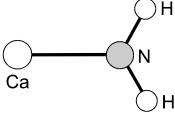


## Structure Data of Free Polyatomic Molecules

<b>111</b> MW	<b>CaH<sub>2</sub>N</b>	<b>Calcium monoamide</b> Calcium(I) amide	<b>C<sub>2v</sub></b> CaNH <sub>2</sub>
	$r_0$ $\text{Ca-N}$ 2.126(3) $\text{N-H}$ 1.018(3)	$\theta_0$ $\text{H-N-H}$ 105.8(5)	

The CaNH<sub>2</sub> radical has  $\tilde{X}^2A_1$  ground electronic state. The observed data are consistent with the molecule being planar and having predominantly ionic bonding.

Brewster, M.A., Ziurys, L.M.: J. Chem. Phys. **113** (2000) 3141.

## LIF

State	$\tilde{X}^2A_1$		$\tilde{A}^2B_2$		$\tilde{B}^2B_1$		$\tilde{C}^2A_1$	
Energy [eV]	0.00	0.00	1.917	1.917	1.970	1.970	2.154	2.154
$r_0(\text{Ca-N}) [\text{\AA}]$	2.140	2.118	2.120	2.098	2.145	2.123	2.125	2.102
$r_0(\text{N-H}) [\text{\AA}]$ <sup>a)</sup>	1.025	1.041	1.025	1.041	1.025	1.041	1.025	1.041
$\theta_0(\text{H-N-H}) [\text{deg}]$	102.9	100.5	103.8	101.3	103.8	101.3	103.5	101.1

CaNH<sub>2</sub> molecules were produced by the reaction of laser-ablated calcium atoms with ammonia seeded in argon under supersonic jet-cooled conditions. The  $\tilde{A}^2B_2 - \tilde{X}^2A_1$ ,  $\tilde{B}^2B_1 - \tilde{X}^2A_1$  and  $\tilde{C}^2A_1 - \tilde{X}^2A_1$  transitions were studied by laser-induced fluorescence. A global fit of the data was carried out yielding molecular constants for the four electronic states together with a complete set of spin-rotation constants for the three excited states.

<sup>a)</sup> The two alternative structures were derived assuming the N-H distances to be 1.025 and 1.041 Å, from NH<sub>2</sub> and NH<sub>2</sub><sup>-</sup>, respectively.

Morbi, Z., Zhao, C., Bernath, P.F.: J. Chem. Phys. **106** (1997) 4860.

Replaces [II/25A\(2, 244\)](#)