

2012

- **Informacja o wykorzystaniu czasu komputerowego w WCSS w roku 2012 przez Zespół Zakładu Modelowania Molekularnego i Chemii Kwantowej wraz ze współpracownikami z innych jednostek Politechniki Wrocławskiej.**

prof. dr hab.	W. Andrzej	Sokalski	profesor
prof. dr hab.	Szczepan	Roszak	profesor
prof. dr hab.	Henryk	Chojnacki	profesor em.
dr hab.	Tadeusz	Andruniów	profesor PWr
dr inż.	Paweł	Kędzierski	adiunkt
dr inż.	Borys	Szefczyk	asystent
prof. dr hab.	Paweł	Kafarski	profesor
dr hab.	Łukasz	Berlicki	adiunkt
dr inż.	Karol	Langner	adiunkt
dr inż.	Tomasz	Misiaszek	adiunkt
dr inż.	Paweł	Szarek	asystent
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mgr inż.	Agnieszka	Dzielendziak	doktorantka
mgr inż.	Paweł	Kadłubański	doktorant
mgr inż.	Rafał	Roszak	doktorant
mgr inż.	Dorota	Ślepieńczuk	doktorantka
mgr inż.	Elżbieta	Walczak	doktorantka
mgr inż.	Łukasz	Wolański	doktorant
inż.	Wiktor	Beker	dyplomant
	Wiktor	Giedroyc-Piasecka	dyplomantka

Robust Predictive Power of the Electrostatic Term at Shortened Intermolecular Distances

Journal of Physical Chemistry Letters, 3, 2785-2789(2012) **IF=6.213**

Karol M. Langner, Wiktor Beker, W. Andrzej Sokalski

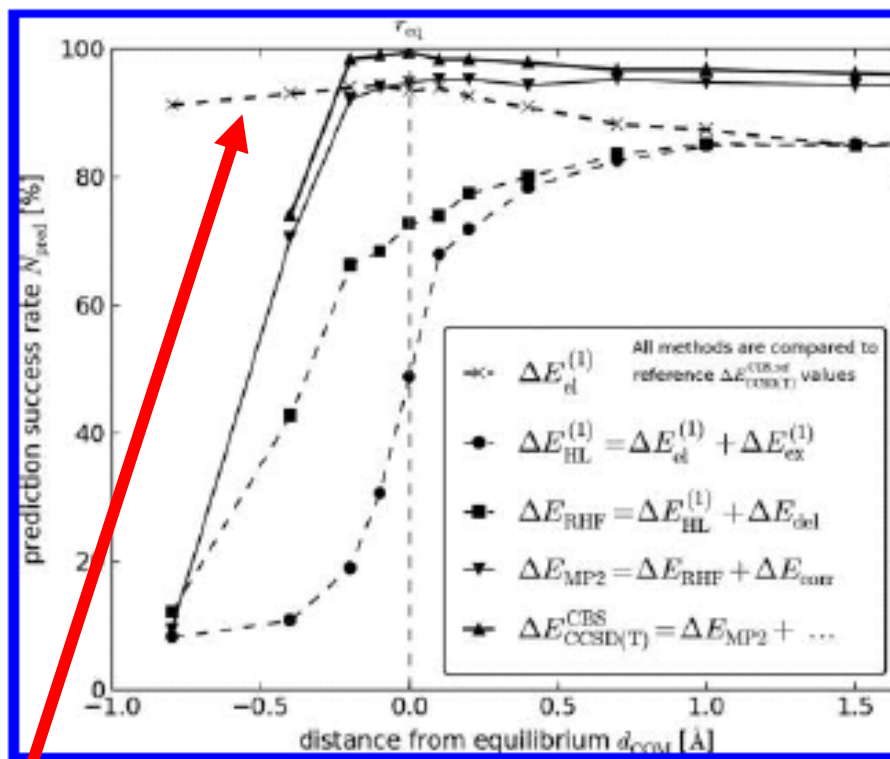
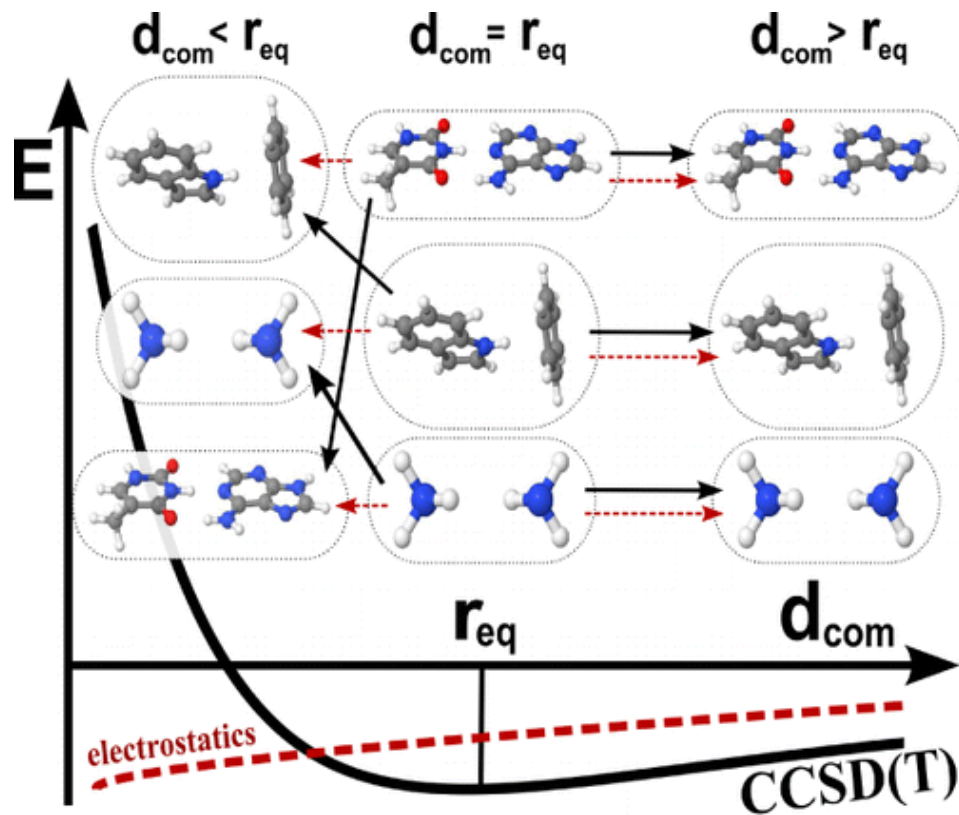


Figure 2. Success rate of predicting the relative stability of molecular dimers at equilibrium, using several levels of theory at various intermolecular distances from equilibrium.



