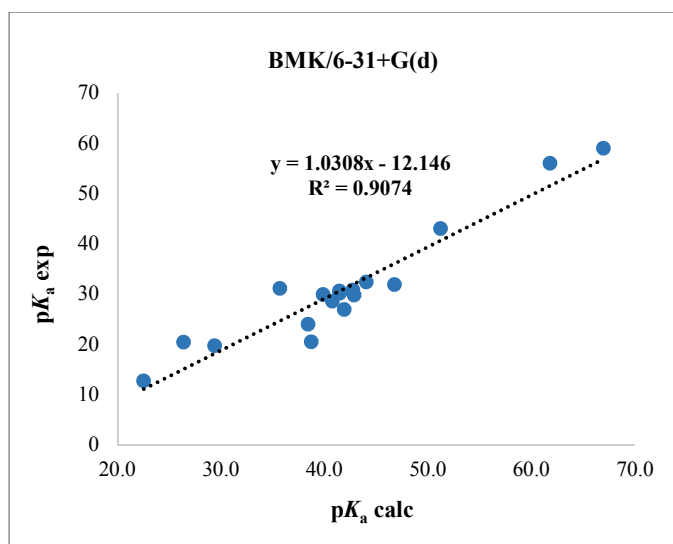
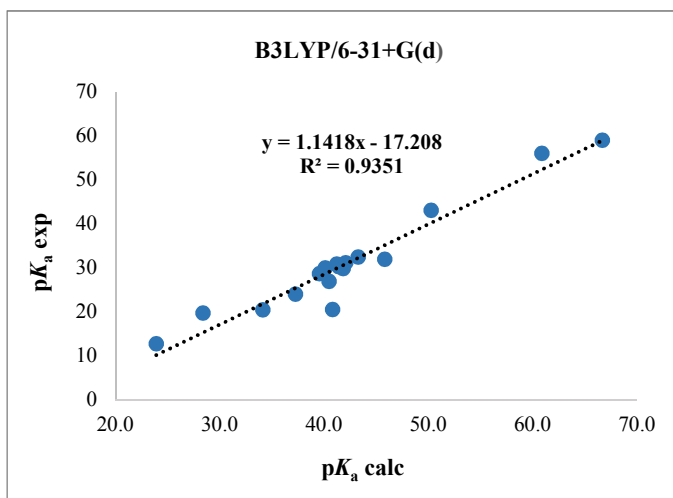
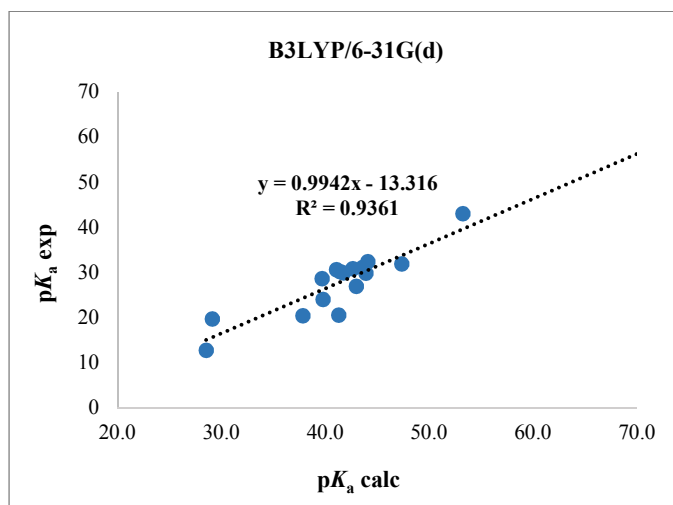


**Supporting Information for**

Control of C-H Bond Activation by Mo-Oxo Complexes:  $pK_a$  or BDFE?

