Supporting Information

A Careful Consideration of the Influence of Structure, Partial charges and Basis Sets on Collision Cross Sections of Monosaccharides when Comparing Values from DFT calculations to those Obtained Experimentally

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Data availability

The interactive IPython (Jupyter) notebooks containing experimental and computational results from this study are available to view on GitHub at https://github.com/BarranLab/ChargePaper_2017. In particular, Figures S2-S6 are included to make viewing of the dataset easier and more comprehensive.

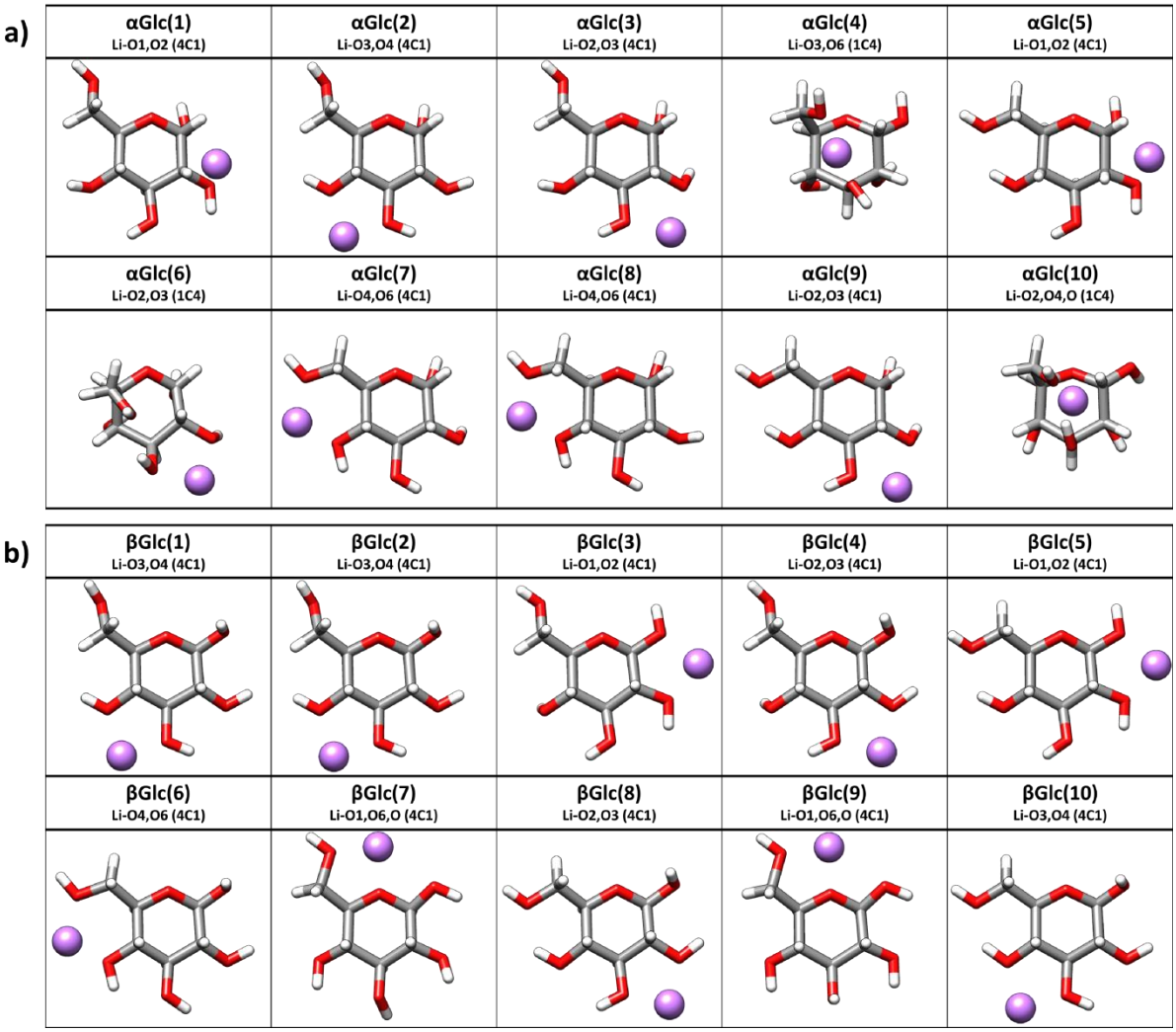

Figure S1. Model structures of a) α-Glc; b) β-Glc with cationic lithium adduct atom (pink) in various positions. Conformers α-Glc(1-10) were assessed in both $^{1}C_{4}$ and $^{4}C_{1}$ conformations, whilst β-Glc(1-10) in the $^{4}C_{1}$. The position of the Li adduct are shown under the titles.