Składowa elektrostatyczna pozwala lepiej niż metody MP2 lub CCSD(T) prognozować względną stabilność kompleksów molekularnych dla odległości mniejszych niż równowagowe

Physical nature of interactions in charge-inverted hydrogen bonds

M. Jabłoński, W.A. Sokalski, Chem.Phys.Lett., 552, 156-161(2012) IF=2.337

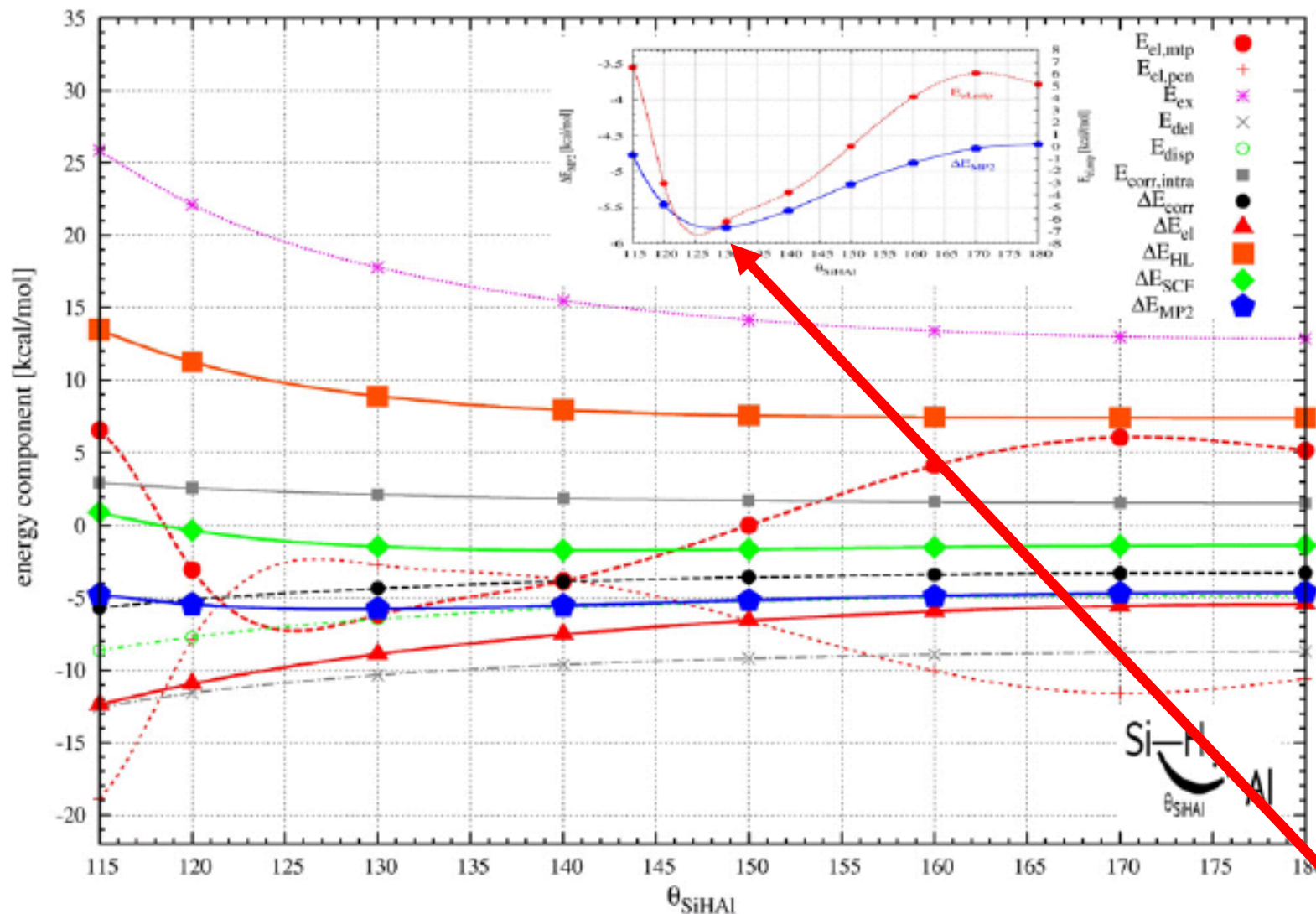
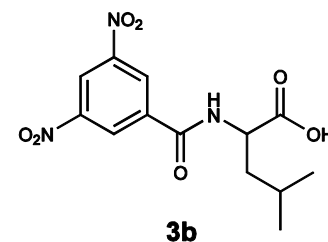
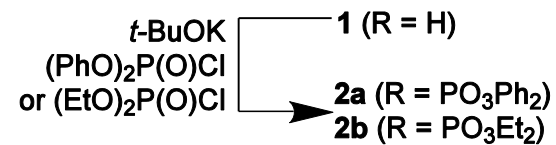
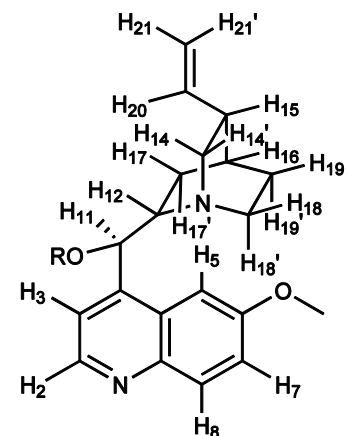
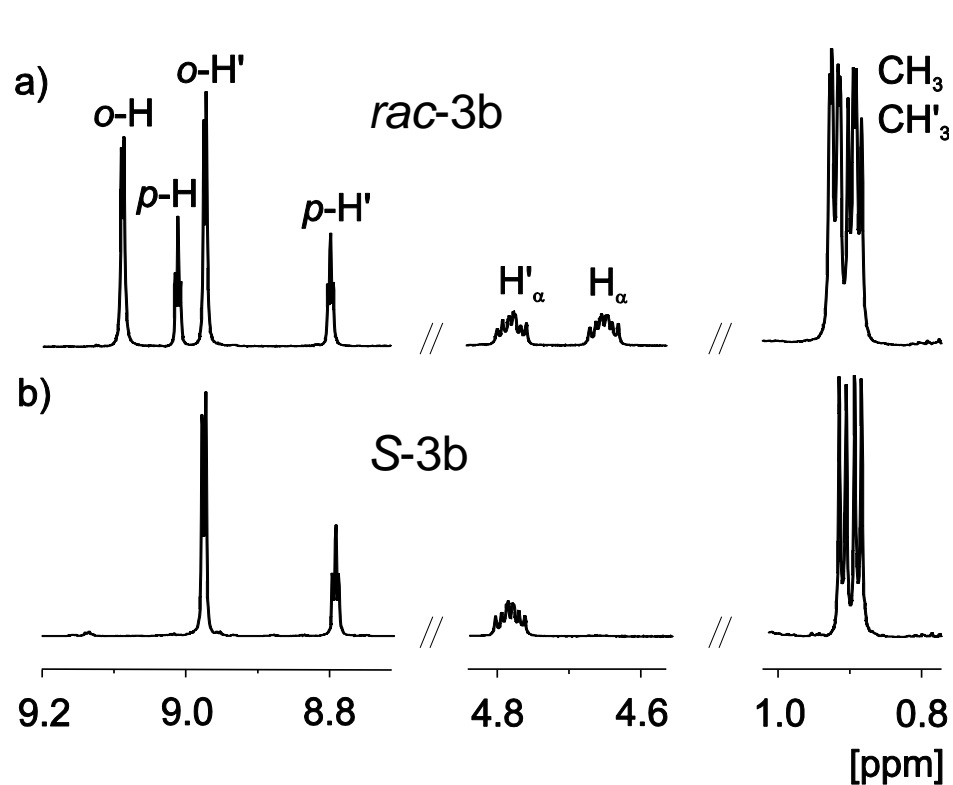


