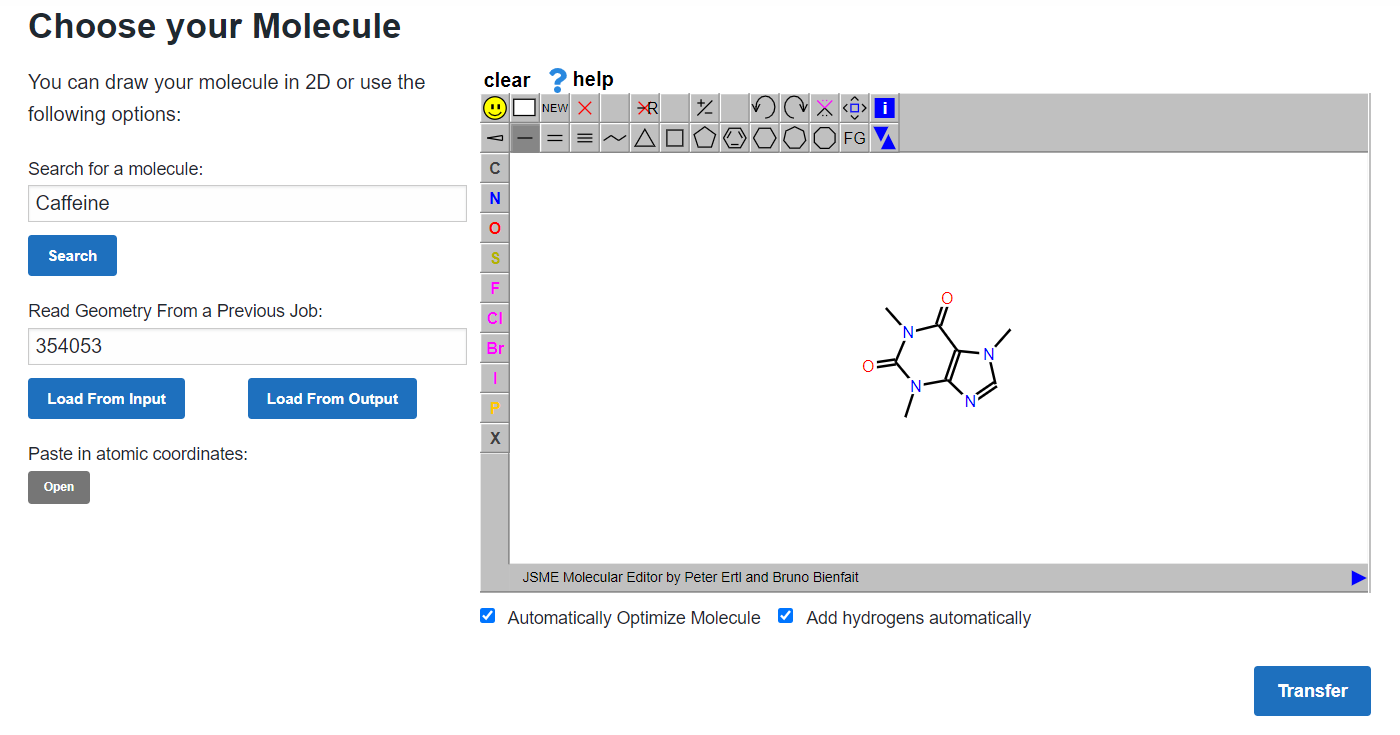
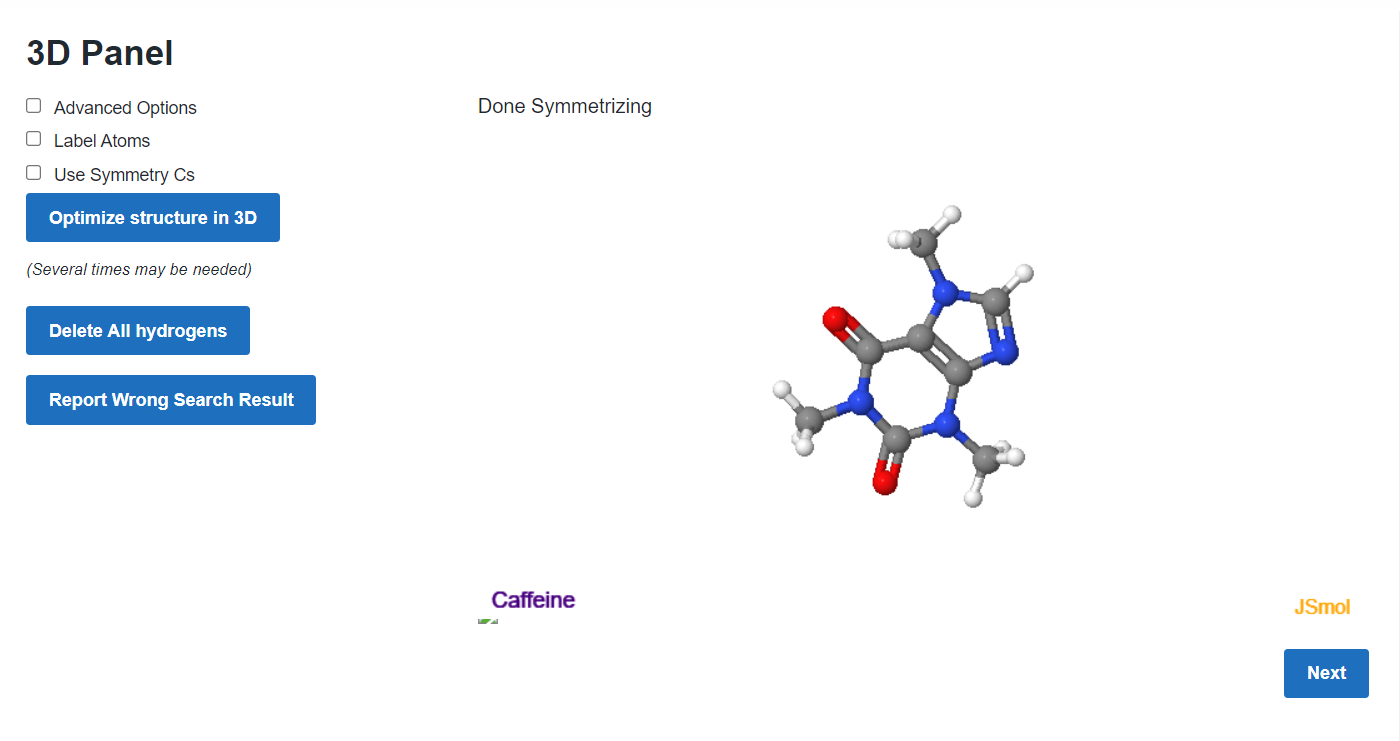
**Energy calculation of Quantum Mechanical model of Caffeine Molecule using Gamess Software**

