

Heavy-Atom Tunnelling in Benzene Isomers: How Many Tricyclic Species are Truly Stable?

Supplementary Information

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Electronic Supplementary Information (ESI) available on the ioChem-BD platform for computational chemistry and materials science teams, at the following link: <https://iochem-bd.bsc.es/browse/handle/100/323394>

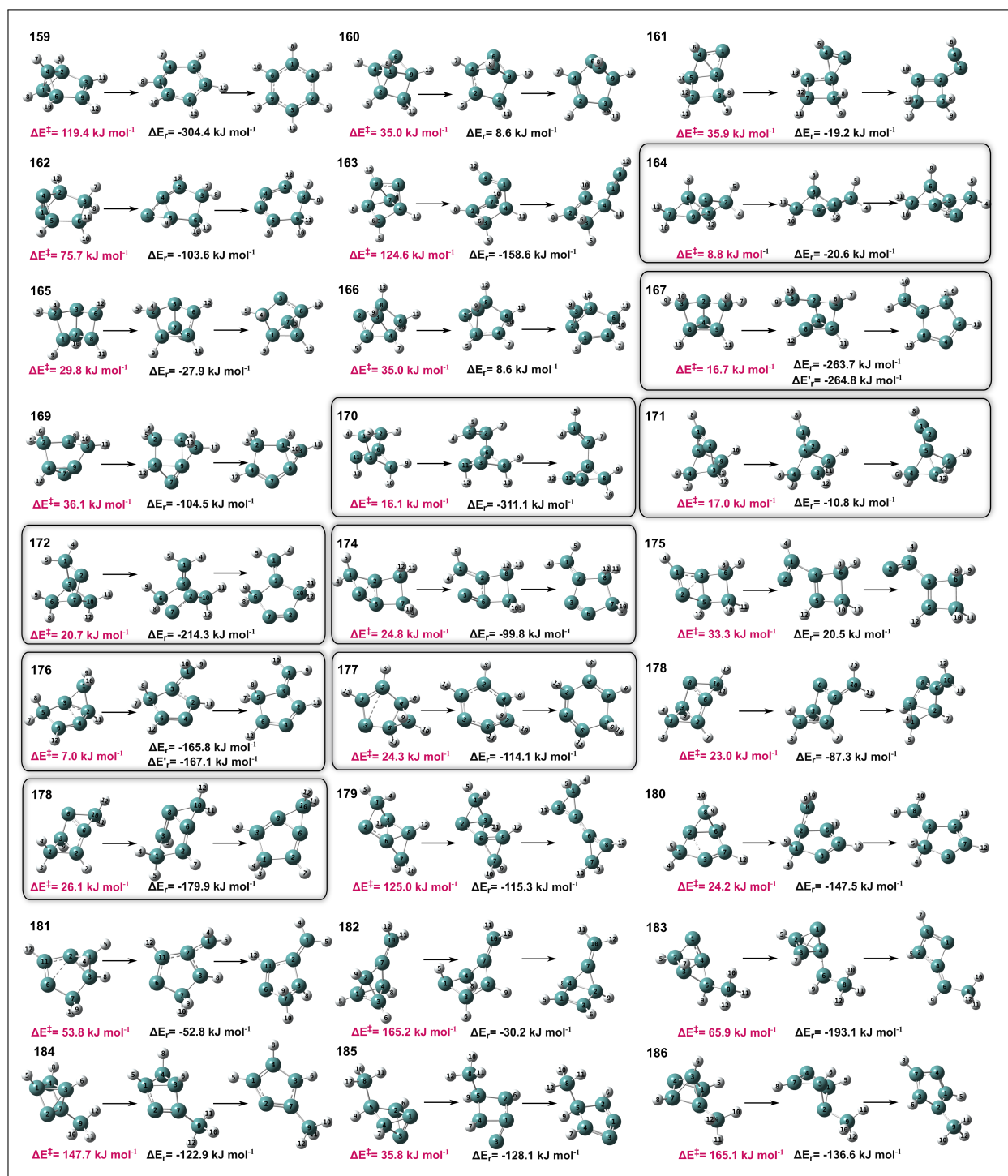


Fig. S1. Optimized geometries of all the 73 tricyclic isomers, including their lowest degradation threshold ($\Delta E^\ddagger$) and reaction energies (ΔE_r) in kJ mol^{-1} , including ZPE (isomer 178 has two decomposition pathways). The QT unstable isomers are highlighted in solid line boxes, and enclosed in dotted lines are the thermodynamically unstable ones. "OSS" indicates open-shell singlet species.