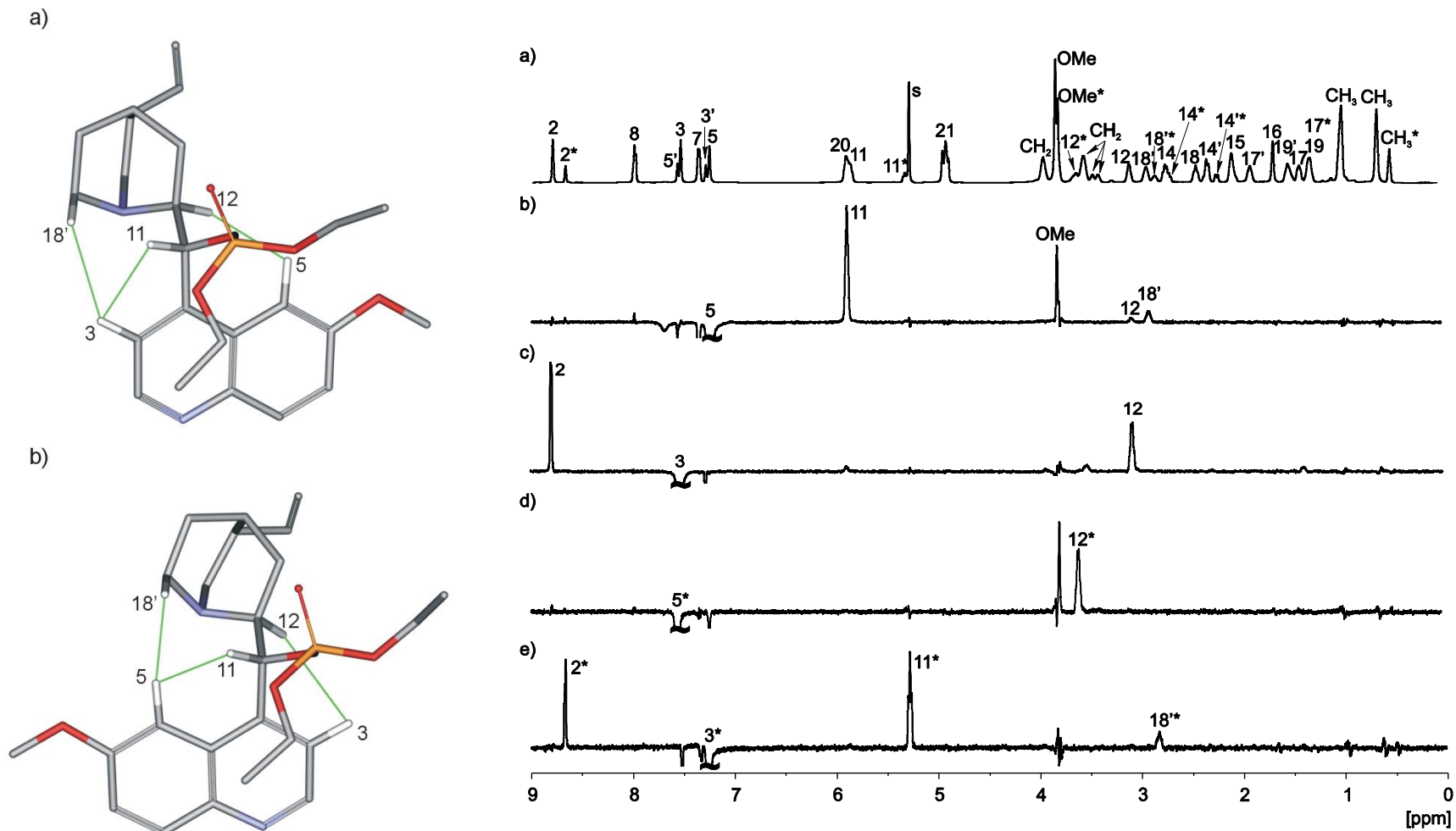
Figure 3. Angular dependence of interaction energy components for $H_3SiH \cdots AlH_3$.

