MS22-P01 | 3D -VISUALIZATION AND -PRINTING OF MOLECULAR SURFACES

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Molecular and other crystal structures are often complex. A three dimensional visualization can help in understanding them and optimizing the applied model to fit the experimental data. A visualization on screen is nice, but some times touching a physical model is a step further to get into the details of some structure properties. Recent Version of *MoleCoolQ*t¹ can not only visualize density iso-surfaces, Hirshfeld surfaces and Voronoi-polyhedra, it is also possible to export three dimensional surfaces in file formats that are suitable for 3D-printers.

[1] C. B. Hübschle and B. Dittrich. J. Appl. Cryst. (2011). 44, 238-240.