Poster Presentation

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The First Covalent Organic Framework solved by Rotation Electron Diffraction

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Covalent organic frameworks (COFs) represent an exciting new type of porous organic materials, which are constructed with organic building units via strong covalent bonds.[1] The structure determination of COFs is challenging, due to the difficulty in growing sufficiently large crystals suitable for single crystal X-ray diffraction, and low resolution and peak broadening for powder X-ray diffraction. Crystal structures of COFs are typically determined by modelling building with the aid of geometry principles in reticular chemistry and powder X-ray diffraction data. Here, we report the single-crystal structure of a new COF (COF-320) determined by 3D rotation electron diffraction (RED),[2] a technique applied in this context for the first time. The RED method can collect an almost complete three-dimensional electron diffraction dataset, and is a useful technique for structure determination of micron- and nanosized single crystals. To minimize electron beam damage, the RED dataset was collected at 89 K. 3D reciprocal lattice of COF-320 was reconstructed from the ED frames using the RED – data processing software[2]. As the resolution of the RED data only reached 1.6 Å, the simulated annealing parallel tempering algorithm in the FOX software package [3] was used to find a starting molecular arrangement from the 3D RED data. Finally, the crystal structure of COF-320 was solved in the space group of I-42d and refined using the SHELXL software package. The single-crystal structure of COF-320 exhibits a 3D extended framework by linking the tetrahedral organic building blocks and biphenyl linkers through imine-bonds forming a highly porous 9-fold interwoven diamond net.

[1] *Uribe-Romo F. J., Hunt J. R., Furukawa H., et al., J. Am. Chem. Soc. 2009, 131, 4570.,* ***[2]*** *Wan W., Sun J. L., Su J., et al., J. Appl. Cryst. 2013, 46, 1863.,* ***[3]*** *Favre-Nicolin, V.; Černý, R. J. Appl. Cryst. 2002, 35, 734*

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