5)
C4	0.021(3)	0.053(4)	0.058(4)	0.005(3)	0.015(3)	0.005(3)
C5	0.031(3)	0.029(3)	0.036(3)	0.008(2)	0.006(3)	-0.003(2)
C6	0.035(3)	0.028(3)	0.049(4)	0.005(2)	0.000(3)	0.008(3)
C7	0.033(3)	0.039(4)	0.067(5)	0.009(3)	0.025(3)	0.013(3)
C8	0.027(3)	0.038(3)	0.051(4)	0.007(3)	0.004(3)	0.004(3)
C9	0.033(3)	0.034(3)	0.042(3)	0.011(2)	0.017(3)	-0.003(3)
C10	0.062(5)	0.058(5)	0.048(4)	0.034(4)	0.032(4)	0.017(3)
C11	0.040(4)	0.047(4)	0.049(4)	0.013(3)	0.005(3)	-0.015(3)
C12	0.033(3)	0.026(3)	0.076(5)	0.003(2)	0.019(3)	-0.003(3)
C13	0.029(3)	0.042(4)	0.054(4)	0.002(3)	-0.004(3)	-0.002(3)
C14	0.037(4)	0.051(4)	0.060(5)	0.020(3)	0.024(3)	0.017(3)
C15	0.051(4)	0.035(3)	0.051(4)	0.005(3)	0.035(4)	0.002(3)
C16	0.046(4)	0.024(3)	0.048(4)	0.000(2)	0.028(3)	0.001(2)
C17	0.041(4)	0.042(4)	0.042(4)	0.005(3)	0.012(3)	0.014(3)
C18	0.039(4)	0.049(4)	0.040(4)	0.003(3)	0.018(3)	-0.006(3)

Table 3 – Main distances (Å) for (I) and (II)

(I)

Mo1-O3	1.685(4)	Mo7-O24	1.685(4)
Mo1-O1	1.722(5)	Mo7-O26	1.697(5)
Mo1-O4	1.874(4)	Mo7-O11	1.904(4)
Mo1-O5	2.075(3)	Mo7-O25	2.045(4)
Mo1-O6^{i}	2.094(4)	Mo7-O23	2.170(3)
Mo1-O2	2.295(4)	Mo7-O12	2.284(3)
aver.	1.958	aver.	1.964
Mo2-O7	1.689(3)	Mo8-O27	1.687(3)
Mo2-O8	1.760(4)	Mo8-O17	1.767(4)
Mo2-O2	1.869(3)	Mo8-O12	1.854(3)
Mo2-O10	1.936(4)	Mo8-O9	1.959(4)
Mo2-O5	2.156(3)	Mo8-O23	2.138(3)
Mo2-O9	2.425(3)	Mo8-O10	2.419(3)
aver.	1.973	aver.	1.971
Mo3-O14	1.686(4)	Mo9-O28	1.687(4)
Mo3-O13	1.702(4)	Mo9-O29	1.701(4)
Mo3-O11	1.916(4)	Mo9-O32^{ii}	1.953(4)
Mo3-O15	1.976(3)	Mo9-O22	2.014(3)
Mo3-O10	2.226(3)	Mo9-O31	2.200(3)
Mo3-O12	2.303(3)	Mo9-O30	2.241(3)
aver.	1.968	aver.	1.966
Mo4-O16	1.697(3)	Mo10-O33	1.686(4)
Mo4-O15	1.874(4)	Mo10-O34	1.760(4)
Mo4-O6	1.758(4)	Mo10-O30	1.865(3)
Mo4-O5	1.913(4)	Mo10-O35	1.939(4)
Mo4-O10	2.218(4)	Mo10-O31	2.150(3)
Mo4-O17	2.221(4)	Mo10-O35^{ii}	2.427(3)
aver.	1.947	aver.	1.971
Mo5-O20	1.694(4)	Mo11-O37	1.695(4)
Mo5-O18	1.700(5)	Mo11-O36	1.706(5)
Mo5-O4	1.952(4)	Mo11-O32	1.926(4)
Mo5-O19	1.957(3)	Mo11-O38	1.964(3)
Mo5-O9	2.259(4)	Mo11-O35	2.210(3)
Mo5-O2	2.273(3)	Mo11-O30^{ii}	2.300(3)
aver.	1.973	aver.	1.967
Mo6-O21	1.691(4)	Mo12-O39	1.697(4)
Mo6-O22	1.792(4)	Mo12-O25	1.760(4)
Mo6-O23	1.888(4)	Mo12-O31	1.880(4)
Mo6-O19	1.888(4)	Mo12-O38	1.896(4)
Mo6-O8	2.236(4)	Mo12-O34^{ii}	2.218(4)
Mo6-O9	2.238(4)	Mo12-O35	2.225(3)
aver.	1.956	aver.	1.946

