

# On The Performance of the RB3-LYP, RMP2 and UCCSD(T) Procedures in Calculating Radical Stabilization Energies for •NHX Radicals

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## SUPPORTING INFORMATION (One Page)

**TABLE S1: Total Energies (Hartrees, Without ZPVEs) for the Ground States (A" or pseudo-A") of •NHX Radicals Calculated at Various Levels of Theory with the 6-31+G(d) Basis Set on UB3-LYP/6-31+G(d) Geometries**

Level	•NH <sub>2</sub>	•NHCF <sub>3</sub>	•NHCHO	•NHCOCH <sub>3</sub>	•NHCONH <sub>2</sub>
UHF	−55.56010	−391.19280	−168.29900	−207.34311	−223.35585
RHF	−55.55576	−391.18826	−168.28303	−207.33242	−223.35019
UB3-LYP	−55.87887	−392.94124	−169.215762	−208.54429	−224.60161
RB3-LYP	−55.87732	−392.93967	−169.21230	−208.54136	−224.59951
UMP2	−55.69658	−391.97390	−168.71486	−207.89827	−223.95632
RMP2	−55.69661	−391.97409	−168.72910	−207.90846	−223.95715
UCCSD(T)	−55.71771	−392.01398	−168.76796	−207.96341	−224.00392
URCCSD(T)	−55.71771	−392.01397	−168.76823	−207.96242	−224.00396