Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Info for:

Formation of water polyhedrons in propofol-water clusters

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KEYWORDS: electronic spectroscopy, jets, hydrogen bond, solvation, anesthetics, IR spectroscopy.

Figure S01. Propofol conformers with their relative energies in kJ/mol, as calculated at MP2/6-311++G(d,p) level.

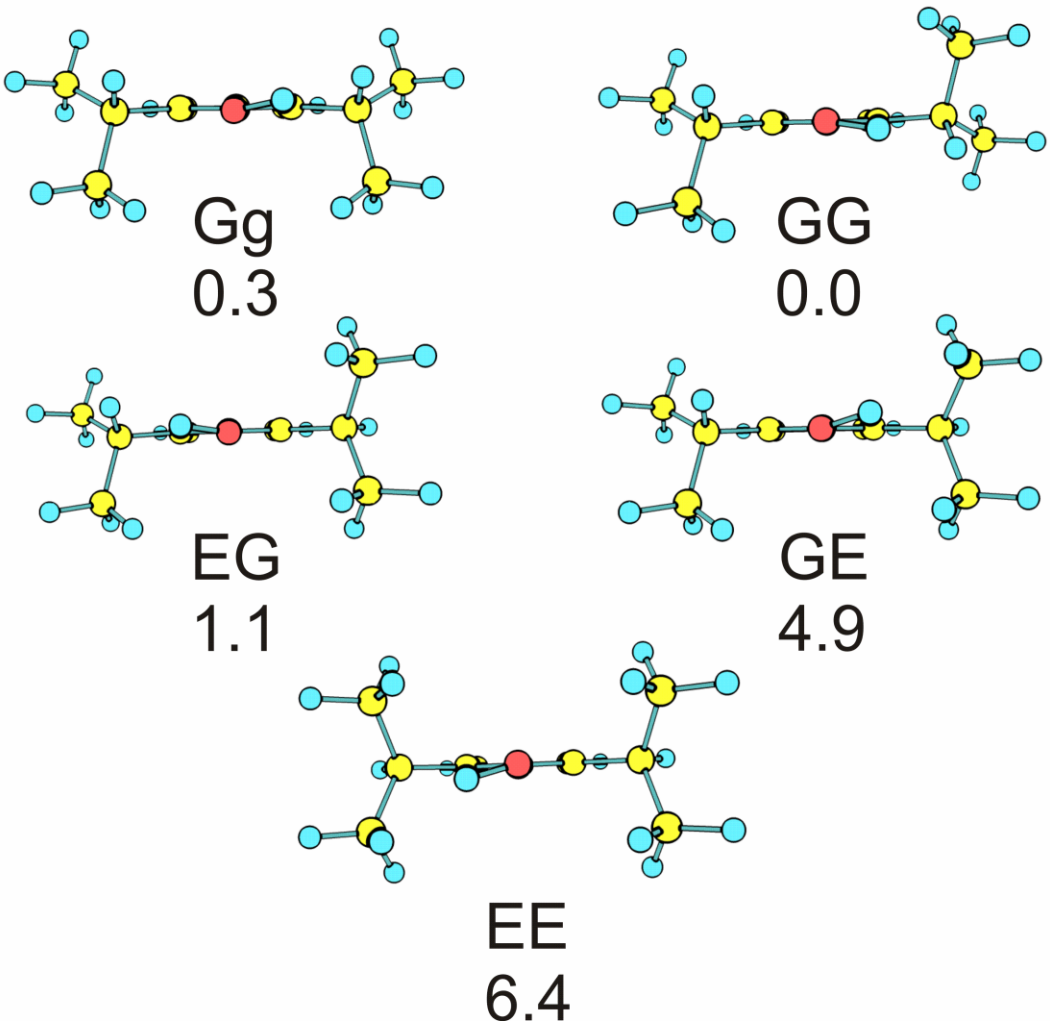


Figure S2. Calculated structures for propofol$_1$(H_2O)$_7$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values

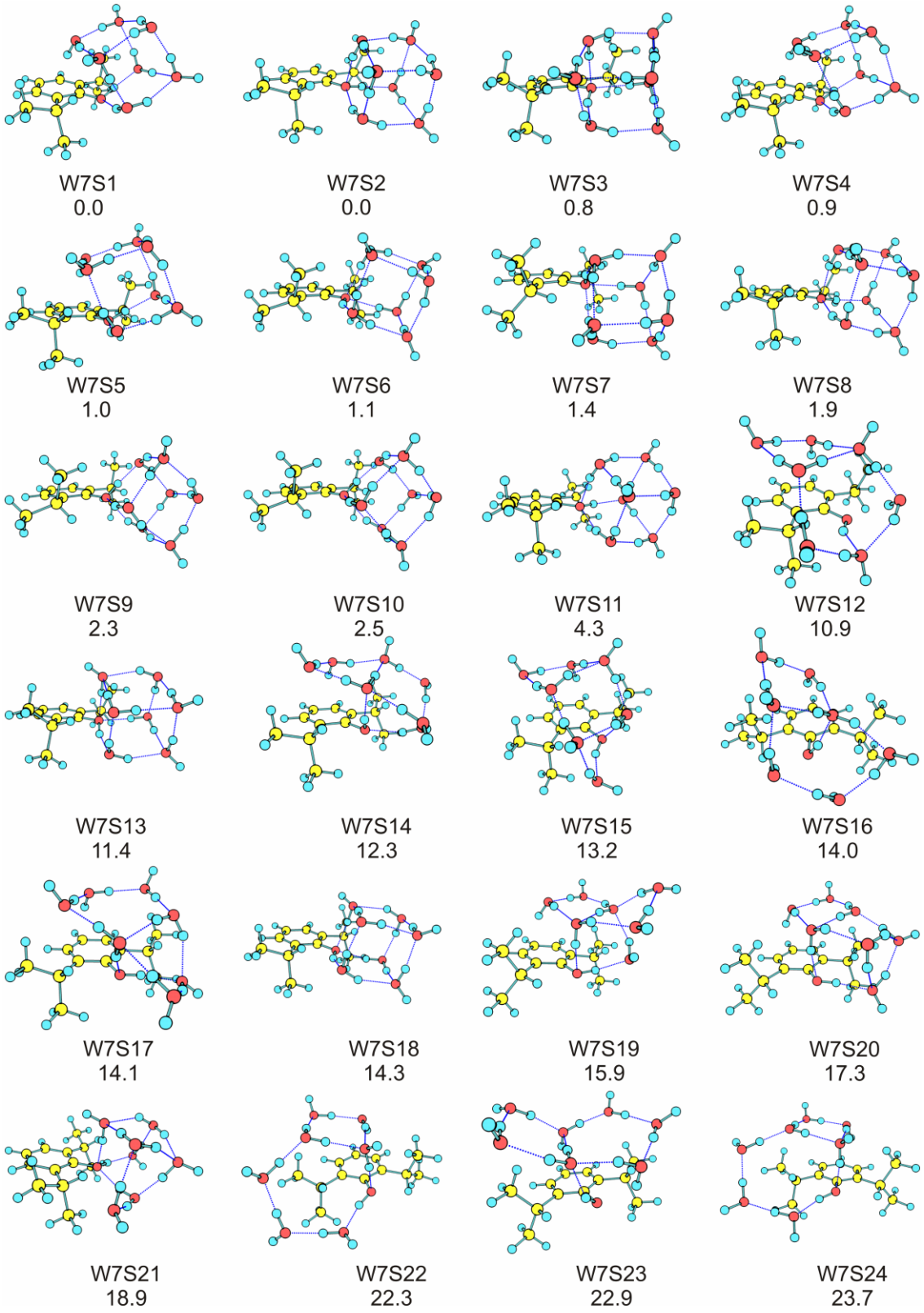


Figure S2.(Cont.)

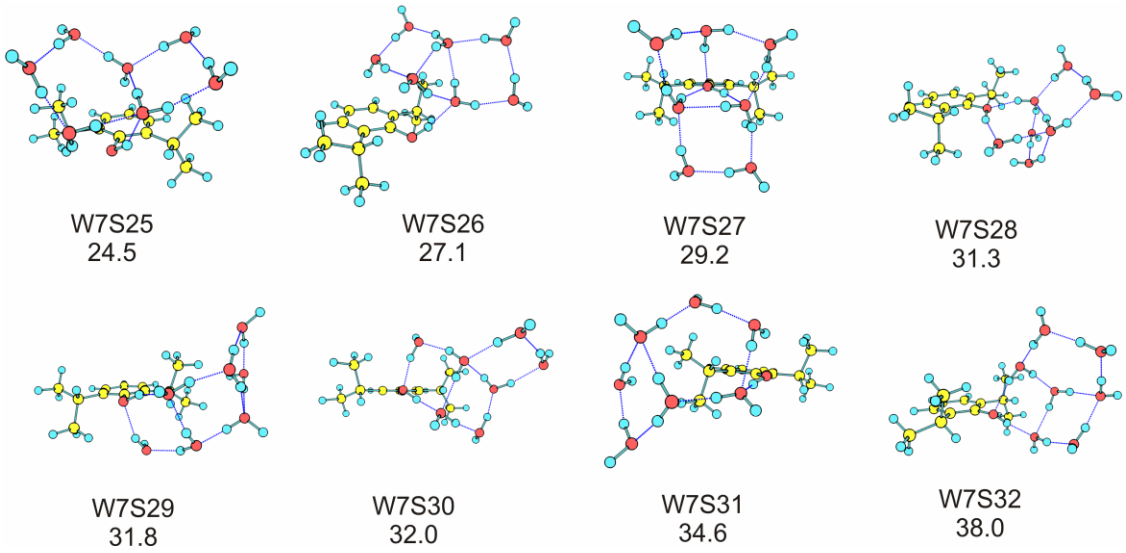


Figure S3. Experimental IDIRS for propofol$_1$(H$_2$O)$_7$ (upper trace) together with the predicted frequencies for each calculated structure. A correction factor of 0.938 was employed.

