

Supporting information for

Ligand effects in gold-carbonyl complexes: evaluation of the bond dissociation energies using blackbody infrared radiative dissociation

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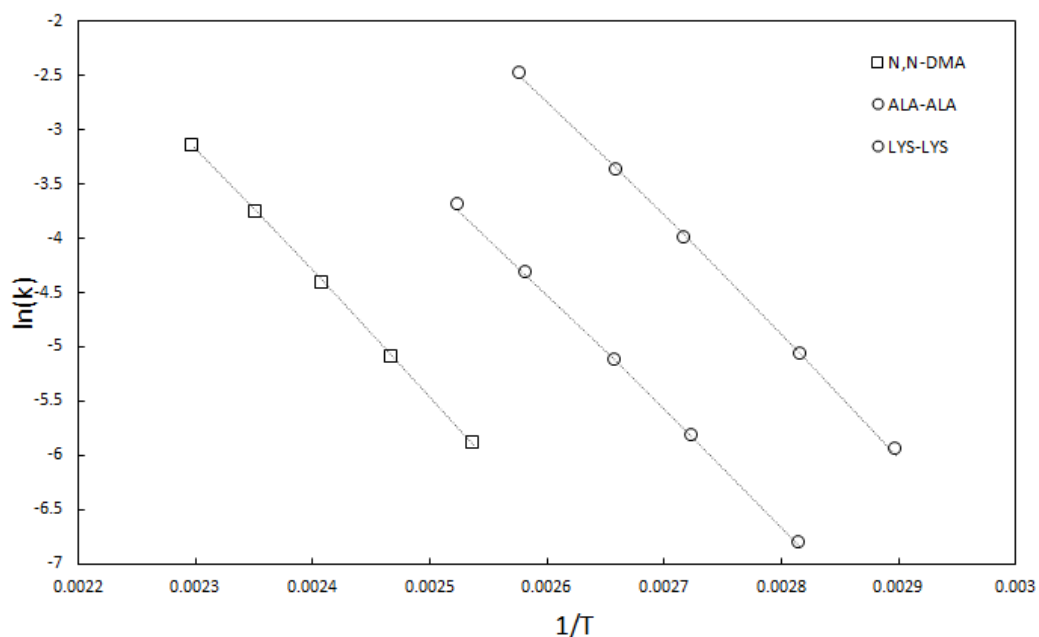


Figure S1. Theoretical Arrhenius plots for the dissociation of the proton-bound dimer of N,N-dimethylacetamide, alanine, and lysine, calculated from data ref 29

