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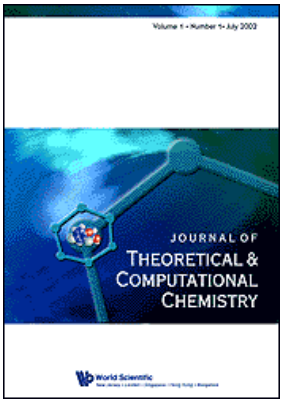


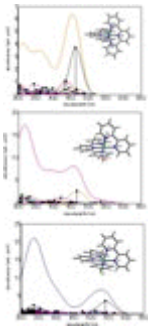
RESEARCH PAPERS

1. **Theoretical investigation of $[Ru(tpy)^{2}]^{2+}2]2+$, $[Ru(tpy)(bpy)(H^{2}O)]^{2+}2+$ and $[Ru(tpy)(bpy)(Cl)]^{+}+$ complexes in acetone revisited: Inclusion of strong spin–orbit couplings to quantum chemistry calculations**

Kenji Mishima, *Takumi Kinoshita*, *Michitoshi Hayashi*, *Ryota Jono*, *Hiroshi Segawa*, *Koichi Yamashita*

1650001

We have theoretically revisited electronic absorption spectra of three kinds of ruthenium polypyridyl complexes $[Ru(tpy)_2]^{2+}$, $[Ru(tpy)(bpy)(H_2O)]^{2+}$, and $[Ru(tpy)(bpy)(Cl)]^{+}$ complexes in acetone (tpy = 2,2′,2″-terpyridine and bpy = 2,2′-bipyridine). For the theoretical calculations, we have used the first-order perturbation theory based on TD-DFT where the first-order perturbation term is the spin-orbit coupling Hamiltonian. It was found that in general the theory including spin-orbit coupling can reproduce experimental data better than the simple quantum chemistry calculation neglecting SO coupling.

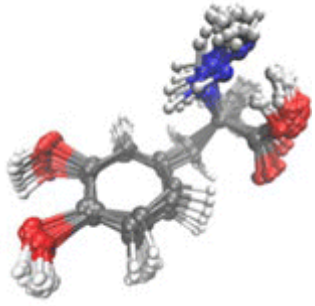


2. **Conformation and electronic structure of Carbidopa. A QM/MD study**

Ghader M. Sukker, *Nuha Wazzan*, *Ashour Ahmed*, *Rifaat Hilal*

1650002

The shallow nature of the PES of CD and the presence of several local minima within a small energy range make it impossible, using routine energy minimization techniques to arrive at the global minimum structure. This is crucial to understand the mode of action of CD as decarboxylase inhibitor. Quantum dynamics simulations seem to be the right approach for this problem.

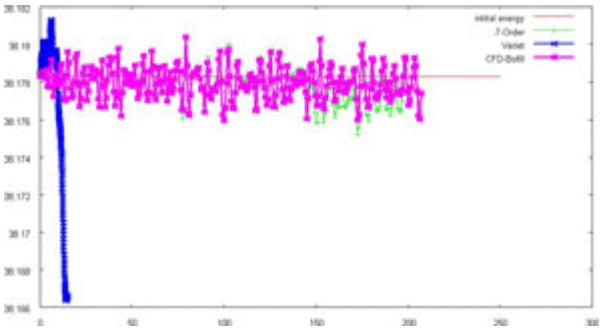


3. **A high order predictor–corrector integration algorithm for first principle chemical dynamics simulations**

Heng Wu, *Shaofei Lu*, *Ningjia Zhu*, *Jialin Liu*, *Eduardo Colmenares*, *Yin Lu*

1650003

This article proposes a High Order (Seventh-Order) Predictor-Corrector approach which uses the two previous points and external interpolation to predict the location of the next time step. The simulation results show the Seventh-Order approach is far better than Velocity Verlet approach and as well as CFD-Bofill for molecules without hydrogen atoms, while new method is simpler than CFD-Bofill. This is due to the Seventh-Order approach which uses two points to predict the next point indirectly, increases the step size and the external interpolation is worse than the internal interpolation.

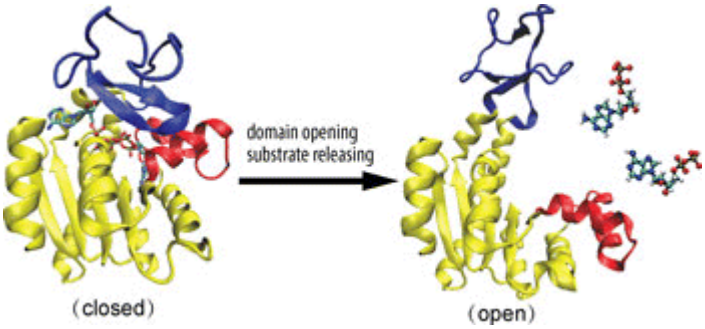


4. **Molecular simulations of substrate release and coupled conformational motions in adenylate kinase**

Dachao Cui, *Weitong Ren*, *Wenfei Li*, *Wei Wang*

1650004

Substrate releasing step of adenylate kinase catalytic cycle was studied by metadynamics simulations. The results showed that the substrate releasing involves full opening of LID domain and partial opening of NMP domain. Protonation of the substrate (ADP) molecule around the NMP domain tends to speed up the substrate releasing.

