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**Separating Electronic, Steric, and Packing Interactions in Crystallographic Structures By Density Functional Theory.** Michael B. Hall, Charles Edwin Webster, Dept. of Chemistry, Texas A&M Univ., Ross and Spence, College Station, TX 77843 USA.

Density functional theory is capable of yielding reasonably accurate fully optimized geometries on small and moderate sized molecules. By comparing the predicted structures for related molecules with different substituents, one can affect a separation of electronic, steric, and packing effects. Examples will be drawn from comparisons on three systems: (1)  $\text{Ir}(\text{H})_2(\text{CO})(\text{Cl})(\text{EPh}_3)_2$ , where the *trans* isomer is observed for  $\text{E}=\text{P}$ , while the *cis* isomer is observed for  $\text{E}=\text{As}$ , the larger ligand; (2)  $(\eta^5\text{-C}_5\text{Me}_5)\text{OsH}_4(\text{PR}_3)$ , where for  $\text{R}=\text{Ph}$  the system is a dihydrogen dihydride complex with the centrally located H-H bond perpendicular to the  $\text{Cp}^*$  ring and for  $\text{R}=\text{Cy}$  the system is a tetrahydride with the central hydrides now parallel to the  $\text{Cp}^*$  ring; and (3)  $\text{ReH}_7(\text{PR}'_3)_2$ , where for  $\text{R}'=p\text{-tolyl}$  an intermediate length H-H bond is observed, while calculations predict two isomers of nearly equal stability, one with a short H-H and one with a long H-H.