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Electronic Structure and Properties of Transition Metal–Benzene Complexes [*J. Am. Chem. Soc.* 2001, 123, 3799–3808]. RAVINDRA PANDEY, BIJAN K. RAO,* PURUSOTTAM JENA, AND MIGUEL ALVAREZ BLANCO

We have found an inconsistency in our recent paper in the definition of the electron affinity of the metal atom, metal–benzene, and metal–(benzene)₂ complexes in Figure 8. A modified Figure 8 is presented here. The definition of the electron affinity to be used is given by $E.A. = E(\text{anion}) - E(\text{neutral})$. With this definition, a negative electron affinity means that the anion is stable. Consequently, the variations of the electron affinities of the metal–benzene complexes and the metal–(benzene)₂ complexes across the 3d series (Sc–Ni) are similar in nature and both Ni–benzene and Ni–(benzene)₂ anions are unstable against autodetachment of the electron. The calculated electron affinity of V–(benzene)₂ is +0.29 eV. The experimental study suggests that the V–(benzene)₂ anion may be unstable in the gas phase.

The remaining discussions in section III.F remain unchanged.

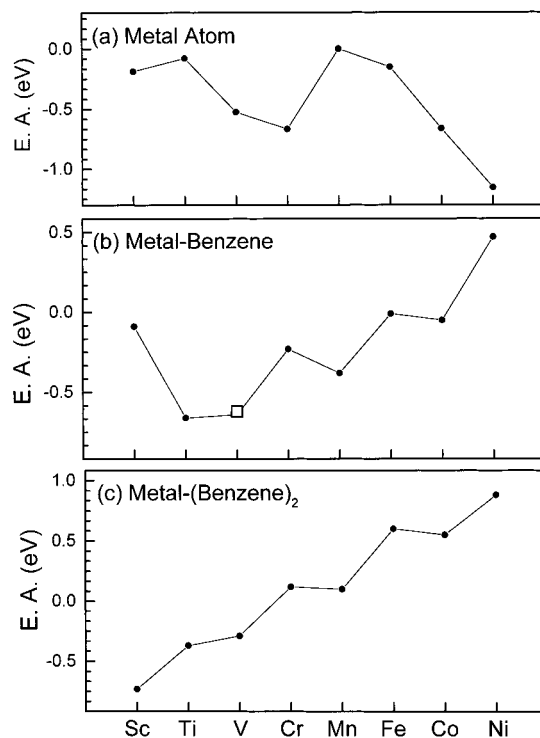


Figure 8.

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