Table S1. Experimental details of the X-ray diffraction analysis

Crystal data	
Chemical formula	$C_6H_6N_2O$
*M*r	122.13
Crystal system, space group	Monoclinic, *P* $2_1/m$
Temperature (K)	295(2)
a, *b*, *c* (Å)	6.798 (3), 6.172 (3), 8.844 (5)
β (°)	110.30 (5)
V (Å^3)	348.0 (3)
Z	2
Radiation type	Mo*Kα*
μ (mm^{-1})	0.08
Crystal size (mm)	0.55 × 0.40 × 0.35
Diffractometer	New Xcalibur, Ruby diffractometer
Absorption correction	Multi-scan *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.33 (release 27-03-2014 CrysAlis171 .NET) (compiled Mar 27 2014,17:12:48) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
No. of measured, independent, and observed [$I > 2\sigma(I)$] reflections	1510, 889, 478
R_{int}	0.018
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.690
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.063, 0.217, 1.06
No. of reflections	889
No. of parameters	61
H-atom treatment	H-atom parameters constrained
$\Delta\varrho_{max}$, $\Delta\varrho_{min}$ (e Å^{-3})	0.14, −0.26