Supplementary Material (ESI) for Chemical Communications
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Trigonal bipyramidal magnetic molecules based on $[Mo^{III}(CN)_6]^{3-}$

Xin-Yi Wang, Matthew G. Hilfiger, Andrey Prosvirin and Kim R Dunbar*

Supporting Information

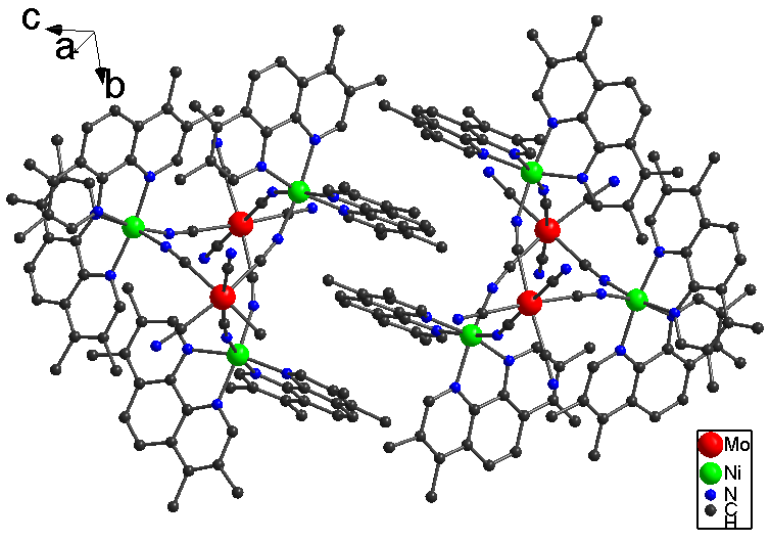

Fig S1. Depiction of π-π stacking between adjacent TBP molecules.

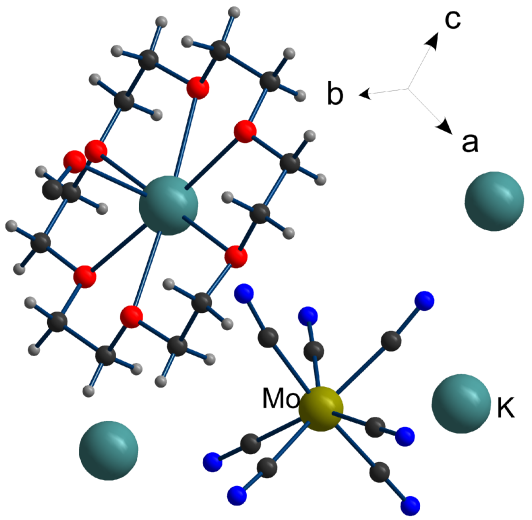

Fig S2. Depiction of the molecular structure of the constituent ions in (18-Crown-6-K)$K_3[Mo(CN)_7]$(MeOH).

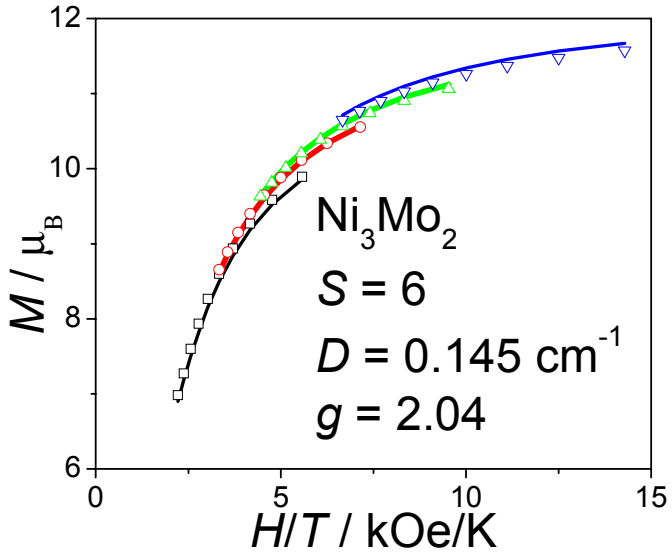

Fig S3 Reduced magnetization data for the compound Ni_3Mo_2 (**2**). The lines represent the fit using Anisofit2.0.

