Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Non-conventional Hydrogen Bonds: Pterins-Metal Anions

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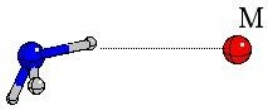
Table 1S. Bond distances (in Å) and angles (in degrees) of $(NH_3\text{-}Au)^{-1}$ optimized at B3LYP/6-311++G(3df,3pd)+LANL2DZ level. Final energy evaluation was done with this optimized geometry at 6-311++G(3df,3pd)+PP level. Available experimental results reported before are included for comparison.



Basis set	Bond Distance		Bond Angle N-H-M	HBE
	H-M	N-M		
B3LYP/ 6-311++G(3df,3pd)+LANL2DZ 6-311++G(3df,3pd)+PP	2.61	3.61	162.8	-5.7
Experimental[1]	2.58	3.63-3.73	158	-6.0

[1] Reference 37 on the paper

Table 2S. Optimized parameters and dissociation energies (De) in the equilibrium geometry of CuOH, AgOH and AuOH, calculated with B3LYP/6-311++G(3df,3pd) for Cu-OH and B3LYP/6-311++G(3df,3pd)+LANL2DZ (for Ag-OH and Au-OH). Final energy evaluation for Ag and Au systems were done at B3LYP/6-311++G(3df,3pd)+PP level. Available experimental results and other theoretical values reported by Ikeda *et al* (Reference 38) are included for comparison.

Method	CuOH			
	De (eV)	R(Cu-O)	R(O-H)	θ (Cu-O-H)
NR-SCF	1.59	1.846	0.943	119.4
NR-CCSD(T)	3.05	1.799	0.973	109.2
DKR3-SCF	1.59	1.826	0.943	117.8
DKR3-CCSD(T)	3.08	1.774	0.974	108.1
Experimental	2.69	1.774	0.964	110.1
B3LYP/6-311++G(3df,3pd)	**2.97**	**1.793**	**0.963**	**110.3**
	AgOH			
	De (eV)	R(Ag-O)	R(O-H)	θ (Ag-O-H)
NR-SCF	1.14	2.101	0.943	120.8
NR-CCSD(T)	2.41	2.084	0.973	109.0
DKR3-SCF	1.00	2.058	0.944	116.4
DKR3-CCSD(T)	2.31	2.035	0.975	106.5
Experimental	-	2.018	0.963	107.8
B3LYP/6-311++G(3df,3pd)+LANL2DZ **B3LYP/6-311++G(3df,3pd)+PP**	**2.27**	**2.057**	**0.985**	**111.0**
	AuOH			
	De (eV)	R(Au-O)	R(O-H)	θ (Au-O-H)
NR-SCF	1.02	2.161	0.943	119.2
NR-CCSD(T)	2.30	2.145	0.974	108.0
DKR3-SCF	0.78	1.981	0.945	109.7
DKR3-CCSD(T)	2.39	1.963	0.977	103.7
B3LYP/6-311++G(3df,3pd)+LANL2DZ **B3LYP/6-311++G(3df,3pd)+PP**	**2.19**	**2.003**	**0.987**	**107.9**