Molecular Orbitals of Nitrogen molecule obtained through Gaussian using Jmol generated input file

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Abstract

The 3D structure of the nitrogen molecule was created in Jmol interface and saved as .mol file. The .mol file was given as the input file to the Gaussian computational engine in the WebMo interface. Using the 3D structure of the nitrogen molecule generated in the Jmol interface the 3D view of molecular orbitals were generated in the Gaussian computational engine. The energies and geometry of the generated 3D molecular orbitals of nitrogen molecule in Gaussian computational engine was compared with the theoretical molecular orbital diagram.

Keyword

Molecular orbital diagram, Jmol, Gaussian, WebMo, 3D molecular orbital