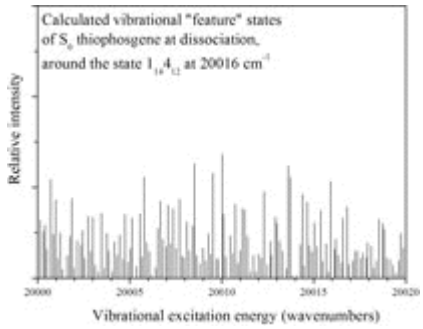


5. **Large scale vibrational calculations on IVR in S^0 thiophosgene**

Svetoslav Rashev, *David C. Moule*

1650005

We calculate the vibrational level structure of S_0 thiophosgene at vibrational excitation energy of ~20000 cm^{-1}(dissociation) using our own variational method based on a specific search/selection algorithm.
The average vibrational density of isolated "feature" states was found to be ~6 lev/cm^{-1}, superimposed on a much denser "dark" background level manifold of about 3000 lev/cm^{-1}.
The statistical analysis of the calculated spectral intensity distributions shows evidence of incomplete IVR and nonergodic behavior.

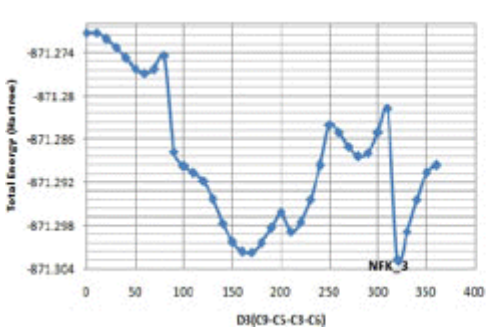


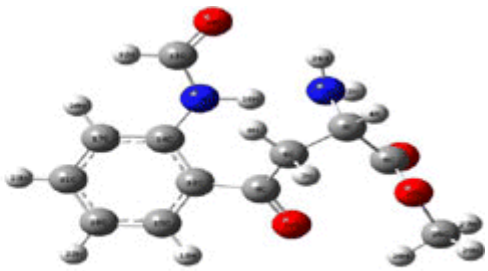
6. ***Ab-initio*** **HF and density functional theory investigations on the synthesis mechanism, conformational stability, molecular structure and UV spectrum of N'-Formylkynurenine**

Nabil Omri, *Mohammed Yahyaoui*, *Ridha Banani*, *Sabri Messaoudi*, *Fathi Moussa*, *Manef Abderrabba*

1650006

The mechanisms of formation of N'-Formylkynurénine (NFK) molecule has been studied by HF and DFT/B3LYP methods with 6-31G(d,p).
Geometric and optimized parameters of the most stable conformation of NFK have been determined and analyzed by DFT/B3LYP/3-21G after a scanning procedure of dihedral angles.
Thermodynamic, electronic and orbital properties of this molecule have been theoretically studied.



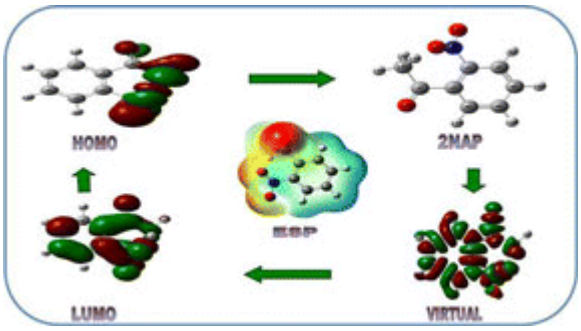


7. **Molecular structure, vibrational spectral assignments (FT-IR and FT-RAMAN), NMR, NBO, HOMO–LUMO and NLO properties of 2-nitroacetophenone based on DFT calculations**

G. Venkatesh, M. Govindaraju, P. Vennila, C. Kamal

1650007

The optimized molecular geometry and vibrations are calculated using DFT method.
The NLO and thermodynamic properties of 2NAP is calculated theoretically.
The redistribution of electron density (ED) and E(2) energies have been calculated by NBO.

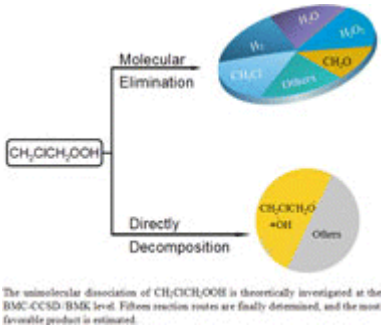


8. **Theoretical study on the unimolecular decomposition of 2-chlorinated ethyl hydroperoxide**

Ya Li, Na Wang, Chunzhang Wang, Xin Wang, Jinglai Zhang, Li Wang

1650008

The mechanism of unimolecular dissociation of 2-chlorinated ethyl hydroperoxide is studied by BMC-CCSD//BMK method. Fifteen pathways are determined. The direct O–O bond cleavage is one of the dominant reaction channels.



9. **Investigation of charge transfer complexes formed between (S, S)-bis-N,N-sulfonyl bis-L-phenylalanine dimethylester donor with tetracyanoethylene and chloranil as ππ-acceptors: Experimental and DFT studies**

Messaouda Mohamdi, *Nadjia Bensouilah*, *Mohamed Abdaoui*

1650009

Two novel charge transfer complexes: [D→TCNE] and [D→CHL] were synthesized, studied and analyzed by elemental analysis: FT-IR and UV-V. Moreover, the experimental studies were supported by quantum chemical calculations at DFT/CAM-B3LYP were applied to provide the geometrical parameters, the electronic spectroscopy, the excited-state properties, the vibrational frequency calculations, the natural population analysis (NPA) and NBO analysis.