

Supporting Information

Magnetic Anisotropy of $[\text{Mo}(\text{CN})_7]^{4-}$ Anions and Fragments of Cyano-Bridged Magnetic Networks

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Table 1S. CASPT2 ligand-field energy levels for a pentagonal bipyramid $\text{Mo}(\text{CN})_7$ (Figure 3)

Table 2S. CASPT2 ligand-field energy levels for a capped trigonal prism $\text{Mo}(\text{CN})_7$ (Figure 4)

Table 3S. CASPT2 ligand-field energy levels for a heptacyanomolybdate fragment of $\text{K}_2[\text{Mn}(\text{H}_2\text{O})_2]_3[\text{Mo}(\text{CN})_7]_2 \cdot 6\text{H}_2\text{O}$ (Figure 5).

Figure 1S. Fragment of the crystal structure of $\text{K}_2[\text{Mn}(\text{H}_2\text{O})_2]_3[\text{Mo}(\text{CN})_7]_2 \cdot 6\text{H}_2\text{O}$ showing a grid-like sheet parallel to the bc plane formed by edge sharing cyano-bridged Mn_2Mo lozenges.

Figure 2S. A view of the crystal structure of $\text{K}_2[\text{Mn}(\text{H}_2\text{O})_2]_3[\text{Mo}(\text{CN})_7]_2 \cdot 6\text{H}_2\text{O}$ in the ab plane. Hydrogen atoms have been omitted for clarity.

Figure 3S. A view of the crystal structure of $\text{K}_2[\text{Mn}(\text{H}_2\text{O})_2]_3[\text{Mo}(\text{CN})_7]_2 \cdot 6\text{H}_2\text{O}$ in the ac plane. Hydrogen atoms have been omitted for clarity.

Table 1S. CASPT2 ligand-field energy levels
for a pentagonal bipyramid $\text{Mo}(\text{CN})_7$ (Figure 3)

PBP		
	CASPT2	D_{5h}
	(cm^{-1})	
$[(xz)(yz)]^3$	0	${}^2E_1''$
	24435	${}^4E_2'$
	27032	${}^2E_1''$
$[(xz)(yz)]^2$	27058	${}^2E_2'$
$[(xy)(x^2-y^2)]^1$	27370	${}^2A_1'$
	28261	${}^2A_2'$
	33027	${}^2E_2'$
$[(xz)(yz)]^2(z^2)^1$	34614	${}^4A_1'$

Table 2S. CASPT2 ligand-field energy levels
for a capped trigonal prism $\text{Mo}(\text{CN})_7$ (Figure 4)

CTP		
C_{2v}	CASPT2 (cm^{-1})	
${}^2\text{B}_1$	0	$[(x^2-y^2)(xz)]^3$
${}^2\text{A}_1$	803	
${}^4\text{A}_2$	20596	
${}^2\text{A}_2$	23144	
${}^2\text{A}_2$	26294	$[(x^2-y^2)(xz)]^2(yz)^1$
${}^2\text{B}_2$	26300	
${}^2\text{B}_2$	29836	
${}^4\text{B}_1$	26908	
${}^2\text{B}_1$	31145	
${}^2\text{B}_1$	33059	$[(x^2-y^2)(xz)]^2(z^2)^1$
${}^2\text{A}_1$	35166	
${}^2\text{A}_1$	38510	
${}^4\text{B}_2$	31841	
${}^2\text{B}_2$	36052	
${}^2\text{B}_2$	36529	$[(x^2-y^2)(xz)]^2(xy)^1$
${}^2\text{A}_2$	39302	
${}^2\text{A}_2$	41999	

Table 3S. CASPT2 ligand-field energy levels
for a heptacyanomolybdate fragment of
 $\text{K}_2[\text{Mn}(\text{H}_2\text{O})_2]_3[\text{Mo}(\text{CN})_7]_2 \cdot 6\text{H}_2\text{O}$ (Figure 5)

fragment		
C_1	CASPT2 (cm^{-1})	CTP notation
2A_1	0	$[(x^2-y^2)(xz)]^3$
2A_1	318	
4A_1	21552	$[(x^2-y^2)(xz)]^2(yz)^1$
2A_1	25233	
2A_1	26698	
2A_1	27880	
2A_1	30082	
4A_1	27067	$[(x^2-y^2)(xz)]^2(z^2)^1$
2A_1	31742	
2A_1	32519	
2A_1	32783	
2A_1	36126	
4A_1	35286	$[(x^2-y^2)(xz)]^2(xy)^1$
2A_1	38758	
2A_1	40333	
2A_1	40952	
2A_1	46158	

