GAS-PHASE ROTATIONAL SPECTRUM OF HZnCN ($X^1\Sigma^+$) BY FOURIER TRANSFORM MICROWAVE TECHNIQUES

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The first gas-phase synthesis of HZnCN was carried out in a pulsed-nozzle DC discharge of a dilute gas mixture of dimethylzinc and cyanogen. The Fourier Transform microwave (FTMW) spectra of this species in its seven isotopologues in their $X^1\Sigma^+$ electronic ground states were studied from 7 GHz to 40 GHz. From the rotational constants of the seven isotopologues, the linear structure of the molecule was precisely determined. Additionally, the electric quadrupole coupling constants were accurately determined, which provide useful information about the bonding properties of this species. The deuterium quadrupole constant was established to be eqQ(D) = 0.08 MHz, indicating weak coupling and a large H-metal distance, which is consistent with our result, 1.495 Å($r_m^{(1)}$). In contrast, the large value of eQq(^{67}Zn) = -104.58 MHz indicates a large electric field gradient across the zinc nucleus and thus a high degree of covalent C-metal bonding.