

Analysis of the double, quadruple and sextuple chemical bonding of diatomic molecules of 2nd row transition metals

Alexandros Androutsopoulos,¹ Theodoros Depastas,¹ Ioannis Karapetsas,¹

Demeter Tzeli^{1,2*}

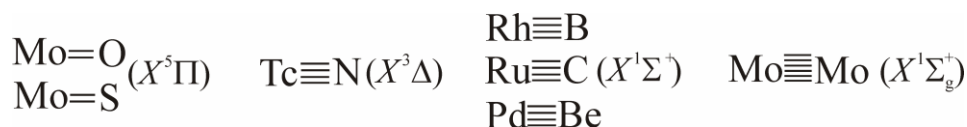
¹Laboratory of Physical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Zografou GR-15784, Greece

²Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens 116 35, Greece

e-mail: alexandrosandroutsopoulos@hotmail.com

The chemical bond is one of the most fundamental concepts in chemistry.[1] Multiple bonds between atoms is one of the aspects of Chemistry that catches the imagination and attracts great interest among chemists. The multiplicity of a chemical bond is determined by the number of electron pairs that occupy the region between the two bonded atoms in bonding molecular orbitals. Nowadays, the maximum bond multiplicity is considered to be six and it has been proposed theoretically for the homonuclear diatomic molecules of transition metals, specifically, Cr₂, Mo₂ and W₂. [2] Quadruple bonds are very rare for the main group elements and they are the bond of highest multiplicity that can form the main group elements.[3]

Here, we present spectroscopic data on the low-lying states of seven diatomic molecules including 2nd row transition metals, i.e., MoO, MoS, Mo₂, TcN, RuC, RhB, and PdBe via high-level multi reference configuration interaction methodology employing the aug-cc-pVnZ(-PP) basis sets, where $n = Q$ and 5. These molecules present a variety of chemical bonding in their ground states, namely, double bonds (MoO, MoS), quadruple bonds (TcN, RuC, RhB, and PdBe) and sextuple bond (Mo₂). We analyzed their bonding in terms of their atomic states. Moreover, we study how the gradual transition from Mo to Pd in the isoelectronic molecules (MoO, TcN, RuC, RhB, PdBe), and from O to S in (MoO, MoS) influence all calculated data, such as bond dissociation energies, bond lengths, dipole moments and frequencies. Finally, we study how the increase of bonding multiplicity affects their spectroscopic data.



References:

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