Multipolowa składowa oddziaływań elektrostatycznych determinuje kątową strukturę kompleksu

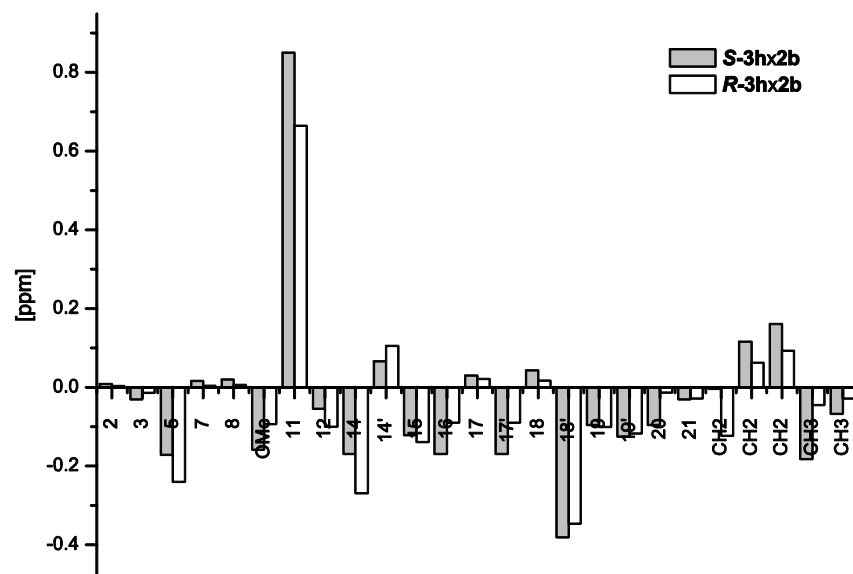
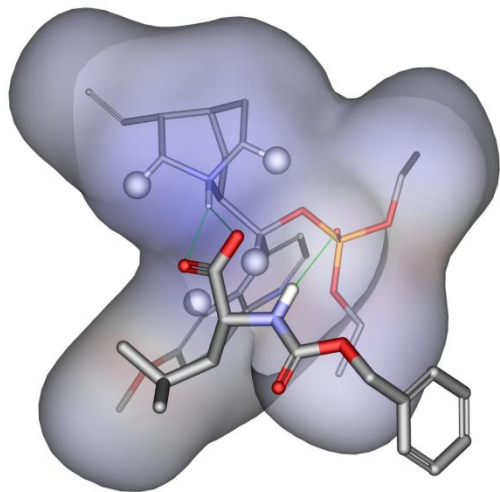
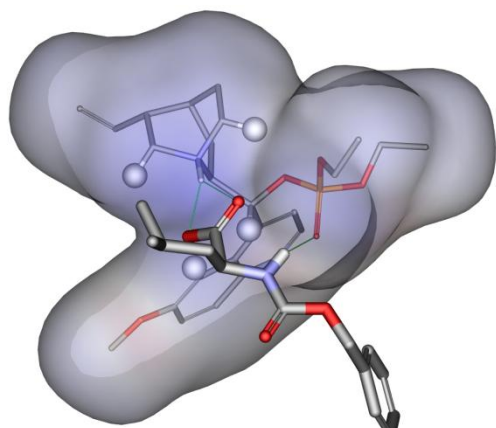
Fosforylowana chinina - konformacje



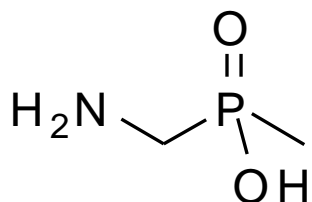
Fosforylowana chinina - konformacje



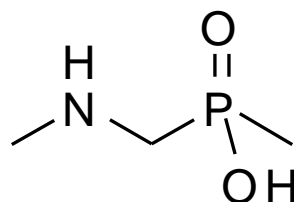
Fosforylowana chinina - kompleksowanie



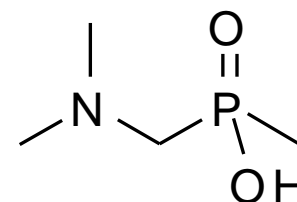
Inhibitory ureazy – kwasy aminofosfinowe