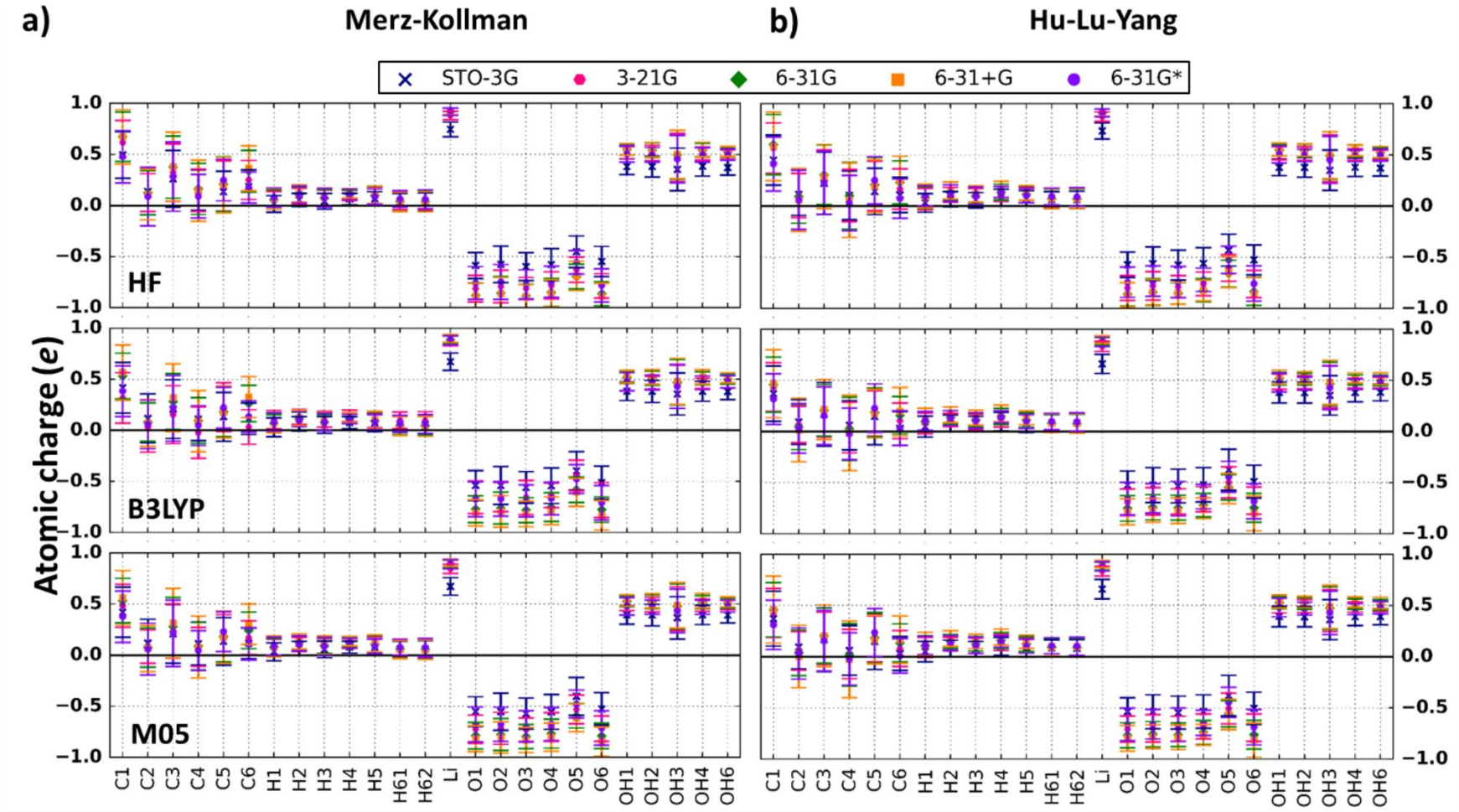

Figure S2. Average partial atomic charges from all conformers of α-/β-Glc ions determined using HF, B3LYP and M05 functionals with several basis sets: STO-3G (blue), 3-21G (magenta), 6-31G (green), 6-31+G (orange) and 6-31G* (purple). a) Partial charges from Merz-Kollman charge scheme; b) Partial charges from Hu-Lu-Yang. Average charges were computed from 20 conformers whereas the standard errors were evaluated by determining the maximum spread of charges on each atom centre due to the conformational differences.

