# S2 Table: DFT energy value in each studied dihedral angle using cc-pvtz(-f) for biaryl (1, 4, 5-7, 15, 23-25, 31, 32, 42, 44) and aryl carbonyl fragments (45-47, 50) and cc-pvtz-pp(-f) for 26.

Tabulated data to build up the Conformational Energy Profiles for biaryl fragments (**1, 4, 5-7, 15, 23-25, 26, 31, 32, 42, 44**) and acetophenone **45-47, 49, 50** with a more complex basis sets.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Fragment | Dihedral Angle | Jaguar Relative Energy (kcal/mol) | QM Basis | QM Method |
| **1****1****1****1****1****1****1****1****1****1** | 020406080100120140160180 | 1.8960.90.0020.8371.931.9290.83600.9011.896 | cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **4****4****4****4****4****4****4****4****4****4** | 020406080100120140160180 | 1.4880.53401.0372.3882.3811.0450.0070.5461.483 | cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **5****5****5****5****5****5****5****5****5****5** | 020406080100120140160180 | 0.16100.512.1933.8193.8152.190.5030.0070.166 | cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **6****6****6****6****6****6****6****6****6****6** | 020406080100120140160180 | 1.8910.7840.0020.7511.8671.8610.72900.7821.889 | cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **7****7****7****7****7****7****7****7****7****7** | 020406080100120140160180 | 1.5050.57400.872.0272.0450.8630.0010.5711.506 | cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **15****15****15****15****15****15****15****15****15****15** | 020406080100120140160180 | 6.9443.5990.73800.30.3110.0040.5463.2646.878 | cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **23****23****23****23****23****23****23****23****23****23** | 020406080100120140160180 | 2.7331.2460.0020.3771.3321.3470.42501.1892.732 | cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **24****24****24****24****24****24****24****24****24****24** | 020406080100120140160180 | 6.8393.5110.73300.350.3750.0120.4873.0836.844 | cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **25****25****25****25****25****25****25****25****25****25** | 020406080100120140160180 | 8.1724.2181.00800.2880.3220.010.733.6238.156 | cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **26****26****26****26****26****26****26****26****26****26** | 020406080100120140160180 | 9.4474.9931.5830.22500.0120.2551.3224.3619.4 | cc-pvtz-pp(-f)cc-pvtz-pp(-f)cc-pvtz-pp(-f)cc-pvtz-pp(-f)cc-pvtz-pp(-f)cc-pvtz-pp(-f)cc-pvtz-pp(-f)cc-pvtz-pp(-f)cc-pvtz-pp(-f)cc-pvtz-pp(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **31****31****31****31****31****31****31****31****31****31** | 020406080100120140160180 | 2.8311.35100.2691.3081.7331.1080.7051.8543.333 | cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **32****32****32****32****32****32****32****32****32****32** | 020406080100120140160180 | 7.4716.8786.4267.1017.8957.2474.9952.330.5570 | cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **42** | 0 | 7.351686 | cc-pvtz(-f) | DFT(b3lyp) |
| **42** | 20 | 7.029949 | cc-pvtz(-f) | DFT(b3lyp) |
| **42** | 40 | 7.040587 | cc-pvtz(-f) | DFT(b3lyp) |
| **42** | 60 | 7.895486 | cc-pvtz(-f) | DFT(b3lyp) |
| **42** | 80 | 8.708973 | cc-pvtz(-f) | DFT(b3lyp) |
