SUPPORTING INFORMATION

Sorption comparison of two indium-organic framework isomers with *syn/anti* configurations

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S1. Crystal Data

Table S1. Summary of Crystal Data and Refinement Results

Name	Formula	Space group	*a/b* (Å)	*c* (Å)	*α/γ* (°)	*β* (°)	*R(F)*
InOF-3	$[Me_2NH_2][In(BPDC)_2]$	***P*2$_1$/n**	14.0612(2)/16.1146(2)	15.5087(2)	90	103.831(2)	0.0360
InOF-4	$[MeNH_3][In(BPDC)_2]$	***P*-42c**	10.74540(10)	14.4927(6)	90	90	0.0511

InOF denotes Indium-Organic Framework; BPDC = Biphenyl-3,3'-dicarboxylic acid; More details see CIF files.

S2. Additional X-ray Crystal Structural Figures

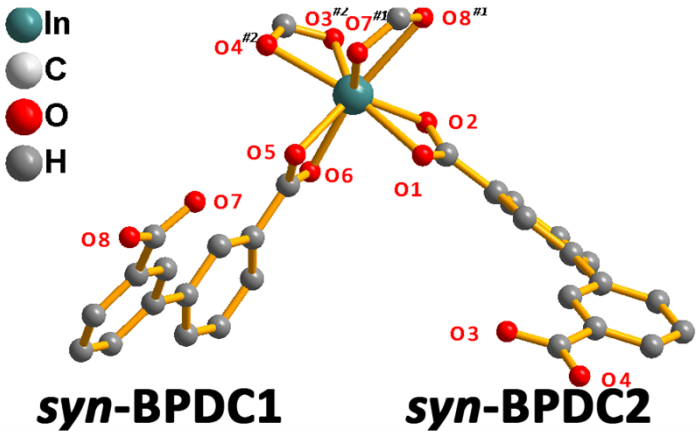

Figure S1. Asymmetric unit of **InOF-3**.

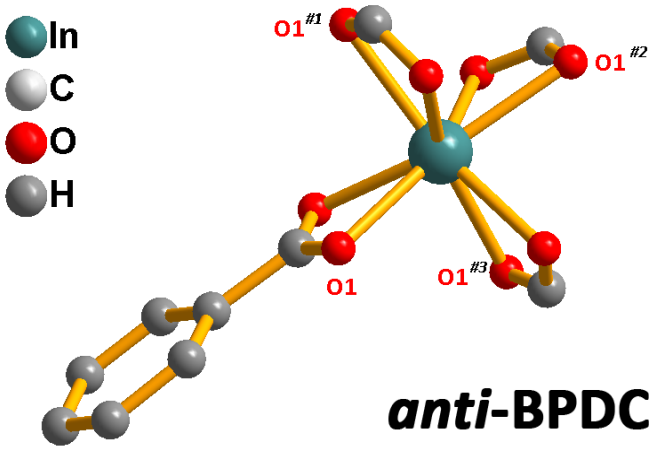

Figure S2. Asymmetric unit of **InOF-4**.

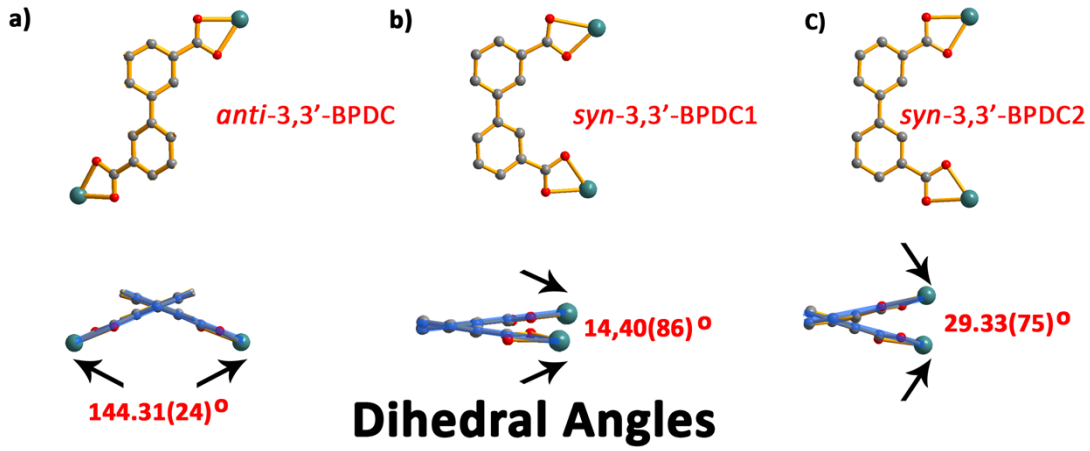

Figure S3. Summary of dihedral angles of BPDC ligands in **InOF-3** (a))and **InOF-4** (b, c).