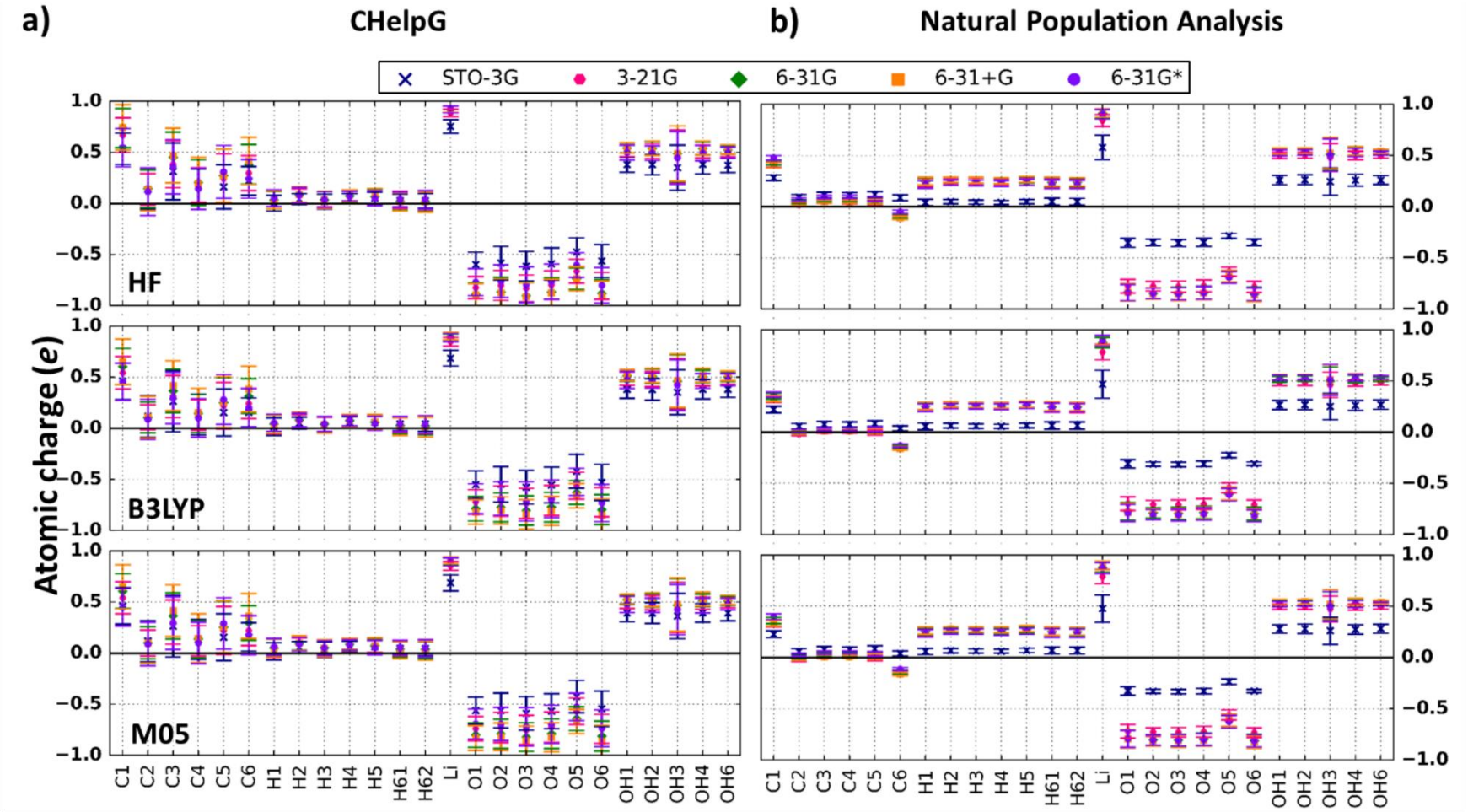

Figure S3. Average partial atomic charges from all conformers of α-/β-Glc ions determined using HF, B3LYP and M05 functionals with several basis sets: STO-3G (blue), 3-21G (magenta), 6-31G (green), 6-31+G (orange) and 6-31G* (purple). a) Partial charges from CHelpG charge scheme; b) Partial charges from Natural Population Analysis. Average charges were computed from 20 conformers whereas the standard errors were evaluated by determining the maximum spread of charges on each atom centre due to the conformational differences