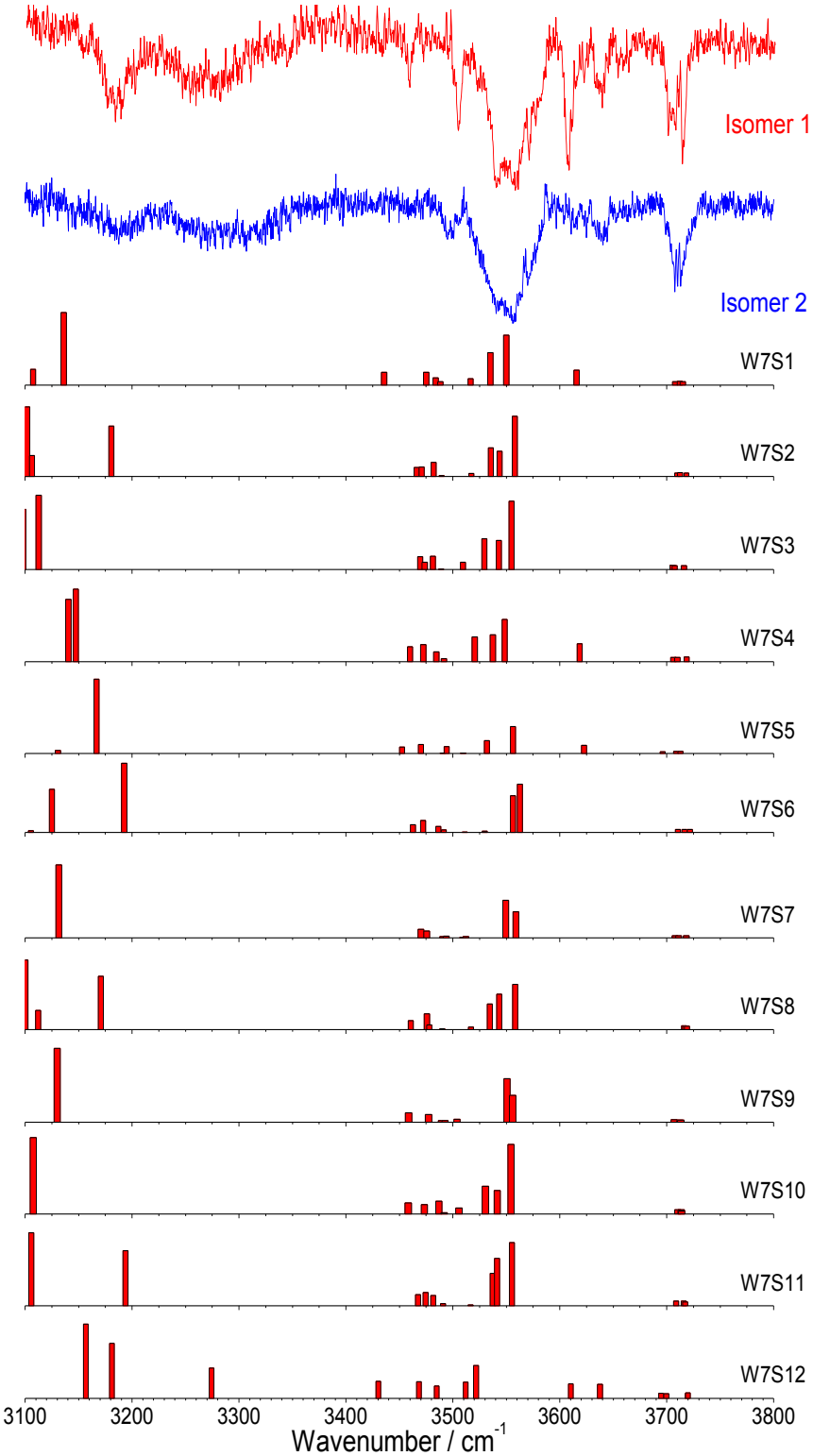


Figure S3.(Cont.)

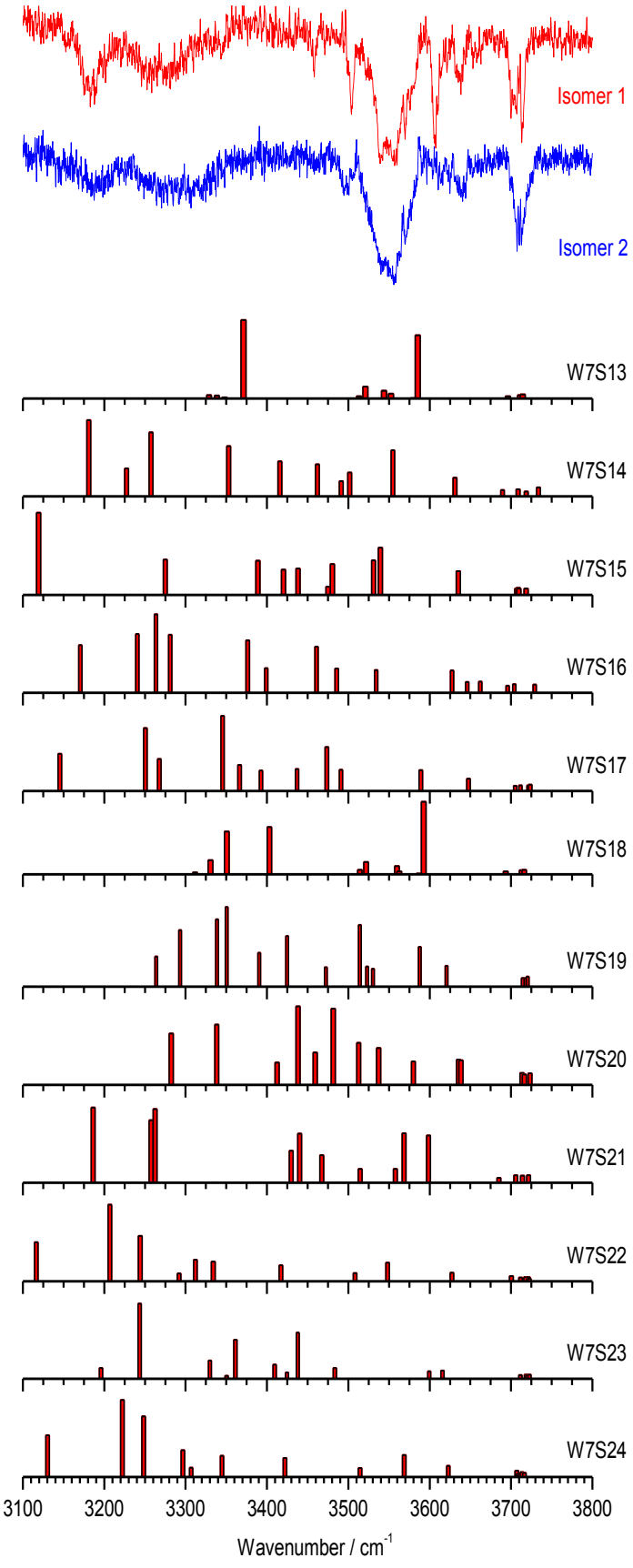
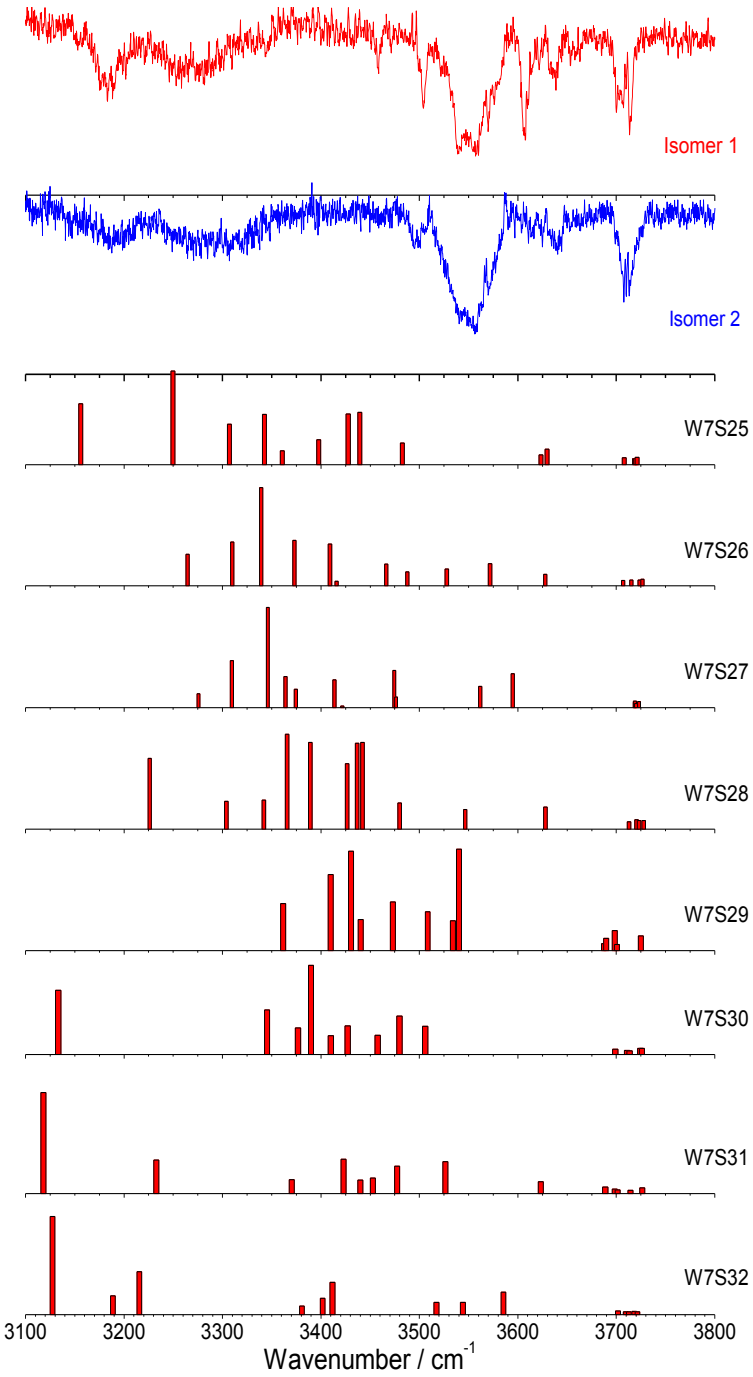