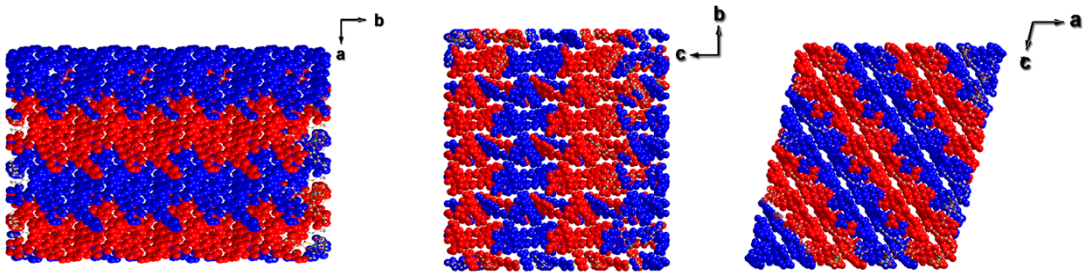

Figure S4. Models of 2D close-stacking layer-by-layer **InOF-3**.

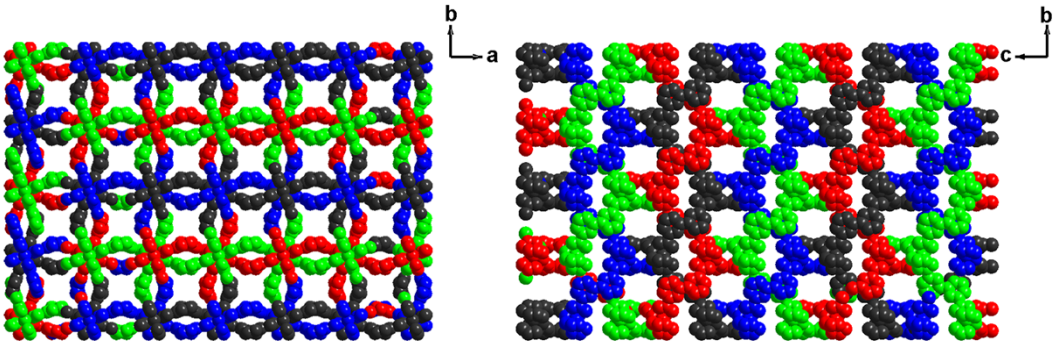

Figure S5. Models of 3D 4-fold microporous **InOF-4**.

