Poster Presentation

IT.P10

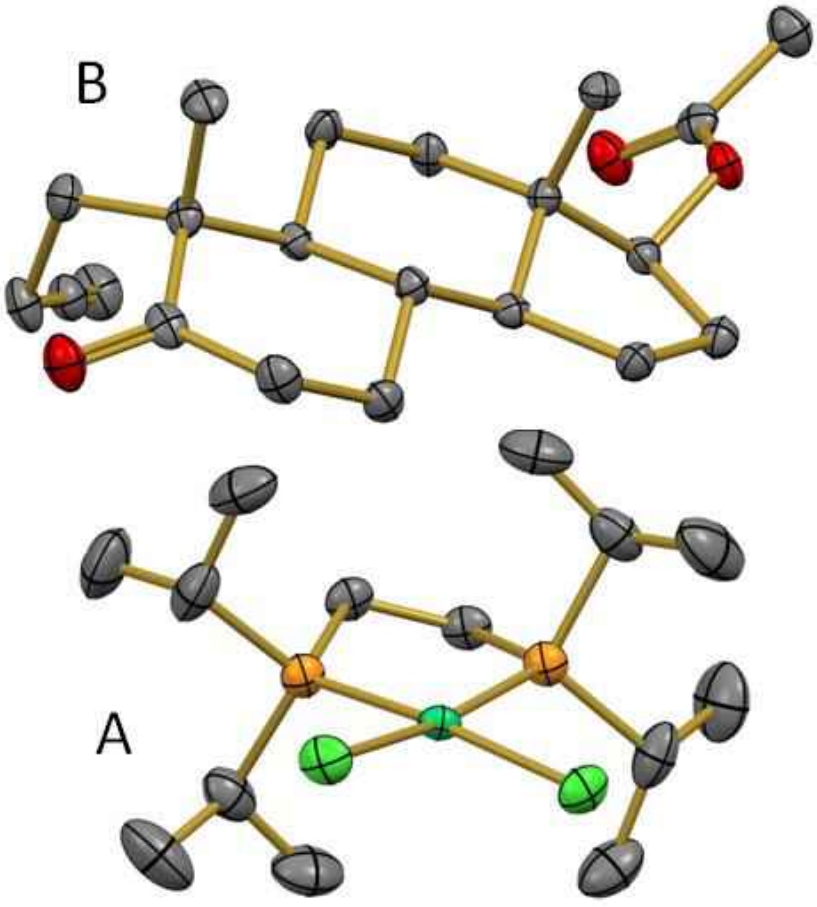
Collecting data for several crystals in a single exposure to X-rays

M. Flores-Alamo[1], A. Maldonado-Hermenegildo[1], H. Gómez-Ruiz[1]

[1]*Universidad Nacional Autónoma de México, Facultad de Química, , Ciudad Universitaria, México, DF, México*

The experimental technique which has been of the greatest importance in revealing the structure of crystals is undoubtedly X-ray diffraction; recently with the CCD detector the time of collection data is most fast, which has given opportunity to explore the option of data collection multiple crystals or twinning crystals of same chemical substance. Considering the Ewald sphere or expression of Bragg's law where it involves the reciprocal lattice in the sphere of reflection and using CrysAlis PRO171 software [1] is possible to identify the number of unit-cells that are present in the material which is composed of multiple crystals (see figure) that have intentionally place in this work. By placing the [1,2-bis(diisopropylphosphanyl)ethane]dichloridonickel(II) (A)[2] and 17β-acetoxy-4,5-secoandrost-3-yn-5-one (B)[3] crystals in the X-ray diffractometer Gemini with Atlas area detector and source of radiation λMo.= 0.7103 to 130 K and collect data for the system of lowest symmetry (2) (laue group: mmm) obtained a total of 15341 reflections in 307 frames and 4 runs with a total time of 2h 17m. Using the lattice wizard tool and Ewald explorer-reciprocal space two groups of data collection is obtained, which the resolve and refine separately R1(obs data) of 0.0255 and 0.0574 for A and B compounds respectively.

[1] *Agilent 2012. CrysAlis PRO and CrysAlis RED. Agilent Technologies, Yarnton, Oxfordshire, England,* ***[2]*** *N.Y. Castellanos-Blanco, J. Garcıa, M. Flores-Alamo, Acta Cryst. 2011. E67, m871,* ***[3]*** *P. Labra-Vazquez, M. Romero-Avila, M. Flores-Alamo, et al, J Chem. Crystallogr 2013 43, 605–609*



Keywords: CrysAlisPRO, Ewald-sphere, multiple-crystals