Supporting information for:

Exploring Microsolvation of the Anesthetics Propofol

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Figure S1. S_1 state lifetimes, for propofol·$(H_2O)_n$, n=0-2 red-most isomer, determined recording the variation in the signal intensity as a function of the delay between pump and probe lasers in a 2-color REMPI experiment. Extraction of the S1 lifetime is performed through an iterative reconvolution procedure that tries to get the values of the parameters which provide the best match between experimental data and calculated decay, while minimizing the deviation. The blue dots in the graphics represent the experimental data, while the dotted red line is the best fit. The lifetime in ns is indicated in an insert for each species.

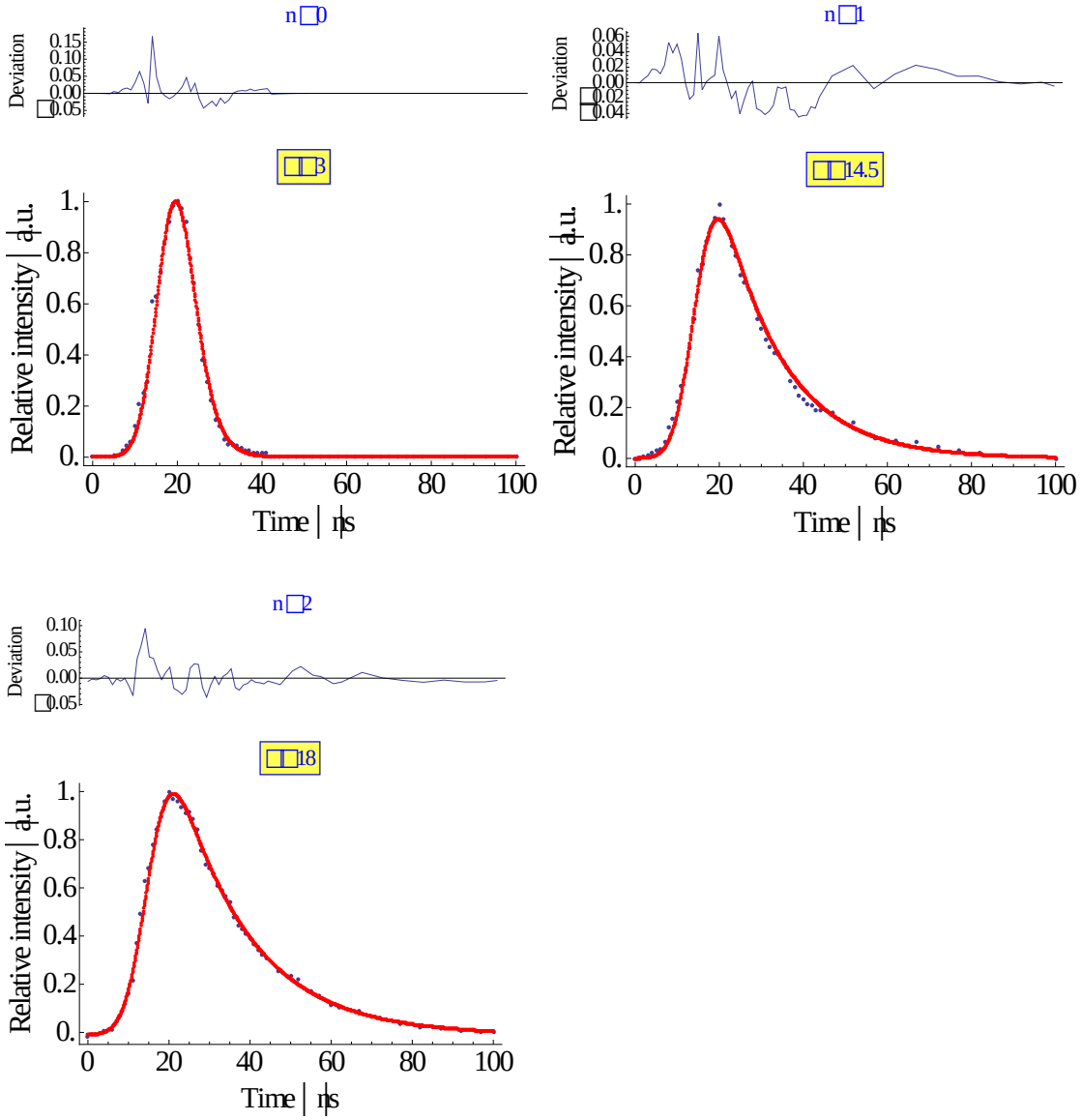
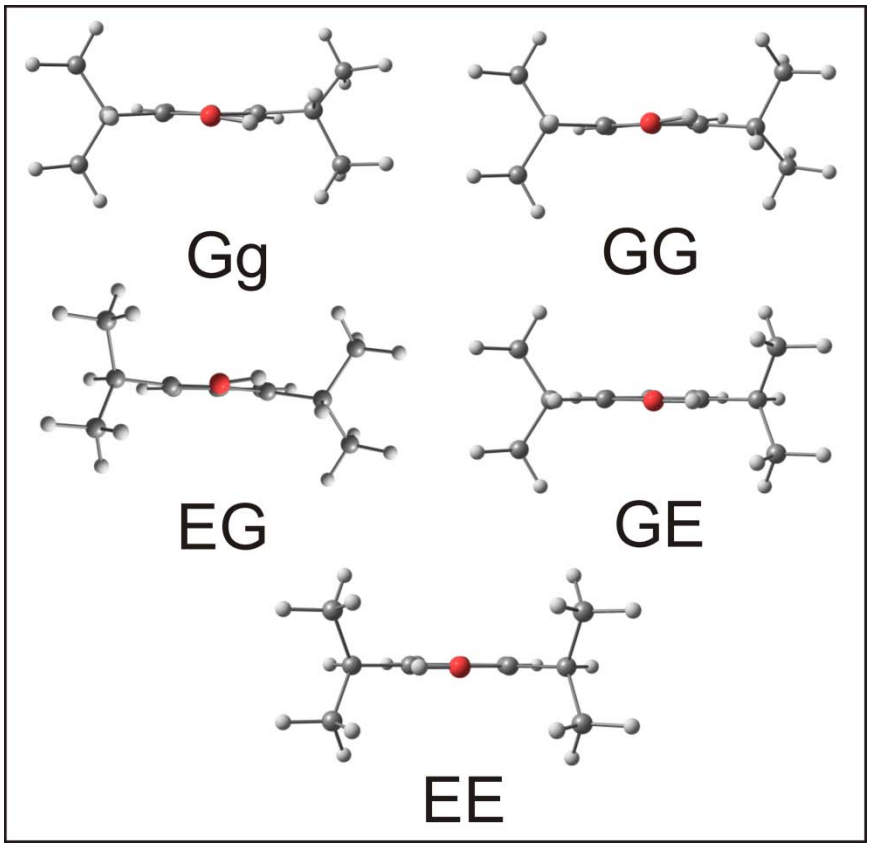