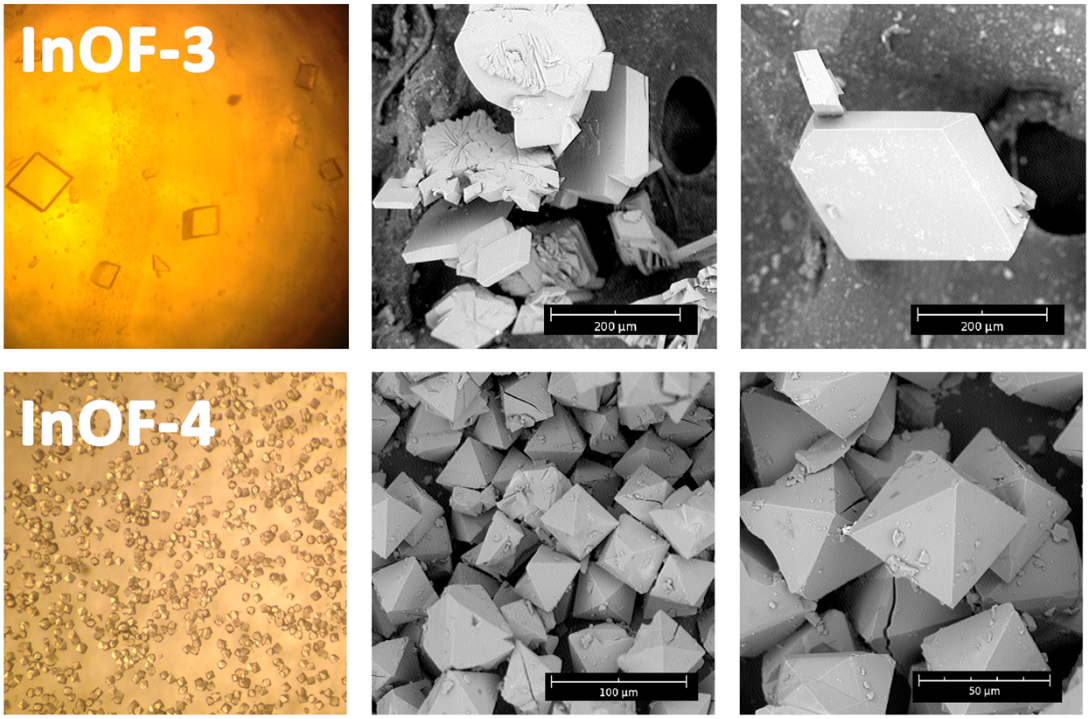

Figure S6. Photographs of the as-obtained **InOF-3** (up) and **InOF-4** (down).

S3. Topological Analysis

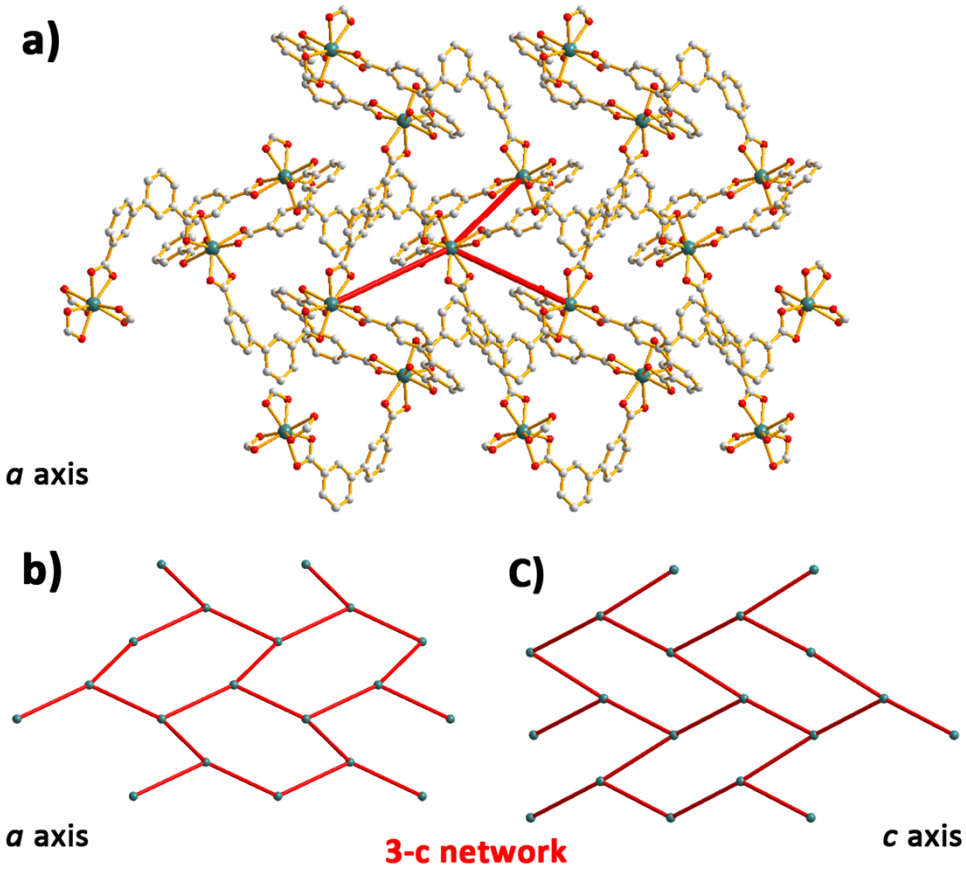

Figure S7. Single layer of **InOF-3** and its topological figures.

