

Comprehensive MARVEL Analysis of Empirical Rovibrational Energy Levels for Twelve Carbon Dioxide Isotopologues

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We present a systematic analysis of empirical rovibrational energy levels for twelve isotopologues of carbon dioxide (CO_2), employing the MARVEL (Measured Active Rotational-Vibrational Energy Levels) protocol. This work integrates over 125,000 experimentally measured transitions compiled from more than 350 literature sources, covering wavenumber ranges from 2 to $14,076 \text{ cm}^{-1}$. The MARVEL approach enables construction of spectroscopic networks and rigorous validation of experimental data, resulting in the extraction of over 58,800 empirical energy levels with quantified uncertainties.

Detailed rovibrational datasets are provided for rare and asymmetric isotopologues including 828 ($^{18}\text{O}^{12}\text{C}^{18}\text{O}$), 728 ($^{17}\text{O}^{12}\text{C}^{18}\text{O}$), 838 ($^{18}\text{O}^{13}\text{C}^{18}\text{O}$), and the third to fifth most abundant species: 628 ($^{16}\text{O}^{12}\text{C}^{18}\text{O}$), 638 ($^{16}\text{O}^{13}\text{C}^{18}\text{O}$), 627 ($^{16}\text{O}^{12}\text{C}^{17}\text{O}$), among others. The number of validated transitions and derived energy levels per isotopologue ranges from hundreds to tens of thousands, spanning polyads up to $P = 17$. Notably, the 626M24 dataset for the parent ($^{12}\text{C}^{16}\text{O}_2$), isotopologue comprises 44,828 line measurements and yields 8,268 empirical energy levels. All MARVEL-generated energy levels were critically compared with established line lists from CDS-296, Ames-2021, and HITRAN2020. The comparisons confirm excellent agreement, while also highlighting areas for potential refinement in the databases. Our results are of direct relevance to high-resolution atmospheric and astrophysical spectroscopy, including the detection and characterization of CO_2 isotopologues in exoplanetary atmospheres.