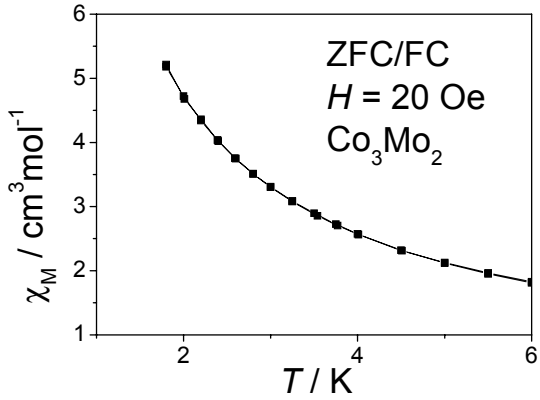

Fig S4. Zero-field-cooled and field-cooled magnetization data for the compound Co_3Mo_2 (**1**).

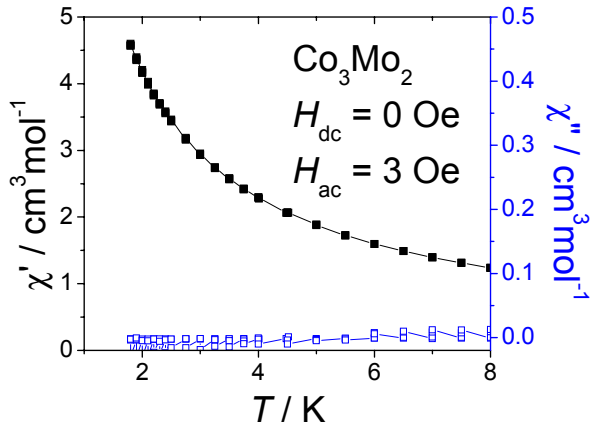

Fig S5. Ac susceptibility data for Co_3Mo_2 (**1**) under a zero dc applied field.

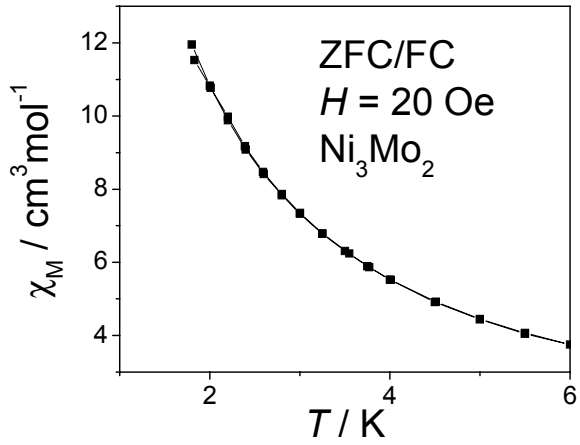

Fig S6. Zero-field-cooled and field-cooled magnetization data for the compound Ni_3Mo_2 (**2**).

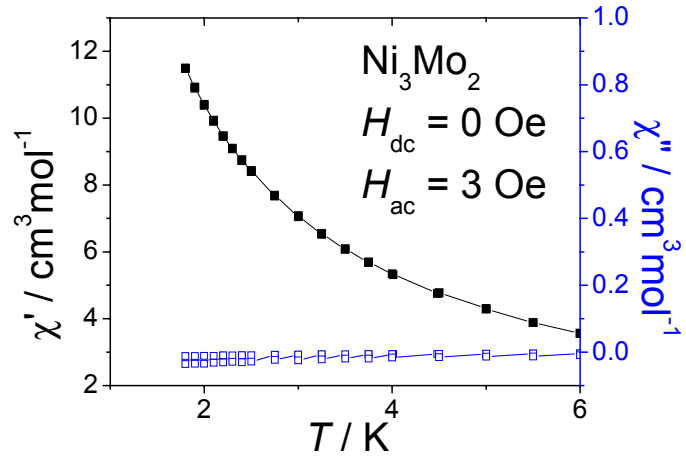

Fig S7. Ac susceptibility data for Ni_3Mo_2 (**2**) under a zero dc field.

Table S1. Bond Distances and Angles for Co_3Mo_2 (**1**) and Ni_3Mo_2 (**2**)

Co_3Mo_2 (1)					
Mo1-C1	2.152(7)	Mo1-C2	2.137(7)	Mo1-C3	2.139(7)
Mo1-C4	2.135(10)	Mo1-C5	2.171(9)	Mo1-C6	2.156(9)
Mo2-C7	2.142(8)	Mo2-C8	2.157(8)	Mo2-C9	2.123(7)
Mo2-C10	2.147(9)	Mo2-C11	2.133(10)	Mo2-C12	2.135(10)

