Subject: Re: Bad Displaying of Complex Polycyclic Molecules
Posted by nbehrnd on Fri, 20 Sep 2024 05:38:02 GMT
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Hell yunforce,

I think your observation refers to a general problem for every program to provide a 2D projection of a 3D molecule. Partial overlap already can be observed for smaller molecules, perhaps especially if DW is used as an interface to access databases with experimentally determined coordinates. The example attached documents a query for rubrenes in the crystallographic open database. For large rings, it can become difficult/impossible to count the number of atoms building this cycle. The depiction can become very busy with if there are «too many» stereochemistry labels ([abs] R/S, P/M, E/Z) per area unit of the array of the structure previews (for which I think there is no toggle-on/off, either), too.

If your sdf data are associated with conformers, the 3D structure window allows to rotate the model of the molecule (dragged right hand mouse button), and change its scale (mouse wheel). This often is helpful when browsing through a stack of structures on a on-by-one basis, complementary to the preview provided by the array.

Norwid

File Attachments

1) search_ruberene.png, downloaded 164 times