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Lattice energies of all known Crystal Structures

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We calculated the Gibb's energy of all known organic and organometallic crystal structures at ambient conditions with FlexCryst (1). Firstly, the implemented data mining force field was validated for the experimental lattice energies of the reference structures. Secondly, the force field was used for the minimization of 100 structures and the error in density and energy was examined. Finally, the Gibb's energy was calculated for all structures. After applying different filters and cleanser did remain 247 344 crystal structures.

In our analysis of the results we concentrated on crystal structures with a Gibbs energy above zero. Obviously these structures violates the second law of thermodynamics. A visualization of the intermolecular interactions did allow us to indicate poor intermolecular potentials and faulty crystal structures. The condition is fulfilled in 96.7 % of structures.

The data mining force field is integrated in the FlexCryst program suite and we tested it crystal structure prediction and in combination with XPRD for crystal structure determination. Since the obtained energies are Gibb's energies, the energies can be used to predict reactions at ambient conditions, for instance solubility (2), co-crystal formation (3), or polymorphism.

References:
1)Hofmann, Detlef WM. "Data mining in organic crystallography." Data Mining in Crystallography. Springer, Berlin, Heidelberg, 2009. 89-134.
2)Hofmann, Detlef Walter Maria, and Ludmila Kuleshova. "New similarity index for crystal structure determination from X-ray powder diagrams." Journal of applied crystallography 38.6 (2005): 861-866.
3)Stepanovs, Dmitrijs, et al. "Cocrystals of pentoxifylline: In silico and experimental screening." Crystal Growth & Design 15.8 (2015): 3652-3660.

Figure 1: The hydrate of the ruthenium complex (CSD reference code: AMUPUU) show strong repulsive interactions between two water molecules. It indicates that water should be placed different in the correct structure.
Figure 2: The co-crystal (CSD reference code: ALARAH) of a platinum complex with methanol show strong repulsive interactions between methanol and it image. It indicates that methanol should be placed different in the correct structure.

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