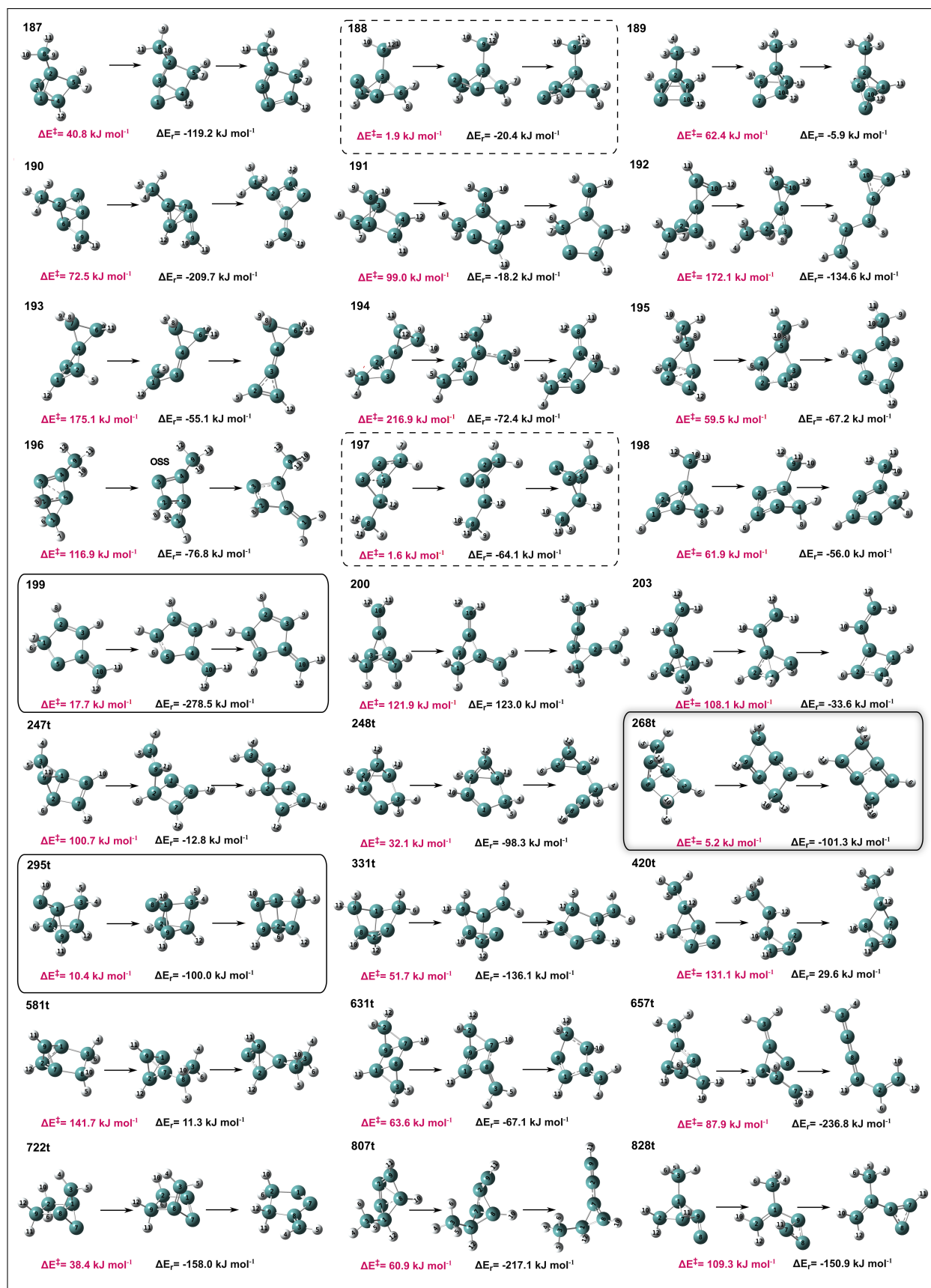


Fig. S1. Continued

