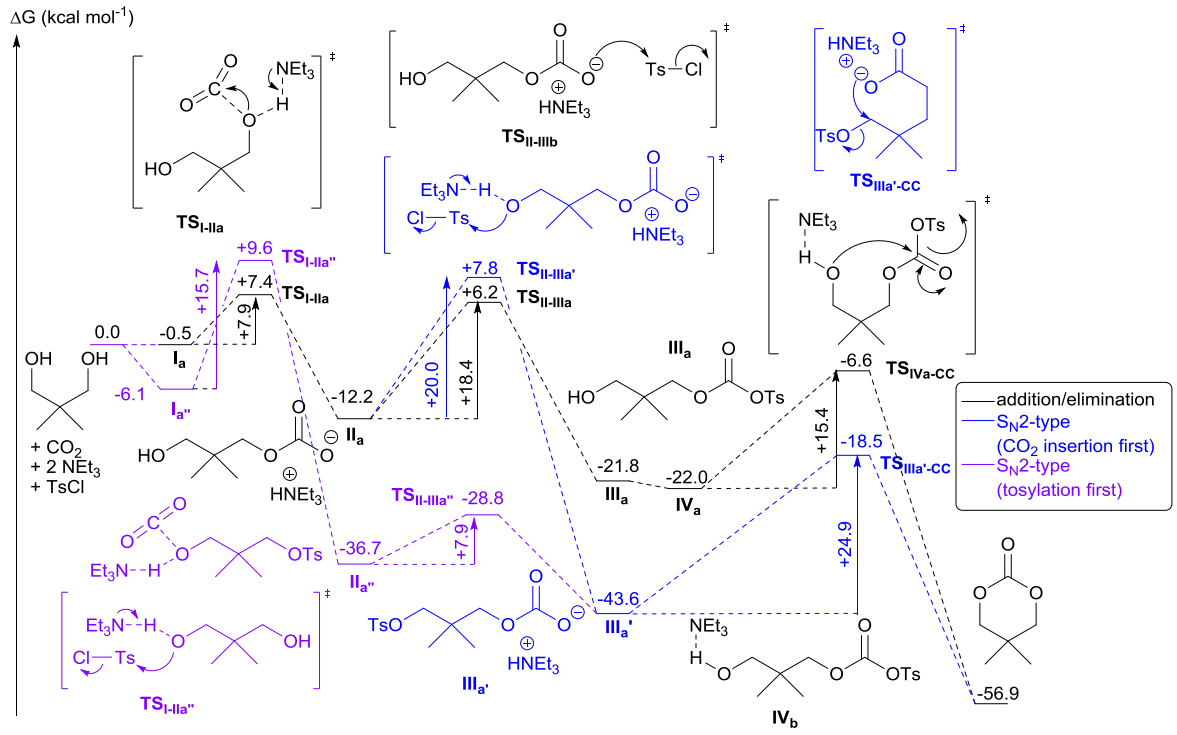

Fig. 1 DFT computed free enthalpy diagram for the cyclocarbonation of 2,2-dimethyl-1,3-propanediol with CO_2 using 2 equiv. of NEt_3 and 1 equiv. of TsCl. Protocol: rωb97xD/6-31+g(d)/cpcm=acetonitrile/298K. Geometries, energies and vibrational data are available for all structures from output files in digital repository DOI: 10.6084/m9.figshare.5831538.