

Title: Fluxional Behavior in Transition Metal Half-Sandwich Complexes of the Phenalenyl Radical

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Abstract: The phenalenyl radical ($P = C_{13}H_9$) is a relatively stable organic radical. It consists of three fused six membered rings sharing a central carbon. We analyze the thermodynamic and kinetic stability of transition metal complexes with P bonded to a range of early transition metals known to form stable half sandwich complexes with radicals. PMX_n ($M = Sc, Ti$; $X = F, Cl$). The MX_n fragments that we employed were chosen because they are similar to known fragments involved in cyclopentadienyl (Cp) or benzene half sandwich complexes - some of which are of continuing interest for catalytic and other potential applications. We report in this poster the outcomes of a series of investigations in the stability of these phenalenyl complexes and the influence of the radical character of the six-membered rings in P on the bonding in those complexes. The systems are especially interesting for us because they combine the properties of six-membered benzene ring and the radical character of Cp – in relatively simple organometallic species, none of which have been prepared to date. We report computed energy barriers and evidence for a mechanism for hopping of the metal fragment from one ring to the next across the surface of the radical. In general, the hapticity of the metal-phenalenyl coordination is very sensitive to the identity of the metal and the barriers to translation are of the order of $6.0 \text{ kcal.mol}^{-1}$.

