

Experimental and calculated bond distances for TPSSh/TZVP method using CPM method with water as solvent

LS systems

Bond distance	(66) exp	(66) calc	(56) exp	(56) calc	(55) exp	(55) calc
Fe(1)–N(1) NH <sub>fac</sub>	2.009(5)		2.020(3)		2.020(2)	
		2.047		2.052		2.050
Fe(1)–N(2) N <sub>centr</sub>	2.128(4)		2.047(3)		2.004(2)	
		2.103		2.059		2.022
Fe(1)–N(3) NH <sub>mer</sub>	2.085(6)		1.969(4)		1.989(2)	
		2.053		2.048		2.006
Fe(1)–N(4) py <sub>centr</sub>	2.049(4)		1.964(3)		1.973(2)	
		1.986		1.973		1.982
Fe(1)–N(5) py <sub>fac</sub>	2.033(5)		1.999(3)		1.984(2)	
		1.993		2.004		2.001
Fe(1)–N(6) py <sub>mer</sub>	2.061(4)		1.997(3)		1.974(2)	
		1.997		2.004		1.988

HS systems

Bond distance	(66) exp <sup>a</sup>	(66) calc	(56) calc	(55) calc
Fe(1)–N(1) NH <sub>fac</sub>	2.208(3)			
		2.240	2.255	2.254
Fe(1)–N(2) N <sub>centr</sub>	2.238(2)			
		2.297	2.253	2.244
Fe(1)–N(3) NH <sub>mer</sub>	2.151/2.217(4)			
		2.218	2.217	2.231
Fe(1)–N(4) py <sub>centr</sub>	2.181(2)			
		2.202	2.193	2.204
Fe(1)–N(5) py <sub>fac</sub>	2.191(2)			
		2.204	2.220	2.201
Fe(1)–N(6) py <sub>mer</sub>	2.235(2)			
		2.277	2.198	2.164