Synthesis, Structural Characterization, and Biological Activities of Organically Templated Cobalt Phosphite (H2DAB)[Co(H2PO3)4]·2H2O

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Supplementary File

Figure S1. Asymmetric unit of (H2DAB)[Co(H2PO3)4]·2H2O. Thermal ellipsoids are shown at 60% probability.

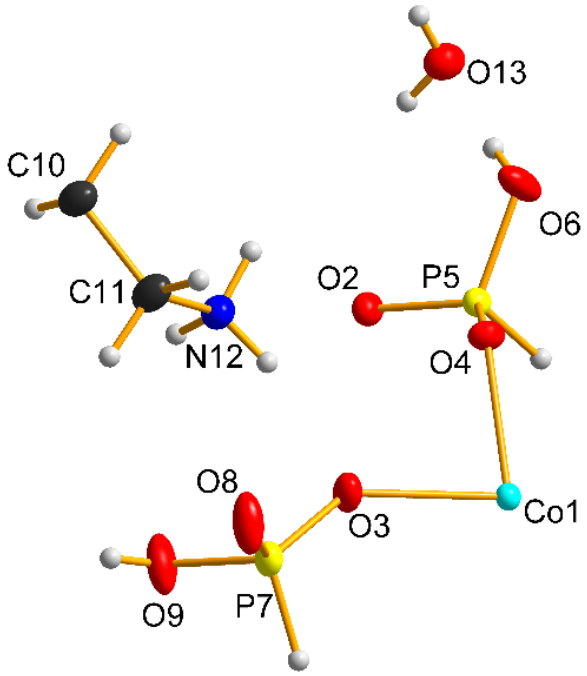

Figure S2. A fragment of the structure of (H2DAB)[Co(H2PO3)4]·2H2O along [010], showing the infinite four-membered ring chain propagating along [100]. Polyhedrons: cyan [CoO6], yellow [H2PO3].

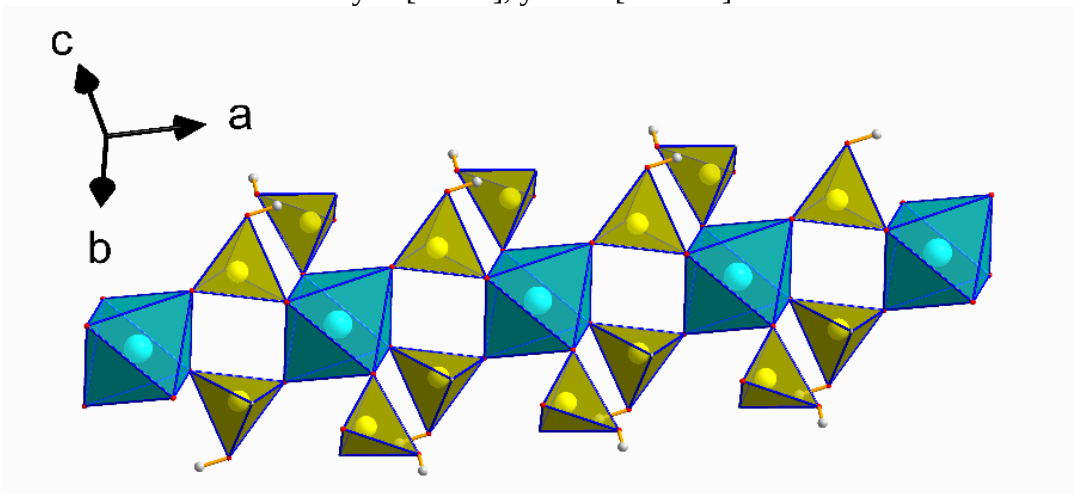

Figure S3. The crystal structure of (H2DAB)[Co(H2PO3)4]·2H2O in a projection along c-axis emphasizing the hydrogen bonds (dashed lines).

