P9. Binding of CO, NO, and O2 to heme: An insight from DFT and CASPT2

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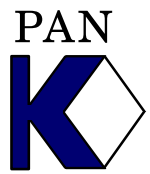
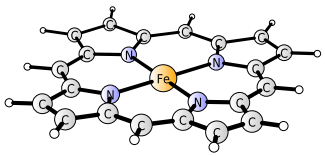
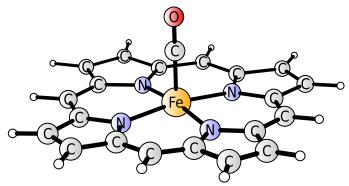
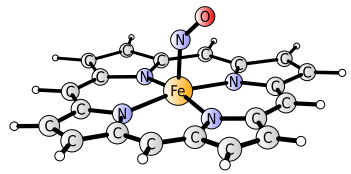
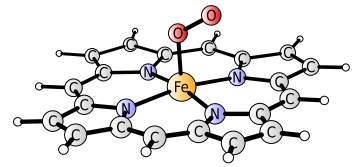
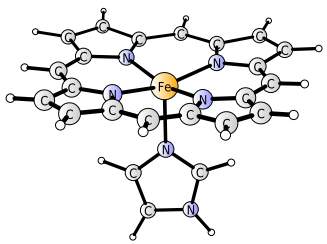
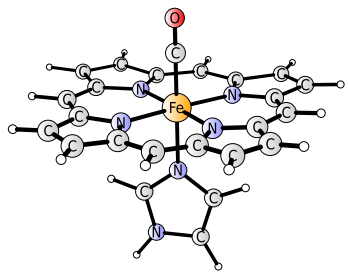
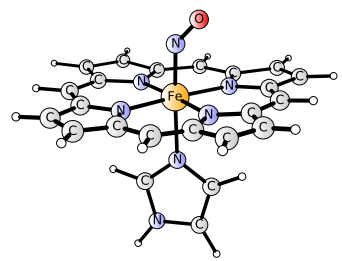
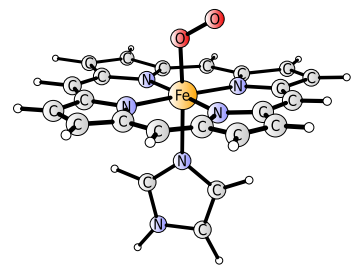
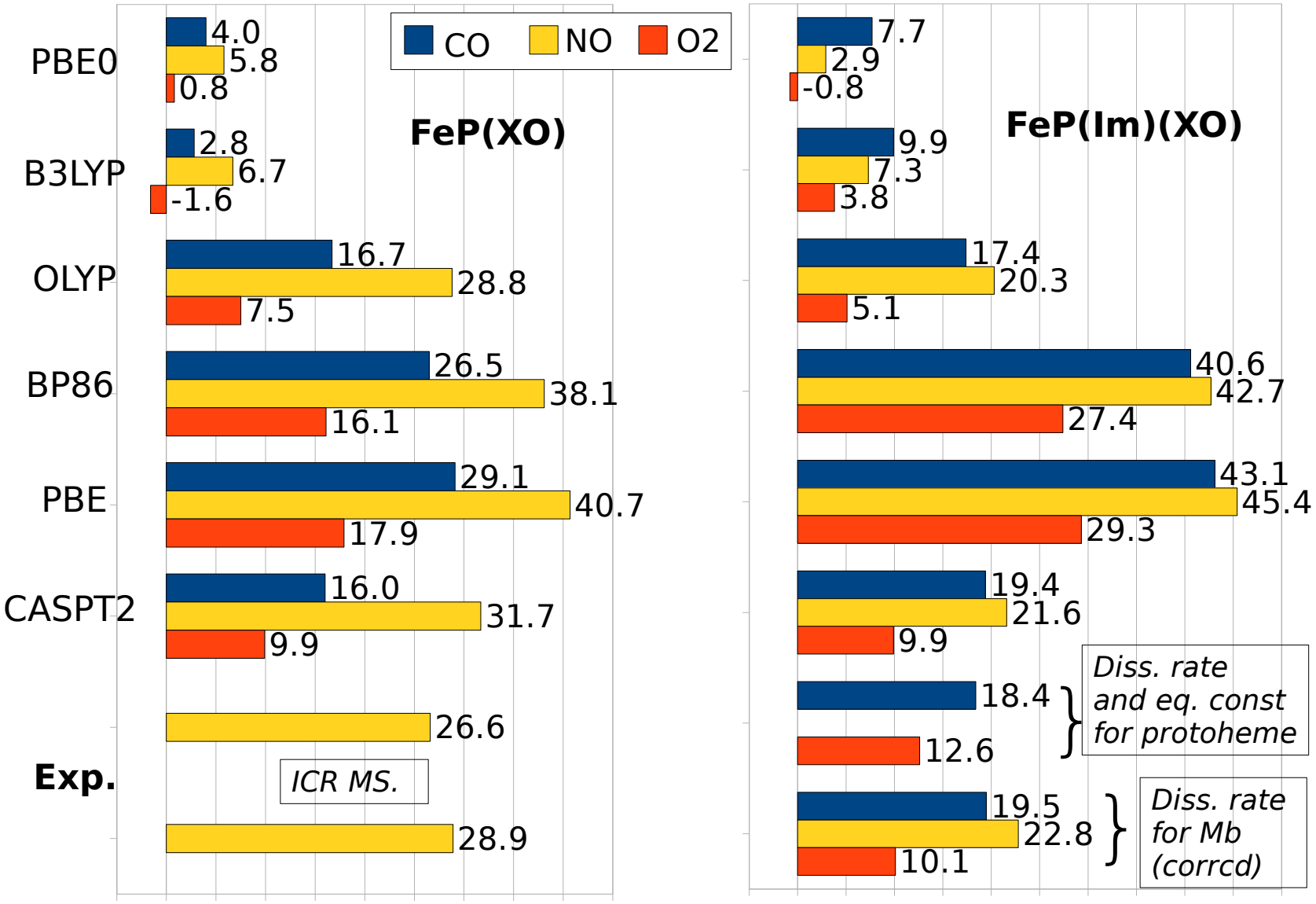


KU KDM, Zakopane 12–13 marca 2009

Model systems

	+CO	+NO	$+O_2$
			
$S = 1$ (?)	$S = 0$	$S = 1/2$	$S = 0$
			
$S = 2$	$S = 0$	$S = 1/2$	$S = 0$

Binding energies [kcal/mol]



Summary

- Ab initio CASSCF/CASPT2 nicely reproduces the experimental binding energies.
- Callibration of DFT against CASPT2 $\Rightarrow$ OLYP.
- How protein effects can be (approximately) accounted for?
- CASSCF and DFT spin densities of the NO complexes.