Figure S2. Propofol excited state minimum energy structures, calculated at CIS/6-31G(d,p) level. The angle between the isopropyl groups and the phenyl ring changes upon excitation resulting in a reduction on the number of isomers, as GG and Gg structures converge to the same structure in the excited state.



Figures S03-05. Animation of propofol's three lowest normal modes, as calculated at MP2/6-311++G(d,p) level (separate .gif files).

Figure S6. Propofol-W_1 isomers calculated at MP2/6-311++G(d,p) level below 10 kJ/mol., with their relative energies in kJ/mol. ip: in plane; oop: out of plane. π: interaction with the π cloud; donor: water acting as a donor; ring: water-ring interaction.

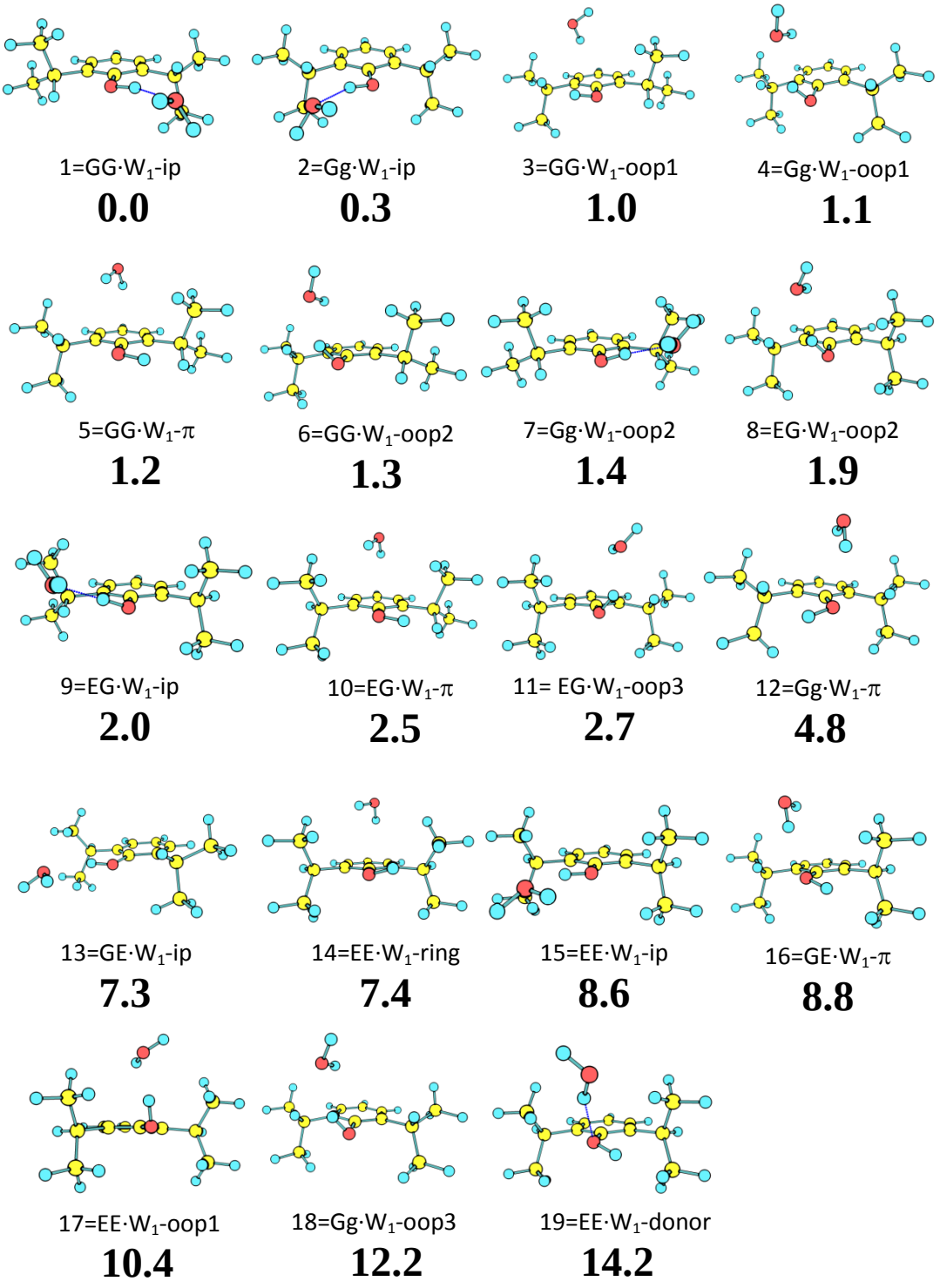


Figure S7. Propofol-W_2 isomers calculated at MP2/6-311++G(d,p) level with relative energies in kJ/mol. ip: in plane; oop: out of plane. π: interaction with the π cloud; donor: water acting as a donor; ring: water-ring interaction.

