

ISOTOPIC RELATIONS FOR TETRAHEDRAL AND OCTAHEDRAL MOLECULES

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The study and analysis of heavy spherical-top molecules is often not straightforward. The presence of hot bands and of many isotopologues can lead to a high line congestion very difficult for assignment.

In this work, using a low-order model we have derived very simple isotopic relations in order to determine initial parameters of the analysis.

We also show that an identical approach can be used for XY_4 and XY_6 molecules and all these results are illustrated by the comparison of numerical computations and experiments for different molecules: CH_4 , GeH_4 , RuO_4 (as shown in the figure on the right) and SF_6 .

Reference: M. Loëte, C. Richard and V. Boudon, *J. Mol. Struct.* **1206**, 127729 (2020).

