

# Cage-Like Structure of Lanthanum Trimer Tetroxide

*Dong-Sheng Yang, Department of Chemistry, University of Kentucky*

Several structures of lanthanum trimer tetroxide ( $\text{La}_3\text{O}_4$ ) were predicted by theory and a minimum-energy cage-like structure was identified by mass-analyzed threshold ionization spectroscopy and spectral simulation.

In this structure, three of the four oxygen atoms are bonded to two lanthanum atoms, while the other oxygen is bonded to three lanthanum atoms. Each lanthanum forms three bonds with oxygens, consistent with the +3 formal oxidation state. The neutral cluster and cation have essentially the same structure, with only small differences in bond lengths and angles. The ionization energy of the  $^2A_1$  neutral ground state is 3.4750(6) eV, and two La-O stretching modes and two O-La-O bending modes of the  $^1A_1$  ion state are 422/533 and 206/252  $\text{cm}^{-1}$ .

