Simulation for excited structure of phenolblue

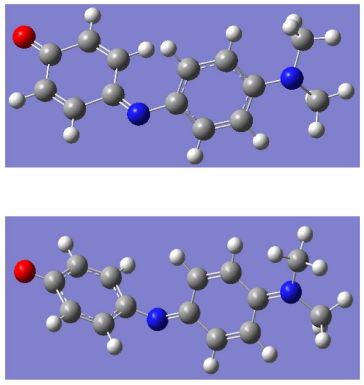
高エネルギー加速器研究機構(KEK) IMSS Dividion name [Shunsuke NOZAWA,v60638]

Purpose Simulation for excited structure of phenolblue using Quantum calculation

Outline X-ray scattering can obtain the molecule structure, we want to compare the exp data and theoretical calculated data

Result We have found some candidate structures, but we are still computing to find a wider variety of candidate structures.

Computing system:	Octopus General Purpose CPU nodes
node-hour	10,230 node-hour (5000 point)
memory used	30 GB
parallelize	4 nodes



Image（the result of simulation）