

# Supporting Information

for

## Linear Absorption Spectra of Solvated Thiouracils Resolved at the Hybrid RASPT2/MM level

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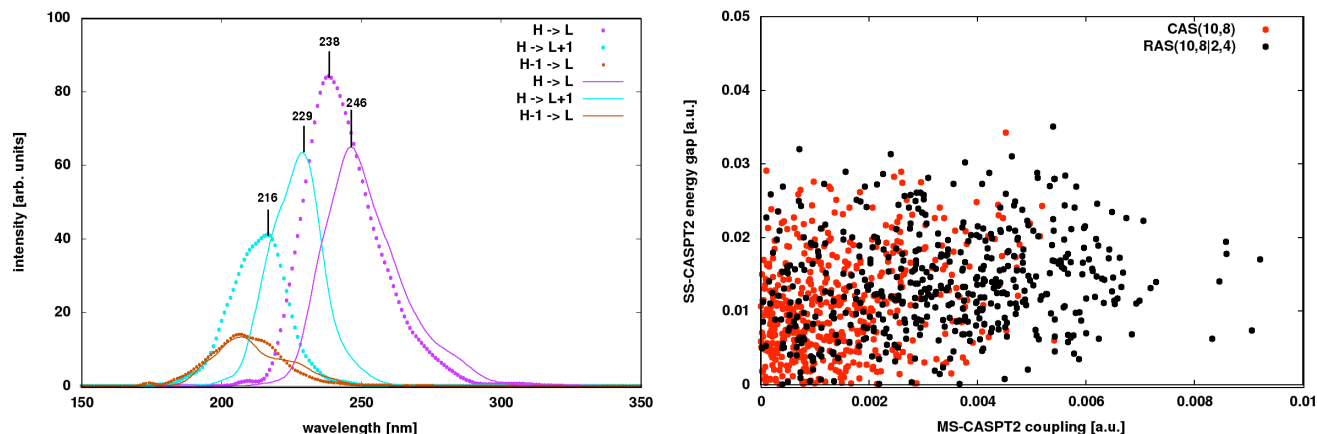
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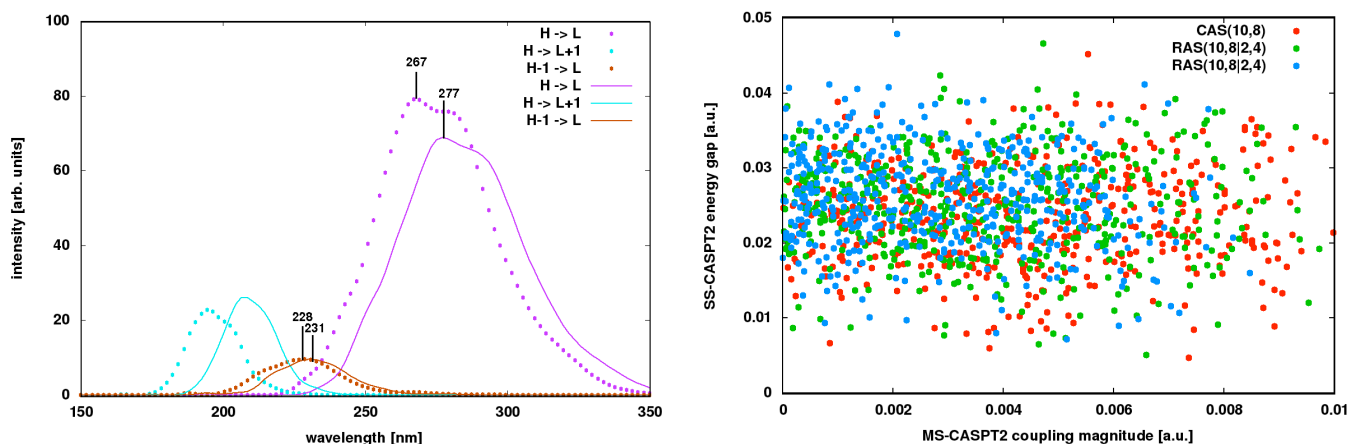
### Table of Contents

