Supporting Information for

Molecular Dynamics of Excited State Intramolecular Proton Transfer: 2-(2′-hydroxyphenyl)-4-methyloxazole in Gas Phase, Solution, and Protein Environments

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Table 1: Modified GROMOS charge parameters corresponding to the S_0 and S_1 states of HPMO. The atom numbers correspond to Figure 1 of the paper.

at. num	S_0	S_1
1	0.398	0.398
2	-0.548	-0.570
3	0.150	0.150
4	-0.100	-0.100
5	0.100	0.100
6	-0.100	-0.180
7	0.100	0.100
8	-0.100	0.000
9	0.100	0.100
10	-0.100	-0.228
11	0.100	0.100
12	0.000	0.100
13	0.300	0.200
14	-0.360	-0.360
15	0.110	0.160
16	0.210	0.230
17	-0.580	-0.540
18	0.210	0.230
19	0.110	0.110

Table 2: Modified GROMOS parameters corresponding to the S_1 state of HPMO. The atom numbers correspond to Figure 1 of the paper. The units for the force constants k_0 are $\left[10^6 \mathrm{kJ} \cdot \mathrm{mol}^{-1} \cdot \mathrm{nm}^{-4}\right]$ for bond distances and $\left[\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right]$ for bond angles and dihedral angles. The units for the equilibrium values q_0 are nm for bond distances and degrees for bond angles and dihedral angles.

atoms	k_0	q_0
C12-C13	0.715E+07	0.14
C3-C12-C13	0.652E+03	145.0
C12-C13-N17	0.630E+03	145.0
H1-O2-C3-C12	12.5	0.0
H1-N17-C13-C12	12.5	0.0