Empirical Rovibrational Energy Levels of Hydrogen Cyanide Isotopologues via MARVEL for High-Resolution Exoplanetary Spectroscopy

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We report high-accuracy empirical rovibrational energy levels for eight isotopologues of hydrogen cyanide (HCN), derived using the MARVEL (Measured Active Rotational-Vibrational Energy Levels) protocol. These include the most astrophysically relevant isotopologues: $H^{12}C^{14}N$ (124), $H^{13}C^{14}N$ (134), $H^{12}C^{15}N$ (125), $D^{12}C^{14}N$ (224), $D^{13}C^{14}N$ (234), $D^{12}C^{15}N$ (225), and $D^{13}C^{15}N$ (235). The MARVEL procedure validates and refines rovibrational transitions collected from a wide range of literature sources spanning seven decades (1952–2019), resulting in an extensive and error-corrected spectroscopic dataset.

For 124 and 134, the two most abundant isotopologues, 29,796 (20,515 unique) and 17,062 (11,719 unique) transitions were analyzed, covering the spectral ranges 500–18,400 cm^{-1} and 522–12,604 cm^{-1}, respectively. The third most abundant, 125, was examined using 13,762 (11,754 unique) transitions over 60–9,700 cm^{-1}, with polyads up to P = 37.

Rare isotopologues $D^{12}C^{14}N$, $D^{13}C^{14}N$, $D^{12}C^{15}N$, and $D^{13}C^{15}N$ yielded 2,493 / 1,321 / 64 / 1,190 empirical energy levels, respectively, based on 8,931 / 3,526 / 407 / 3,427 measured transitions. After critical evaluation, subsets of questionable transitions were removed (e.g., 1,322 transitions from 224), ensuring dataset integrity. The energy levels span wavenumber ranges from below 1 cm^{-1} to over 5,000 cm^{-1}, across up to 77 vibrational bands depending on the isotopologue.

Cross-comparison with ExoMol, Ames-2021, HITRAN, and CDMS databases demonstrates strong agreement, while also identifying areas for refinement, especially for the deuterated isotopologues. The validated datasets produced here enhance the precision of molecular line lists essential for the detection and modeling of exoplanetary atmospheres rich in HCN and its isotopic variants.