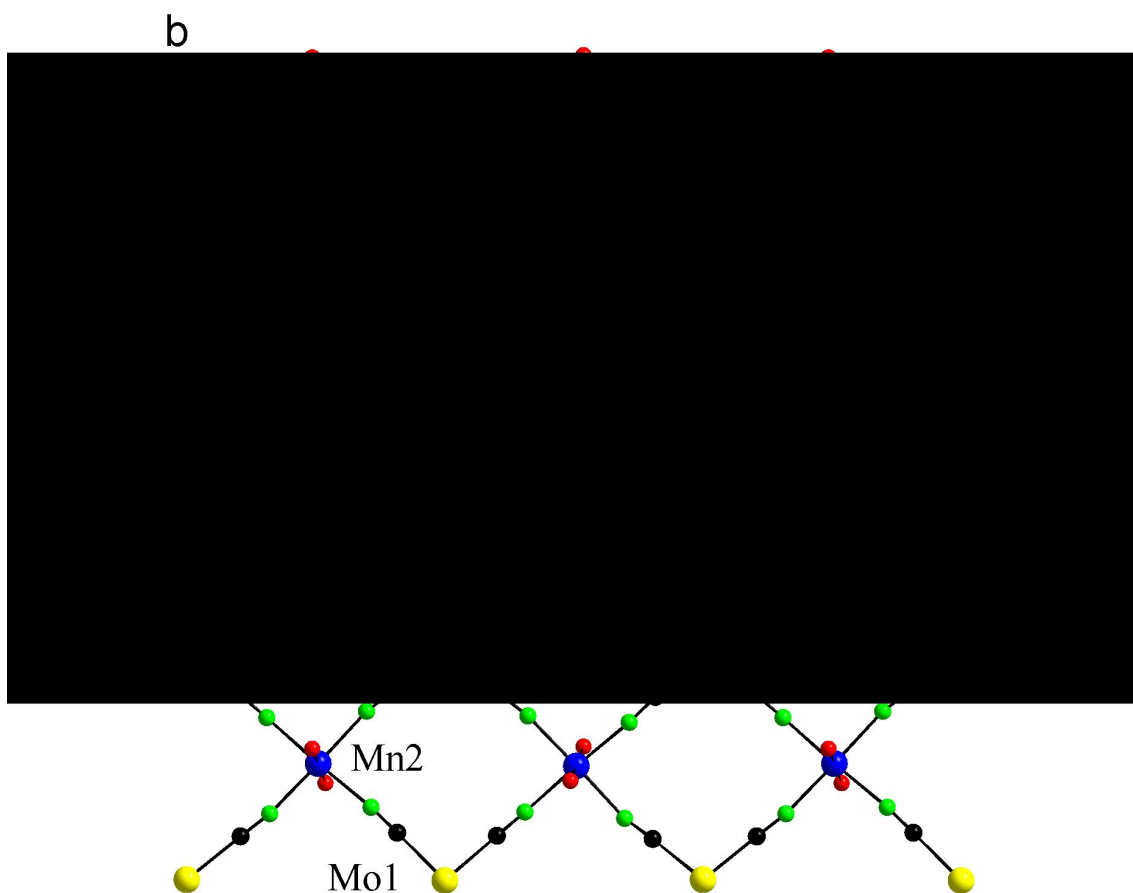


Figure 1S. Fragment of the crystal structure of $\text{K}_2[\text{Mn}(\text{H}_2\text{O})_2]_3[\text{Mo}(\text{CN})_7]_2 \cdot 6\text{H}_2\text{O}$ showing a grid-like sheet parallel to the bc plane formed by edge sharing cyano-bridged Mn2Mo lozenges.

