Crystal data and structure refinement parameters for ISE-1.

Parameter / Code	**ISE-1**
CCDC	2237254
Empirical formula	$C_{12}H_9N_5$
Formula weight	223.24
Temperature/K	100(2)
Crystal system	monoclinic
Space group	I2/a
a/Å	20.8450(9)
b/Å	4.6353(2)
c/Å	22.7163(11)
α/°	90
β/°	107.329(5)
γ/°	90
Volume/Å^3	2095.29(17)
Z	8
ρ_{calc}g/cm^3	1.415
μ/mm^{-1}	0.744
F(000)	928.0
Crystal size/mm^3	0.12 × 0.04 × 0.02
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.154 to 138.37
Index ranges	$-25 \leq h \leq 25$, $-5 \leq k \leq 3$, $-27 \leq l \leq 27$
Reflections collected	7480
Independent reflections	1949 [R_{int} = 0.0263, R_{sigma} = 0.0262]
Data/restraints/parameters	1949/0/154
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0386, wR_2 = 0.0966
Final R indexes [all data]	R_1 = 0.0433, wR_2 = 0.0996
Largest diff. peak/hole / e Å^{-3}	0.17/-0.18

A suitable crystal was studied using Rigaku «XtaLAB Synergy-S» diffractometer (monochromated Cu Kα radiation, λ= 1.54184 Å). The temperature was kept at 100 K throughout the experiment. Empirical absorption correction was applied in CrysAlisPro (Agilent Technologies, 2014) program complex using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The structures were solved by SHELXT[1] program, using least squares minimization in anisotropic (for non-hydrogen atoms) approximation and refined with the SHELXL package[2] incorporated in the Olex2 program package[3]. The hydrogen atoms were introduced to the geometrically calculated positions and refined by attaching themselves to the corresponding parent atoms.
Supplementary crystallographic data for this paper have been deposited at Cambridge Crystallographic Data Centre (CCDC 2237254) and can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

[1] Sheldrick, G.M. SHELXT – Integrated space-group and crystal-structure determination. Acta Crystallogr. Sect. A Found. and Adv. Crystallogr. 2015, 71, 3–8 (DOI:10.1107/S2053273314026370)
[2] Sheldrick, G. M. Crystal structure refinement with SHELXL. Acta Crystallogr., Sect. C: Struct. Chem. 2015, 71, 3−8 (DOI: 10.1107/S2053229614024218)
[3] Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Crystallogr. 2009, 42, 339−341. (DOI: 10.1107/S0021889808042726)