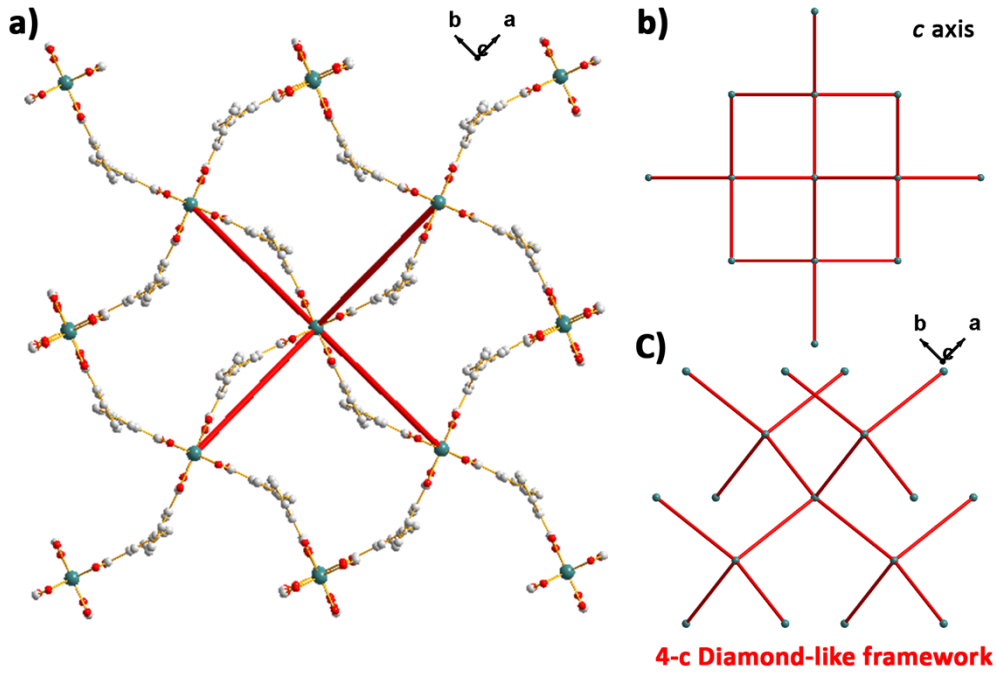

Figure S8. Single network of **InOF-4** and its topological figures.

S4. TGA data and PXRD patterns

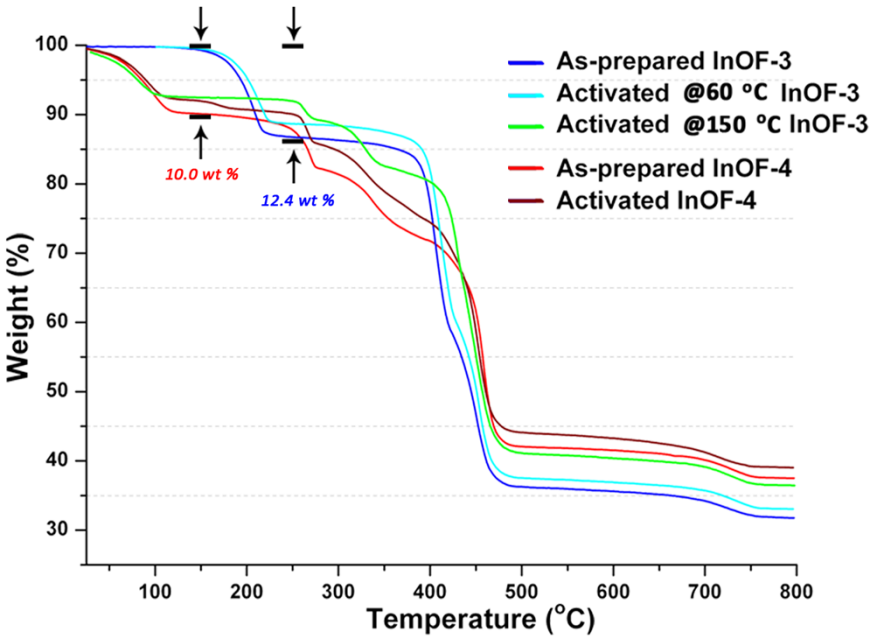

Figure S9. TGA curves for **InOF-3** and **InOF-4** before and after activation process.