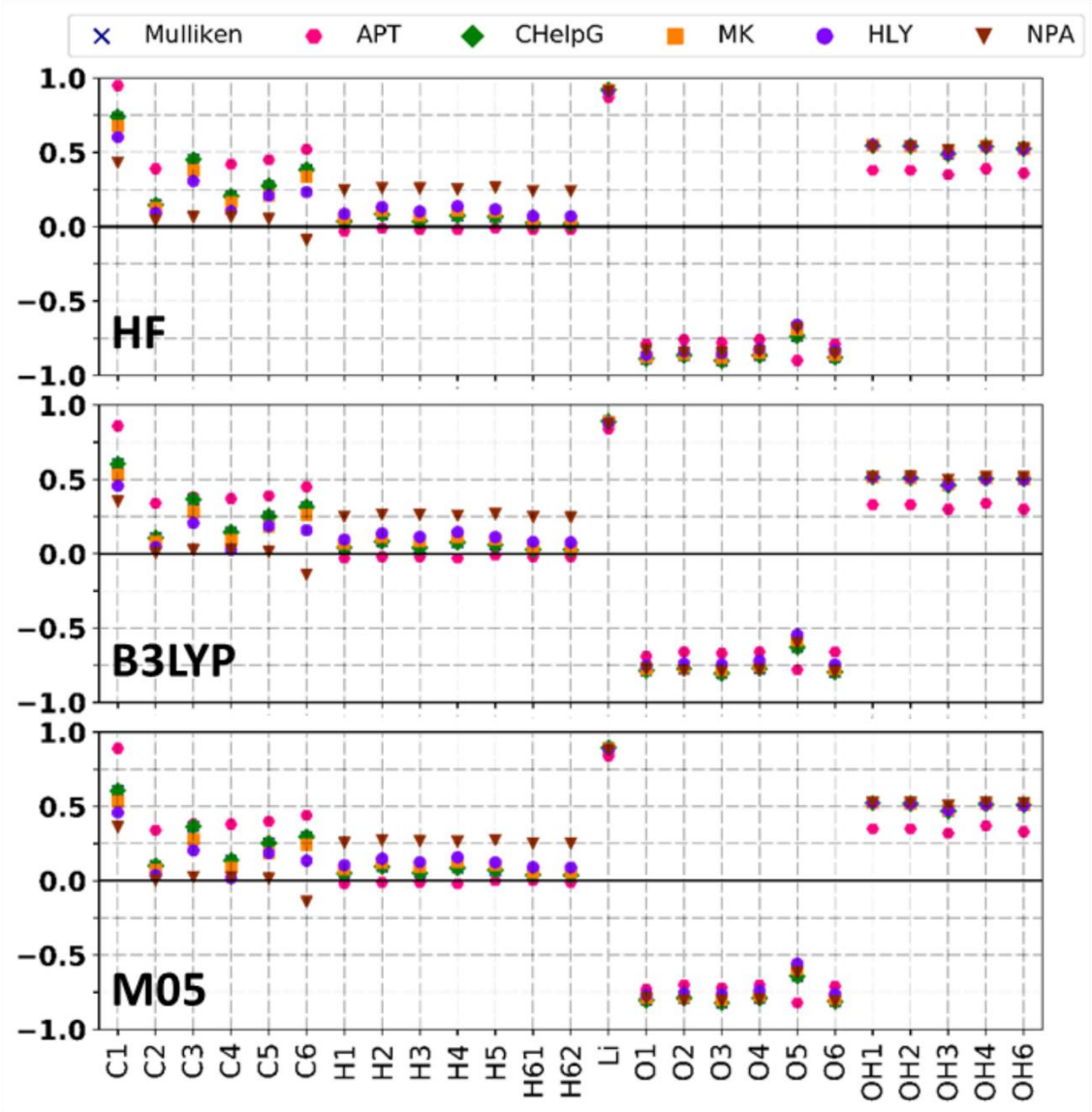

Figure S4. Average partial charges from all charge schemes calculated for each functional (top: HF, middle: B3LYP and bottom: M05) using the 6-31G basis set. Charge schemes shown: Mulliken (blue), APT (magenta), CHelpG (green), MK (orange), HLY (purple) and NPA (brown).

