

Table S1. Positional and Isotropic Thermal Parameters for Fe[C₆H₅PO₃]·H₂O.

Atom	X	Y	Z	U _i /U _e *100 (Å ²)	FRAC
Fe	.00000	.01770	.06100	.78	1.0000
P	.00000	.87400	.59100	1.93	1.0000
O1	.00000	.91190	.30860	5.16	1.0000
O2	.19840	.92690	.71730	6.91	1.0000
O3	.00000	.09895	.46165	28.55	1.0000
C1	.00000	.75050	.62730	.96	1.0000
C4	.00000	.55230	.69990	2.21	1.0000
C2	.71206	.30428	.13241	19.40	.4322
C3	.29380	.39597	.17350	2.50	.4907
C3A	.00000	.70830	.88810	10.79	1.0000
C4A	.00000	.61230	.92080	9.32	1.0000
C5A	.00000	.59630	.44650	4.03	.5100
C6A	.00000	.69240	.40730	33.01	.5678

$$U_{iso}=B_{iso}/(8\pi^2)$$