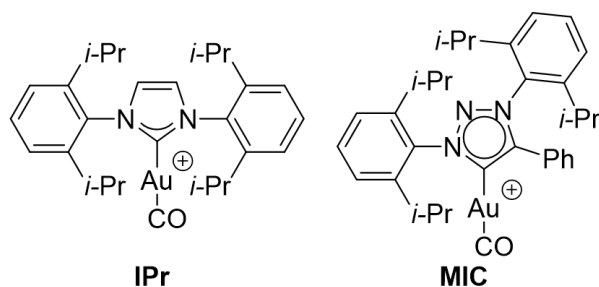
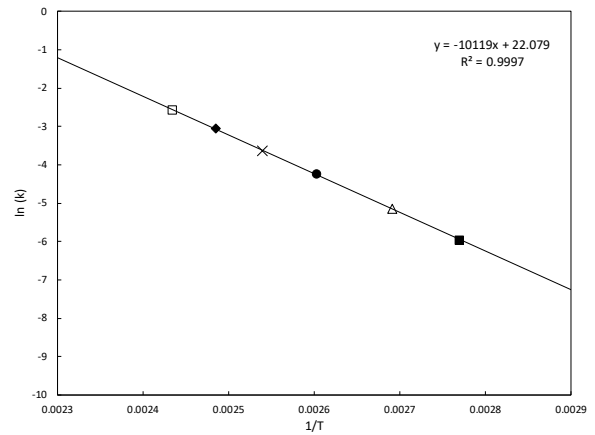
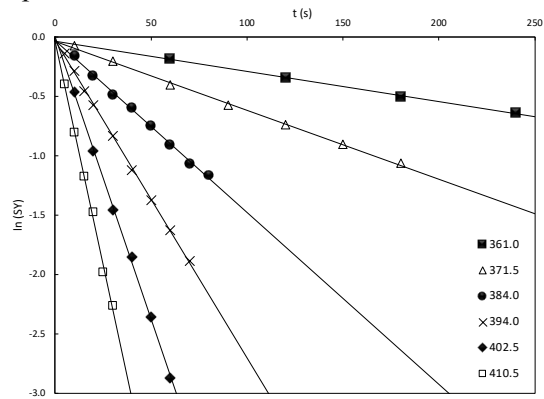
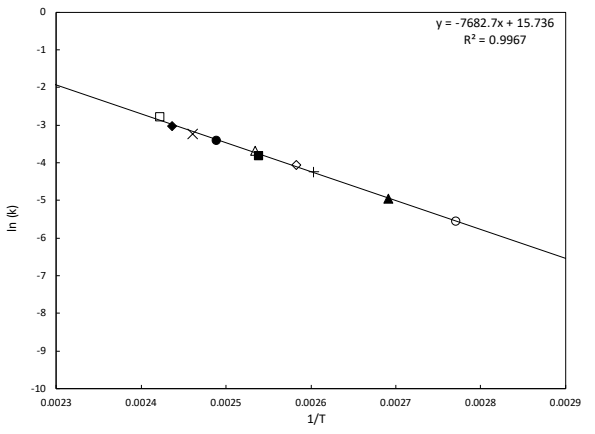
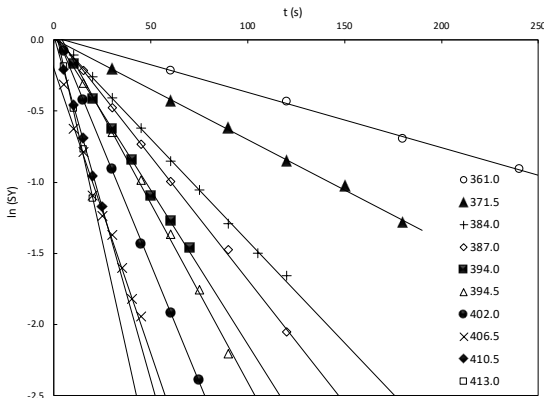


Figure S2. Chemical structure of carbenes IPr and MIC

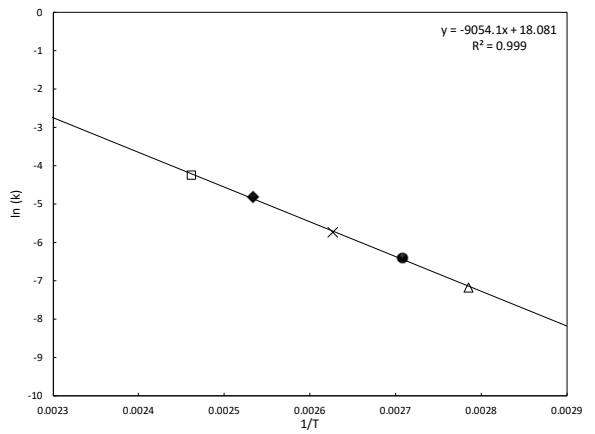
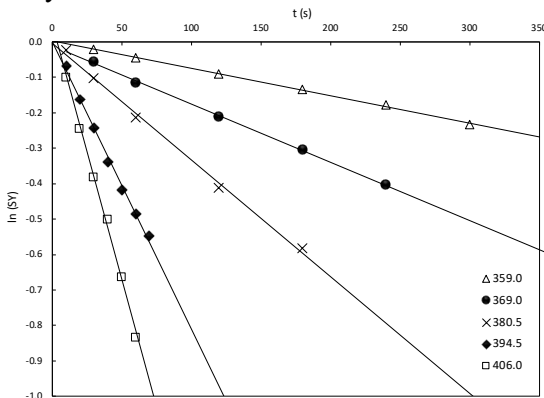
1-pOMe



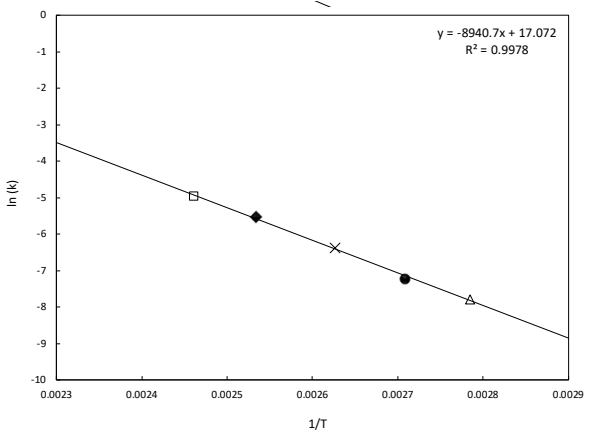
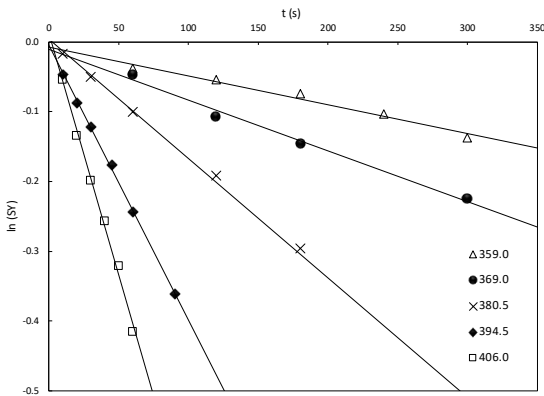
2-biPh



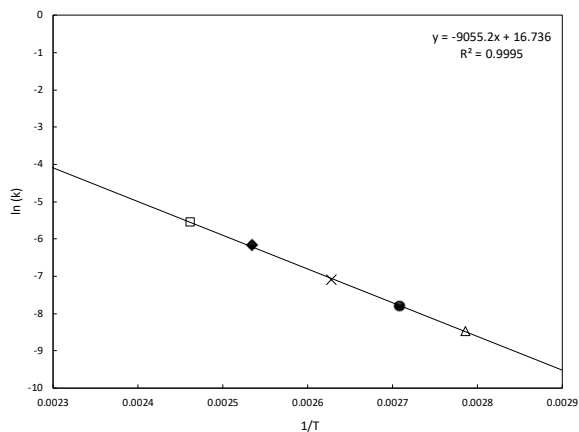
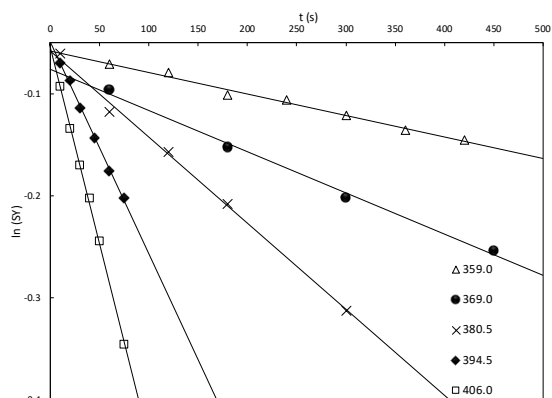
3-Cy



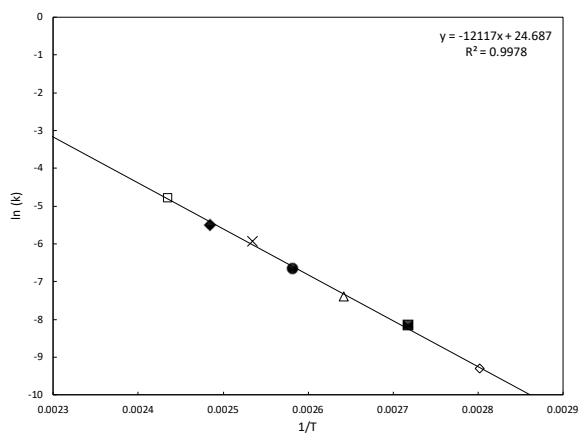
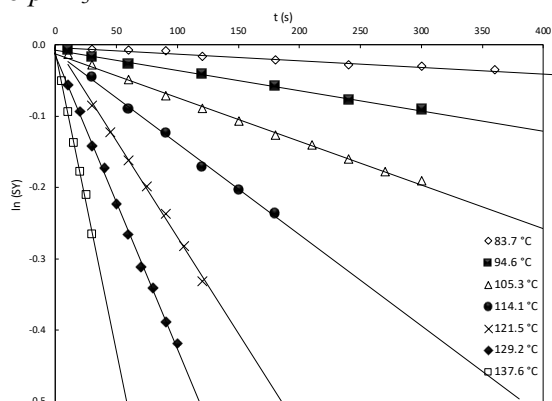
4-tBu



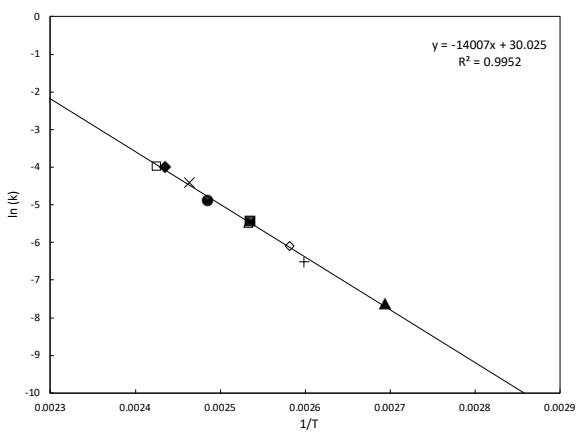
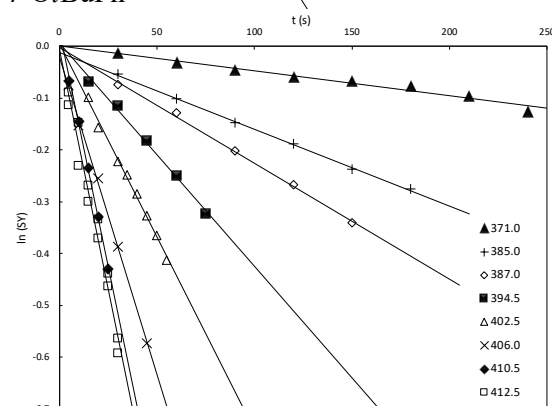
5-Ph



6-pCF₃



7-OtBuPh



8-OPh

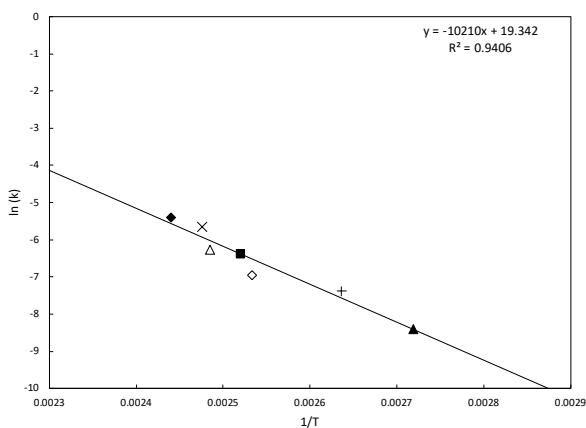
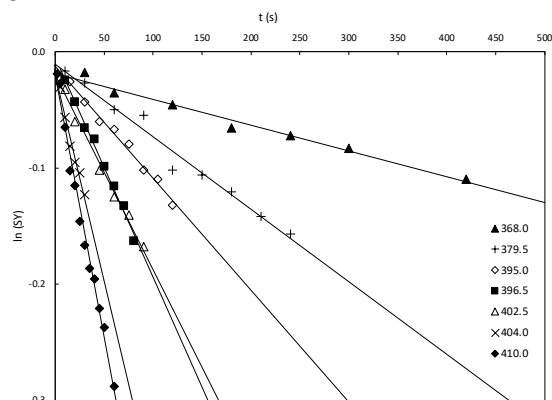


Figure S3. Plots of the natural logarithms of the survival yield of complexes as a function of reaction time for different temperatures and corresponding Arrhenius plots for the dissociation

of the seven $[LAu-CO]^+$ complexes studied. **1**-*p*OMe, **2**-*bi*Ph, **3**-*Cy*, **4**-*t*Bu, **5**-*Ph*, **6**-*p*CF₃, **7**-*O**t*BuPh, **8**-*O*Ph

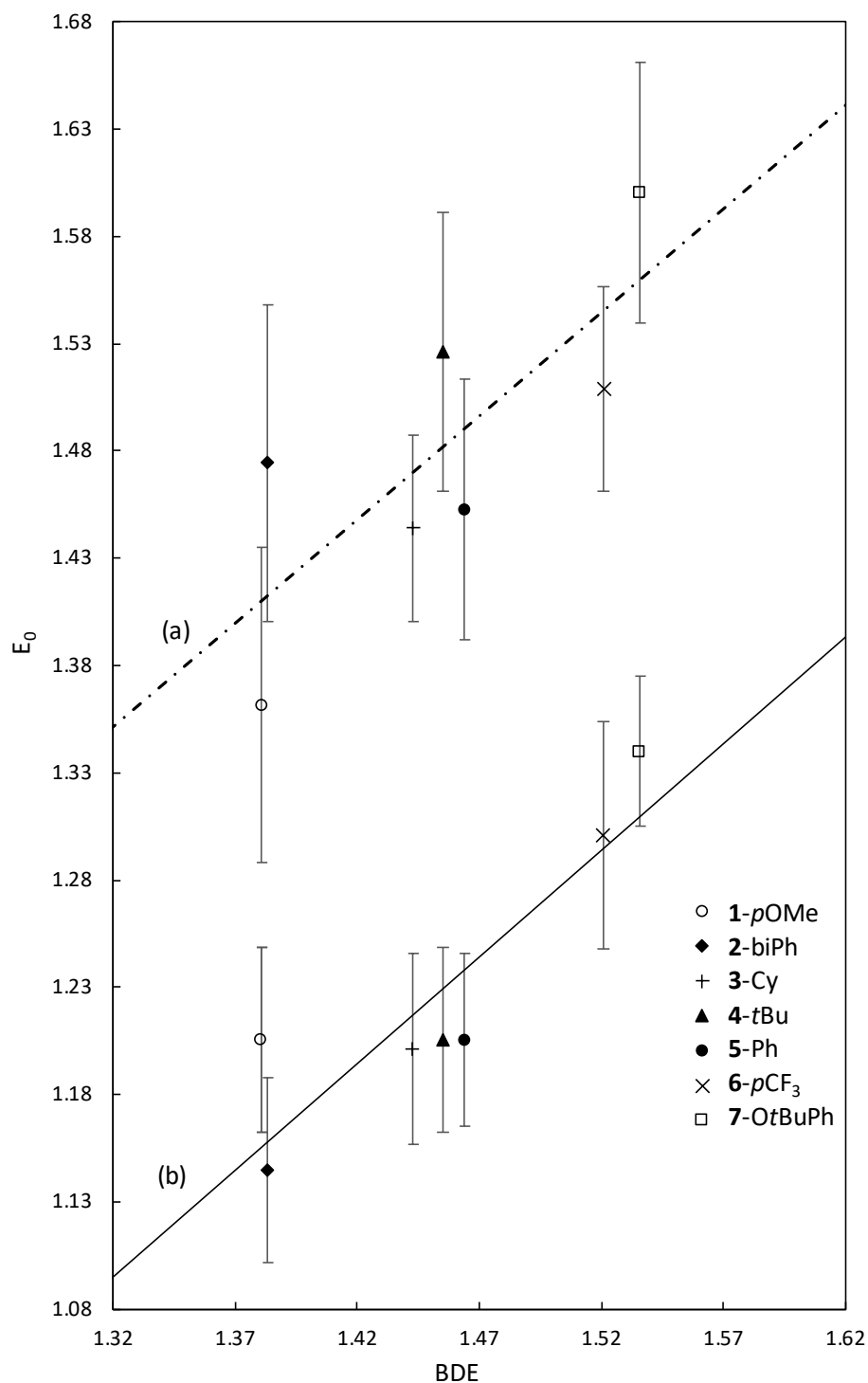


Figure S4. Comparison of calculated BDE (eV) at the PBE0-D3BJ/def2-TZVP level with E_0 a) obtained by CID high pressure (ref. 5), correlation dash dot line, b) and E_0 obtained by RRKM modeling from BIRD experiments, correlation full line

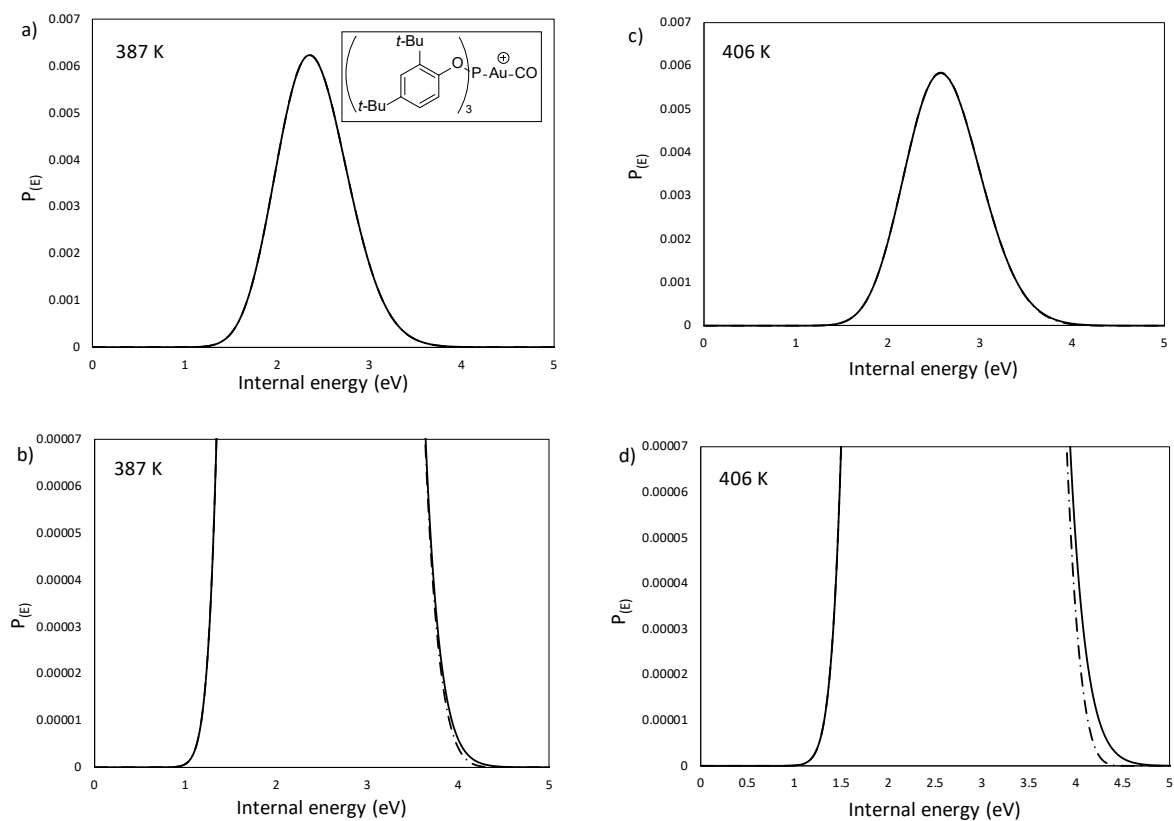
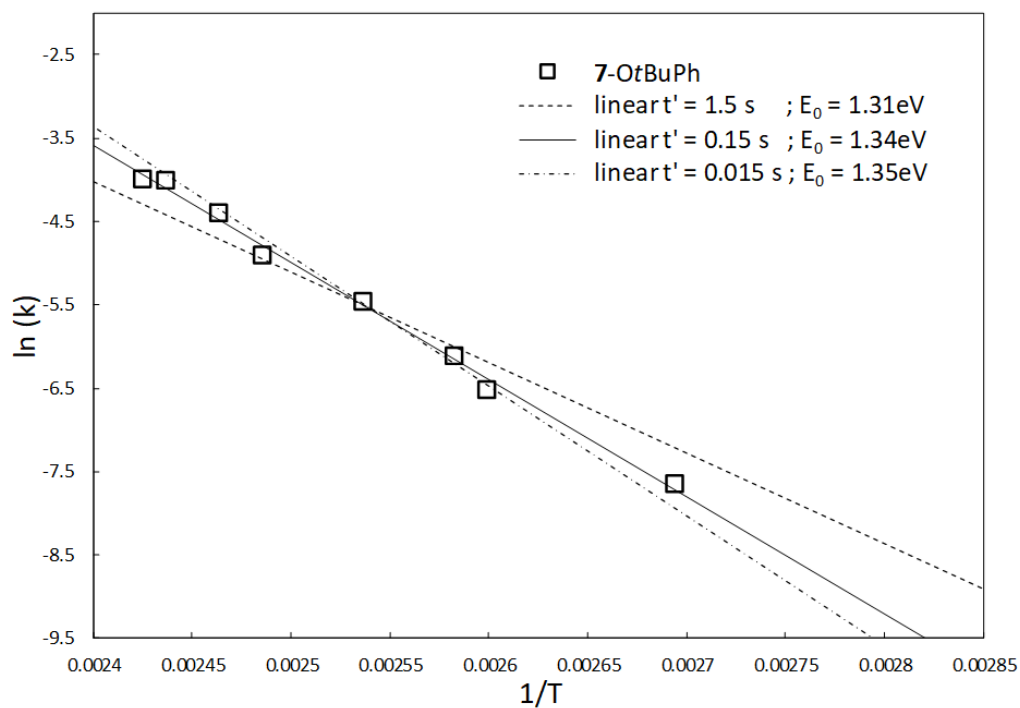


Figure S5. a) Thermal internal energy distribution for complex 7-OtBuPh calculated at $T = 387$ K before depletion (line) and after depletion of $t' = 0.15$ s (dash-dot line), this truncation corresponds to 0,0004% of the initial population b) magnification x100. c) Similar curves for $T = 406$ K, this truncation corresponds to 0.0022% of the initial population d) magnification x100.

a)



b)

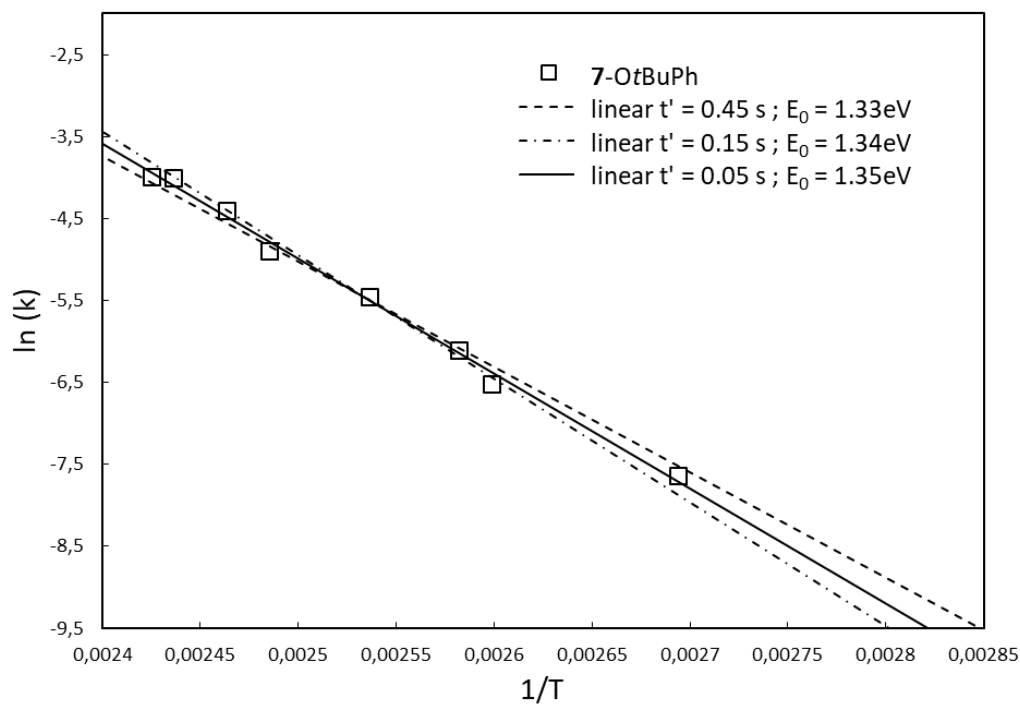


Figure S6. Arrhenius plots for the dissociation of 7-OtBuPh complex. Calculated lines obtained by ETT modeling using $A=10^{15.6} \text{ s}^{-1}$ a) for depletion time t' equal to 0.015 s, 0.15 s and 1.5 s b) for depletion time t' equal to 0.05 s, 0.15 s and 0.45 s, and corresponding critical energy values (E_0)