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Supporting information for article:

An inorganic–organic hybrid supramolecular framework based on the γ-$[Mo_8O_{26}]^{4-}$ cluster and cobalt complex of aspartic acid: X-ray structure and DFT study

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Table S1 Hydrogen-bond geometry (Å, º) for **1**.

D—H···A	D—H (Å)	H···A (Å)	D···A (Å)	D—H···A (°)
O18—H18A···O15i	0.87	1.96	2.781 (3)	156
O18—H18B···O8ii	0.87	1.90	2.745 (3)	163
O19—H19A···O12iii	0.87	2.00	2.800 (3)	151
O19—H19B···O11iv	0.87	1.96	2.779 (3)	157
O20—H20B···O16	0.87	1.89	2.641 (3)	144
O20—H20A···O23v	0.87	2.01	2.838 (3)	158
O21—H21A···O6vi	0.87	1.90	2.772 (3)	178
O21—H21B···O23i	0.87	1.89	2.749 (3)	171
O22—H22A···O4iii	0.87	1.94	2.809 (3)	173
O22—H22B···O2vii	0.87	2.29	3.104 (3)	155
O22—H22B···O5vii	0.87	2.60	3.258 (3)	134
N1—H1A···O6vi	0.91	2.11	2.912 (3)	147
N1—H1B···O17iii	0.91	2.10	2.913 (3)	149
N1—H1C···O14	0.91	2.29	2.919 (3)	126
N1—H1C···O19iii	0.91	2.18	2.902 (3)	136
C2—H2A···O6vi	0.99	2.34	3.134 (4)	136
C3—H3···O3viii	1.00	2.33	3.240 (4)	150
O23—H23A···O4ix	0.87	2.32	3.024 (3)	138
O23—H23B···O15	0.87	1.81	2.679 (3)	175
O24—H24A···O1viii	0.87	2.20	2.892 (3)	137
O24—H24A···O2viii	0.87	2.28	2.992 (3)	140
O24—H24B···O21v	0.87	2.16	2.914 (3)	144

Symmetry code(s): (i) *x*, −*y*+3/2, *z*−1/2; (ii) *x*, *y*, *z*−1; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*+1, *y*−1/2, −*z*+3/2; (v) −*x*, −*y*+1, −*z*+1; (vi) −*x*+1, *y*+1/2, −*z*+3/2; (vii) *x*−1, *y*, *z*−1; (viii) −*x*+1, −*y*+1, −*z*+2; (ix) *x*−1, −*y*+3/2, *z*−1/2.