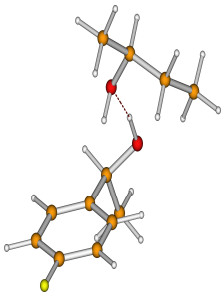
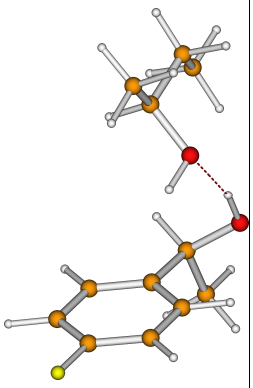
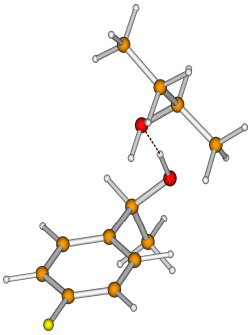
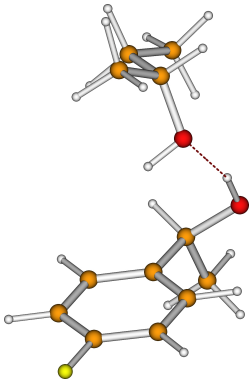
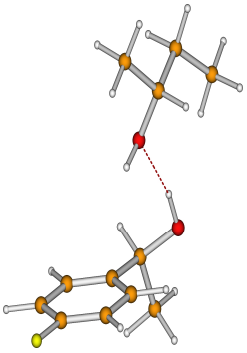
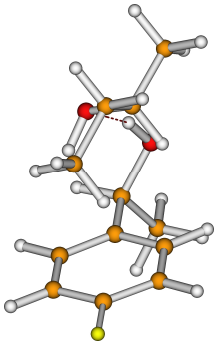
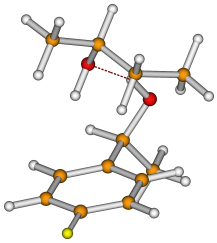
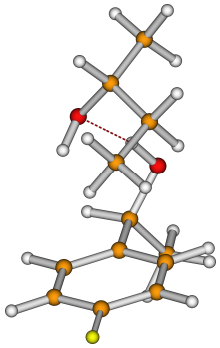
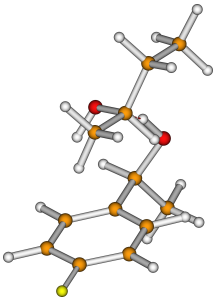
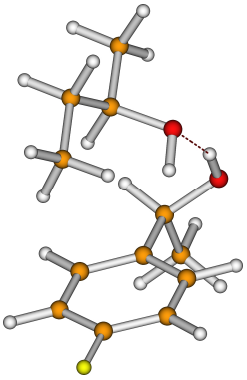
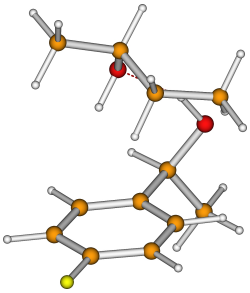
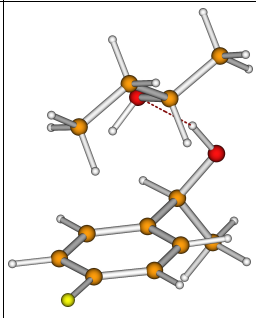
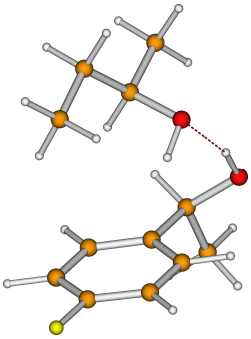
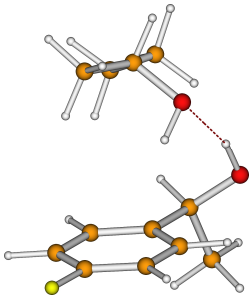
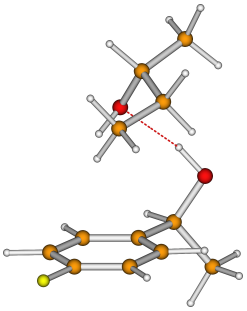
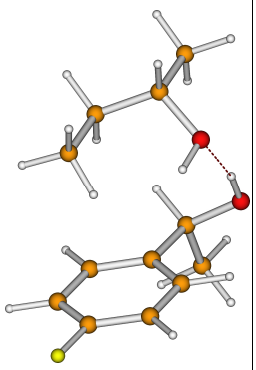
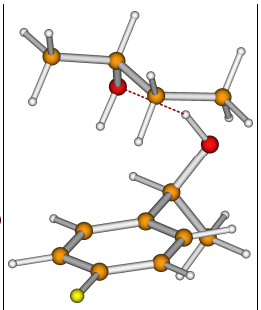
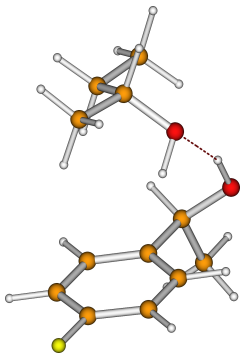
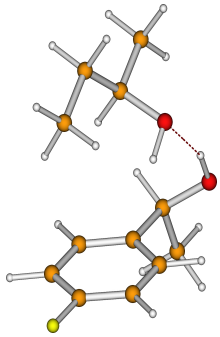
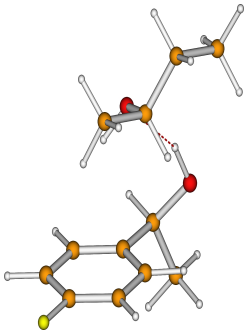
Structures of the most stables conformers of homochiral [FE_S·B_S] and heterochiral [FE_S·B_S] complexes and energies relative to the most stable adduct.

	Homochiral		Heterochiral		
	A_{homo}	B_{homo}	A_{hetero}	B_{hetero}	C_{hetero}
B3LYP	 +0.20 Kcal/mol	 0.00 Kcal/mol	 +0.30 Kcal/mol	 +0.46 Kcal/mol	 +0.63 Kcal/mol
D-B3LYP	 0.0 Kcal/mol	 +0.32 Kcal/mol	 +0.50 Kcal/mol	 +0.56 Kcal/mol	 +0.74 Kcal/mol
B97D	 +0.29 Kcal/mol	 +0.29 Kcal/mol	 0.00 Kcal/mol	 +0.56 Kcal/mol	 +0.89 Kcal/mol

WB97XD	 +0.11 Kcal/mol	 +0.38 Kcal/mol	 0.00 Kcal/mol	 +0.39 Kcal/mol	 +0.46Kcal/mol

νO^bH calculated vibrational frequencies for the S_0 ground state

	A_{homo}	B_{homo}	A_{hetero}	B_{hetero}	C_{hetero}
B3LYP	3623	3621	3617	3662	3651
D-B3LYP	3635	3602	3672	3659	3612
B97D	3517	3552	3558	3530	3553
XB97XD	3751	3664	3700	3714	3700
exp	3637		3610		

Supplementary Material (ESI) for Physical Chemistry Chemical Physics