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Keywords: intermolecular interactions, density-functional theory, cambridge structural database

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Understanding disorder in a Z'=4 structure with computationally cheap tools

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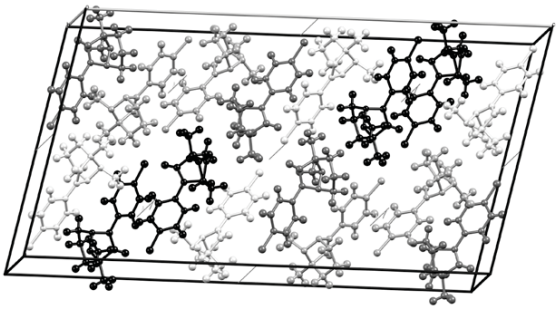
As computationally cheap tools have recently become available to better understand crystal packing, we have applied the CE-B3LYP method as implemented in Crystal Explorer 17 [1] to an interesting structure with Z'=4, and whole molecule disorder in each of the four molecules in the asymmetric unit.

The structure itself contains many subtle features which are interesting to discuss all by themselves, but we are interested to see whether the energy calculations will aid in providing a reasonable explanation why the structure crystallizes as it does.

The average nature of the coordinates obtained from the crystallographic experiment will obviously be the largest challenge, as it conflicts with the basic premise of a calculation that does not optimize the atomic coordinates before calculating energies.



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Keywords: whole molecule disorder, crystal explorer, high Z'