

Electronic Supplemental Information:

Table S1. Crystal data and structure refinement for glutardiamidoxime (H₂B)

Identification code	H ₂ B-H ₂ O	
Chemical formula	C ₅ H ₁₄ N ₄ O ₃	
Formula weight	178.20	
Temperature	100(2) K	
Radiation, wavelength	synchrotron, 0.77490 Å	
Crystal system, space group	triclinic, P $\bar{1}$	
Unit cell parameters	a = 8.3203(9) Å	$\alpha = 74.802(2)^\circ$
	b = 11.6780(13) Å	$\beta = 89.821(2)^\circ$
	c = 18.750(2) Å	$\gamma = 88.107(2)^\circ$
Cell volume	1757.1(3) Å ³	
Z	8	
Calculated density	1.347 g/cm ³	
Absorption coefficient μ	0.110 mm ⁻¹	
F(000)	768	
Crystal colour and size	colourless, 0.20 × 0.17 × 0.04 mm ³	
Reflections for cell refinement	9380 (θ range 3.27 to 33.61°)	
Data collection method	Bruker APEX II CCD diffractometer	
	ω rotation with narrow frames	
θ range for data collection	2.93 to 33.64°	
Index ranges	h -11 to 11, k -15 to 16, l 0 to 26	
Completeness to $\theta = 30.00^\circ$	99.4 %	
Intensity decay	.%	
Reflections collected	144482	
Independent reflections	10633 ($R_{\text{int}} = 0.0409$)	
Reflections with $F^2 > 2\sigma$	9808	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.94 and 0.95	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0622, 0.3971	
Data / restraints / parameters	10633 / 0 / 560	
Final R indices [$F^2 > 2\sigma$]	R1 = 0.0377, wR2 = 0.1034	
R indices (all data)	R1 = 0.0407, wR2 = 0.1059	
Goodness-of-fit on F^2	1.029	
Extinction coefficient	0	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.491 and -0.252 e Å ⁻³	