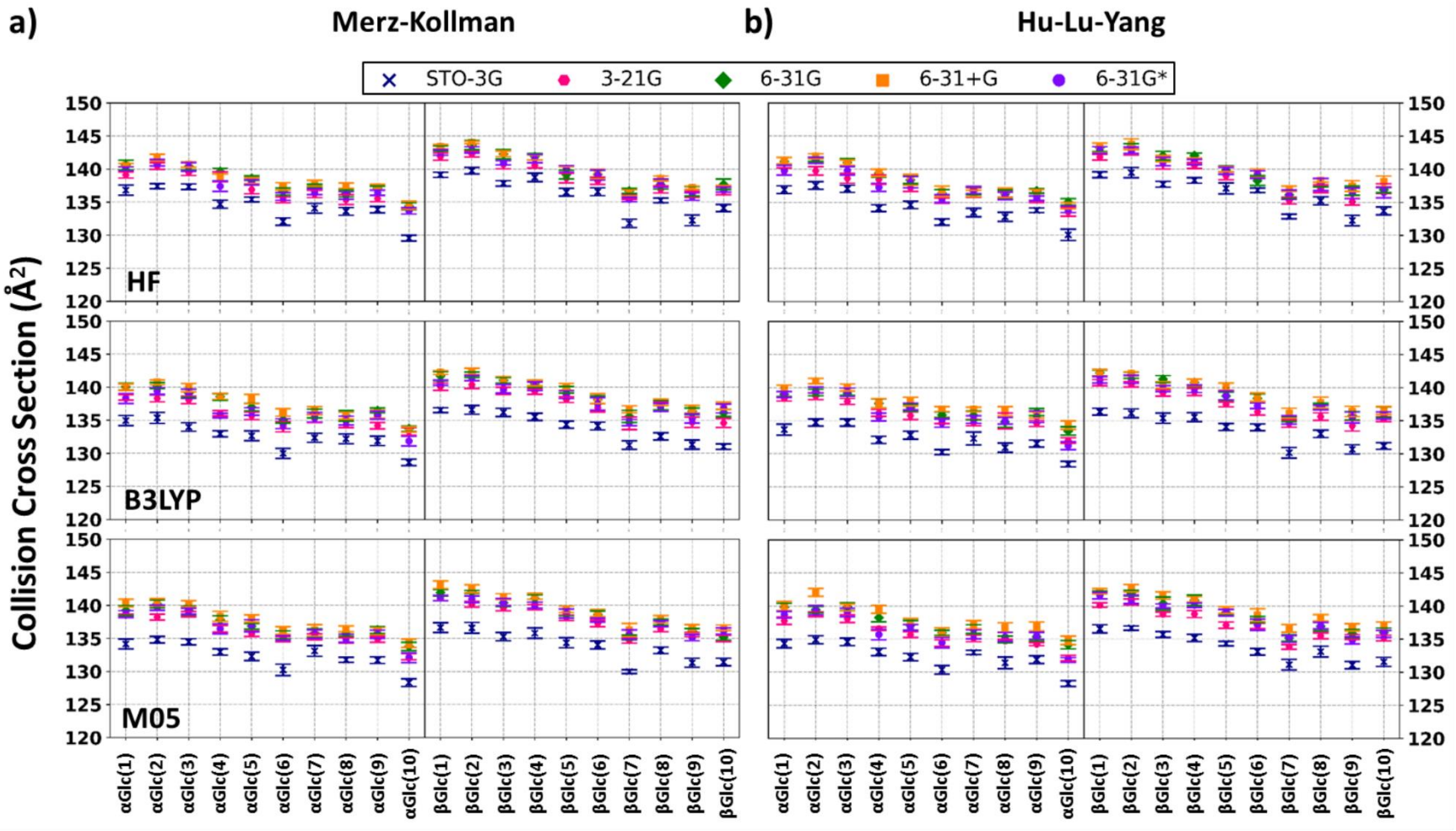

Figure S5. Rotationally averaged collision cross sections calculated using the Trajectory Method with partial charges calculated using either HF, B3LYP or M05 hybrid functional with several basis sets, namely: STO-3G (blue), 3-21G (magenta), 6-31G (green), 6-31+G (orange) and 6-31G* (purple) for a) Merz-Kollman, and b) Hu-Lu-Yang charge schemes. Error bars on each data point represent the standard deviation from Trajectory Method calculation, typically less than 0.5 %, and always less than 1.2 %.