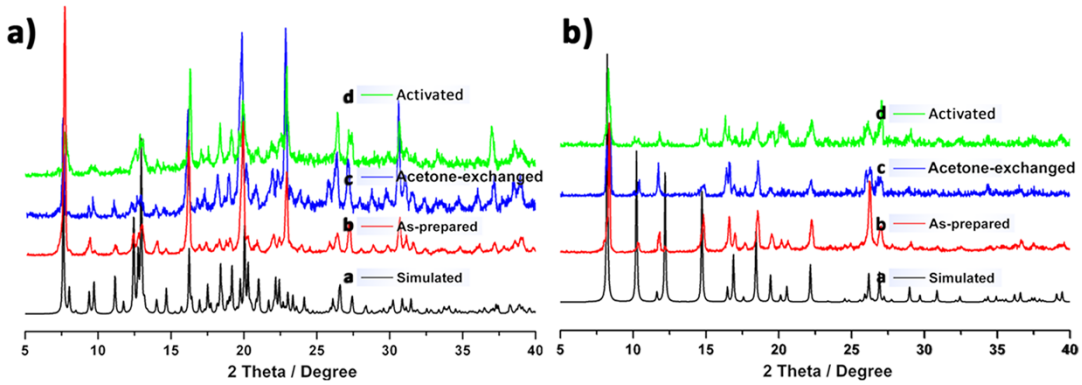

Figure S10. PXRD patterns for **InOF-3** (a) and **InOF-4** (b).

S5 Sorption Isotherms and Pore Size Distributions

N_2, H_2 and CO_2 Isotherms. All the N_2, H_2 and CO_2 isotherms for **InOF-3** and **InOF-4** were determined using an IGA gravimetric adsorption apparatus at the Fujian Institute of Research on the Structure of Matter in a clean ultra high vacuum system. Before measurements, about 100 mg acetone-exchanged samples were loaded into the sample basket within the adsorption instrument (ASAP 2020) and then degassed under dynamic vacuum for 10 h to obtain the fully desolvated samples.

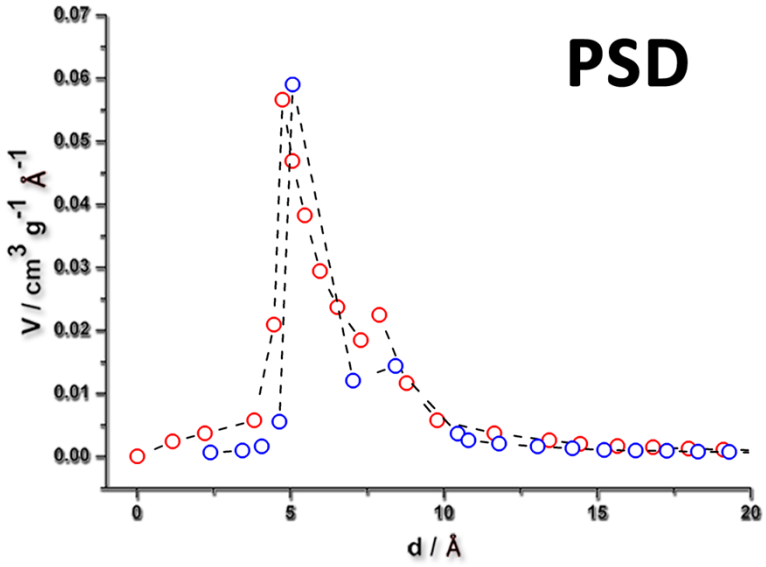

Figure S11. The pore size distribution incremental pore volume (V) vs. pore width (d) conducted by Horvath-Kawazoe method.

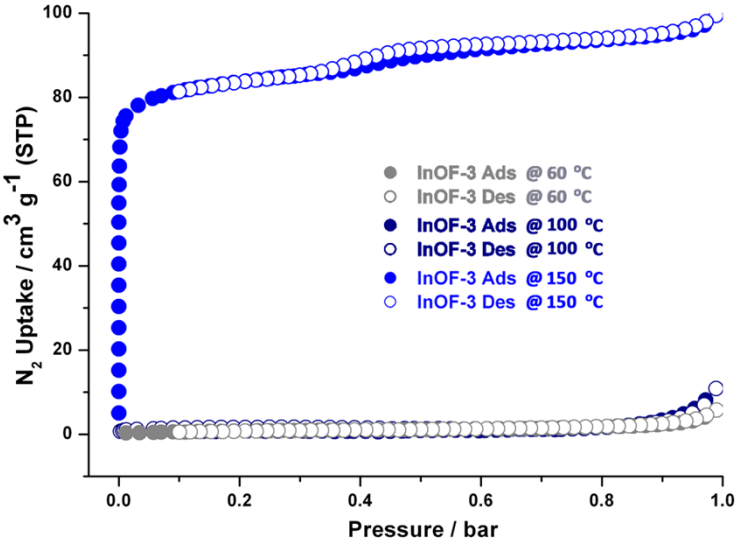

Figure S12. N_2 isotherms at 77 K for **InOF-3** samples activated at different temperature (60 °C, 100 °C, 150 °C).