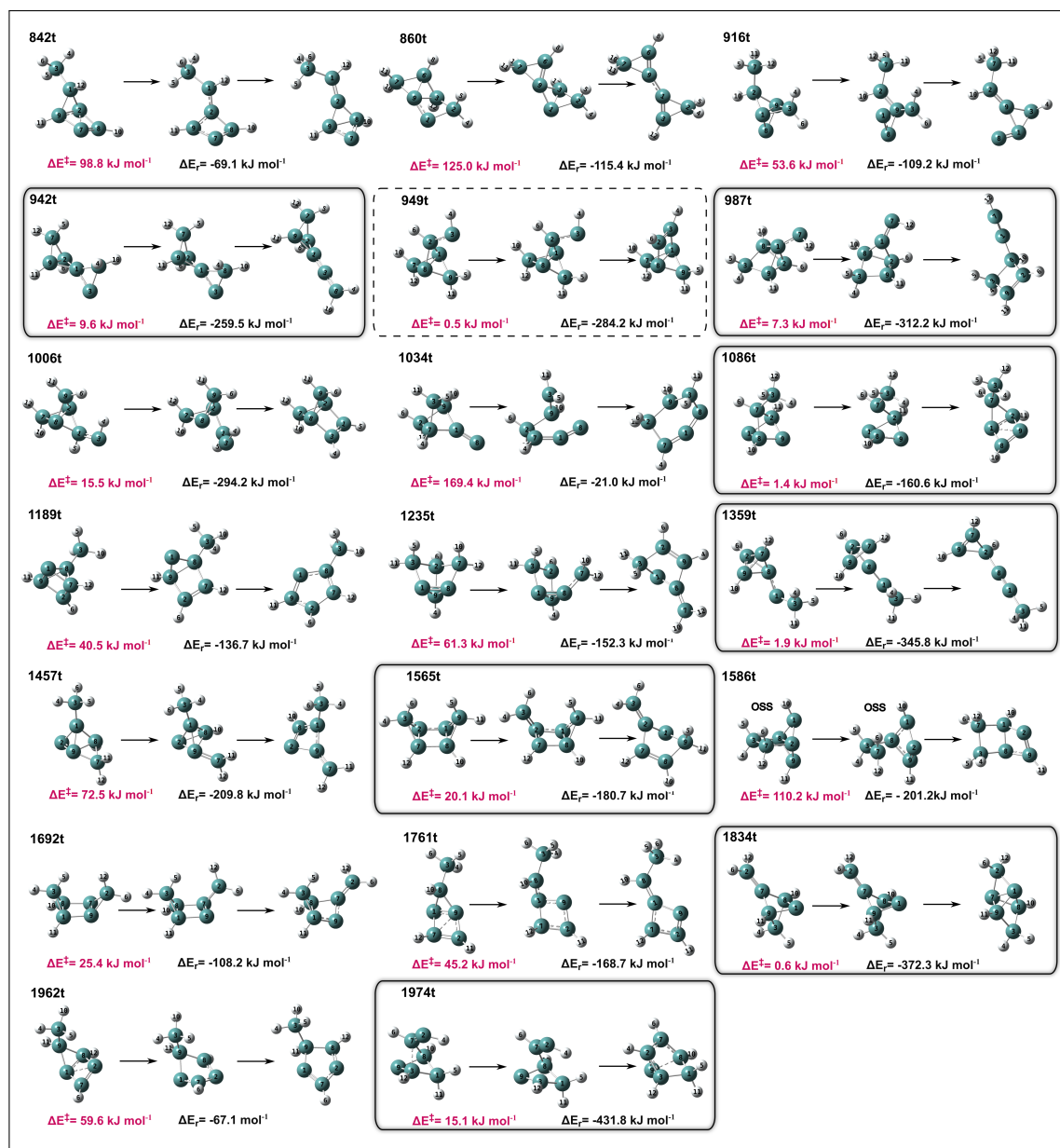


Fig. S1. Continued