Figure S3 (cont.)



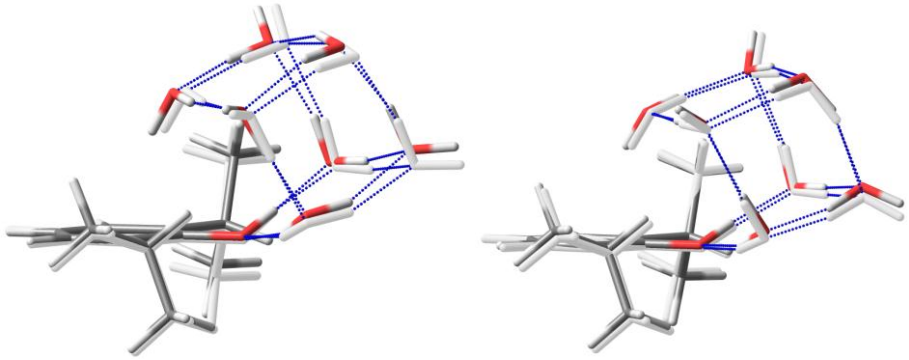


Figure S4. Comparison between the structures of W7S1 (left) and W7S4 (right) calculated at M06-2X/G-311++G(d,p) and at M06-2X/AUG-cc-pVTZ (in white). Small differences between the two structures are found.

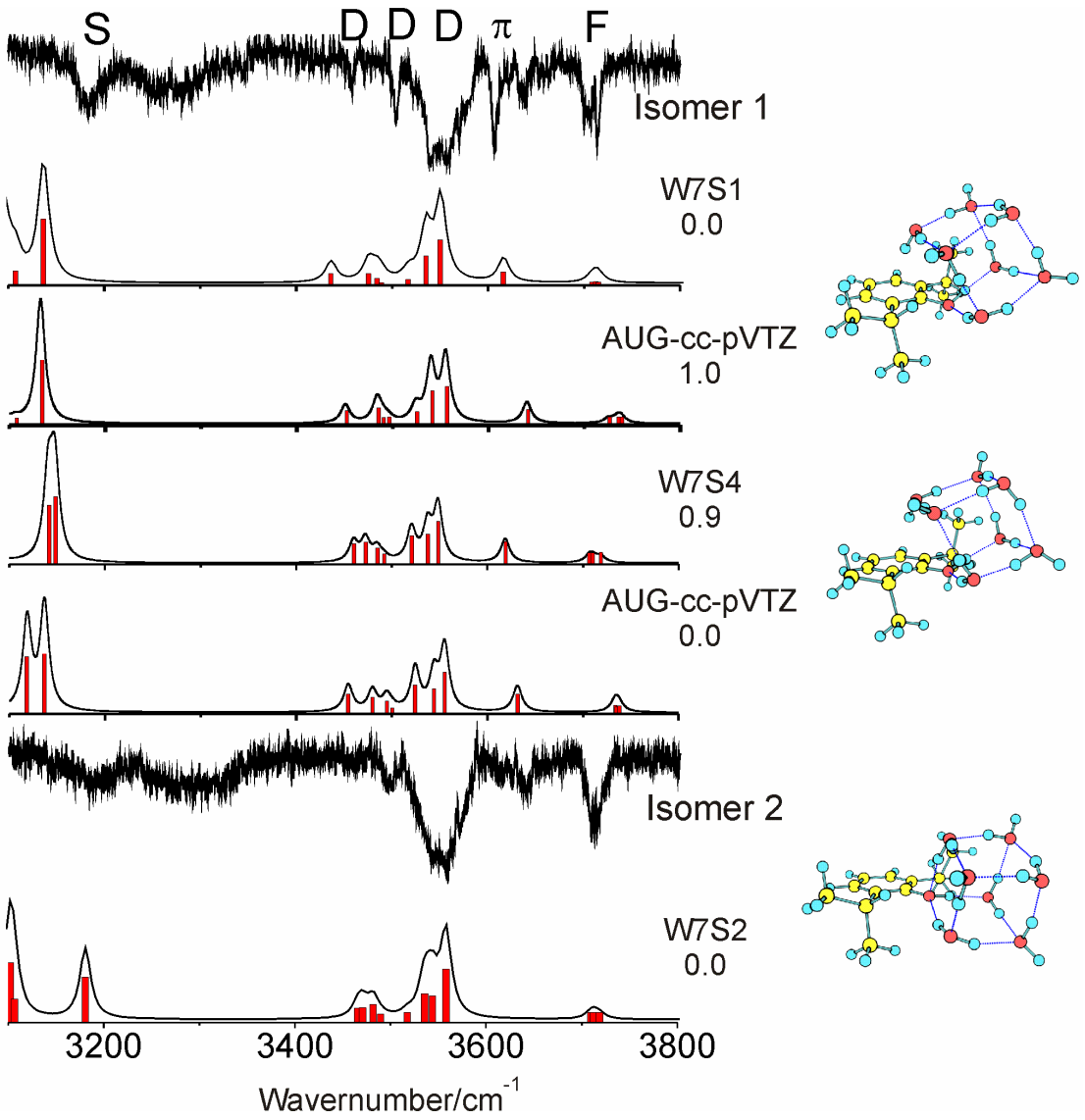


Figure S5. Comparison between the experimental IDIRS of the two propofol$_1$(H$_2$O)$_7$ isomers and the spectra predicted for W7S1 and W7S4 using two basis sets: 6-311++G(d,p) and AUG-cc-pVTZ. A correction factor of 0.950 was used for the second basis set.

