Invariom Modeling for Improving Absolute Structure Determination

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A reliable determination of the Flack parameter [1] for structures of organic molecules, containing only the elements H, C, N, and O usually fails. The reason for this is the very weak anomalous signal obtained from the light atoms [2]. Recently we have introduced invarioms [3] and here we try to improve the absolute structure determination by replacing the independent atom model with the aspherical invariom scattering model. The determination of the Flack parameter was included in the program XDLSM [4]. Alternatively, its calculation has been attempted via a hole-in-one procedure. A precise data set on a steroid compound was collected using copper radiation and CCD detection, and first results are reported.

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