| **42** | 100 | 7.886998 | cc-pvtz(-f) | DFT(b3lyp) |
| **42** | 120 | 5.407367 | cc-pvtz(-f) | DFT(b3lyp) |
| **42** | 140 | 2.661321 | cc-pvtz(-f) | DFT(b3lyp) |
| **42** | 160 | 0.681038 | cc-pvtz(-f) | DFT(b3lyp) |
| **42** | 180 | 0 | cc-pvtz(-f) | DFT(b3lyp) |
| **44** | 0 | 5.265324 | cc-pvtz(-f) | DFT(b3lyp) |
| **44** | 20 | 4.137904 | cc-pvtz(-f) | DFT(b3lyp) |
| **44** | 40 | 3.016876 | cc-pvtz(-f) | DFT(b3lyp) |
| **44** | 60 | 2.832477 | cc-pvtz(-f) | DFT(b3lyp) |
| **44** | 80 | 3.222141 | cc-pvtz(-f) | DFT(b3lyp) |
| **44** | 100 | 2.957982 | cc-pvtz(-f) | DFT(b3lyp) |
| **44** | 120 | 1.806889 | cc-pvtz(-f) | DFT(b3lyp) |
| **44** | 140 | 0.545514 | cc-pvtz(-f) | DFT(b3lyp) |
| **44** | 160 | 0 | cc-pvtz(-f) | DFT(b3lyp) |
| **44** | 180 | 0.180905 | cc-pvtz(-f) | DFT(b3lyp) |
| **45****45****45****45****45****45****45****45****45****45** | 020406080100120140160180 | 00.5412.1094.1385.5815.5273.9491.9690.4960.001 | cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f)cc-pvtz(-f) | DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp)DFT(b3lyp) |
| **46** | 0 | 7.169479 | cc-pvtz(-f) | DFT(b3lyp) |
| **46** | 20 | 5.857237 | cc-pvtz(-f) | DFT(b3lyp) |
| **46** | 40 | 6.426921 | cc-pvtz(-f) | DFT(b3lyp) |
| **46** | 60 | 7.073685 | cc-pvtz(-f) | DFT(b3lyp) |
| **46** | 80 | 7.15263 | cc-pvtz(-f) | DFT(b3lyp) |
| **46** | 100 | 6.086282 | cc-pvtz(-f) | DFT(b3lyp) |
| **46** | 120 | 3.831731 | cc-pvtz(-f) | DFT(b3lyp) |
| **46** | 140 | 1.557378 | cc-pvtz(-f) | DFT(b3lyp) |
| **46** | 160 | 0 | cc-pvtz(-f) | DFT(b3lyp) |
| **46** | 180 | 0.241454 | cc-pvtz(-f) | DFT(b3lyp) |
| **47** | 0 | 3.534475 | cc-pvtz(-f) | DFT(b3lyp) |
| **47** | 20 | 3.53196 | cc-pvtz(-f) | DFT(b3lyp) |
| **47** | 40 | 3.921453 | cc-pvtz(-f) | DFT(b3lyp) |
| **47** | 60 | 4.644052 | cc-pvtz(-f) | DFT(b3lyp) |
| **47** | 80 | 5.200438 | cc-pvtz(-f) | DFT(b3lyp) |
| **47** | 100 | 4.547122 | cc-pvtz(-f) | DFT(b3lyp) |
| **47** | 120 | 2.996514 | cc-pvtz(-f) | DFT(b3lyp) |
| **47** | 140 | 1.435697 | cc-pvtz(-f) | DFT(b3lyp) |
| **47** | 160 | 0.304533 | cc-pvtz(-f) | DFT(b3lyp) |
| **47** | 180 | 0 | cc-pvtz(-f) | DFT(b3lyp) |
| **49** | 0 | 10.710103 | cc-pvtz(-f) | DFT(b3lyp) |
| **49** | 20 | 9.45325 | cc-pvtz(-f) | DFT(b3lyp) |
| **49** | 40 | 9.014258 | cc-pvtz(-f) | DFT(b3lyp) |
| **49** | 60 | 9.238873 | cc-pvtz(-f) | DFT(b3lyp) |
| **49** | 80 | 9.472443 | cc-pvtz(-f) | DFT(b3lyp) |
| **49** | 100 | 8.457581 | cc-pvtz(-f) | DFT(b3lyp) |
| **49** | 120 | 5.93886 | cc-pvtz(-f) | DFT(b3lyp) |
| **49** | 140 | 2.993026 | cc-pvtz(-f) | DFT(b3lyp) |
| **49** | 160 | 0.748132 | cc-pvtz(-f) | DFT(b3lyp) |
| **49** | 180 | 0 | cc-pvtz(-f) | DFT(b3lyp) |
| **50** | 0 | 6.836167 | cc-pvtz(-f) | DFT(b3lyp) |
| **50** | 20 | 5.190938 | cc-pvtz(-f) | DFT(b3lyp) |
| **50** | 40 | 4.459623 | cc-pvtz(-f) | DFT(b3lyp) |
| **50** | 60 | 4.686366 | cc-pvtz(-f) | DFT(b3lyp) |
| **50** | 80 | 5.139618 | cc-pvtz(-f) | DFT(b3lyp) |
| **50** | 100 | 4.814349 | cc-pvtz(-f) | DFT(b3lyp) |
| **50** | 120 | 3.388368 | cc-pvtz(-f) | DFT(b3lyp) |
| **50** | 140 | 1.594644 | cc-pvtz(-f) | DFT(b3lyp) |
| **50** | 160 | 0.384232 | cc-pvtz(-f) | DFT(b3lyp) |
| **50** | 180 | 0 | cc-pvtz(-f) | DFT(b3lyp) |