Figure S6. Calculated structures for propofol$_1$(H_2O)$_8$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values

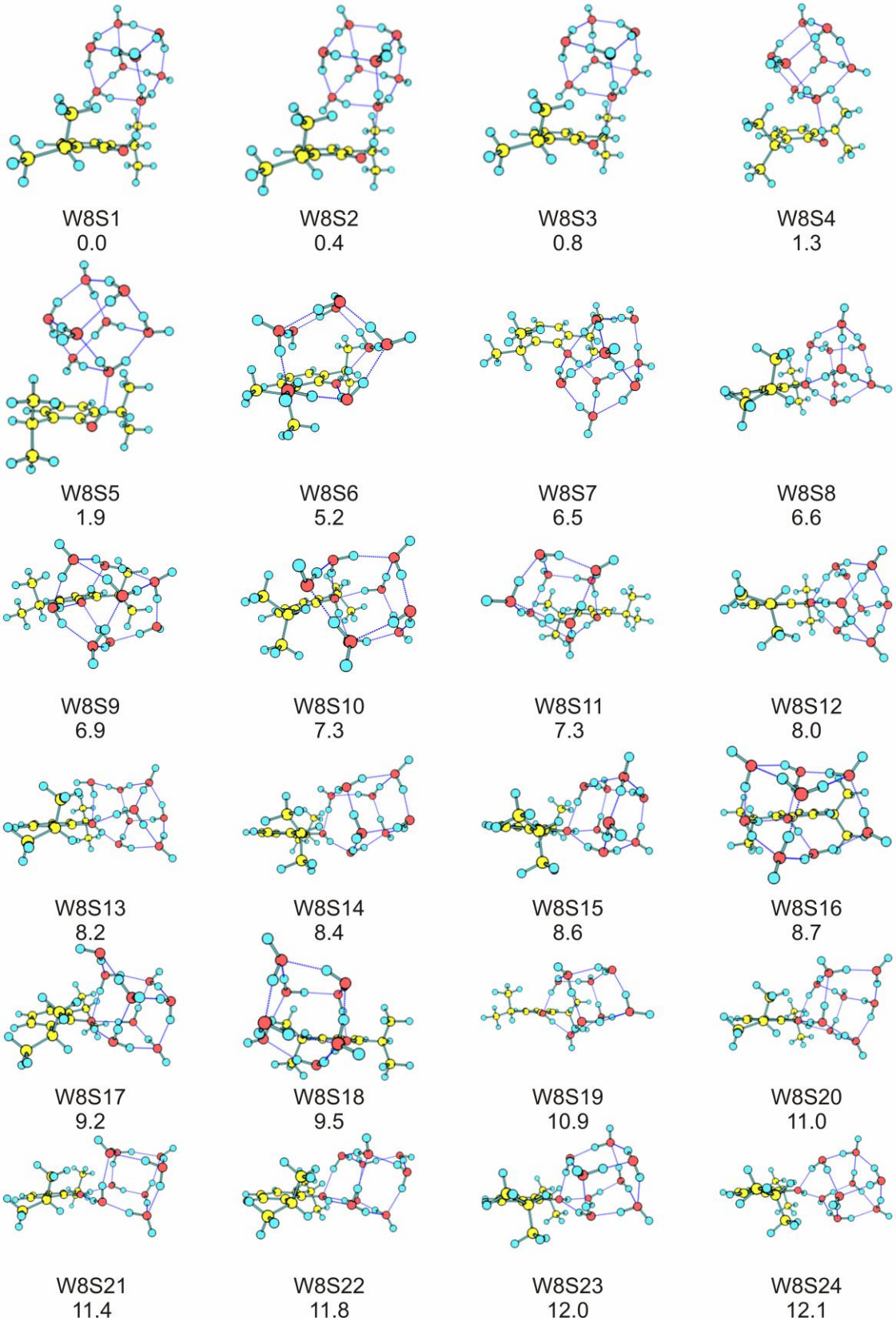


Figure S6. (Cont.)

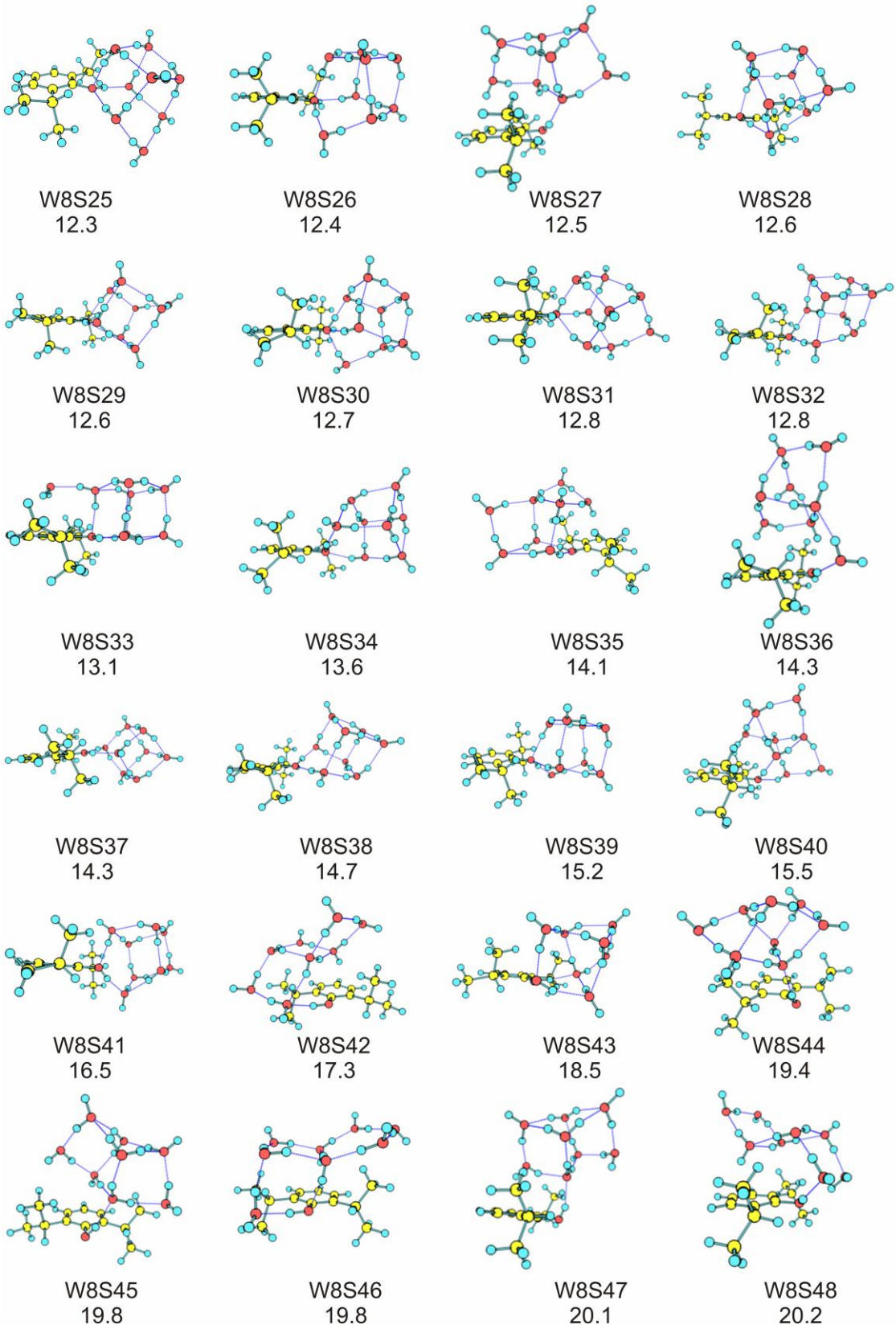


Figure S6. (Cont.)

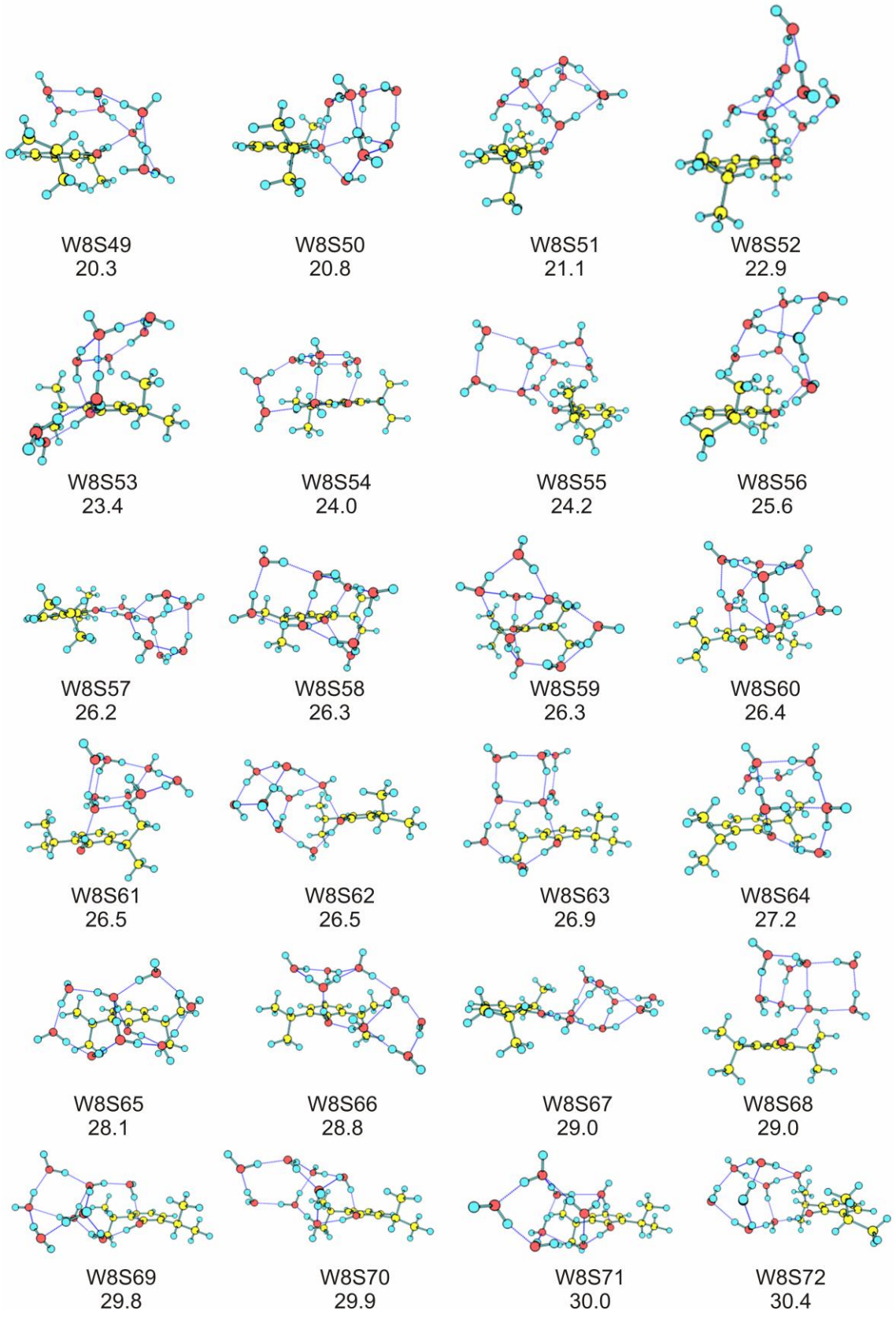


Figure S6. (Cont.)

