NUCLEAR HYPERFINE STRUCTURE IN THE $X^3\Sigma^+$ STATE OF ^{91}ZrC

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Electronic bands of zirconium monocarbide, ZrC, can be observed following the reaction of laser-ablated Zr atoms with methane under supersonic free-jet conditions. In our experiments some of the bands near 17000 cm^{-1} are strong enough for nuclear hyperfine structure from the ^{91}Zr isotope (I = 5/2, 11.22% abundance) to be assignable. Hyperfine splittings of up to 0.2 cm^{-1} are found in some of the rotational lines. Analysis shows that the principal hyperfine effects are in the $^3\Sigma$ ground state, where $b = -0.03132 \pm 0.00015$ cm^{-1} and $c = -0.00122 \pm 0.00038$ cm^{-1} (3σ error limits). The large Fermi contact parameter, b, indicates that an unpaired Zr $5s\sigma$ electron is present, which, taken together with the small value of λ (0.5139 cm^{-1}), means that the ground state must be a $^3\Sigma^+$ state, from the electron configuration (Zr $5s\sigma)^1$ (C $2p\sigma)^1$. Internal hyperfine perturbations occur between the F_1 and F_3 electron spin components of the ground state in the range $N = 2 - 4$, producing extra lines in some of the branches; the perturbations are of the type $\Delta N = 0$, $\Delta J = \pm 2$, and are a second order effect arising because the F_1 and F_3 spin components ($J = N + 1$ and $J = N - 1$, respectively) both interact with the F_2 component ($J = N$) through $\Delta N = 0$, $\Delta J = \pm 1$ matrix elements of the Fermi contact operator.