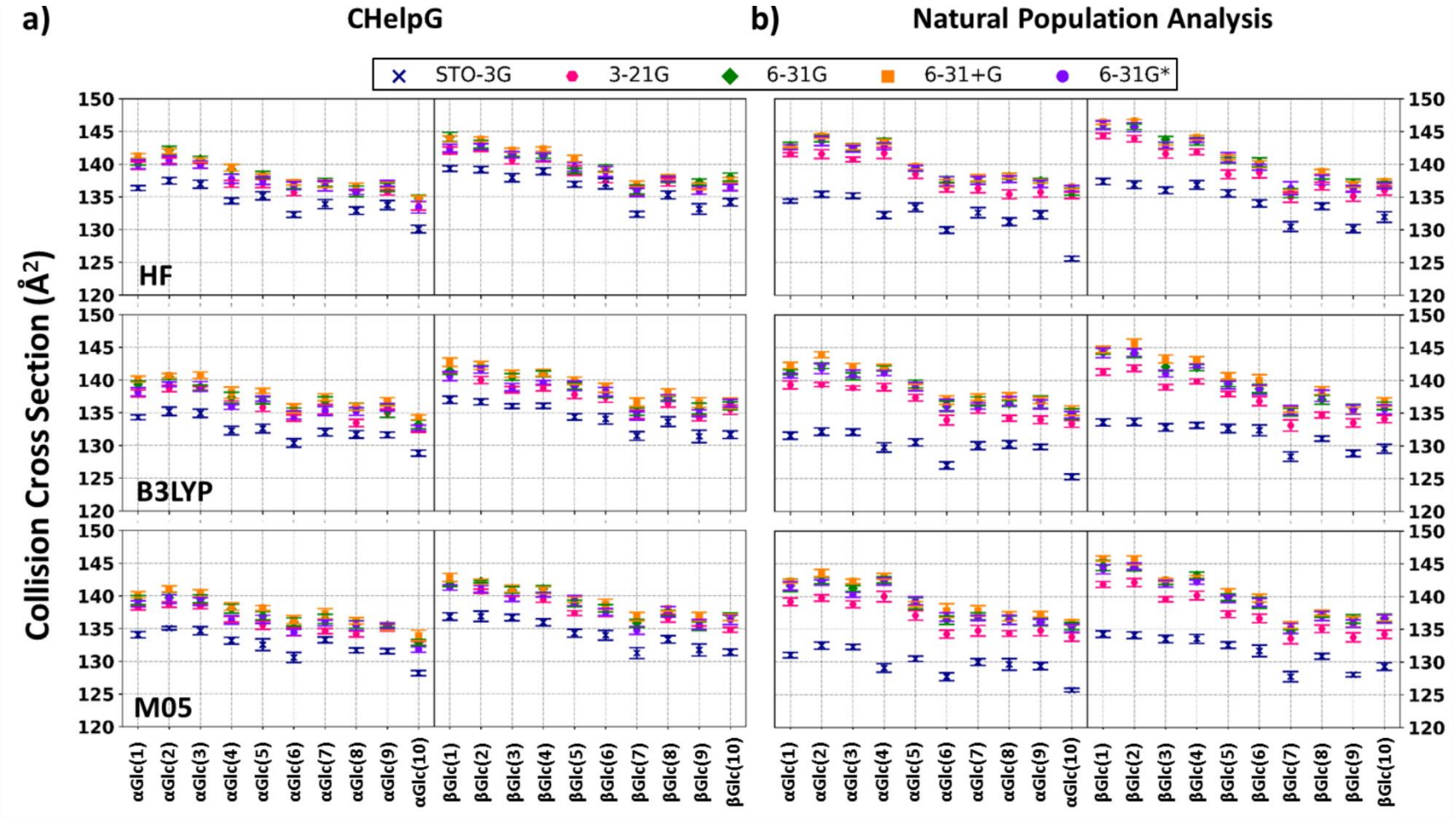

Figure S6. Rotationally averaged collision cross sections calculated using the Trajectory Method with partial charges calculated using either HF, B3LYP or M05 hybrid functional with several basis sets, namely: STO-3G (blue), 3-21G (magenta), 6-31G (green), 6-31+G (orange) and 6-31G* (purple) for a) CHelpG, and b) NPA charge schemes. Error bars on each data point represent the standard deviation from Trajectory Method calculation, typically less than 0.5 %, and always less than 1.2 %.