SPECTROSCOPIC IDENTIFICATION OF $Y(C_4H_6)$ ISOMERS FORMED BY YTTRIUM-MEDIATED C-H BOND ACTIVATION OF BUTENES

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$Y(C_4H_6)$ was observed from the reactions of laser-vaporized Y atom with 1-butene (CH_2=$CHCH_2CH_3$) and iso-butene (CH_2=$C(CH_3)_2$) in a pulsed molecular beam source, and its structural isomers were investigated with mass-analyzed threshold ionization spectroscopy combined with electronic structure calculations and spectral simulations. $Y(C_4H_6)$ was identified as a five-membered metallacycle [$Y(CH_2$-CH=CH-$CH_2)$] from the Y + 1-butene reaction and a tetrahedral structure [$YC(CH_2)_3$] from the Y + iso-butene reaction. The metallacycle has a C_s structure with Y binding to the two terminal carbon atoms, whereas the tetrahedron has C_{3v} symmetry with Y binding to the tertiary carbon atom of trimethylenemethane. Both isomers have a doublet ground state with the highest molecular orbital being largely a Y 5s character. Ionization removes the metal based electron, and the resultant singlet ion has a similar structure to the neutral complex. However, the adiabatic ionization energy [46309(5) cm^{-1}] of the tetrahedron is considerably higher than that [43473(5) cm^{-1}] of the cyclic structure.