STRUCTURE AND SPECTRA OF THE CALCIUM MONOMETHOXIDE RADICAL

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Laser excitation spectra of the origin bands of the $A\,^2\mathrm{E} \leftarrow X\,^2\mathrm{A}_1$ system (around 635 nm) and $B\,^2\mathrm{A}_1 \leftarrow X\,^2\mathrm{A}_1$ system (around 565 nm) of four isotopomers of calcium methoxide have now been recorded at the University of New Brunswick. The aim of the experiments was to use isotope effects to examine changes in the structure of the molecule on excitation. 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 using a tunable, single-mode cw dye laser (CR 699 + autoscan), operating with DCM, Kiton red and Rhodamine 6G dyes. The analysis used an effective Hamiltonian given in the literature.[a] The fits to both spectroscopic and structural parameters build on earlier work on the A-X system,[b] and include spectroscopic data for the $B \leftarrow X$ system given in the literature.[c,d] We present the results of our analysis, outlining some of the difficulties encountered with the $B \leftarrow X$ spectra, particularly for the $^{13}\mathrm{CD_3OD}$ molecule.

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