EMPIRICAL ENERGY LEVELS OF METHANE UP TO POLYAD 6

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An extensive analysis of the available spectroscopic data on methane is being performed. The MARVEL (Measured Active Rotational-Vibrational Energy Levels) algorithm by Furtenbacher et al is used to provide accurate empirical rovibrational energy levels for methane.

Experimental data are collected from 159 sources; these are evaluated and then added to a database of measured transitions with their experimental uncertainties. Each transition must have assigned quantum numbers for their upper and lower states and an uncertainty. The database is being built starting from lower and moving towards higher polyads and used as an input for MARVEL. The self-consistency of the input transitions is evaluated during the MARVEL procedure, and the uncertainties are adjusted accordingly until a self-consistent network of energy levels is achieved. As part of this process, a constant cleansing of the database of incorrect and wrongly assigned transitions is performed.

The output of the procedure is a set of empirical energy levels with their respective uncertainties, derived from the inversion of the input measured lines which will be used to update our calculated line lists. At the same time, the resulting energy levels will be used for the attribution of quantum numbers to unassigned experimental transitions.