ON THE A-X SYSTEM OF THE CALCIUM MONOMETHOXIDE RADICAL

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Laser excitation spectra of the $A\ ^2\mathrm{E} \leftarrow X\ ^2\mathrm{A}_1$ system of four isotopomers of calcium methoxide were recorded at the University of New Brunswick. The radicals were produced in a laser ablation source, using a 1.2 % mixture of methanol ($^{12}\mathrm{CH_3OH}$, $^{13}\mathrm{CH_3OH}$, $^{12}\mathrm{CD_3OD}$ and $^{13}\mathrm{CD_3OD}$) in He as a precursor. High resolution spectra were recorded in the range 15870 - 15985 cm^{-1} and 16320 - 16500 cm^{-1}(F.W.H.M. 250 MHz) using a tunable, single-mode cw dye laser (CR 699 + autoscan), operating with DCM and Kiton red dyes. The transitions were assigned to the two spin-orbit components $A\ ^2\mathrm{E}_{3/2} \leftarrow X\ ^2\mathrm{A}_1$ and $A\ ^2\mathrm{E}_{1/2} \leftarrow X\ ^2\mathrm{A}_1$ of the origin band, and of a band with $\mathrm{v'}_4$(Ca-[$\mathrm{OCH_3}$] stretch) = 1. Resolved J and K structures are observed. The analysis used an effective Hamiltonian given in the literature[a]. The fits build on earlier work on the main isotopomer[b], and include spectroscopic data for the $B \leftarrow X$ system given in the literature.[cd] We obtain structural parameters for the calcium monomethoxide radical from the rotational constants obtained from the different isotopomers.

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