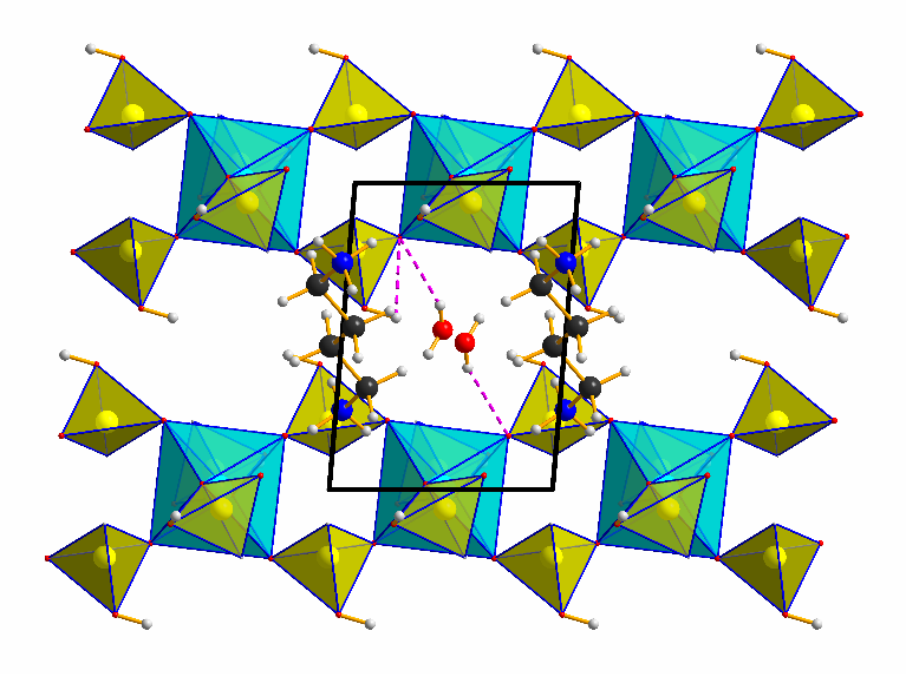

Figure S4. Infrared spectrum of (H2DAB)[Co(H2PO3)4]·2H2O.

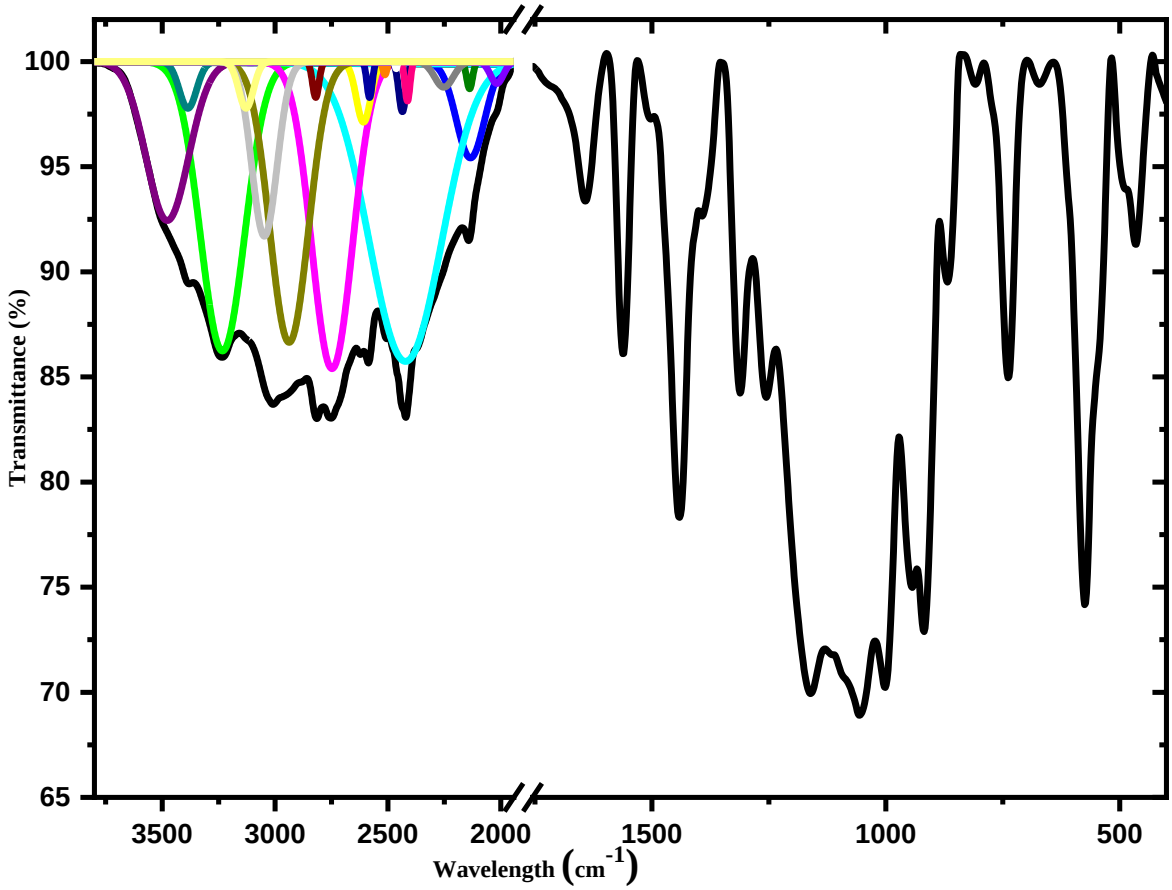

Figure S5. Thermogravimetric (TG) and differential thermal analysis (TDA) curves of (H2DAB)[Co(H2PO3)4] ·2H2O.

