C-O AND O-H BOND ACTIVATION OF METHANOLE BY LANTHANUM

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The interaction between methanol (CH_3OH) molecules and laser-vaporized La atoms resulted in the cleavage of C-O and O-H bonds and the formation of three major products, LaH_2O_2, $LaCH_4O_2$ and $LaC_2H_6O_2$, in a supersonic molecular beam. These products were identified by time-of-flight mass spectrometry, and their electronic spectra were obtained using mass-analyzed threshold ionization (MATI) spectroscopy. From the MATI spectra, adiabatic ionization energies of the three complexes were measured to be 40136 (5), 39366 (5) and 38685 (5) cm^{-1} for LaH_2O_2, $LaCH_4O_2$ and $LaC_2H_6O_2$, respectively. The ionization energies of these complexes decrease as the size of the coordinated organic fragments increases. The most active vibrational transitions of all three complexes were observed to be the M-O stretches in the ionic state. A metal-ligand bending mode with a frequency of 127 cm^{-1} was also observed for $[LaH_2O_2]^+$. However, the spectra of the other two complexes were less resolved, due to the existence of a large number of low frequency modes, which could be thermally excited even in the supersonic molecular beams, and of multiple rotational isomers formed by the free rotation of the methyl group in these systems. The electronic transitions responsible for the observed spectra were identified as $^1A_1$ (C_{2v}) $\leftarrow$ $^2A_1$ (C_{2v}) for LaH_2O_2 and ^1A (C_1) $\leftarrow$ ^2A (C_1) for $LaCH_4O_2$ and $LaC_2H_6O_2$.