SHEET-09

96378: C16H16-4,
NMR - Gaussian

0.2505 Debye

-607.777203437 Hartree

Symmetry C1

96383: 2-C16H16-3,
NMR - Gaussian

0.0002 Debye

-607.776591063 Hartree

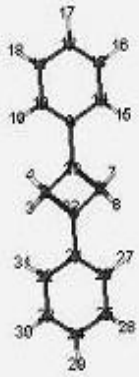
Symmetry C1

96386: 3-C16H16-1,
NMR - Gaussian

0.0030 Debye

-607.772788927 Hartree

Symmetry C1

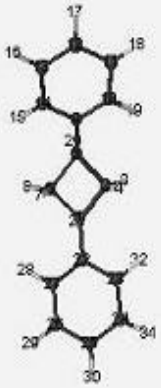


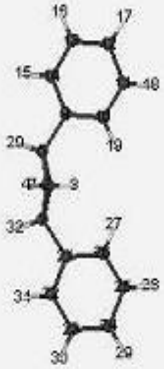
96390: 4-C16H16-2,
NMR - Gaussian

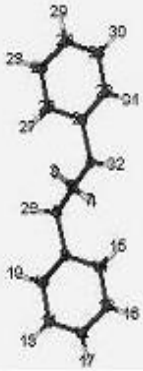
0.3362 Debye

-607.775552439 Hartree

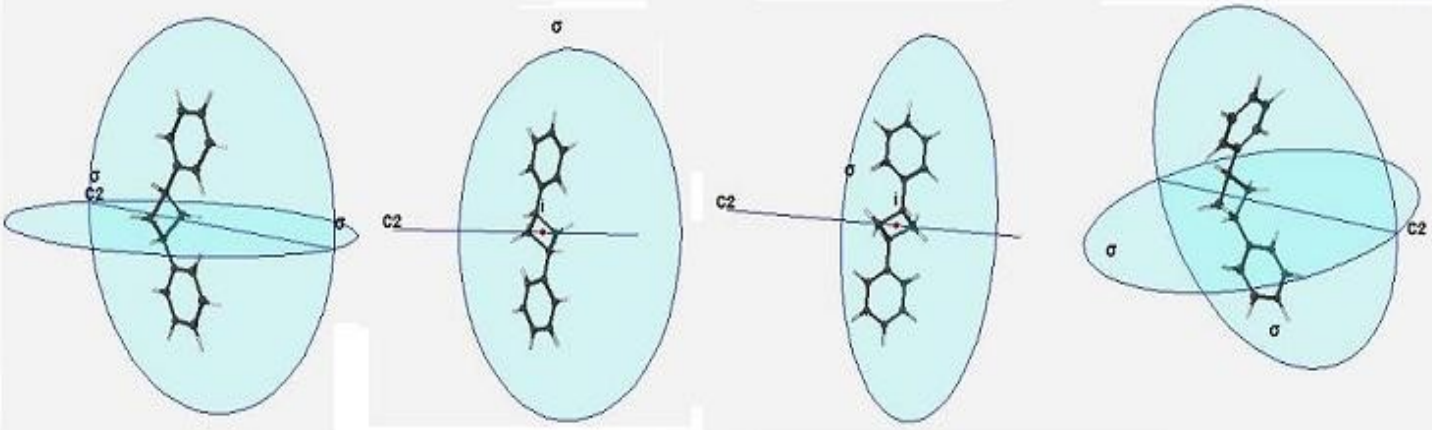
Symmetry C1







Display with symmetry elements by symmetrizing to the nearest point group (the optimized quantities are the same)



Energy Values and the Symmetry aspects for an assessment of the Theoretical findings on the Dimes at present considered merely as hypothetical to explain how the book-keeping geometries can be validated with the experimental J-coupling constants.