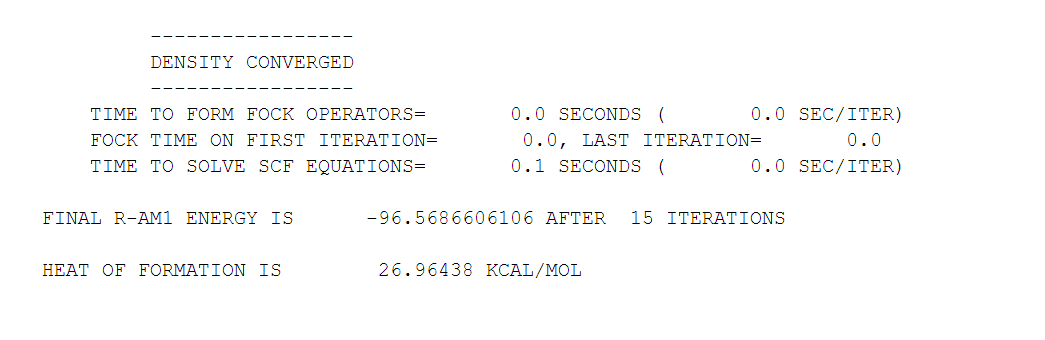


Optimized Structure:

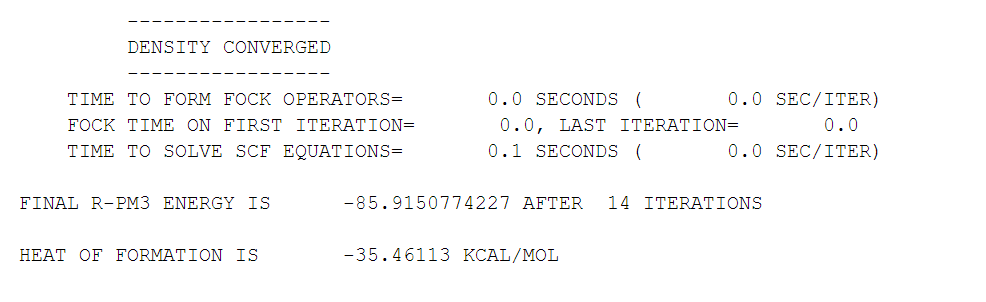


Energies of various Basis set:

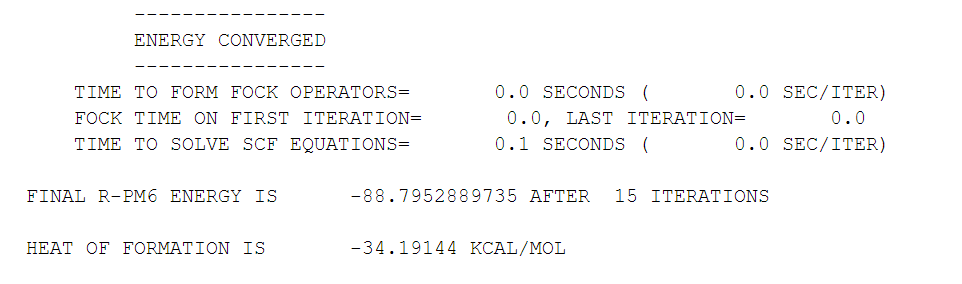
i) AM1:



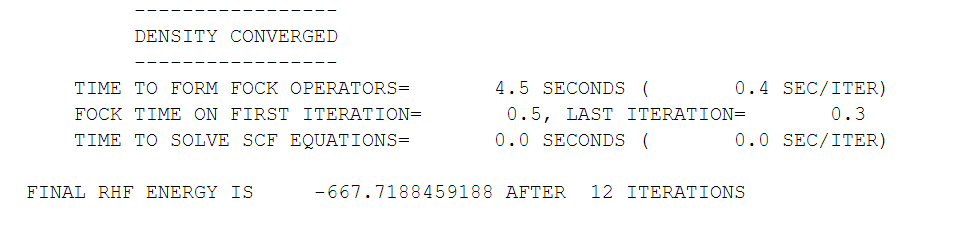
ii) PM3:



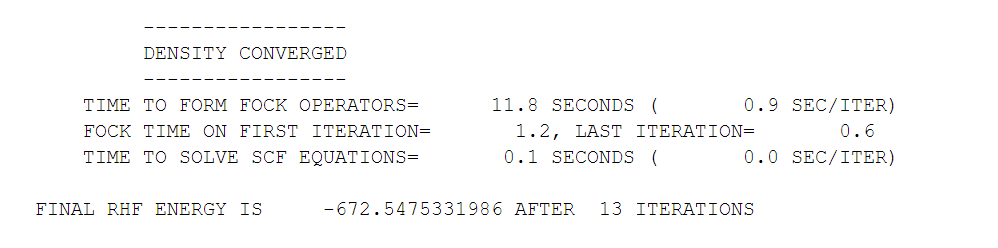
iii) PM6:



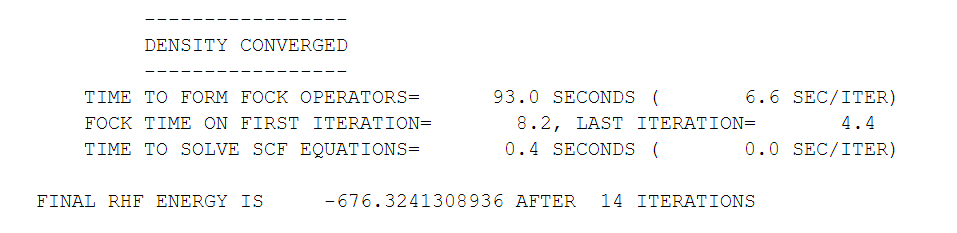
iv) STO-3G:



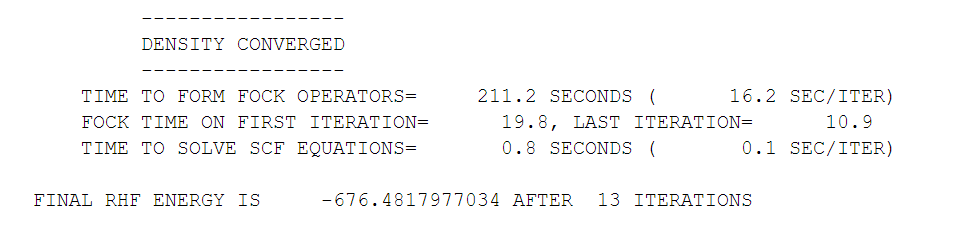
v) 3-21G:



vi) 6-31G\*:



vii) 6-311G\*\*:



viii) 6-311G\*\*+:

