Supporting Information for

Energetics and Mechanism for the Deamination of Lithiated Cysteine

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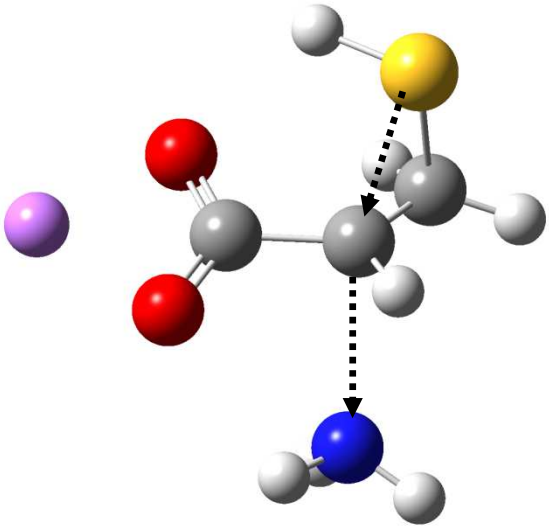
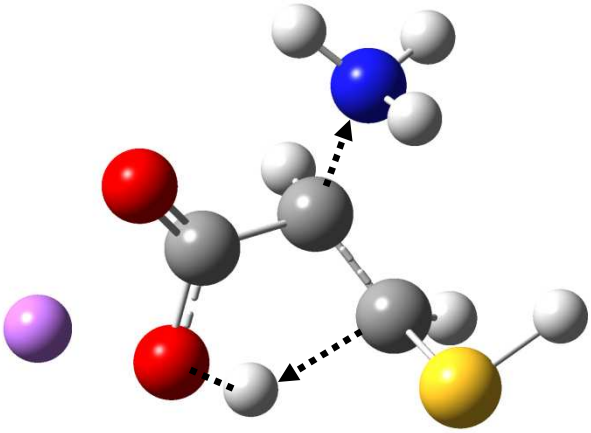
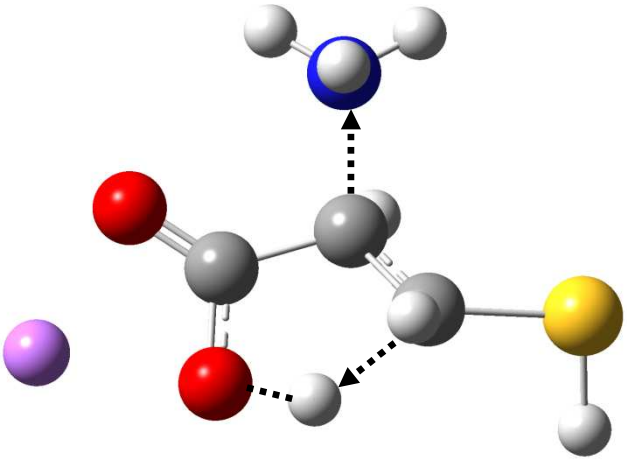
Figure showing the transition states for deamination of Li^+(Cys) discussed in the main text. Species are identified by the transformation discussed in the text along with the energies (in kJ/mol) relative to the Li^+(Cys) [N,CO,S] $tggg_+$ ground state reactants calculated at the B3LYP, B3P86, and MP2(full) levels of theory using the 6-311+G(2d,2p) basis set and geometries and vibrational frequencies calculated at a B3LYP/6-311G(d,p) level of theory. The imaginary frequency (unscaled) in cm^{-1} is also indicated.



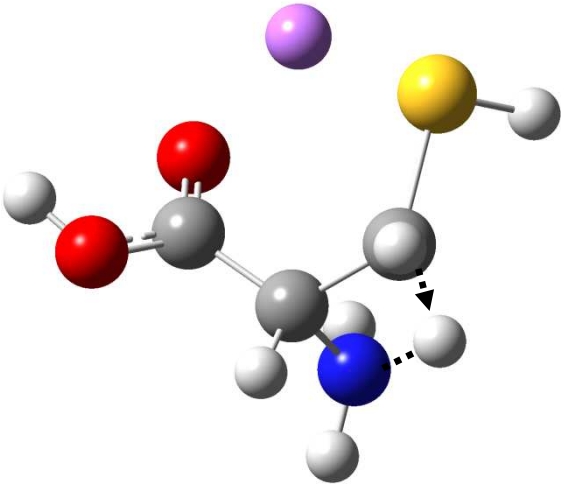
Li^+(Cys) $[CO_2^-]$ ctg_+g_- →
$(NH_3)Li^+$(Tica) $[CO_2^-]$cc
143.0, 151.7, 156.9 kJ/mol
-175 cm^{-1}



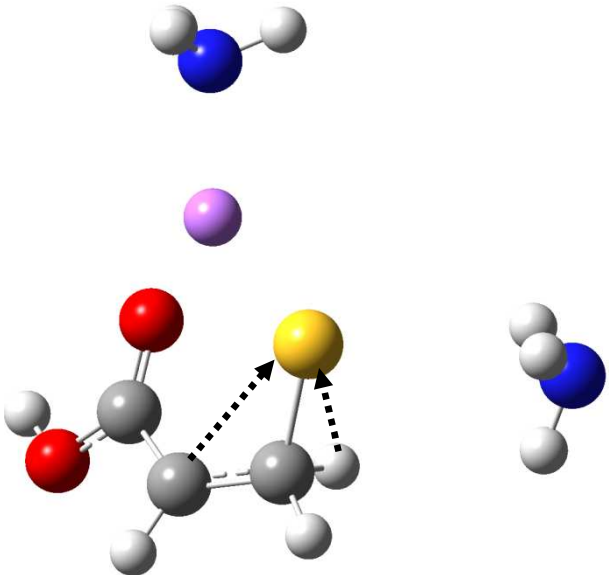
Li^+(Cys) $[CO_2^-]$ ctg_-g_- →
$(NH_3)Li^+$(Tpa) [CO,S] ttct
253.3, 249.7, 265.4
-663 cm^{-1}



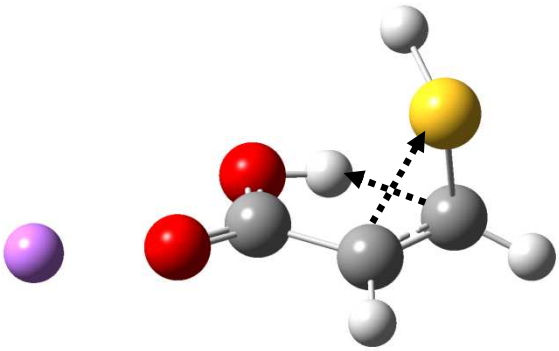
Li^+(Cys) [CO_2^-] cgtg →
$(NH_3)Li^+$(Tpa) [CO]tctc
255.0, 252.8, 273.4 kJ/mol
-1062 cm^{-1}



Li^+(Cys) [CO,S] ttgt →
$(NH_3)Li^+$(Tpa) [CO,S] ttct
281.2, 275.8, 300.6 kJ/mol
-1436 cm^{-1}



$(NH_3)Li^+$(Tica) [CO,S]tg →
$(NH_3)Li^+$(Tpa) [CO,S]ttct
206.1, 235.0, 275.4 kJ/mol
-783 cm^{-1}



$(NH_3)Li^+$(Tica) [CO_2^-] cc →
$(NH_3)Li^+$(Tpa) [CO] ccct
237.8, 250.8, 271.2 kJ/mol
-578 cm^{-1}