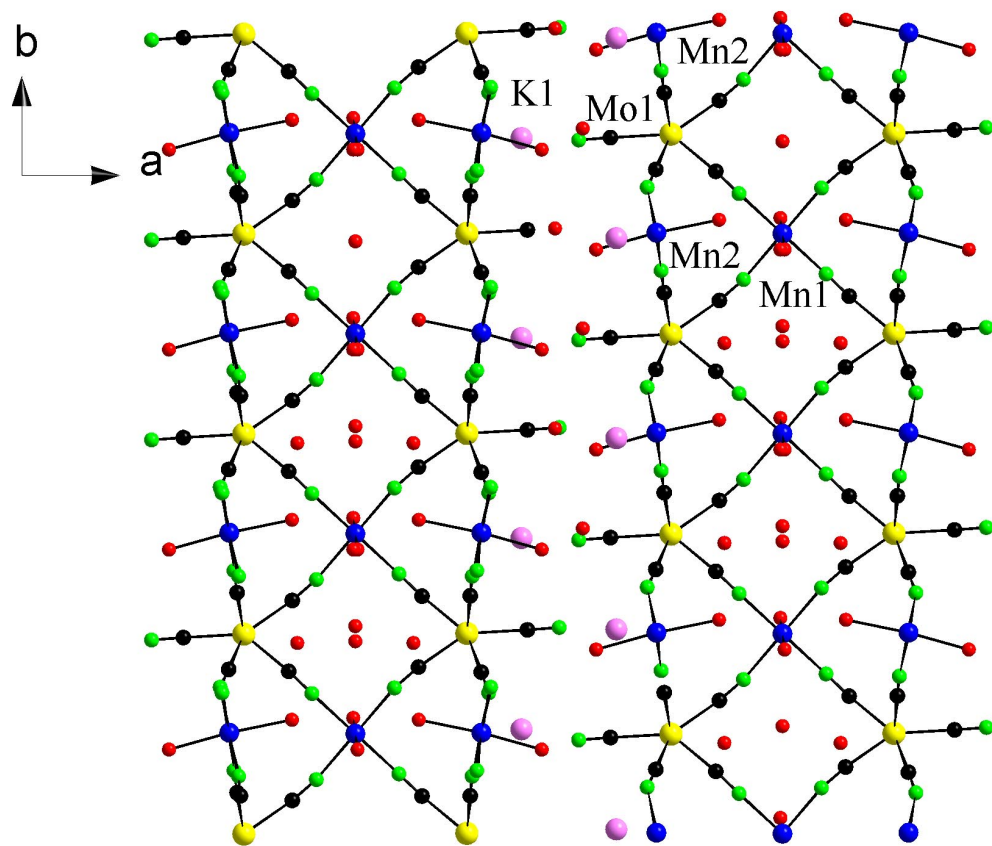


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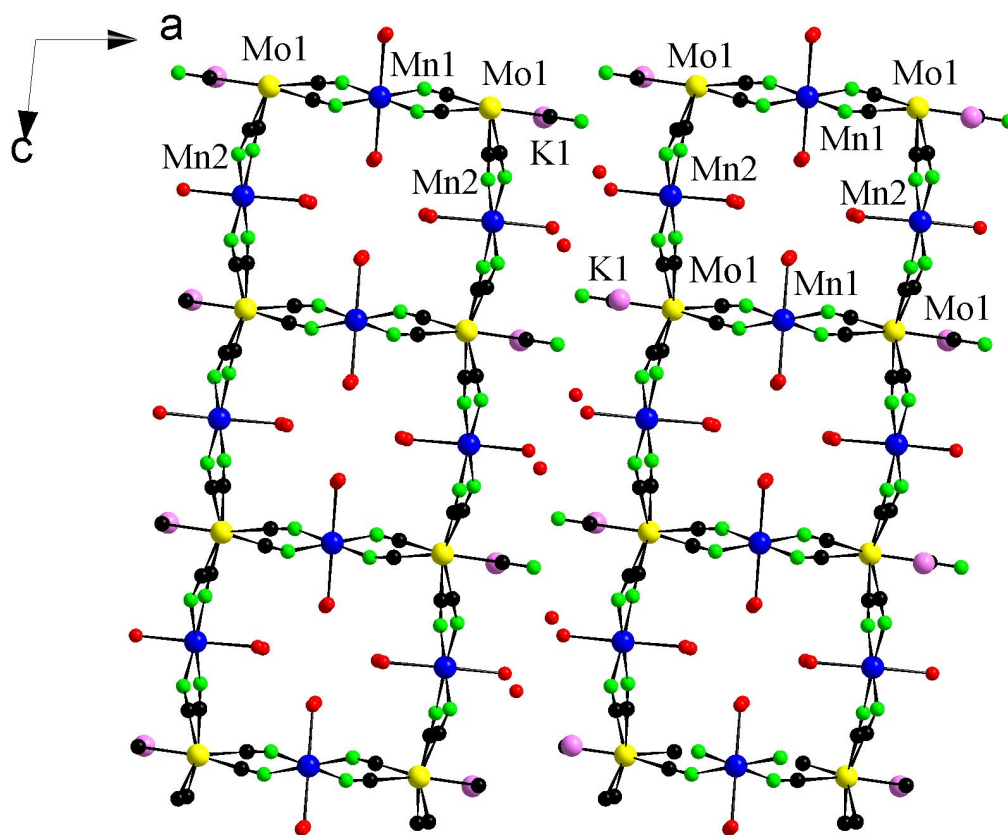


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