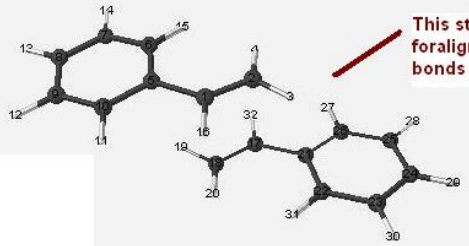
SHEET-11

input str step 0 -607.492875516
output str step 4 -607.604200501



This structure was edited foralignment of the double bonds and optimized

Symmetry C1

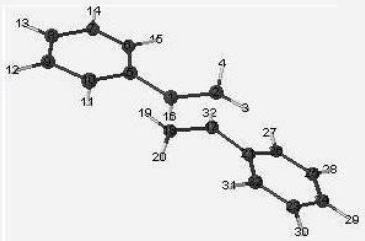
Basis STO-3G

RHF Energy -607.604200501 Hartree

Dipole Moment 0.0790 Debye

90739: C16H16-C1sym, Geometry Optimization - Gaussian

input str step 0 -607.067169480 Hartree
output str step 4 -607.559590187



Symmetry C1

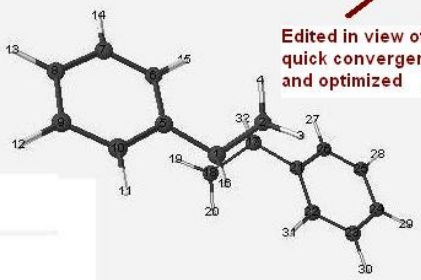
Basis STO-3G

RHF Energy -607.559590187 Hartree

Dipole Moment 0.2321 Debye

90741: C16H16-C1sym, Geometry Optimization - Gaussian

input str step 0 -607.596191599 Hartree
output str step 5 -607.747574943



Edited in view of the quick convergence and optimized

Symmetry C1

Basis STO-3G

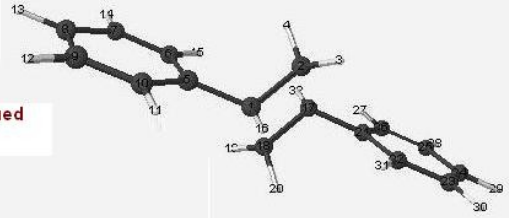
RHF Energy -607.747574943 Hartree

Dipole Moment 0.1297 Debye

90742: C16H16-C1sym, Geometry Optimization - Gaussian

input str step 0 -607.747574920 Hartree
output str step 4 -607.776219908

Optimiztion continued without editing



Symmetry C1

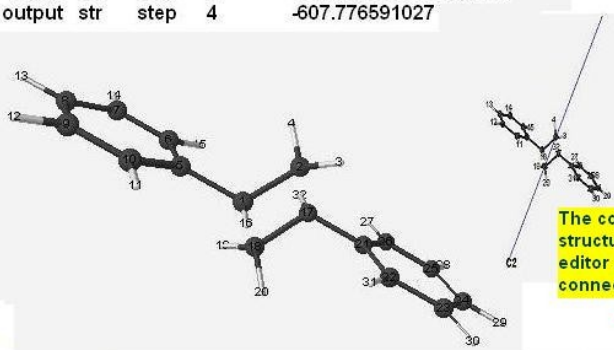
Basis STO-3G

Dipole Moment 0.0649 Debye

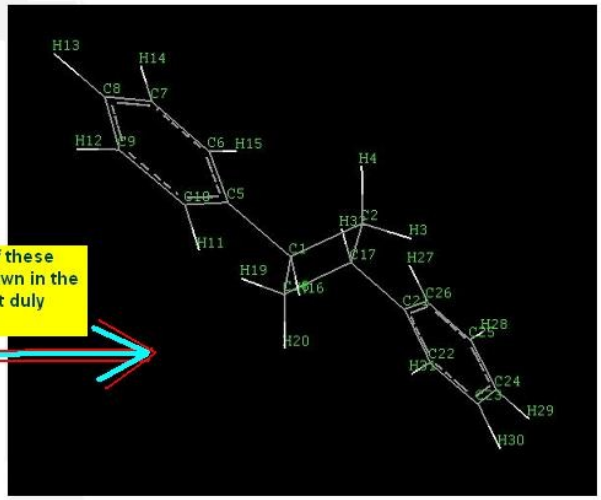
RHF Energy -607.776219908 Hartree

90743: C16H16-C1sym, Geometry Optimization - Gaussian

input str step 0 -607.776513382 Hartree
output str step 4 -607.776591027



The coordinates of these structure are redrawn in the editor all bonds get duly connected



RHF Energy -607.776591027 Hartree

Basis STO-3G

Symmetry C2

Dipole Moment 0.0001 Debye

90744: C16H16-C1sym, Geometry Optimization - Gaussian