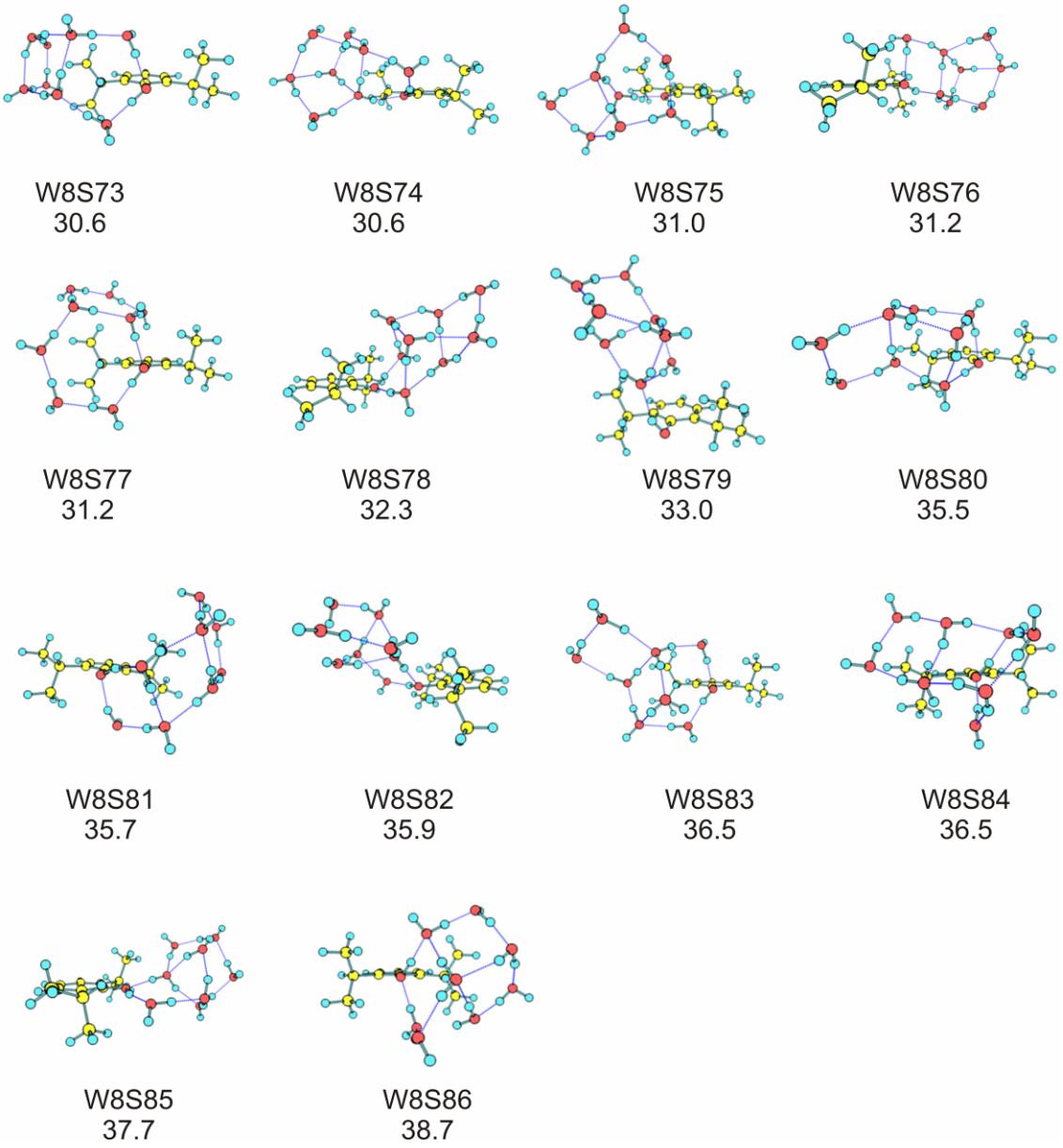


Figure S7. Experimental IDIRS for propofol$_1$(H_2O)$_8$ (upper trace) together with the predicted frequencies for each calculated structure. A correction factor of 0.938 was employed.

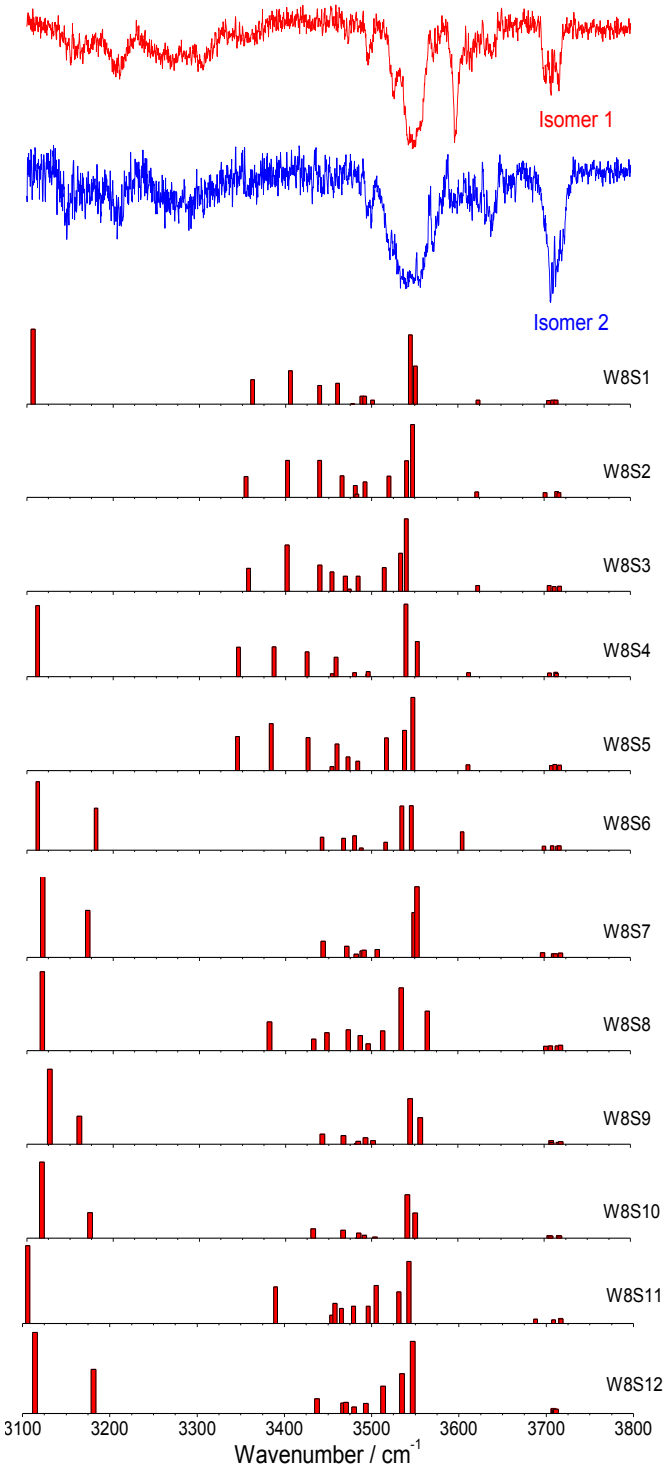


Figure S7.(Cont.)