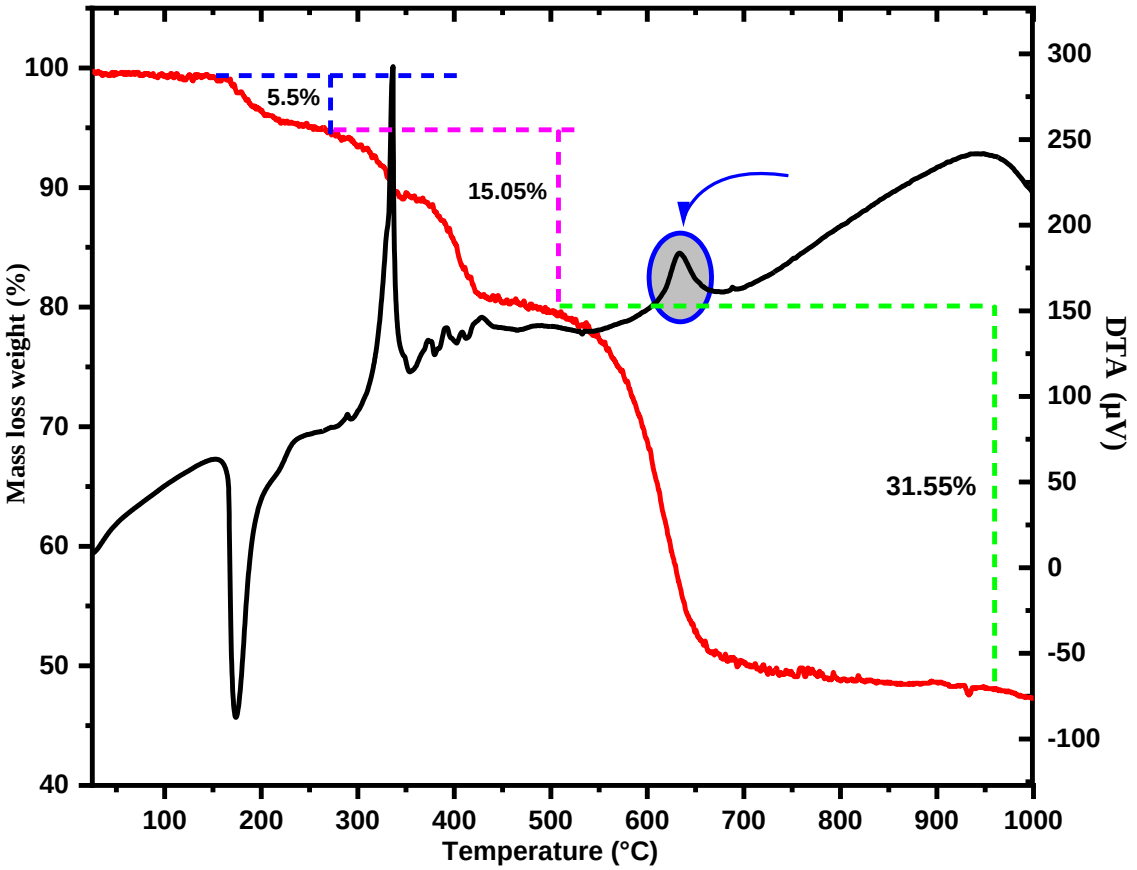

Figure S6. Antimicrobial activity of (H2DAB)[Co(H2PO3)4]·2H2O against Candida albicans, Saccharomyces cerevisiae, Escherichia coli, Staphylococcus epidermidis and Steinernema feltiae.

