



HAL
open science

SPECTROSCOPIC DETERMINATION OF Lin ([MATH]) CLUSTERS STRUCTURE

Ph. Dugourd, J. Chevaleyre, M. Broyer, J. Blanc, L. Wöste, J. Wolf

► **To cite this version:**

Ph. Dugourd, J. Chevaleyre, M. Broyer, J. Blanc, L. Wöste, et al.. SPECTROSCOPIC DETERMINATION OF Lin ([MATH]) CLUSTERS STRUCTURE. Journal de Physique IV Proceedings, 1991, 01 (C7), pp.C7-563-C7-563. 10.1051/jp4:19917150 . jpa-00250825

HAL Id: jpa-00250825

<https://hal.science/jpa-00250825>

Submitted on 4 Feb 2008

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

SPECTROSCOPIC DETERMINATION OF Li_n ($3 \leq n \leq 8$) CLUSTERS STRUCTURE

Ph. DUGOURD, J. CHEVALEYRE, M. BROYER, J. BLANC*, L. WÖSTE* and J.P. WOLF*

*Laboratoire de Spectrométrie Ionique et Moléculaire (associé au CNRS n° 171), Université Lyon I, 43 boulevard du 11 novembre 1918, F-69622 Villeurbanne cedex, France***Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-1000 Berlin, Germany*

Lithium clusters up to Li_{100} are produced in a seeded molecular beam using a special oven able to sustain temperatures up to 1800 K. Optical spectra were recorded by Two Photon Ionization Spectroscopy for Li_3 and by Depletion Spectroscopy for larger clusters because of fast dissociation in excited states. For Li_3 , clear vibronic and rotational structures have been measured leading to a complete determination of the geometry and potential surfaces of the ground state of the two observed excited states. For larger clusters, no vibronic structure was observed except in Li_4 for which a residual vibronic pattern was obtained.

Optical spectra have been compared to SCF-CI calculations [1]. Since the calculated spectra strongly depend on the ground state geometry, it is possible to determine the cluster geometry. In Li_4 , the experimental absorption spectrum is in complete agreement with the theoretical spectrum obtained for the planar rhombus geometry while the theoretical spectrum calculated for the other isomer slightly higher in energy (deformed tetrahedron) is completely different. This is the first confirmation of the planar rhombus geometry of Li_4 . For Li_7 and Li_8 , the experimental results are also in agreement with the geometries calculated by the SCF-CI method. In Li_6 , the calculations lead to three isomers having very similar energy [2]: the planar D_{3h} structure, the quasi planar C_{5v} pentagonal pyramid and the 3D tripyramidal C_{2v} geometry. Only this last geometry gives a theoretical absorption spectrum in agreement with the experimental one. The two other structures lead mainly to a huge peak at 2.1 eV in complete contradiction with the experimental results. Experiments are in progress to extend our measurements up to Li_{40} .

[1] V. Bonacic-Koutecky, P. Fantucci and J. Koutecky, *Chem. Phys. Lett.* **166**, 32 (1988).

[2] J. Koutecky, I. Boustani and V. Bonacic-Koutecky, *Int. J. of Quant. Chem.* **38**, 146 (1990).