(i) 1-x,1-y,-z; (ii) 1-x,-y,1-z; (iii) 1-x,-y,-z

Shortest A-B contacts for possible A-H...B hydrogen bonds:

//-like H_2DABCO^{2+}			⊥-like H_2DABCO^{2+}	
N1-O3w	2.683(8)		N5-O32	2.666(5)
N2-O1w	2.678(7)		N6-O1	2.945(6)
N3-O5w	2.664(10)		N6-O2	3.028(7)
N4-O2w	2.664(9)			
O1w-O39	2.767(5)		O2w-O16	2.951(6)
O1w-O16	2.894(7)		O2w-O39	3.026(8)
O3w-O36	2.716(7)		O4w-O5w	2.842(9)

O3w-O38	2.726(7)		O4w-O24	2.989(8)
O5w-O13	2.768(6)		O6w- O3	2.706(9)
O5w-O4w	2.842(9)		O6w-O32	2.947(10)

(II)

	basic structure	average	min	max
Mo1-O2	1.692(2)	1.697(7)	1.654(7)	1.753(7)
-O4	1.706(2)	1.711(8)	1.640(7)	1.778(8)
-O6	1.9231(15)	1.924(5)	1.872(5)	1.983(5)
-O3	1.9873(13)	1.990(5)	1.927(5)	2.054(5)
-O1	2.2053(15)	2.208(5)	2.135(5)	2.269(5)
-O5	2.3080(15)	2.310(5)	2.256(5)	2.351(5)
Mo2-O9	1.6933(19)	1.695(6)	1.652(6)	1.734(6)
-O7	1.696(2)	1.699(8)	1.662(8)	1.751(8)
-O6	1.9243(16)	1.925(6)	1.899(6)	1.947(6)
-O8	2.0356(16)	2.037(6)	2.017(6)	2.061(6)
-O10	2.1612(14)	2.162(5)	2.117(5)	2.203(5)
-O5	2.2585(13)	2.260(5)	2.209(5)	2.311(5)
Mo3-O11	1.6986(16)	1.701(5)	1.685(6)	1.716(5)
-O8	1.7779(16)	1.779(6)	1.744(6)	1.813(6)
-O3	1.8797(16)	1.882(6)	1.845(6)	1.916(5)
-O10	1.8888(17)	1.891(6)	1.840(6)	1.933(6)
-O12	2.2214(15)	2.223(5)	2.183(5)	2.256(5)
-O1	2.2418(13)	2.243(5)	2.234(5)	2.254(5)
Mo4-O13	1.6904(18)	1.692(6)	1.662(6)	1.722(6)
-O12	1.7678(14)	1.769(5)	1.748(5)	1.793(5)
-O5	1.8710(14)	1.873(5)	1.830(5)	1.913(5)
-O1	1.9400(17)	1.942(6)	1.905(6)	1.983(6)
-O10	2.1461(14)	2.148(5)	2.136(5)	2.160(5)
-O1	2.4208(14)	2.422(5)	2.379(5)	2.465(5)

Shortest A-B contacts for possible A-H...B hydrogen bonds:

	basic structure	average	min	max
N1(1)-O1w	2.633(5)	2.672(14)	2.651(15)	2.689(14)
N2(1)-O2w	2.715(6)	2.650(14)	2.608(13)	2.693(13)
N1(2)-O6	2.808(5)	2.705(7)	2.600(7)	2.895(7)
N2(2)-O5	2.872(8)	2.830(10)	2.760(10)	2.911(10)
-O4	3.303(7)	3.099(10)	2.991(10)	3.332(10)
O1w -O11	2.907(5)	2.917(17	2.886(16)	2.960(17)
-O13	2.890(4)	2.905(12)	2.823(12)	2.951(13)
O2w -O4	2.709(5)	2.753(16)	2.595(14)	2.867(15)
-O3	2.771(6)	2.770(19)	2.662(18)	3.00(2)
O3w -O9	2.769(7)	2.787(12)	2.755(11)	2.840(12)
-O6	3.026(7)	3.028(12)	2.970(12)	3.075(12)