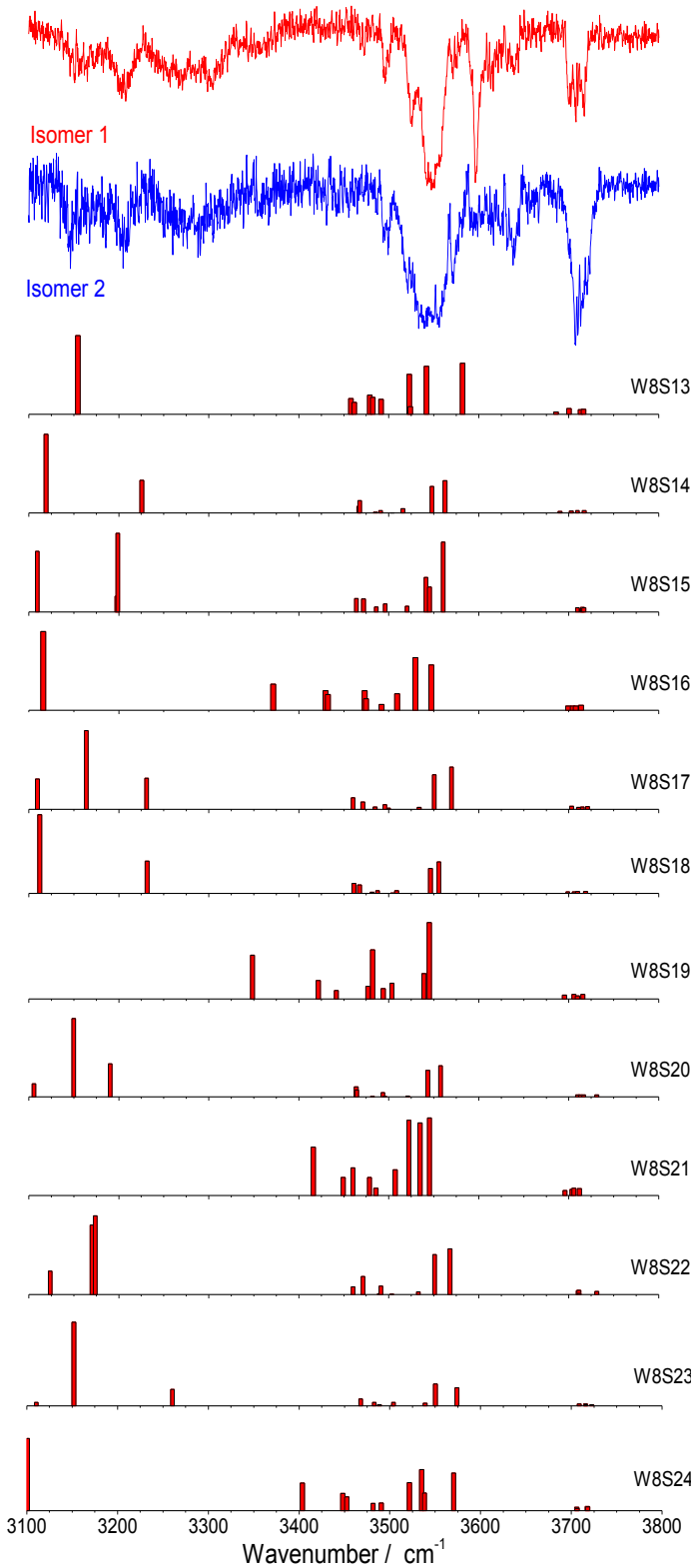


Figure S7.(Cont.)

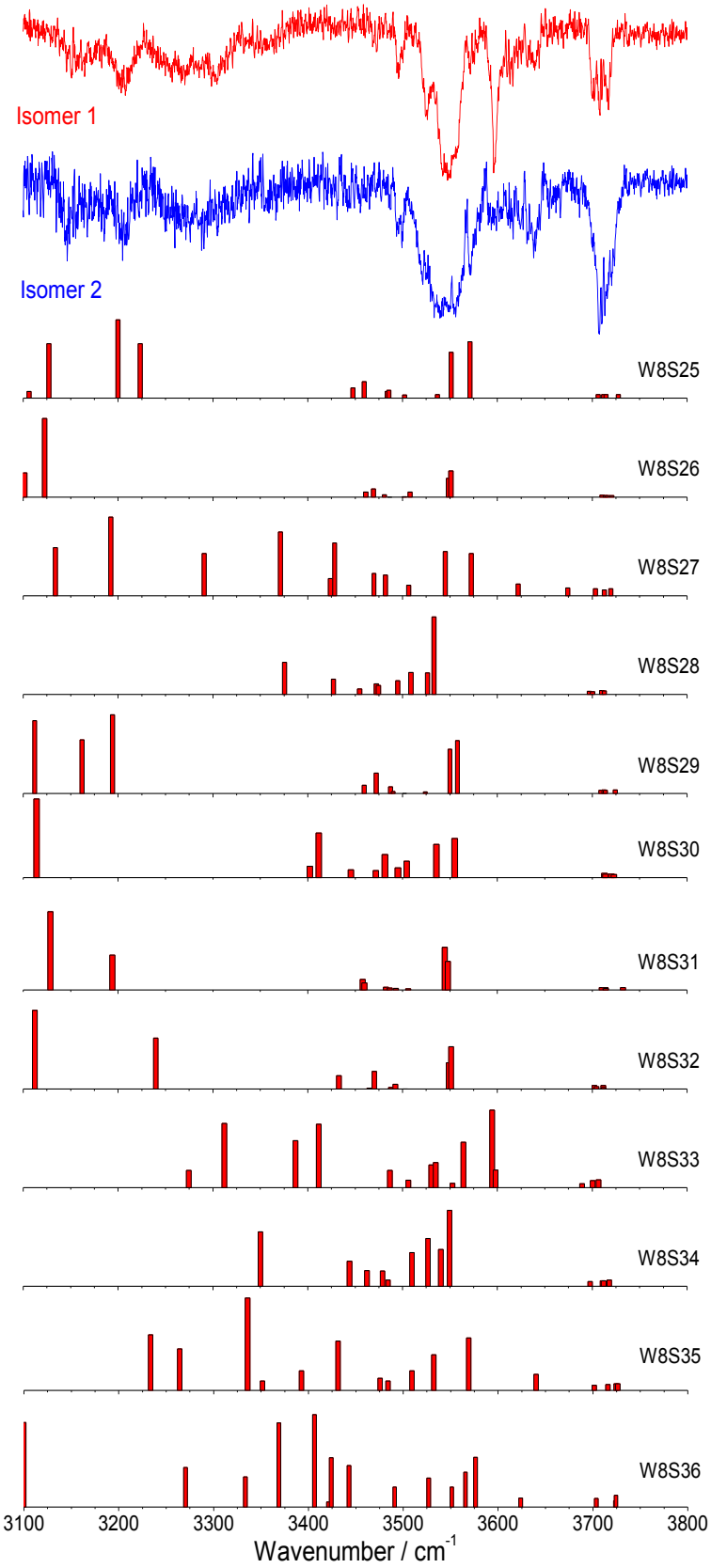


Figure S7.(Cont.)

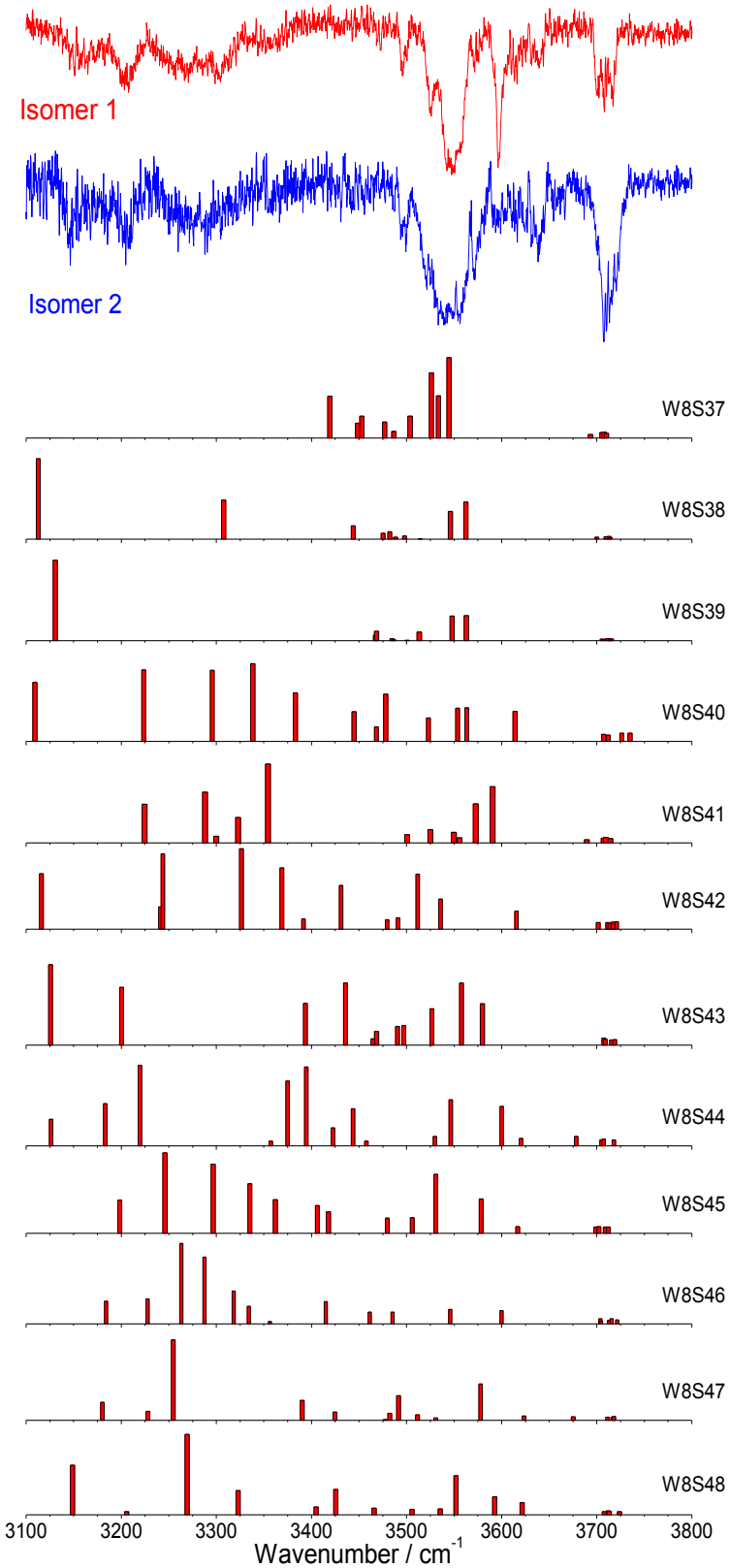


Figure S7.(Cont.)