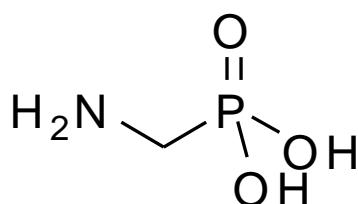
$$K_i = 340 \mu\text{M}$$



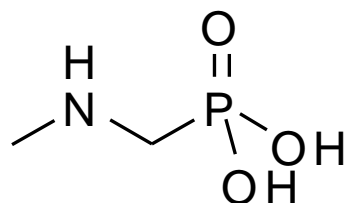
$$K_i = 18 \mu\text{M}$$



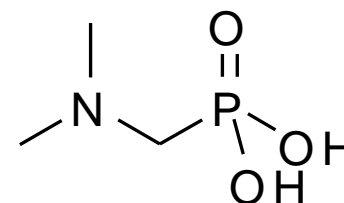
$$K_i = 0.62 \mu\text{M}$$



$$K_i = 314 \mu\text{M}$$

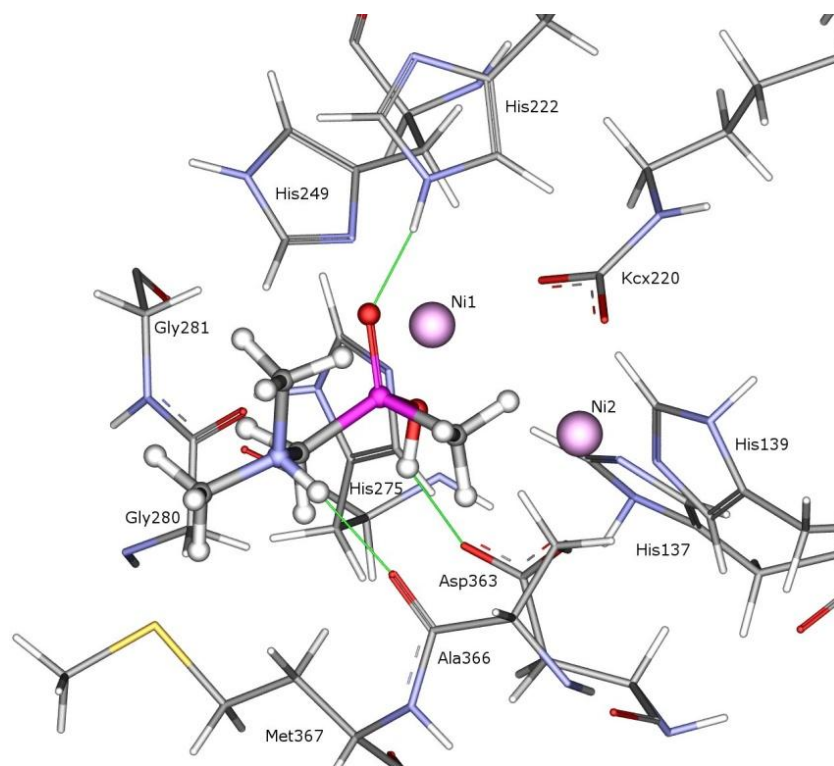


$$K_i = 70 \mu\text{M}$$



$$K_i = 13 \mu\text{M}$$

Inhibitory ureazy – kwasy aminofosfinowe

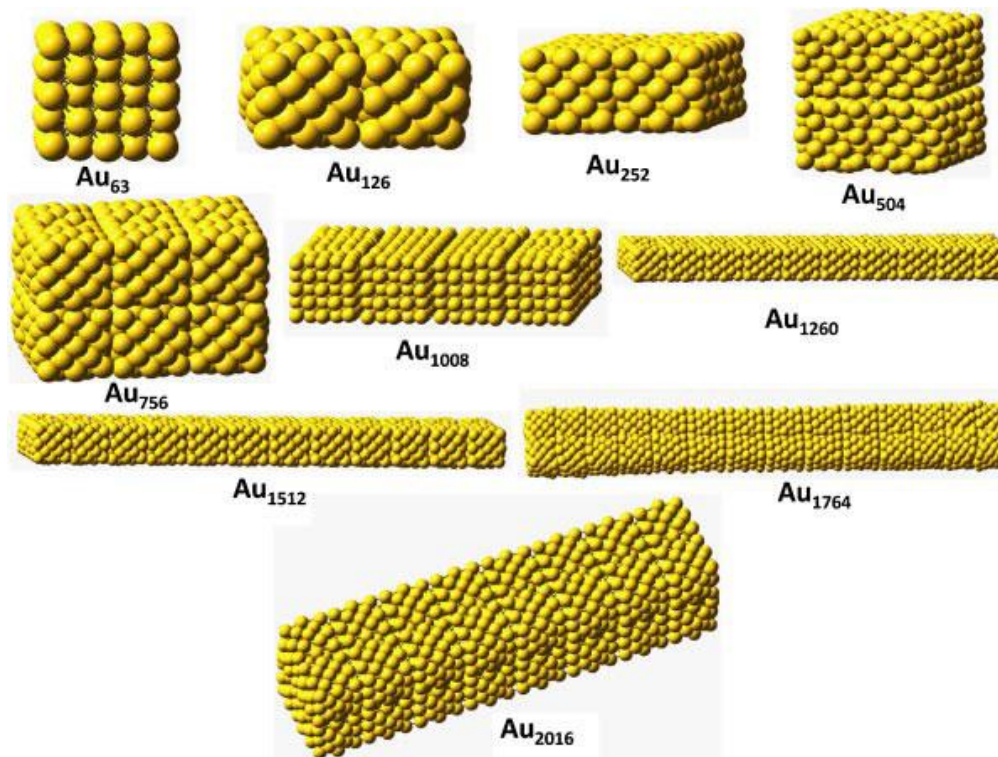


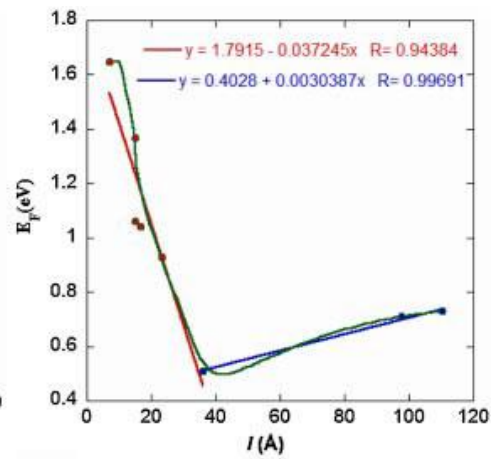
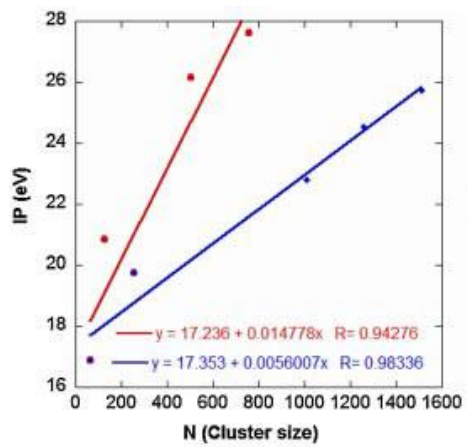
Vassiliou, S.; Grabowiecka, A.; Kosikowska, P.; Yiotakis, A.; Kafarski, P.; **Berlicki, Ł.** *J. Med. Chem.* **2008**, *51*, 5736;
Berlicki, Ł.; Bochno, M.; Grabowiecka, A.; Białas, A.; Kosikowska, P.; Kafarski, P. *Amino Acids* **2012**, *42*, 1937–1945.

