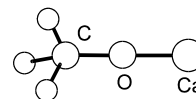


**113**      **CH<sub>3</sub>CaO**      **Calcium(I) methoxide**      **C<sub>3v</sub>**  
 LIF      Methoxycalcium      Ca–O–CH<sub>3</sub>

State	$\tilde{X}^2A_1$	$\tilde{A}^2E$	$\tilde{B}^2A_1$
Energy [eV]	0.00	1.974	2.912
$r_0(\text{Ca–O})$ [Å]	1.9945 <sup>a)</sup>		1.9730 <sup>a)</sup>
$r_0(\text{C–H})$ [Å]	1.10(2) <sup>b)</sup>	1.10 <sup>b)</sup>	
$\theta_0(\text{H–C–H})$ [deg]	105.6(30) <sup>b)</sup>	105.7(30) <sup>b)</sup>	
Reference	[1,2]	[2]	[1]



CaOCH<sub>3</sub> molecules were produced by the reaction of laser-ablated calcium atoms with methanol in argon, under supersonic jet-cooled conditions. The  $\tilde{A}^2E - \tilde{X}^2A_1$  and  $\tilde{B}^2A_1 - \tilde{X}^2A_1$  transitions were studied by laser-induced fluorescence. Some structural information was deduced from the rotational constants. The Ca–O–C framework remains linear in all three electronic states.

<sup>a)</sup> From the *B*-rotational constants, assuming that the structural parameters for the OCH<sub>3</sub> group are the same as those derived from the MW work.

<sup>b)</sup> From the *A*-rotational constants, assuming that the C–H bond lengths are the same as those in related compounds.

[1] Whitham, C.J., Beaton, S.A., Ito, Y., Brown, J.M.: J. Mol. Spectrosc. **191** (1998) 286.

[2] Crozet, P., Martin, F., Ross, A.J., Linton, C., Dick, M.J., Adam, A.G.: J. Mol. Spectrosc. **213** (2002) 28.

MW, MW-optical double  
 resonance

Pure rotational transitions in the  $\tilde{X}^2A_1$  state were recorded using the pump/probe MW-optical double resonance technique, by monitoring the  $\tilde{B}^2A_1 - \tilde{X}^2A_1$  electronic transition. The proton magnetic hyperfine splitting pattern confirms a C<sub>3v</sub> symmetry of the ground electronic state.

Namiki, K.C., Robinson, J.S., Steimle, T.C.: J. Chem. Phys. **109** (1998) 5283.