



**Fig. 9** Catalytic cycle involving one amine (data<sup>29</sup> sub-collection DOI: [10.14469/hpc/1854](https://doi.org/10.14469/hpc/1854)). The total computed free energy for each stationary point is shown in Hartree, with the relative energies shown in parentheses in kcal mol<sup>-1</sup>. The DOI for data repository entries for individual species are shown in the form e.g. [10.14469/hpc/1885](https://doi.org/10.14469/hpc/1885). Energies in blue are for the pre-assembly stage, in black for the cycle proper and in red for the regeneration step to initiate a new cycle. All DOIs in this figure are available as clickable links (final paginated PDF only).