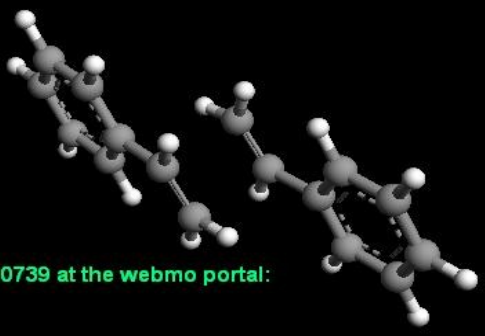
SHEET-12

Typical Input: An optimized structure of an isolated Styrene molecule:
Two such molecules are drawn placed conveniently for the cycloaddition

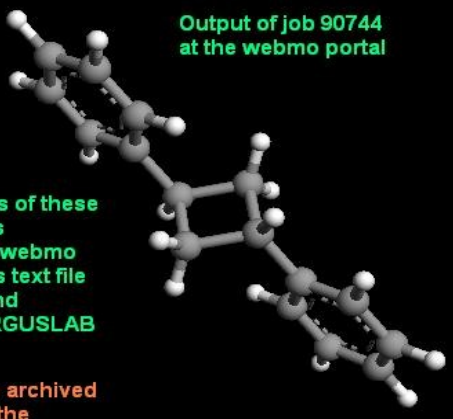


Input to job 90739 at the webmo portal:

The coordinates of these systems as was available at the webmo editor copied as text file in xyz format and displayed in ARGUSLAB

The two molecule cluster is subjected to Optimization/energy minimization until this final dimer results as output structure:

Output of job 90744 at the webmo portal



The details about the calculations in these jobs can be retrieved from the archived internet sources of this author. The necessary instructions and some of the results are in display sheets "SHEET-06" and "SHEET-11" of thsi poster.

CONCLUSIONS

It is obvious that several jobs became necessary before the final structure. WEBMO site has the free working demo which enables free access for jobs of not more than one minute duration. It is obvious that the contents of several jobs cannot be obtained simply by submitting by a single job. There is provison at the webmo job manager to continue the unfinished task of optimization by a resubmission of the job output. Even with the STO-3G minimal basis set, the ***ab initio*** SCF calculation for this system could not proceed beyond 4 to 8 iterations depending upon the input structure. Thus the strategy was to submit an Initial Guess structure, and at the end of one minute the remote server returns the interim result by stopping the CPU from continuing the job beyond one minute. Then this job is resubmitted by the appropriate button (there are three buttons including the **view** button)at the job manager. This procedure is continued untll the job returns with "completed" message instead of the "failed" message for incomplete job due to time limit.

If one had the access to the unlimited time feature usually only what results at the end of convergence would be analyzed. Since the jobs required for continuing till convergence were too many, every time the job was returned after 5-6 iterations (steps)due to the constraint of one-minute limit, it was possible to consider editing the structure after the five – six iterations before resubmission. By this it was possible to reduce the number of iterations required. An examination of the animated output of the sequence of structures generated during the iteration of the jobs, it was possible to visualize what the kind interaction which governs minimizing energy to the next step. This could give a indication as to how one can hasten the process of convergence by manually editing and incorporating the required emphasis on interactions in the system. Thus it was possible to monitor the state of hybridizations, the charges on the atoms etc., and alter the structure for appropriate cahges in geometries and set appropriate formal charges at atoms. For example if there is tendency for increase in electronic charge at one atom by transfer from another atom in the interim result, then it was possible to place appropriately a positive charge on donor atom and a negative charge on the acceptor atom and hasten the process instead of the program proceeding stage by stage in small steps of charge transfer. Thus the visualization with the intuition of chemist based on the experiences in theoretical calculations, it was possible to realize the dimerization in 5 one minute jobs which otherwise would have taken much longer even to estimate.