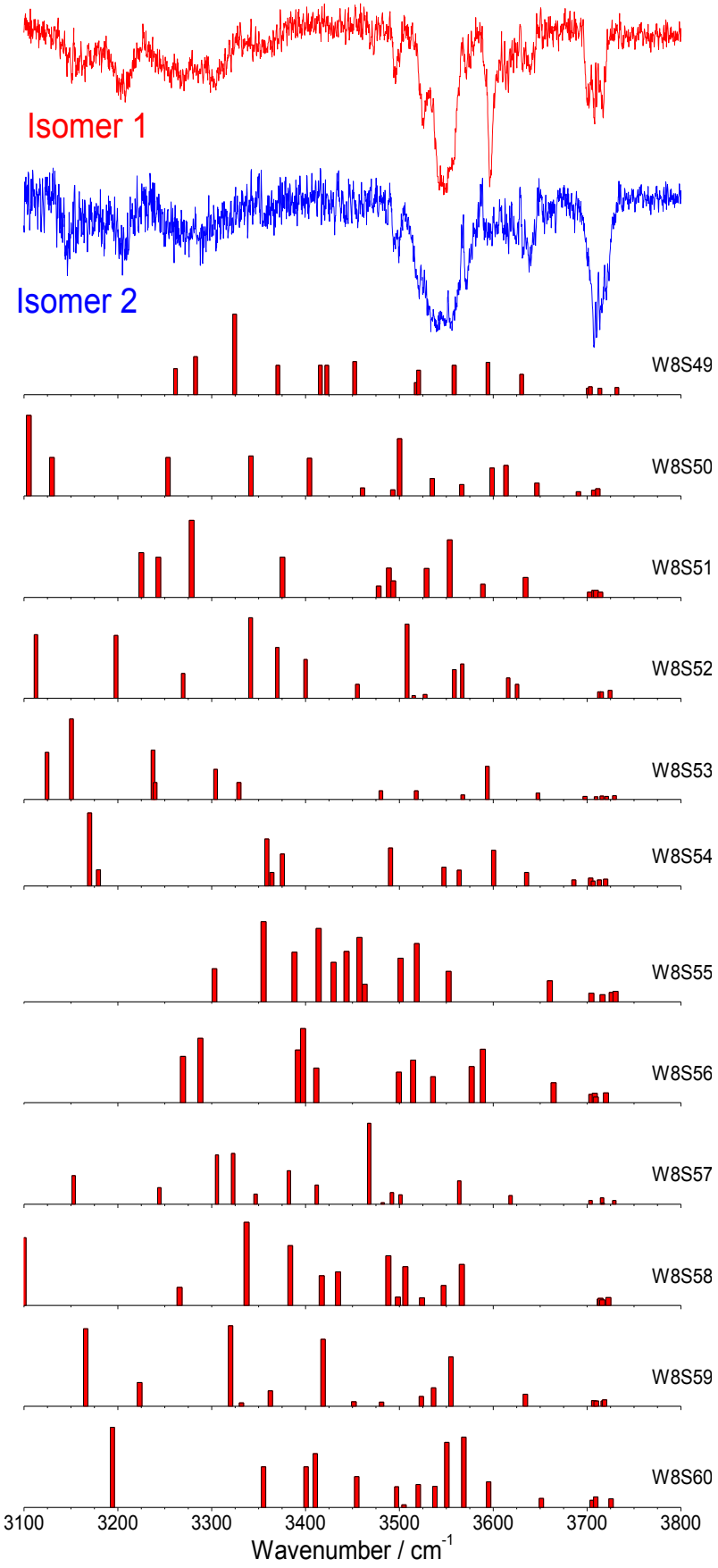


Figure S7.(Cont.)

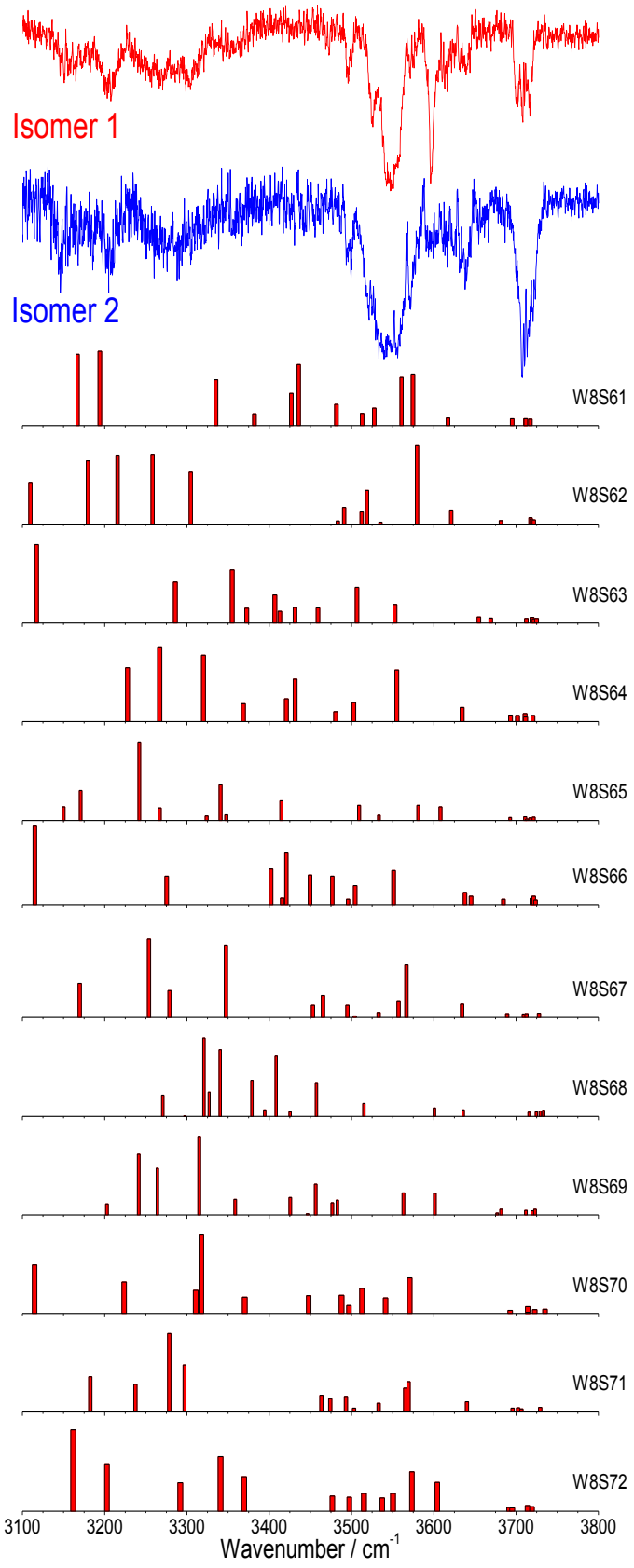


Figure S7.(Cont.)

