

# Oral Contributions

**[MS30] Beyond Harmonic Treatment**  
*Co-Chairs: Birger Dittrich (DE), Simon Grabowsky (AU)*

**[MS30-01] Anharmonic Motion in Experimental Charge Density Investigations.**  
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In the charge density study of 9-diphenylthiophosphinoyl-anthracene the thermal motion of several atoms needed an anharmonic description via Gram-Charlier coefficients even for data collected at 15 K. As several data sets at different temperatures were measured this anharmonic model could be proved to be superior to a disorder model.[1] The refined multipole parameters were distorted, when the anharmonic motion was not properly refined. Therefore this study reveals the importance of detecting and properly handling of anharmonic motion. Unrefined anharmonic motion leads to typical shashlik-like residual density pattern.[2] Therefore careful analysis of the residual density and the derived probability density function after the refinement of the Gram-Charlier coefficients proved to be the most useful tools to indicate the presence of anharmonic motion.

Herbst-Irmer R., Henn J., Holstein J. J., Hübschle C. B., Dittrich B., Stern D., Kratzert D., Stalke D. (2013). *J. Phys. Chem A.* **117**, 633-641. [2] Meindl K., Herbst-Irmer R., Henn (2010). *Acta Cryst. A* **66**, 362-371.

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