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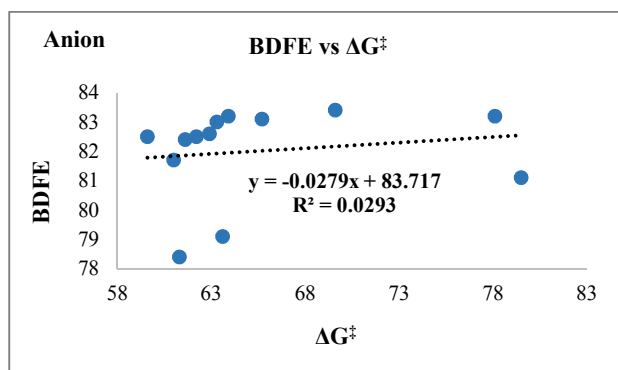
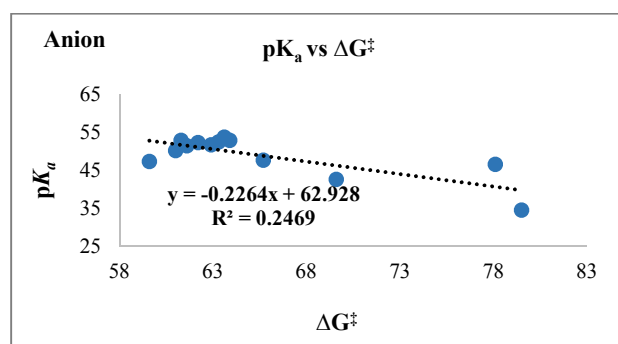
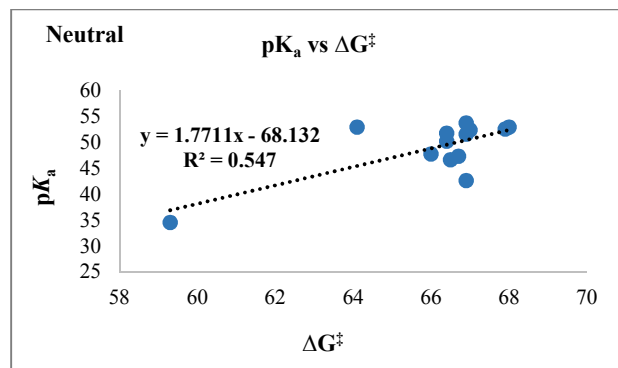
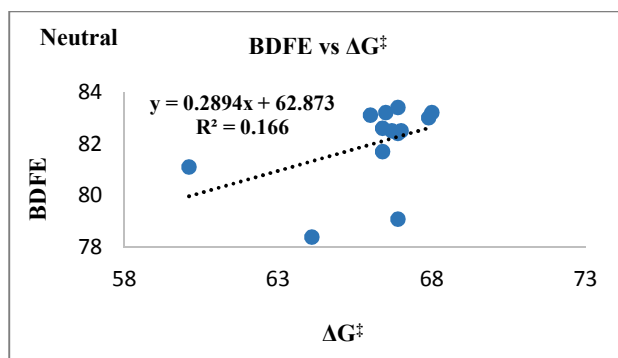
**Figure S-1.** Experimental versus calculated  $pK_a$  values at three levels of theory.

**Table S-1.** Calculated relative free energies of plausible multiplicities for ground state neutral (singlet vs. triplet) an anionic (doublet vs. quartet) dadi-Mo-oxo complexes.

Multiplicity	Charge	G <sub>rel</sub> (kcal/mol)
Double	0	7.3
Quartet	0	0
Singlet	1-	0
Triplet	1-	30.9

**Table S-2.** Calculated relative free energies of plausible multiplicities for ground state of neutral (doublet vs. quartet) an anionic (singlet vs. triplet) dadi-Mo-hydroxy complexes.

Multiplicity	Charge	G <sub>rel</sub> (kcal/mol)
Double	0	0
Quartet	0	4.0
Singlet	1-	0
Triplet	1-	6.8



**Figure S-2.** BDFEs and  $pK_a$  versus calculated activation energy barriers for neutral and anionic MoO(dadi).  $\Delta G^\ddagger$ s and BDFEs are reported in kcal/mol.