Subject: Re: Generate 2D atom coordinates gives overlapping atoms
Posted by nbehrnd on Fri, 03 Feb 2023 21:32:10 GMT
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Dear mcmc,

I speculate an underlying contribution to the issue is the discrepancy between identifying a good orientation for a 3D object in space for a 2D projection, on one hand, and retaining a consistent pattern of single / double / triple bond lengths, on the other. A substituted briged piperazines may be an example where a chemist might consider to draw one single bond longer, than others to move and rearrange a (sub) motif on the paper/black board further away from the centre of the molecule to keep all well intelligible. On the other hand, a computer algorithm (like the one in DW, but equally in Marvin) may yield overlaps. The approach starting from 2D and a sketcher like ChemDraw/ChemDoodle is different as all work is in 2D only.

Because you mentioned the structure import into DW used .sdf, it was possible to identify COD 1513802 of the Crystallographic Open Database as an entry where DW faces a similar problem to the one reported by you. But it isn't unique to DW; the same structure eventually imported into Marvin equally has no orientation without a (partial) overlap of the atoms.

With regards,

Norwid

File Attachments

1) 1513802_DW.png, downloaded 515 times
2) 2023-02-03_DW_2D_overlap.zip, downloaded 201 times