Co1-N1	2.038(8)	Co1-N7	1.997(8)	Co1-N13	2.143(6)
Co1-N14	2.079(6)	Co1-N15	2.094(6)	Co1-N16	2.158(6)
Co2-N2	2.008(7)	Co2-N8	2.036(8)	Co2-N17	2.102(6)
Co2-N18	2.145(6)	Co2-N19	2.154(6)	Co2-N20	2.089(6)
Co3-N3	1.996(9)	Co3-N9	1.994(8)	Co3-N21	2.155(6)
Co3-N22	2.072(7)	Co3-N23	2.045(7)	Co3-N24	2.143(6)
C3-Mo1-C5	91.1(3)	C1-Mo1-C5	88.5(3)	C6-Mo1-C5	93.3(3)
C2-Mo1-C1	92.0(2)	C3-Mo1-C1	85.7(2)	C2-Mo1-C3	87.2(2)
C4-Mo1-C1	95.0(3)	C4-Mo1-C2	91.1(3)	C2-Mo1-C6	86.0(3)
C3-Mo1-C6	89.4(3)	C4-Mo1-C5	90.7(3)	C4-Mo1-C6	89.8(3)
C1-Mo1-C6	174.8(3)	C4-Mo1-C3	178.1(3)	C2-Mo1-C5	178.2(3)
C7-Mo2-C8	89.0(2)	C9-Mo2-C7	87.2(3)	C7-Mo2-C10	86.0(3)
C11-Mo2-C7	89.8(3)	C9-Mo2-C8	85.7(2)	C10-Mo2-C8	94.4(3)
C12-Mo2-C8	86.3(4)	C9-Mo2-C11	88.9(3)	C9-Mo2-C12	94.6(3)
C11-Mo2-C10	90.9(3)	C12-Mo2-C10	92.2(3)	C11-Mo2-C12	95.0(4)
C12-Mo2-C7	174.9(4)	C11-Mo2-C8	174.5(3)	C9-Mo2-C10	173.2(3)
N7-Co1-N1	89.3(2)	N15-Co1-N16	77.1(2)	N1-Co1)-N14	90.0(2)
N7-Co1-N15	94.7(2)	N14-Co1-N16	91.8(2)	N14-Co1-N15	87.1(2)
N7-Co1-N13	94.8(2)	N1-Co1-N13	98.4(2)	N14-Co1-N13	78.1(2)
N15-Co1-N13	89.5(2)	N7-Co1-N16	95.5(2)	N1-Co1-N16	94.3(2)
N1-Co1-N15	170.8(2)	N7-Co1-N14	172.7(3)	N13-Co1-N16	163.7(2)
N9-Co3-N3	92.1(3)	N22-Co3-N21	78.3(2)	N3-Co3-N23	91.2(3)
N9-Co3-N22	91.9(3)	N23-Co3-N21	97.1(3)	N23-Co3-N22	86.7(3)
N9-Co3-N24	92.1(2)	N3-Co3-N24	94.1(2)	N23-Co3-N24	77.9(3)
N22-Co3-N24	96.6(2)	N9-Co3-N21	92.6(2)	N3-Co3-N21	90.7(2)
N9-Co3-N23	169.7(3)	N3-Co3-N22	168.4(3)	N24-Co3-N21	173.2(2)

