

## 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).

