DETERMINATION OF THE BOND LENGTHS IN MgCCH, CaCCH and SrCCH

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To determine the three bond lengths in a linear four atom molecule, one requires spectral data from three isotopologues of that molecule. By combining information from previously published analyses with new high resolution isotopically substituted spectra, we have determined the bond lengths for MgCCH, CaCCH and SrCCH. In each case, the $\tilde{A}^2\Pi - \tilde{X}^2\Sigma^+$ spectra of the M-^{12}C^{12}CH, M-^{12}C^{12}CD and M-^{13}C^{13}CH isotopologues were considered, where M refers to Mg, Ca and Sr. This study is of particular interest since it shows how the structure of this family of molecules evolves as we change the alkaline earth atom attached to the CCH ligand. In MgCCH, the structure of the CCH ligand is nearly the same as it is in acetylene, HCCH[a]. Surprisingly, the bonding in the ligand is quite different from that of acetylene for the two heavier acetylide molecules, with the triple bond between the two carbon atoms experiencing the greatest change.

[a] J. Overend, Trans. Faraday Soc. 56 (1960) 310-314