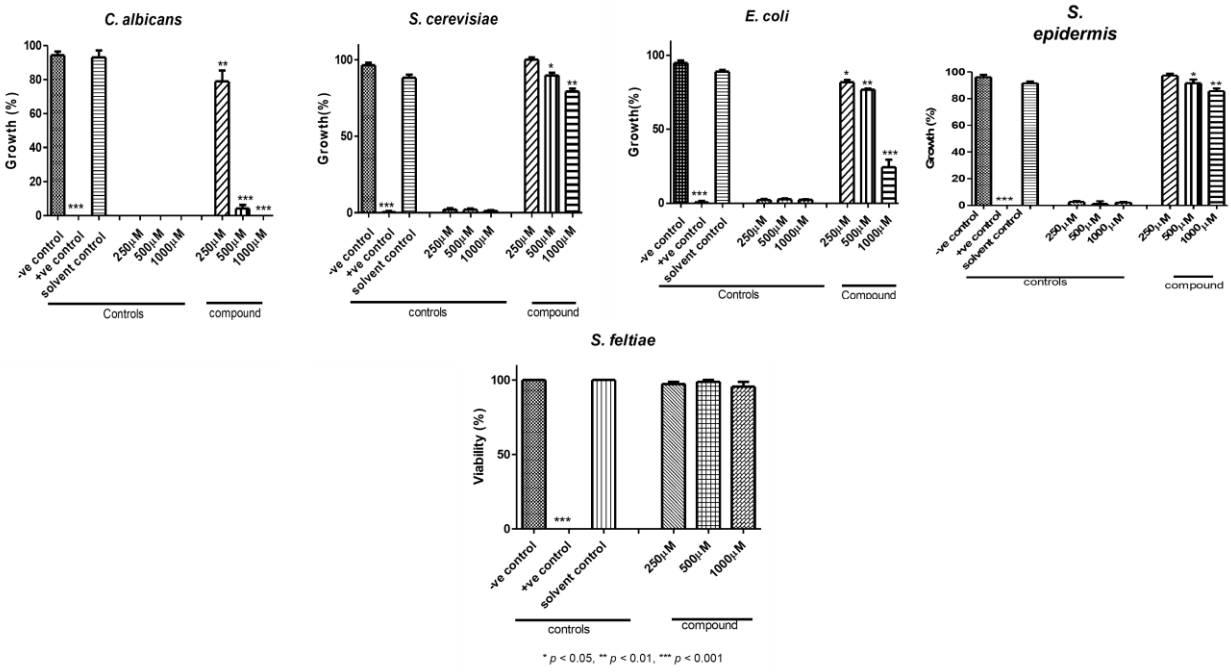

Table S1. Experimental X-ray data collection from (H2DAB)[Co(H2PO3)4]·2H2O.

Chemical Formula	$(C_4H_{14}N_2)[Co(H_2PO_3)_4]\cdot 2H_2O$
Mr (g/mol)	509.08
F(000)	263.9
Symmetry, S.G.	Triclinic P-1 (n. 2)
Cell parameters/V	A = 5.4814 (3) Å, b = 7.5515 (4) Å, c = 10.8548 (6)Å, α = 88.001 (4)°, β = 88.707 (5)°, γ = 85.126 (5)°/447.33 (4) $Å^3$
Z	1
λ (Mo Kα radiation) (Å)	0.71073
T(K)/μ(mm^{-1})	298/1.39
Crystal size (mm)	0.25 × 0.25 × 0.3
Measured reflections/independent reflections (reflections with I ≥ 2u(I))/parameters	9480/2005 (1878)/137
Θmin—θmax (°)/Rint	1.9–27.8/0.024
Reciprocal space limiting indices	h: −6–7, k: −9–9, l: −13–14
R[F2 > 2σ(F2)]/wR(F2)/G.O.F.	0.026/0.072/1.03

Table S2. Hydrogen bonding network in the framework of (H2DAB)[Co(H2PO3)4]·2H2O.

D-H···A	**D-H/Å**	**H···A/Å**	**D···A/Å**	**DHA/°**
O6-H6···O13	0.80 (3)	1.80 (3)	2.605 (2)	175 (3)
O9-H9···O8	0.82 (1)	1.77 (1)	2.574 (2)	169(1)
N12-H12A···O6	0.89 (1)	2.16 (1)	2.900 (2)	140 (1)
N12-H12B···O3	0.89 (1)	2.02 (1)	2.887 (2)	166 (1)
N12-H12C···O8	0.89 (1)	1.91 (1)	2.776 (2)	165 (1)
O13-H13A···O2	0.71 (3)	2.22 (3)	2.888 (2)	159 (3)
O13-H13B···O4	0.76 (3)	2.11 (3)	2.863 (2)	179 (4)