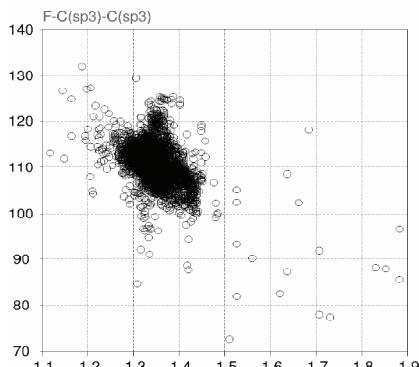


$R \leq 0.05$. In spite of this restraints, the following scattergram shows that the dispersion of F-C distances and F-C-F angles is very broad, indicating that, in a large number of cases, disorder was possibly present but ignored by the authors. As a conclusion same typical cases of disorder will be discussed.



Keywords: weak interactions; analysis of disordered structures; fluorine compounds

FA4-MS10-P04

Absolute Configuration Determination: Is There More Information in the Data? David J. Watkin^a, Amber L. Thompson^a. ^a*Chemical Crystallography, Department of Inorganic Chemistry, Oxford.*

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A sample of unknown enantiopurity can be regarded as containing a mole fraction of a given hand equivalent to $1-x$, and x mole fraction of the other. Because the Flack x parameter [1] is a parameter in the refinement, its standard uncertainty $u(x)$ can also be determined giving a measure of the confidence in the assignment of the absolute structure. Flack & Bernardinelli [2] give confidence intervals for the assignment of the absolute structure of materials of new samples: For a sample of unknown enantiopurity, the value of $u(x)$ must be less than about 0.04 for x to be a reliable assignment of the chirality of the major component. If the material is known to be enantiopure, then the condition on $u(x)$ can be relaxed to 0.10 and x in the range 0.3 to -0.3 would be considered as confirming the stated configuration.

Increasingly, there has been a suspicion that these conditions are over-cautious. By examining the distribution of the Friedel differences, Hooft et al. [3] have derived a parameter, y , which lies in the interval 0 to 1 and behaves something like the Flack x parameter. Because the calculation is working with distributions, there is the possibility of estimating the probability, for a known enantiopure material, that the assigned hand is correct. Hooft et al. remark, "These probabilities can be surprisingly decisive, even when the resonant scattering signal is very weak".

Examination of the Flack x and the Hooft y parameters for the natural product, epiallexine (below) raised some interesting questions [4]. In order to get a snap-shot of the performance of the Flack and Hooft parameters, 120 recent data sets collected on known enantiopure light atom

materials measured using molybdenum radiation [5] have been examined and results will be presented.

[1] Flack H.D. **1983**. *Acta Cryst.*, A39, 876-881. [2] Flack H.D. & Bernardinelli G. **2000**. *J. Appl. Cryst.*, 33, 1143-1148. [3] Hooft, R.W.W., Straver, L.H. & Spek A.L. **2008**. *J. Appl. Cryst.*, 41, 1, 96-103. [4] Thompson, A.L., Watkin, D.J., Gal, Z.A., Jones, L., Hollinshead, J., Jenkinson, S.F., Fleet G.W.F. & Nash R.J. **2008**. *Acta Cryst.*, C64, o649-o652. [5] Thompson A.L. & Watkin, D.J., *Tet. Asym.*, in press.

Keywords: absolute configuration determination; chirality; small-molecule crystallography

FA4-MS10-P05

The Coordination Mode of the Carboxylate Ligands in Copper Complexes. Goran A. Bogdanović^a, Sladjana B. Novaković^a. ^a*VINČA Institute of Nuclear Sciences, Laboratory of Theoretical Physics and Condensed Matter Physics, P.O. Box 522, 11001 Belgrade, Serbia.*

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Oxygen atoms from the carboxylate group possess four free electron pairs what enables the formation of different coordination modes with different number of metal atoms. Over 5000 crystal structures of copper complexes with carboxylate ligands have been analyzed using the Cambridge Structural Database (CSD) [1]. We have performed the classification of Cu carboxylate complexes based on geometrical parameters and frequency of structural motifs related to different coordination modes. The majority of crystal structures extracted from CSD can be described by two structural motifs: a) the carboxylate group is a part of chelate ring (five- or six-membered) with one carboxyl oxygen coordinated to the Cu atom, b) the carboxylate group is a bridging ligand connecting two Cu atoms. The second group of crystal structures has been analyzed in more details using different geometrical parameters. We found some preferential Cu...Cu interatomic distances related to different coordination modes of the carboxylate group.

[1] Allen F.H., *Acta Crystallogr.*, **2002**, B58, 380.

Keywords: Cambridge structural database; chemistry of complex compounds; carboxylates

FA4-MS10-P06

Conformational Analysis of Bidentate Tetra-Aryl Diphosphines. Claire L. McMullin^a, Natalie Fey^a, A. Guy Orpen^a. ^a*Department of Chemistry, University of Bristol, UK.*

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Phosphine ligands play an important role in many homogeneous catalytic reactions, including hydroformylation and asymmetric hydrogenation. In particular, bidentate tetra-aryl-substituted diphosphines allow fine-tuning of catalyst properties by modification