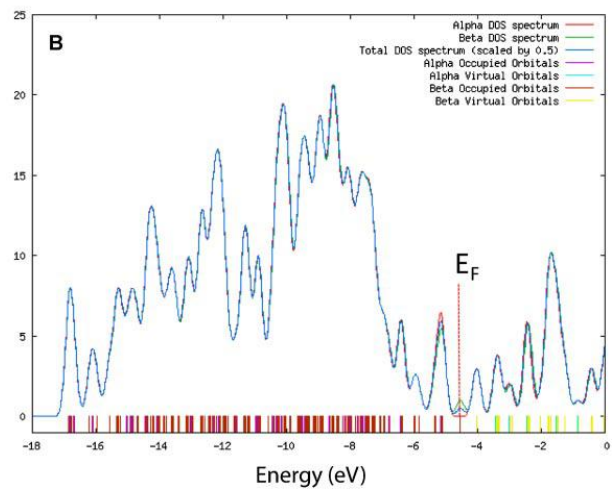
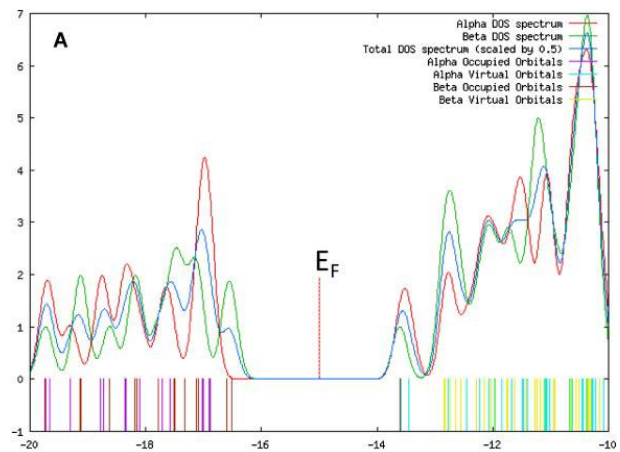
THE CANADIAN JOURNAL OF CHEMICAL ENGINEERING|

Theoretical Studies on the Structure and Electronic Properties of Cubic Gold Nanoclusters

D. Majumdar, Szczepan Roszak and Jerzy Leszczynski



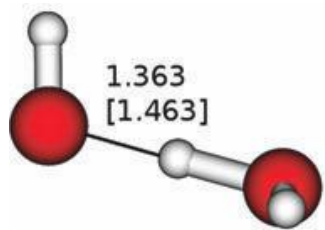




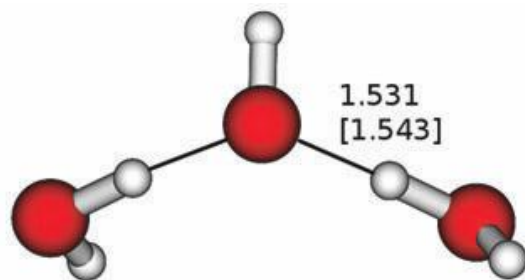
International Journal of Quantum Chemistry 2012, 112, 3046–3051

The Theoretical Studies of Interactions of the $\text{OH}-(\text{H}_2\text{O})_n$ Clusters Evolution Toward the Hydroxide Anion Hydration

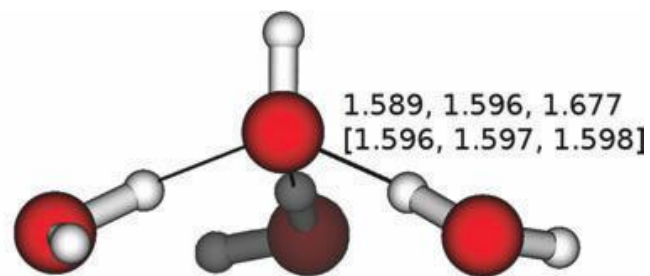
Rafał Roszak, Robert W. Gora, and Szczepan Roszak



