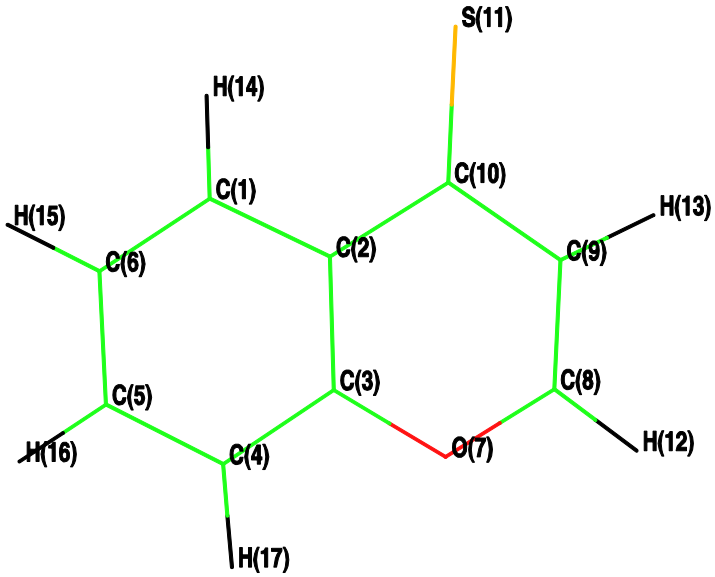
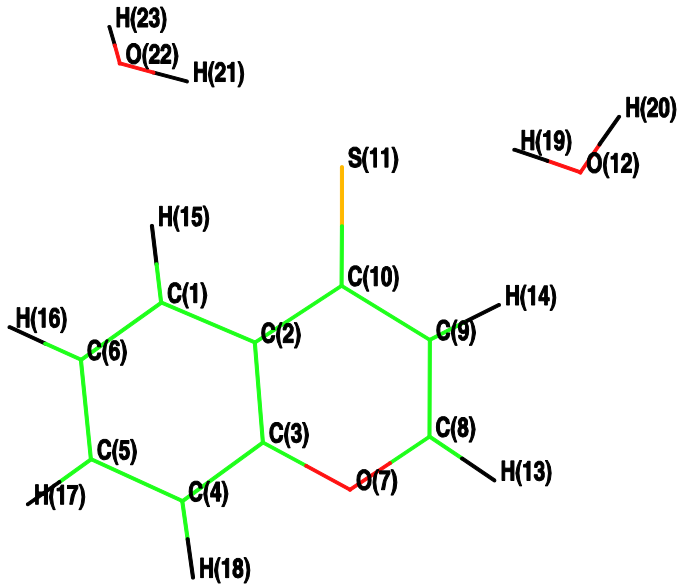


Atomic charges q (in e) for the ground state S_0 of the BPT molecule and changes in the atomic charges Δq due to excitation to the states S_1 and S_2

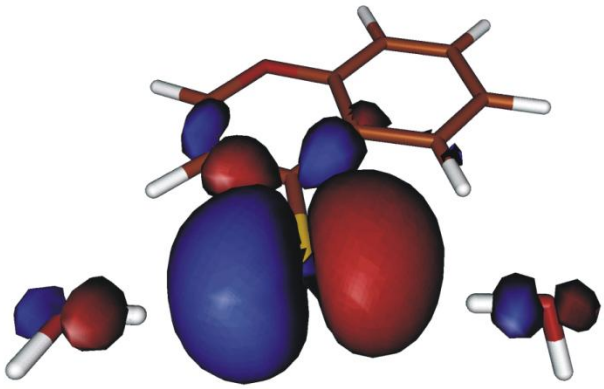
Atom	Number	q (S_0)	Δq (S_1)	Δq (S_2)
C	1	-0.191	0.071	0.064
C	2	-0.128	-0.279	-0.031
C	3	0.313	0.008	-0.047
C	4	-0.226	-0.015	0.031
C	5	-0.214	0.011	0.006
C	6	-0.198	0.019	-0.036
O	7	-0.482	-0.009	0.051
C	8	0.208	-0.018	-0.003
C	9	-0.310	-0.039	-0.037
C	10	-0.203	0.379	0.138
S	11	-0.002	-0.011	-0.106
H	12	0.216	-0.018	-0.006
H	13	0.256	-0.029	0.004
H	14	0.253	-0.053	-0.024
H	15	0.233	-0.005	0.005
H	16	0.232	-0.010	-0.004
H	17	0.244	-0.003	-0.006



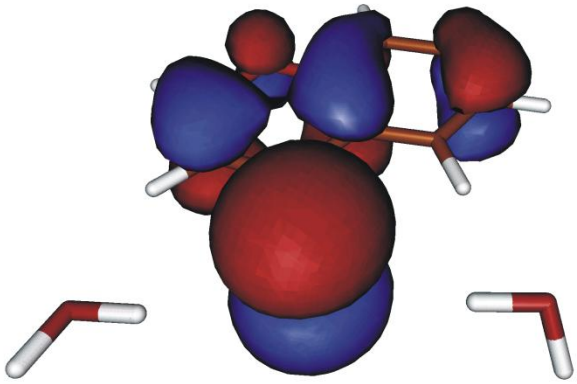
Atomic charges q (in e) for the ground state S_0 of the **a**&**b** BPT-water complex and changes in the atomic charges Δq due to excitation to the states S_1 and S_2

