

Interacting Quantum Atoms Analysis of Covalent and Collective Interactions in Single Elongated Carbon–Carbon Bonds

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XYZ files

In this link

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the interested reader can download the XYZ files and AIMAll outputs (in sumviz format) corresponding to the molecules addressed in this investigation as well as the Python scripts used to compute the LHS of equations (15) and (16), i.e., the approximations to $E_{\text{cl}}^{\text{AB}}$ and $E_{\text{xc}}^{\text{AB}}$ respectively, along with the dispersion contributions to the IQA interaction energies.

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Benchmark of exchange-correlation functionals

Table S1: Computed changes in energy for the process $(\text{Ph})_3\text{C}\cdot \rightleftharpoons (\text{Ph})_3\text{C}-\text{C}(\text{Ph})_3$ with different exchange-correlation functionals and basis sets.

PBE/Def2-SVP	8.80
PBE/Def2-TZVP	14.10
PBE+D3BJ/Def2-SVP	-12.00
PBE+D3BJ/Def2-TZVP	-6.80
PBEh-3c	-6.10
PBE0/Def2-SVP	5.70
PBE0/Def2-TZVP	11.10
M06-2X/Def2-SVP	-16.60
M06-2X/Def2-TZVP	-11.10
PBE0+D3BJ/Def2-SVP	-14.70
PBE0+D3BJ/Def2-TZVP	-9.40
PBE0+D3BJ/aug-cc-pVTZ	0.00
B3LYP/Def2-SVP	20.60
B3LYP/Def2-TZVP	26.40
B3LYP +D3BJ/Def2-SVP	-11.50
B3LYP +D3BJ/Def2-TZVP	-5.70
DLPNO-CCSD(T)/cc-pVTZ	-22.40