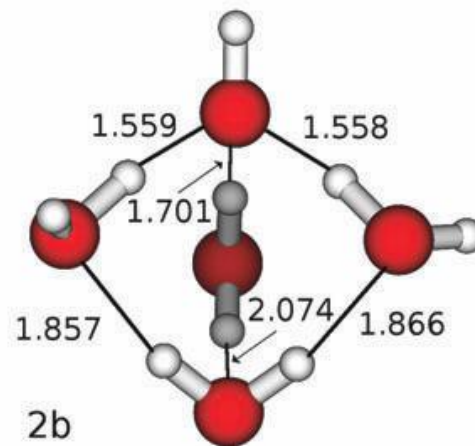
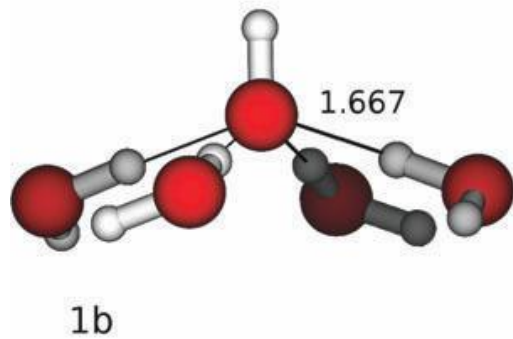
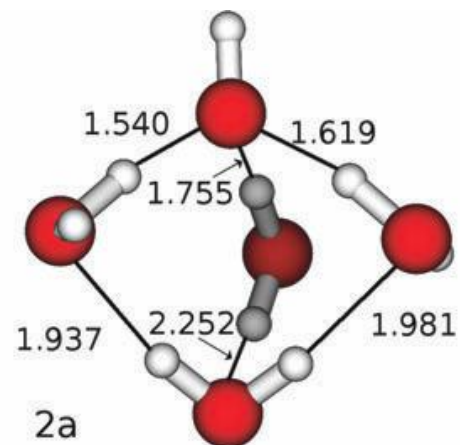
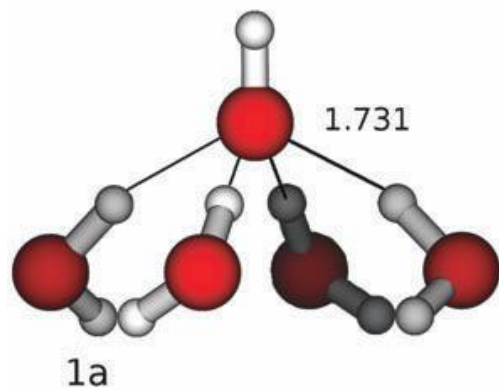
a



b



c

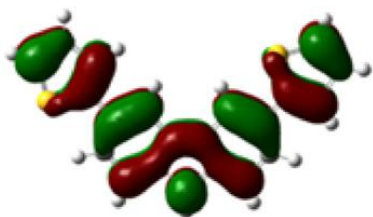


Materials Chemistry and Physics 131 (2012) 757– 763

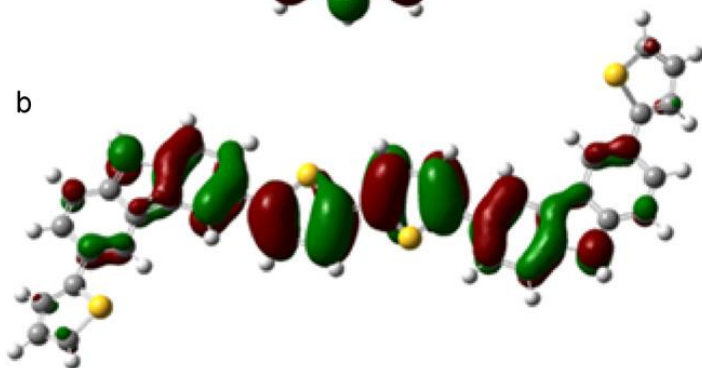
Electrochemical characterization of alternate
conducting carbazole–bisthiophene units

Mieczysław Łapkowski, Przemysław Data,
Anna Nowakowska-Oleksy, Jadwiga
Sołoducho, Szczepan Roszak

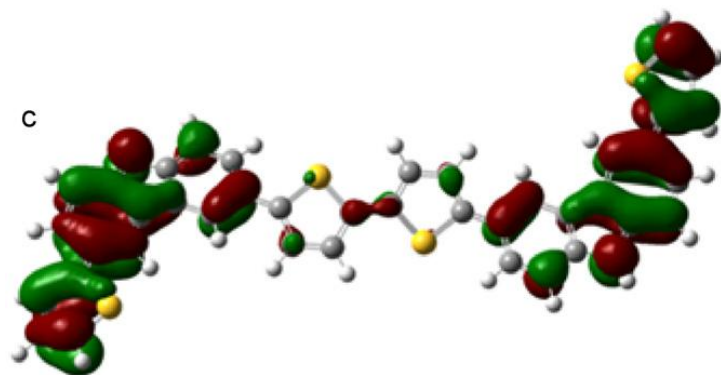
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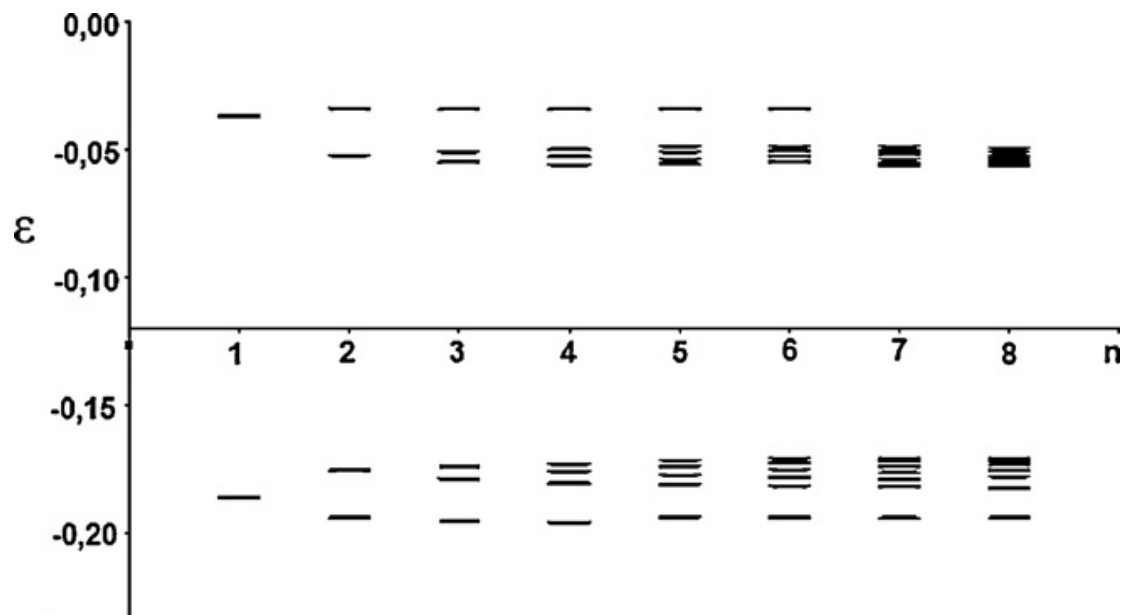