Atom	Number	q (S_0)	Δq (S_1)	Δq (S_2)
C	1	-0.191	0.106	0.085
C	2	-0.126	-0.302	-0.060
C	3	0.316	0.012	-0.030
C	4	-0.225	-0.019	0.018
C	5	-0.211	0.007	0.009
C	6	-0.189	-0.002	-0.048
O	7	-0.470	-0.014	0.041
C	8	0.222	-0.018	-0.004
C	9	-0.311	-0.047	-0.057
C	10	-0.166	0.336	0.176
S	11	-0.087	0.054	-0.107
O	12	-0.991	0.021	0.001
H	13	0.220	-0.020	-0.010
H	14	0.274	-0.025	0.005
H	15	0.254	-0.040	-0.011
H	16	0.237	-0.008	0.004
H	17	0.233	-0.011	-0.003
H	18	0.245	-0.004	-0.003
H	19	0.487	-0.038	-0.003
H	20	0.487	0.012	0.000
H	21	0.486	-0.023	-0.002
O	22	-0.977	0.011	-0.001
H	23	0.482	0.012	0.000

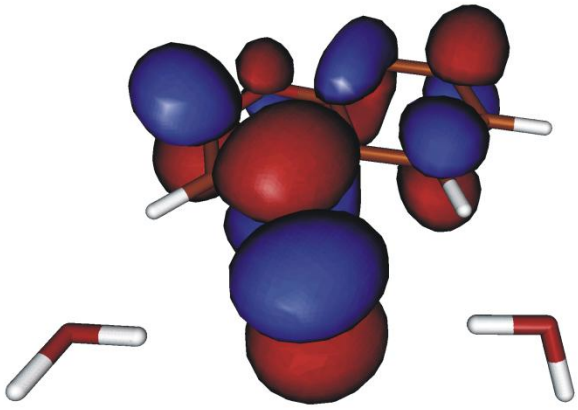
Molecular orbitals of the hydrogen-bonded BPT-water complex



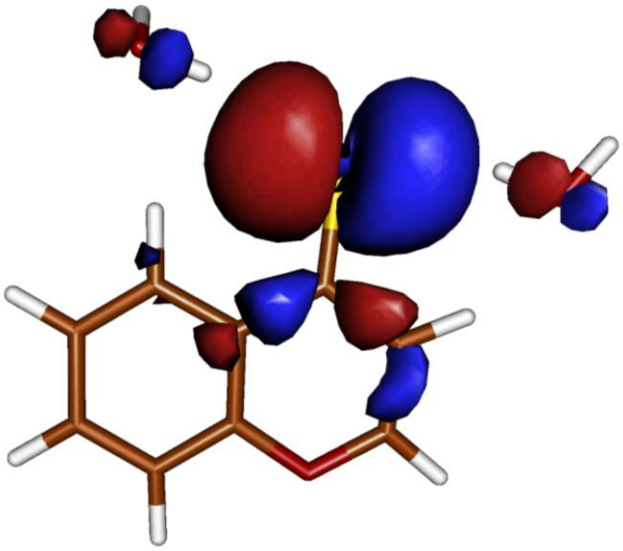
Orbital no 51 (HOMO-1, *n*)



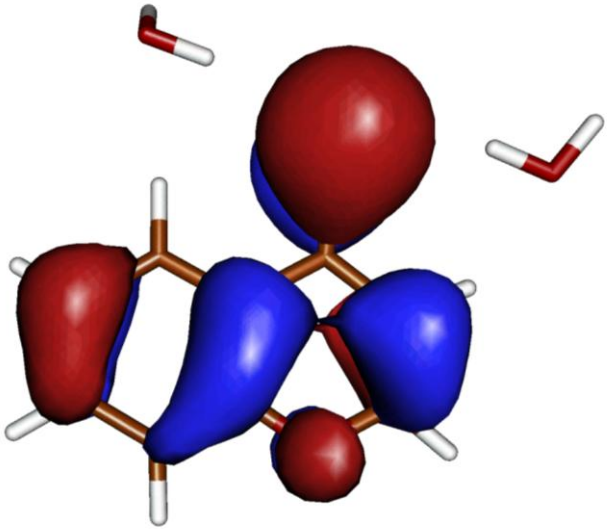
Orbital no 52 (HOMO, π)



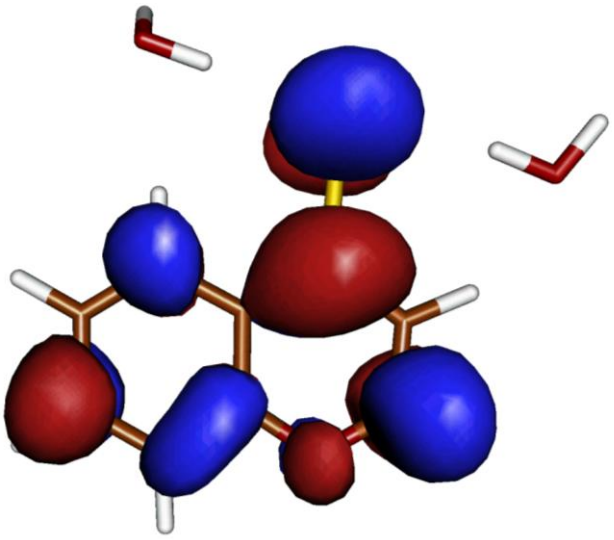
Orbital no 53 (LUMO, π*)



Orbital no 51 (HOMO-1, *n*)



Orbital no 52 (HOMO, π)



Orbital no 53 (LUMO, π*)