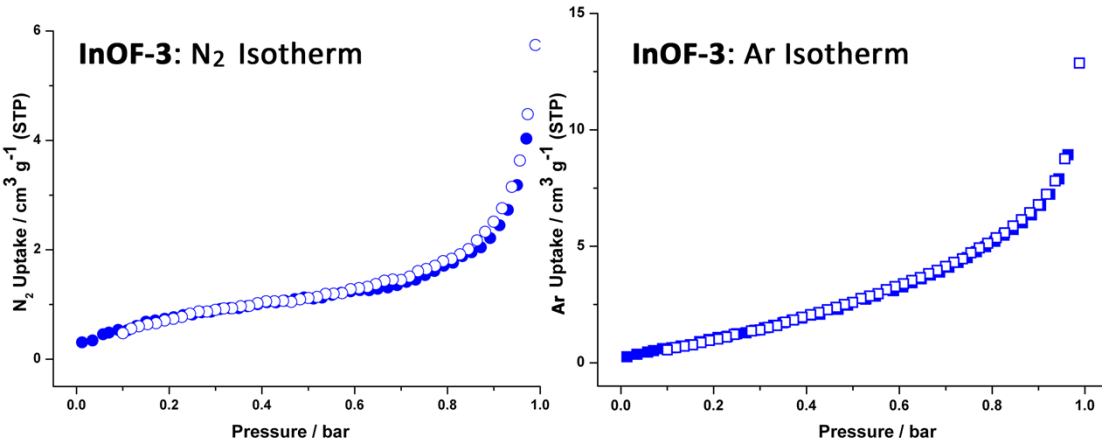

Figure S13. N_2 and Ar isotherms at 77 K for **InOF-3** samples activated at 60 °C.

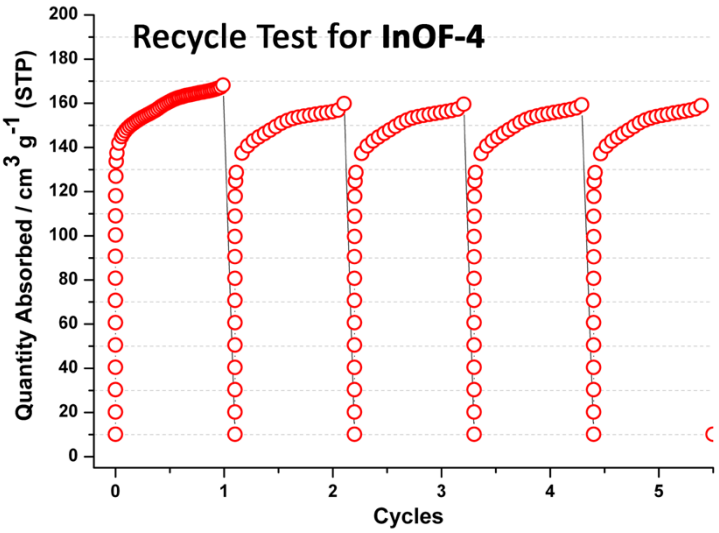

Figure S14. Cycling of N_2 uptake for the activated **InOF-4** sample at 77 K without reactivation process between cycles.

S6. References.

[S1] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.* **2009**, *42*, 339.

[S2] SHELXS, G.M. Sheldrick, *Acta Cryst*. **2008**, *A64*, 112.

[S3] SHELXL, G.M. Sheldrick, *Acta Cryst*. **2008**, *A64*, 112.

[S4] (a) A. L. Spek, *J. Appl. Crystallogr.* **2003**, *36*, 7; (b) P. v.d. Sluis and A. L. Spek, *Acta Crystallogr., Sect. A*, **1990**, *46*, 194.