S1. Supporting pictures	2
S2. Cartesian coordinates	4

## S1. Supporting pictures

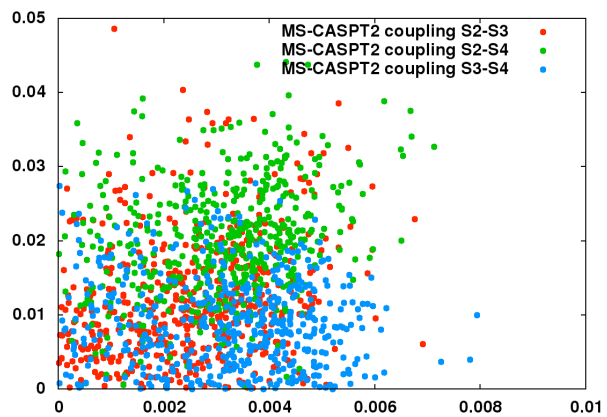


**Figure S1.** left: State assignment in 2-thiouracil at the SA-4-CASSCF(10,8) (dotted lines) and at the SA-4-RASSCF(10,8|2,4) (solid lines) levels. right: cross-correlation of the MS-CASPT2 off-diagonal Hamiltonian matrix elements and the energy gaps between the  $\pi_{S_2} \rightarrow \pi_1^*$  and the  $\pi_{S_2} \rightarrow \pi_2^*$  states of 2-thiouracil with CAS(10,8) and RAS(10,8|2,4). Representation for all 500 snapshots generated through the Wigner sampling procedure.



**Figure S2.** State assignment in 4-thiouracil at the SA-4-CASSCF(10,8) (dotted lines) and at the SA-4-RASSCF(10,8|2,4) (solid lines) levels.

**Figure S3.** Cross-correlation of the MS-CASPT2 off-diagonal Hamiltonian matrix elements and the energy gaps between the  $\pi_4 \rightarrow \pi_1^*$  and the  $\pi_{S_4} \rightarrow \pi_2^*$  states of 4-thiouracil as a function of the AS size. Representation for all 500 snapshots generated through the Wigner sampling procedure.



**Figure S4.** Cross-correlation of the MS-CASPT2 S2-S3, S2-S4 and S3-S4 off-diagonal Hamiltonian matrix elements and the energy gaps in 2,4-thiouracil at the RASPT2/SA-5-RASSCF(10,8|2,8) level. Representation for all 500 snapshots generated through the Wigner sampling procedure.

## S2. Cartesian coordinates

### 2-Thiouracil (S<sub>0</sub> Minimum)

N	18.403170	17.249006	14.500337
C	18.611751	16.345328	15.513426
N	17.621679	16.327180	16.452333
C	16.493380	17.076727	16.358125
C	16.283901	17.914671	15.312977
C	17.267459	18.000450	14.275570
S	19.948320	15.379308	15.565652
O	17.157652	18.685947	13.241634
H	15.362773	18.467244	15.229863
H	15.781898	16.954058	17.161785
H	19.119936	17.240754	13.771182
H	17.701283	15.659527	17.224323

### 4-Thiouracil (S<sub>0</sub> Minimum)

C	17.803042	18.030324	16.491376
N	18.661627	17.002731	16.231633
C	18.410827	16.057711	15.278065
C	17.318758	16.138658	14.477283
C	16.426965	17.250824	14.598700
N	16.752104	18.128950	15.609377
H	17.124179	15.377005	13.740260
S	15.077605	17.502492	13.673507
O	17.941570	18.789844	17.447464
H	19.124280	15.250151	15.226637
H	16.118840	18.911060	15.770608
H	19.485142	16.940630	16.830954

### 2,4-Thiouracil (S<sub>0</sub> Minimum)

C	17.758255	16.301952	14.599252
N	18.131406	17.579555	14.275703
C	18.362323	18.552336	15.193147
C	18.263599	18.303582	16.524489
C	17.939243	16.986060	16.971374
N	17.663609	16.092118	15.958477
H	18.477678	19.068402	17.253527
S	17.895142	16.522788	18.563300
S	17.459143	15.141300	13.472565
H	18.646595	19.512943	14.789113
H	17.358842	15.157812	16.223297
H	18.249552	17.797764	13.287043