Table S1: Relevant bond distances of the neutral (S_0) structures shown in Figure 5.

Bonds	Distances (Å)				
	Structure I	Structure II	Structure III	Structure IV	Structure V
O1-H1	0.98008	1.27489	1.48338	1.56939	1.94759
H1-O2	1.80630	1.15986	1.03418	1.00782	0.97239
O2-H2	0.98751	1.41996	1.63620	1.75610	2.18399
H2-N1	1.86535	1.14371	1.06031	1.03876	1.02098
N1-H3	1.01929	1.05704	1.11313	1.21945	1.81828
H3-O1	2.41828	1.71447	1.53563	1.33608	0.99313

Table S2: Relevant bond distances of the neutral (S_0) structures shown in Figure 8.

Bonds	Distances (Å)					
	Structure I	Structure II	Structure III	Structure IV	Structure V	Structure VI
O1-H1	1.05477	1.28557	1.51636	1.67023	1.90102	4.20898
H1-O2	1.43269	1.13623	1.02012	0.98976	0.97566	0.96416
O2-H2	1.01977	1.10133	1.43075	1.65049	1.70589	1.74378
H2-N1	1.67533	1.44746	1.12529	1.05917	1.04972	1.04411
N1-H3	1.01766	1.01863	1.02120	1.04025	1.04965	1.07005
H3-O1	4.51866	4.11680	3.86105	1.89171	1.76684	1.57982