

## The WEBMO JOBS Related to this cycloaddition:

SHEET-05

These jobs enlisted below are from the contents of the displayable list at the author's Web Subdirectory: [http://www.ugc-inno-nehu.com/cycloaddition\\_export90718/](http://www.ugc-inno-nehu.com/cycloaddition_export90718/)  
Once the above subdirectory contents are on display in the browser window, any of the jobs archived can be displayed by clicking on the html file with the specific jobnumber.

Any particular Job below, to begin with job90727, can be retrieved and displayed from the internet browser by typing the address as per this format: The **Web Subdirectory** as per the link above followed by **filename** consisting of the specific job.

[http://www.ugc-inno-nehu.com/cycloaddition\\_export90718/job\\_90727.html](http://www.ugc-inno-nehu.com/cycloaddition_export90718/job_90727.html)

**All these jobs were run at the remote server  
at the *computational chemistry* Portal: <http://www.webmo.net/>**

**90727:** C16H16, Geometry Optimization – Gaussian  
Initial setting of two Styrene molecules  
#N HF/STO-3G OPT(NewEstmFC) Geom=Connectivity

Basis	STO-3G
RHF Energy	-607.654172606 Hartree
Dipole Moment	0.0520 Debye

**90729:** C16H16, Geometry Optimization – Gaussian

Route	#N HF/STO-3G OPT(NewEstmFC) Geom=Connectivity
Basis	STO-3G
RHF Energy	-607.654172607 Hartree
Dipole Moment	0.0520 Debye

**90731:** C16H16, Geometry Optimization – Gaussian

Route	#N HF/STO-3G OPT(NewEstmFC) Geom=Connectivity
Basis	STO-3G
RHF Energy	-607.621097851 Hartree
Dipole Moment	0.0111 Debye

Of all the jobs archived only the files relevant for visualizing the cycloaddition are listed out in the next sheet