ELECTRONIC SUPPORTING INFORMATION

Supramolecular lone pair–π / π-π / π–anion assembly in a Mg(II)-malonate–2-aminopyridine–nitrate ternary system

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Table S1. Crystallographic data for compound 1

Compound	**1**
Formula	$C_{26}H_{36}N_{10}O_{16}Mg$
M	768.96
Crystal system	triclinic
Space group	*P*$\bar{1}$ (No. 2)
a/ Å	7.1006(1)
b/ Å	10.7532(2)
c/ Å	11.4468(2)
A	89.280(1)º
B	86.005(1)º
Γ	77.384(1)º
F(000)	402
V/ Å^3	850.83(3)
Z	1
T/K	150
Theta Min-Max [˚]	1.8 to 28.6°
λ(Mo Kα)/ Å	0.71073 Å
μ(Mo Kα)/ mm^{-1}	0.141
*R*1, *I*> *2σ(I)* (all)	0.0339
w*R*2, *I* > 2σ(*I*) (all)	0.0975
S(GOF)	1.10
Total reflections	10708
Independent reflections	4358
Observed data [*I* > 2σ(*I*)]	3544
Min. and Max. Resd. Dens. [e/ Å^3]	–0.26, 0.25

Table S2. Selected Bond Lengths (Å) and Angles (deg) for 1

Mg(1)–O1	2.0064(8)	O(4)–C(1)	1.2507(14)
Mg(1)–O2	2.0343(8)	O(5)–C(3)	1.2324(13)
Mg(1)–O3	2.1080(8)	C(1)–C(2)	1.5223(15)
O(1)–C(3)	1.2808(14)	C(2)–C(3)	1.5287(15)
O(2)–C(1)	1.2684(14)		
O(1)–Mg(1)–O(2)	88.34(3)	Mg(1)–O(1)–C(3)	130.27(7)
O(1)–Mg(1)–O(3)	87.97(3)	Mg(1)–O(2)–C(1)	129.47(7)
O(1)–Mg(1)–O(2)$^{\#}$	91.66(3)	O(2)–C(1)–O(4)	122.81(10)
O(1)–Mg(1)–O(3)$^{\#}$	92.04(3)	C(1)–C(2)–C(3)	119.82(9)
O(2)–Mg(1)–O(3)	87.84(3)	O(1)–C(3)–O(5)	123.58(10)
O(2)–Mg(1)–O(3)$^{\#}$	92.17(3)	O(4)–C(1)–C(2)	118.01(10)

Symmetry code: # = –x,1–y,1–z

Table S3. Relevant H-bonds in compound 1

D–H···A	D–H [Å]	H···A [Å]	D···A [Å]	D–H···A [º]
N2–H2C···O4[a]	0.86	2.09	2.9333(13)	171
N2–H2D···O7[b]	0.84	2.20	3.0148(15)	165
N3–H3···O1[c]	0.88	1.89	2.7491(12)	164
O3–H3A···O6[d]	0.87	1.97	2.8310(13)	172
O3–H3B···O4[a]	0.88	1.84	2.7168(12)	175
N4–H4A···O5[c]	0.88	1.97	2.8401(14)	169
N4–H4B···O8[e]	0.88	2.13	2.9774(14)	162
N6–H6A···O2[a]	0.88	1.91	2.7796(12)	171
C5–H5···O8[b]	0.95	2.53	3.3982(18)	152
C7–H7···O5[f]	0.95	2.32	3.1991(16)	154
C13–H13···O7[a]	0.95	2.59	3.3877(16)	142

Symmetry codes: [a] = 1–x,1–y,1–z; [b] = 1–x,2–y,1–z; [c] = –x,1–y,1–z; [d] = –1+x,y,z; [e] = 1–x,1–y, –z; [f] = 1–x,1–y,2–z.