Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic supplementary information

The Non-Covalent Nature of the Molecular Structure of the Benzene Molecule

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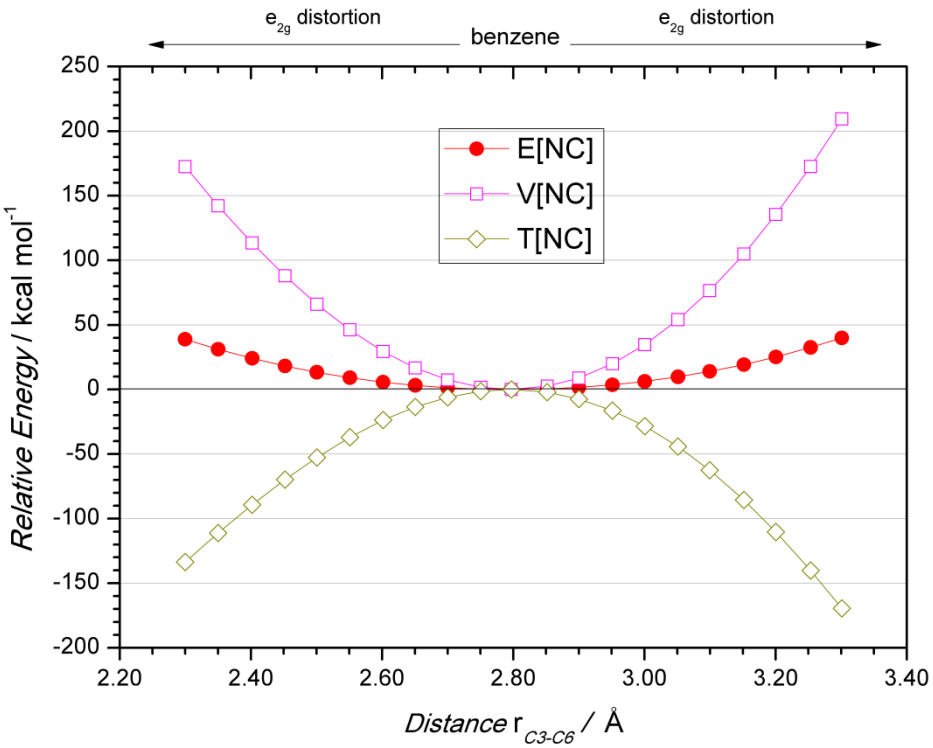

Fig. S1 Non-covalent energy partition into kinetic, T[NC], and potential, V[NC] contributions for the molecule along the e_{2g} vibration mode.

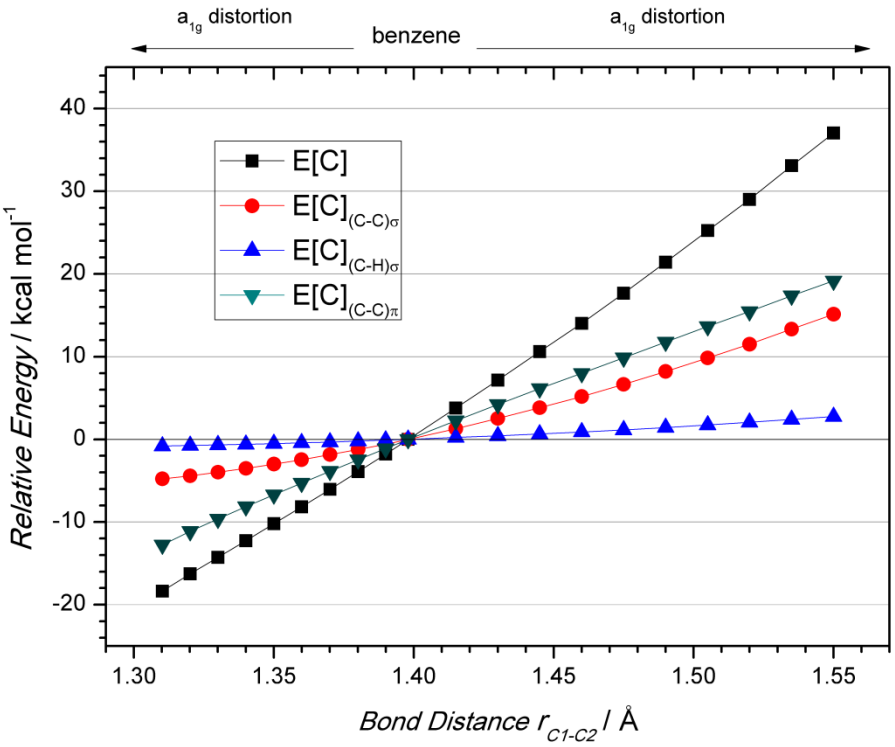

Fig. S2 Covalent energy partition into C-H, (C-C)σ and (C-C)π contributions for the molecule along the a_{1g} vibration mode.

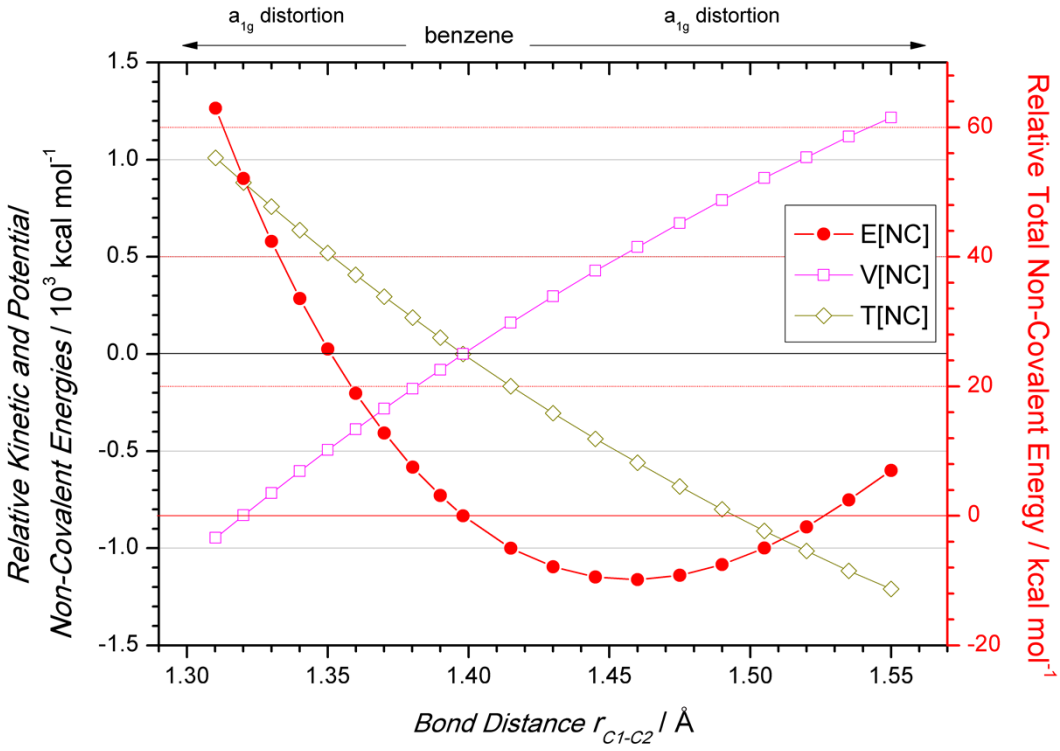

Fig. S3 Non-covalent energy partition into kinetic, T[NC], and potential, V[NC] contributions for the molecule along the a_{1g} vibration mode.