# Improving semi-experimental structures of molecules with near-axis atoms

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In the process of experimental and semi-experimental determination of molecular structure, presence of atoms near inertial axes leads to inaccuracies and uncertainties in bond distances and angles. This study deals with two different approaches that could be used in determining a semi-experimental structure of such molecules. One approach is obtaining a kraitchman substitution structure using a reference coordinate system where the inertial axes are slightly rotated away from the atoms, thus leading to a better estimation of its coordinates. This method has been applied to two molecules, pyridazine and 1,2,4-triazole with excellent results. An attempt to use this technique for thiophene fails. Another technique involves studying the sensitivity of different semi-experimental structural parameters with respect to change in rotational constants. This analysis helps in identifying parameters that are most affected by the proximity of atoms to the inertial axes. These values are then fixed to the best available ab initio number, before doing a least squares fitting of the remaining parameters. This method is applied to three molecules namely methacrylonitrile, oxazole, and thiophene with varying degrees of success.