Electronic Supplementary Material (ESI) for Chemical Communications.


# ELECTRONIC SUPPLEMENTARY INFORMATION

## Reply to the 'Comment on "Exploiting electronic strategies to stabilize a planar tetracoordinate carbon in cyclic aromatic hydrocarbons"' by V. S. Thimmakondu, *ChemComm*, 2019, DOI: 10.1039/C9CC04639A

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Cartesian coordinates of the ptC-containing $Si_2C_5H_2$ cluster optimized at different levels:

**PBE0/def2-TZVP**

| | | | |
|---|---|---|---|
| C | 0.000000000 | 1.154328000 | -0.514245000 |
| C | 0.000000000 | 0.689157000 | -1.847993000 |
| Si | 0.000000000 | 1.755115000 | 1.123858000 |
| H | 0.000000000 | 1.326436000 | -2.723540000 |
| C | 0.000000000 | 0.000000000 | 0.387651000 |
| C | -0.000000000 | -1.154328000 | -0.514245000 |
| C | -0.000000000 | -0.689157000 | -1.847993000 |
| Si | -0.000000000 | -1.755115000 | 1.123858000 |
| H | -0.000000000 | -1.326436000 | -2.723540000 |

**CCSD/cc-pVDZ***

| | | | |
|---|---|---|---|
| C | 0.000000000 | 0.000000000 | 0.345625000 |
| C | 0.000000000 | -1.168284000 | -0.559120000 |
| C | 0.000000000 | 1.168284000 | -0.559120000 |
| Si | 0.000000000 | -1.808056000 | 1.088963000 |
| Si | 0.000000000 | 1.808056000 | 1.088963000 |
| C | 0.000000000 | -0.695706000 | -1.917122000 |
| C | 0.000000000 | 0.695706000 | -1.917122000 |
| H | 0.000000000 | -1.339007000 | -2.802742000 |
| H | 0.000000000 | 1.339007000 | -2.802742000 |

**CCSD/cc-pVTZ***

| | | | |
|---|---|---|---|
| C | 0.000000000 | 0.000000000 | 0.341212000 |
| C | 0.000000000 | -1.159967000 | -0.557953000 |
| C | 0.000000000 | 1.159967000 | -0.557953000 |
| Si | 0.000000000 | -1.769091000 | 1.081367000 |
| Si | 0.000000000 | 1.769091000 | 1.081367000 |
| C | 0.000000000 | -0.689582000 | -1.900762000 |
| C | 0.000000000 | 0.689582000 | -1.900762000 |
| H | 0.000000000 | -1.323982000 | -2.774318000 |
| H | 0.000000000 | 1.323982000 | -2.774318000 |

***** Cartesian coordinates reported by Thimmakondu, *ChemComm*, 2019, DOI: 10.1039/C9CC04639A