

Supplementary materials

New data on crystal phases in the system $\text{MgSO}_4 - \text{OC}(\text{NH}_2)_2 - \text{H}_2\text{O}$

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Table S1. Distances (Å) and angles (°) describing hydrogen bonds in $\text{Mg}(\text{SO}_4)\cdot\text{OC}(\text{NH}_2)_2\cdot 2\text{H}_2\text{O}$.

D-H A	d(D-H)	d(H...A)	< D-H...A	d(D...A)
N1-H1A...O6	0.860	2.342	147.22	3.100
N1-H1B...O4 ⁱ	0.860	2.261	178.11	3.121
N2-H2A...O2 ⁱⁱ	0.860	2.439	148.95	3.207
N2-H2B...O3 ⁱ	0.860	2.384	155.88	3.188
O6-H6A...O4 ⁱⁱⁱ	0.881	2.224	157.51	3.054
O6-H6B...O ^{iv}	0.935	2.144	148.77	2.983
O7-H7A...O2	0.937	2.798	151.23	2.733
O7-H7B... O2 ⁱⁱ	0.893	2.131	139.29	2.868

i) x,y-1,z; ii) x-1,y,z; iii) -x+2,-y+1,-z+1; iv) x+1,y,z; v) x,y-1,z; vi) x+1, y, z.

Table S2. Distances (Å) and angles (°) describing hydrogen bonds in $\text{Mg}(\text{SO}_4)\cdot\text{OC}(\text{NH}_2)_2\cdot 3\text{H}_2\text{O}$.

D-H A	d(D-H)	d(H...A)	< D-H...A	d(D...A)
N1-H1B...O2 ⁱ	0.860	2.201	160.00	3.023
N2-H2A...O7	0.860	2.342	145.78	3.091
N2-H2B...O4 ⁱⁱ	0.860	2.181	148.51	2.949
O5-H5A...O2 ⁱⁱⁱ	0.952	1.814	177.02	2.765
O5-H5B...O ⁱⁱⁱ	0.903	1.954	167.60	2.842
O6-H6B...O2 ^{iv}	0.827	2.132	149.71	2.876

O6-H6B...O3 ^{iv}	0.827	2.592	131.70	2.876
O7-H7A...O4 ^v	0.971	1.778	167.07	2.733
O7-H7B...O6 ^{vi}	0.903	2.161	176.64	3.063

i)-x,-y-1/2,-z+1; ii) -x+1,y-1/2,-z+1; iii) x+1,y,z; iv)- x,y-1/2,-z+2; v)x,y-1,z; vi)x+1, y, z.

Table S3. Coordination polyhedral of Mg atoms in the known $\text{MgSO}_4 \cdot n\text{OC}(\text{NH}_2)_2 \cdot m\text{H}_2\text{O}$ compounds.

compound	Coordination number of Mg polyhedra	Type and number of SO ₄ , Urea and H ₂ O ligands
$\text{MgSO}_4 \cdot \text{OC}(\text{NH}_2)_2 \cdot 2\text{H}_2\text{O}$	6	4SO ₄ , 2H ₂ O;
	6	2SO ₄ , 2Urea, 2H ₂ O
$\text{MgSO}_4 \cdot \text{OC}(\text{NH}_2)_2 \cdot 3\text{H}_2\text{O}$	6	2SO ₄ , 3H ₂ O; 1Urea
$\text{MgSO}_4 \cdot 4\text{OC}(\text{NH}_2)_2 \cdot \text{H}_2\text{O}$	6	1SO ₄ , 4Urea, 1H ₂ O
$\text{MgSO}_4 \cdot 6\text{OC}(\text{NH}_2)_2 \cdot 0.5\text{H}_2\text{O}$	6	6Urea

Figure S1 – 3D packing of $\text{MgSO}_4 \cdot \text{OC}(\text{NH}_2)_2 \cdot 2\text{H}_2\text{O}$ The hydrogen bonding contacts are marked with dashed lines.

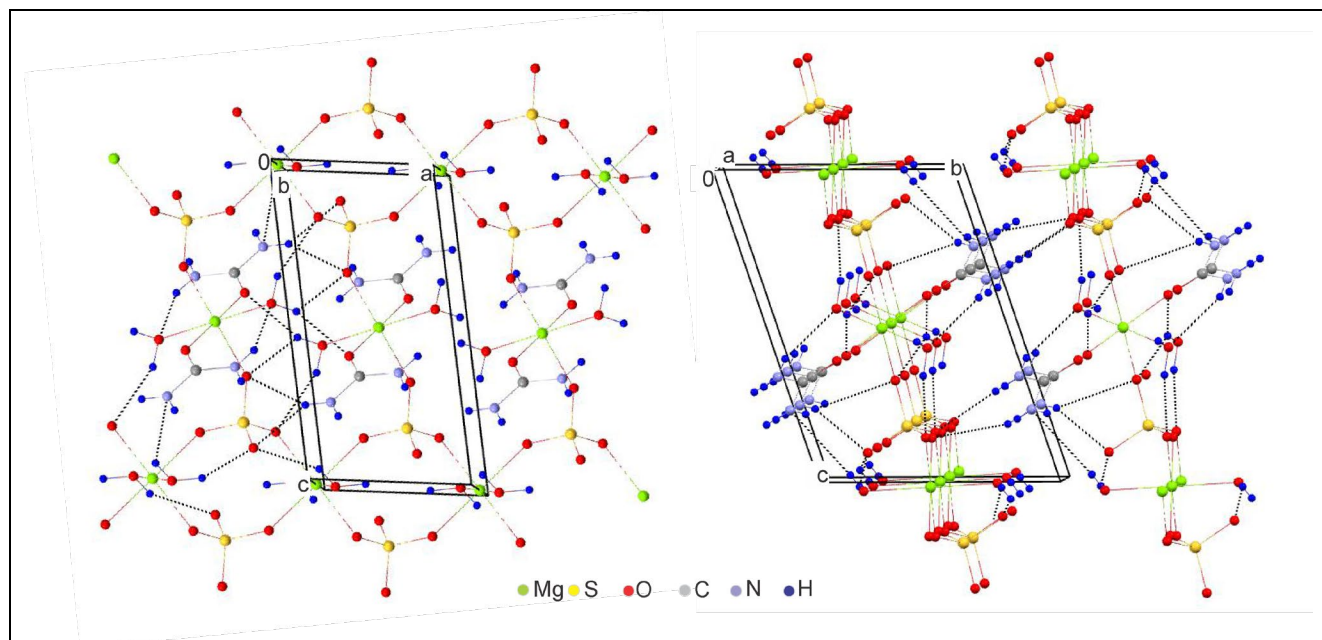


Figure S2 – 3D packing of $\text{MgSO}_4 \cdot \text{OC}(\text{NH}_2)_2 \cdot 3\text{H}_2\text{O}$. The hydrogen bonding contacts are marked with dashed lines.