C7-N7-Co1	169.4(7)	C1-N1-Co1	164.6(6)	C8-N8-Co2	166.6(6)
C2-N2-Co2	159.5(6)	C3-N3-Co3	167.7(6)	C9-N9-Co3	170.2(6)
N1-C1-Mo1	166.7(6)	N2-C2-Mo1	178.7(6)	N3-C3-Mo1	171.0(6)
N4-C4-Mo1	176.3(9)	N5-C5-Mo1	179.3(8)	N6-C6-Mo1	174.8(7)
N7-C7-Mo2	174.0(7)	N8-C8-Mo2	170.3(6)	N9-C9-Mo2	167.6(6)
N10-C10-Mo2	177.4(8)	N11-C11-Mo2	177.2(9)	N12-C12-Mo2	178.2(11)
Ni_3Mo_2 (2)					
Mo1-C1	2.176(12)	Mo1-C2	2.167(11)	Mo1-C3	2.150(11)
Mo1-C4	2.117(13)	Mo1-C5	2.125(11)	Mo1-C6	2.141(14)
Mo2-C7	2.155(11)	Mo2-C8	2.190(9)	Mo2-C9	2.183(10)
Mo2-C10	2.153(11)	Mo2-C11	2.145(11)	Mo2-C12	2.166(11)
Ni1-N1	2.044(10)	Ni1-N7	2.008(9)	Ni1-N13	2.108(8)
Ni1-N14	2.103(8)	Ni1-N15	2.104(8)	Ni1-N16	2.064(8)
Ni2-N2	2.031(8)	Ni2-N9	2.026(8)	Ni2-N17	2.086(7)
Ni2-N18	2.082(7)	Ni2-N19	2.091(8)	Ni2-N20	2.089(7)
Ni3-N3	2.002(9)	Ni3-N8	2.056(7)	Ni3-N21	2.093(7)
Ni3-N22	2.103(7)	Ni3-N23	2.079(7)	Ni3-N24	2.082(7)
C4-Mo1-C5	92.9(4)	C4-Mo1-C6	98.0(6)	C5-Mo1-C6	92.3(5)
C4-Mo1-C3	89.0(4)	C5-Mo1-C3	84.8(4)	C6-Mo1-C3	172.6(5)
C4-Mo1-C2	87.6(4)	C5-Mo1-C2	171.9(4)	C6-Mo1-C2	95.6(4)
C3-Mo1-C2	87.1(3)	C4-Mo1-C1	171.1(4)	C5-Mo1-C1	94.9(4)
C6-Mo1-C1	86.0(5)	C3-Mo1-C1	87.5(3)	C2-Mo1-C1	84.1(3)
C11-Mo2-C10	88.6(4)	C11-Mo2-C7	85.3(4)	C10-Mo2-C7	92.0(4)
C11-Mo2-C12	94.8(4)	C10-Mo2-C12	90.5(4)	C7-Mo2-C12	177.4(4)
C11-Mo2-C9	88.5(3)	C10-Mo2-C9	176.7(3)	C7-Mo2-C9	86.2(3)
C12-Mo2-C9	91.2(3)	C11-Mo2-C8	173.1(4)	C10-Mo2-C8	97.9(3)
C7-Mo2-C8	92.1(3)	C12-Mo2-C8	87.5(3)	C9-Mo2-C8	84.9(3)
N7-Ni1-N1	89.3(3)	N7-Ni1-N16	96.4(3)	N1-Ni1-N16	91.4(3)

N7-Ni1-N14	169.1(3)	N1-Ni1-N14	90.1(3)	N16-Ni1-N14	94.5(3)
N7-Ni1-N15	94.7(3)	N1-Ni1-N15	169.2(3)	N16-Ni1-N15	78.2(3)
N14-Ni1-N15	87.8(3)	N7-Ni1-N13	90.6(3)	N1-Ni1-N13	97.5(3)
N16-Ni1-N13	168.8(3)	N14-Ni1-N13	78.6(3)	N15-Ni1-N13	92.5(3)
N9-Ni2-N2	92.4(3)	N9-Ni2-N18	91.6(3)	N2-Ni2-N18	92.2(3)
N9-Ni2-N17	169.8(3)	N2-Ni2-N17	91.4(3)	N22-Ni2-N17	78.7(3)
N9-Ni2-N20	93.0(3)	N2-Ni2-N20	93.2(3)	N22-Ni2-N20	172.8(3)
N17-Ni2-N20	96.2(3)	N9-Ni2-N19	91.0(3)	N2-Ni2-N19	171.0(3)
N22-Ni2-N19	96.0(3)	N17-Ni2-N19	86.7(3)	N20-Ni2-N19	78.3(3)
N3-Ni3-N8	89.9(3)	N3-Ni3-N23	173.7(3)	N8-Ni3-N23	89.4(3)
N3-Ni3-N24	95.1(3)	N8-Ni3-N24	97.0(3)	N23-Ni3-N24	78.8(3)
N3-Ni3-N21	95.2(3)	N8-Ni3-N21	94.3(3)	N23-Ni3-N21	91.1(3)
N24-Ni3-N21	164.7(3)	N3-Ni3-N22	94.1(3)	N8-Ni3-N22	172.1(3)
N23-Ni3-N22	87.4(3)	N24-Ni3-N22	89.5(3)	N21-Ni3-N22	78.5(3)
C1-N1-Ni1	163.8(8)	C7-N7-Ni1	158.0(8)	C2-N2-Ni2	166.9(8)
C9-N9-Ni2	165.9(7)	C3-N3-Ni3	169.1(8)	C8-N8-Ni3	161.5(7)
N1-C1-Mo1	173.2(8)	N2-C2-Mo1	171.1(8)	N3-C3-Mo1	176.7(9)
N4-C4-Mo1	174.3(11)	N5-C5-Mo(1)	174.7(9)	N6-C6-Mo1	179.2(15)
N7-C7-Mo2	178.6(9)	N8-C8-Mo2	169.8(8)	N9-C9-Mo2	172.4(8)
N10-C10-Mo2	177.0(10)	N11-C11-Mo2	175.9(9)	N12-C12-Mo2	176.7(10)