b



c

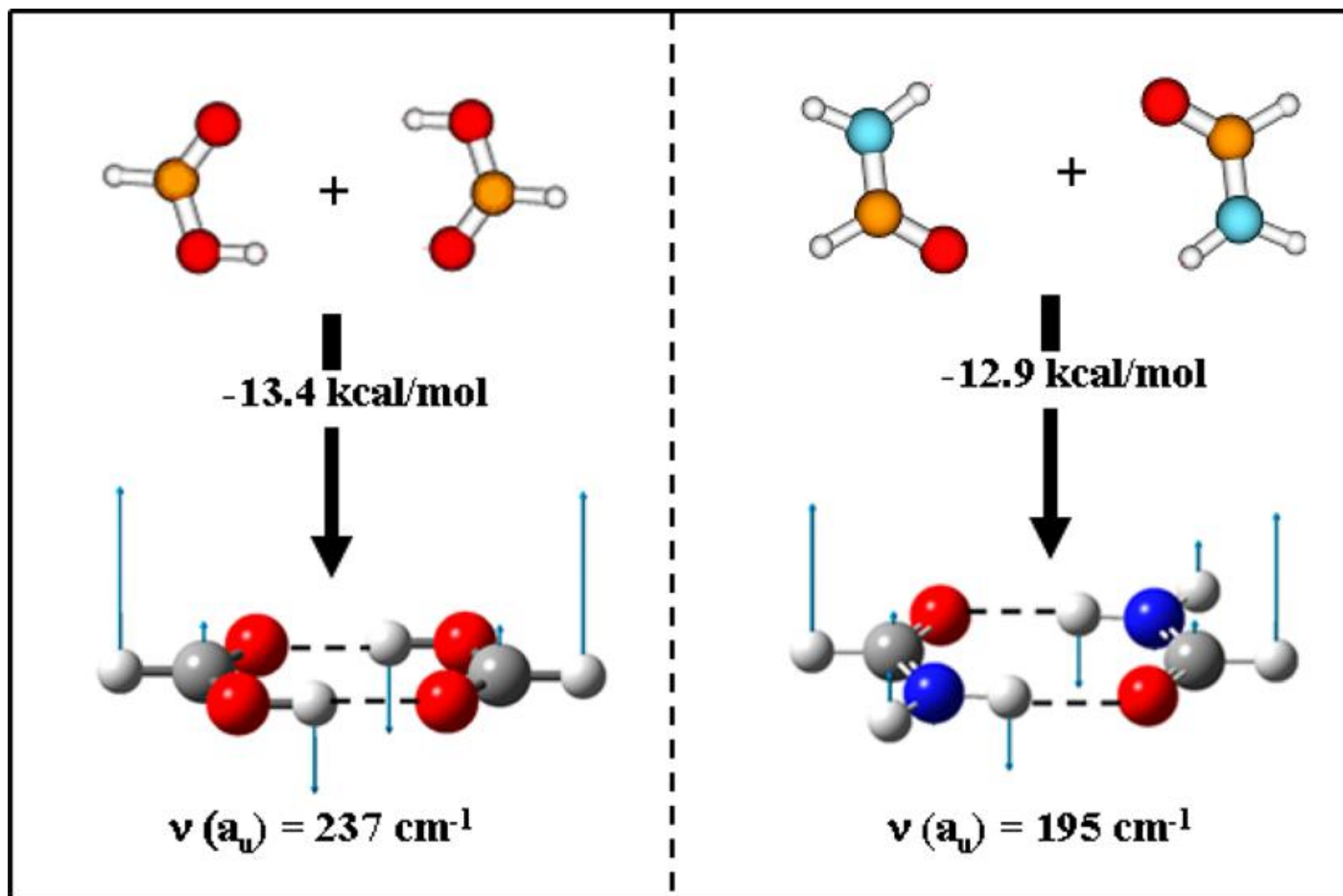


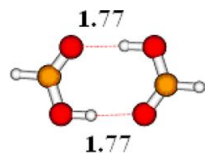


Journal of Theoretical Chemistry and Computation

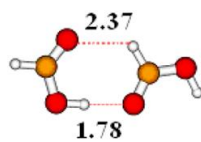
Exploring Relative Thermodynamic
Stabilities of Formic Acid and Formamide
Dimers – Role of Low-Frequency
Hydrogen-Bond Vibrations

Michael Cato, D. Majumdar, Szczepan
Roszak, and Jerzy Leszczynski

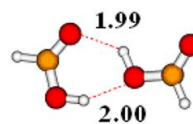




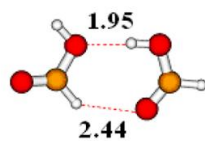
TT-1



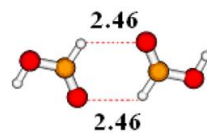
TT-2



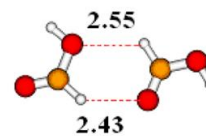
TT-3



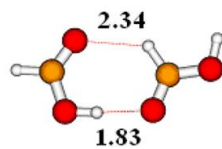
TT-4



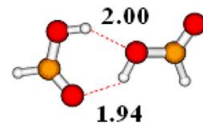
TT-5



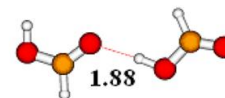
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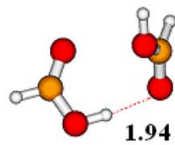
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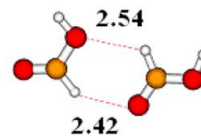
TC-2



TC-3



TC-4



TC-5