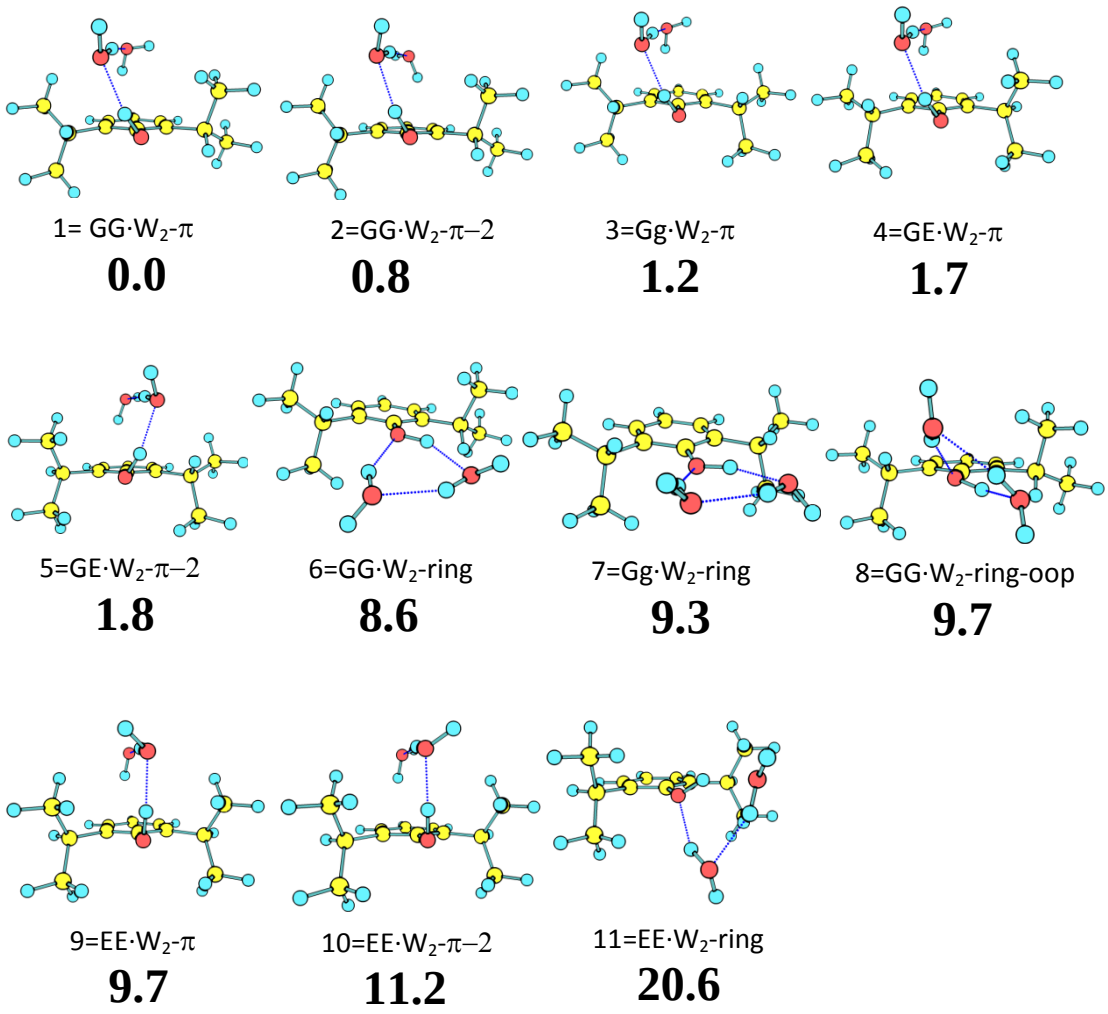


Figure S8. Comparison between the IRID spectra of propofol-W_1 recorded tuning the probe laser at 36030, 36064 and 36120 cm^{-1} and the predicted IR spectra for the calculated isomers.

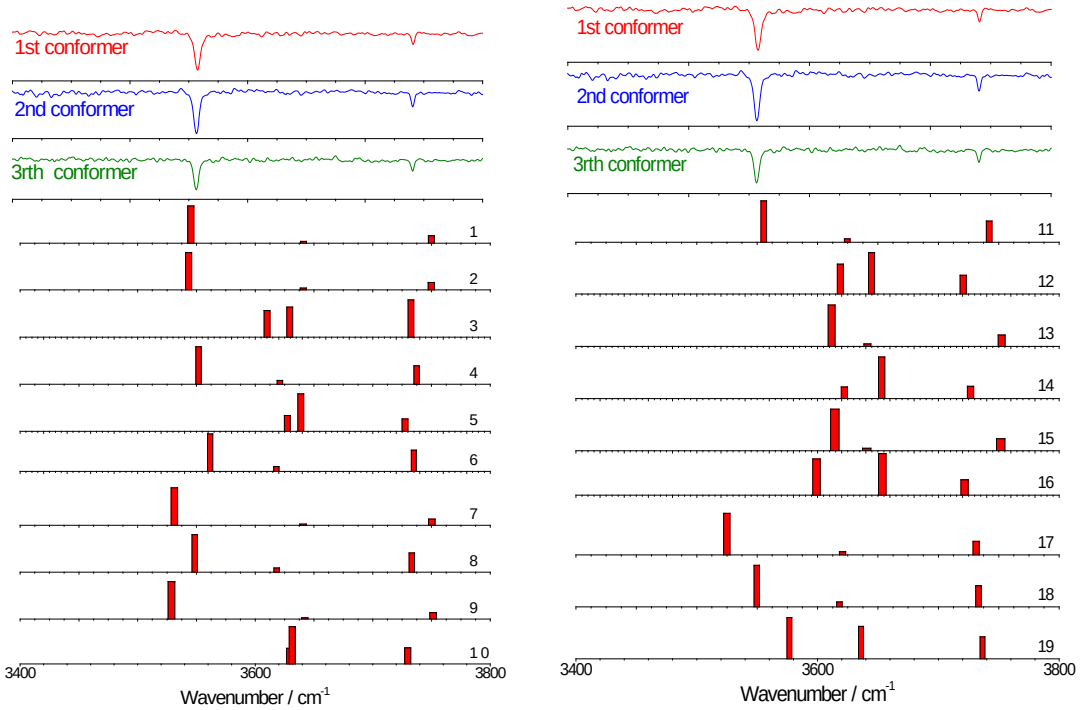


Figure S9. Comparison between the IRID spectra of propofol-W_2 recorded tuning the probe laser at 36030, 36064 and 36120 cm^{-1} and the predicted IR spectra for the calculated isomers.