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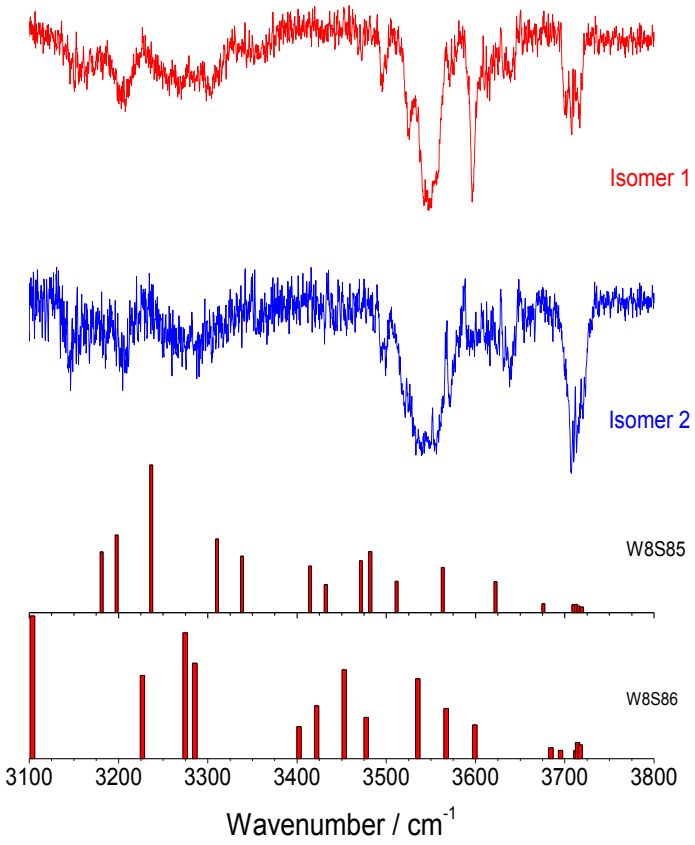


Figure S8. Experimental IDIRS for propofol$_1$(H_2O)$_8$ isomer 1(upper trace) obtained in the fingerprint region, together with the predicted frequencies for the 11 lowest energy calculated structure. A correction factor of 0.938 was employed

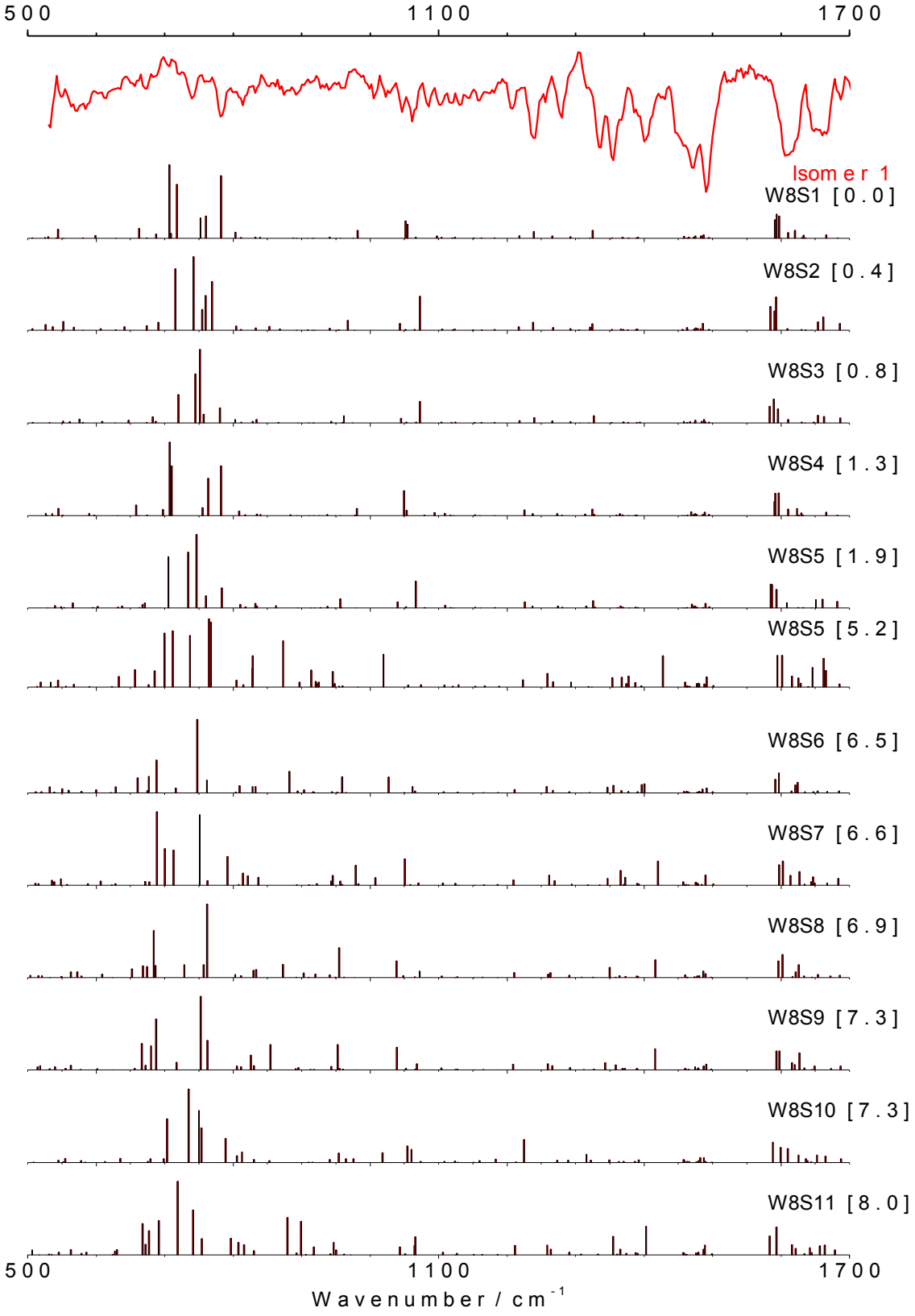


Figure S8. Calculated structures for propofol$_1$(H$_2$O)$_9$ at M06-2X/6-311++G(d,p) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values

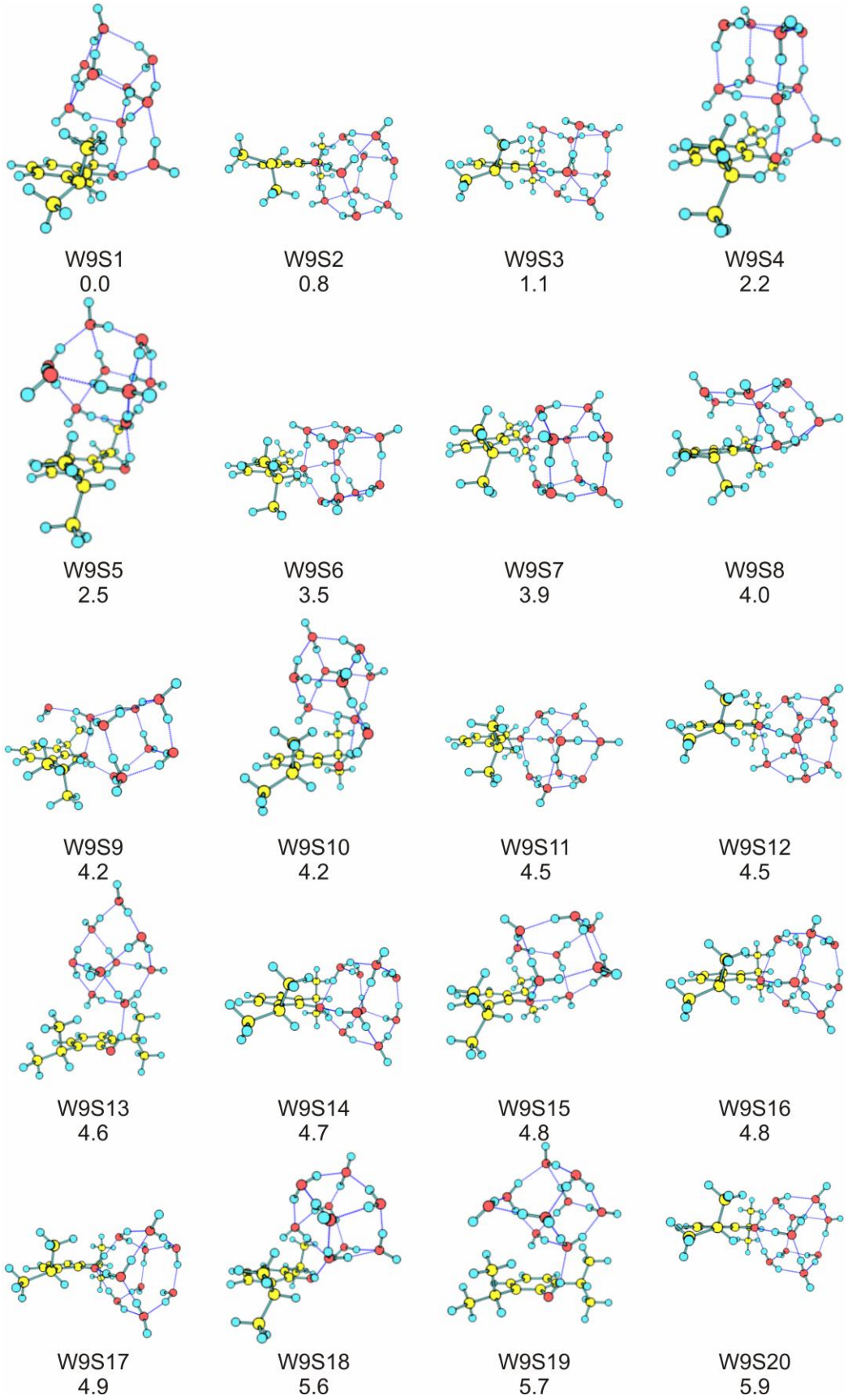


Figure S9. (Cont.)

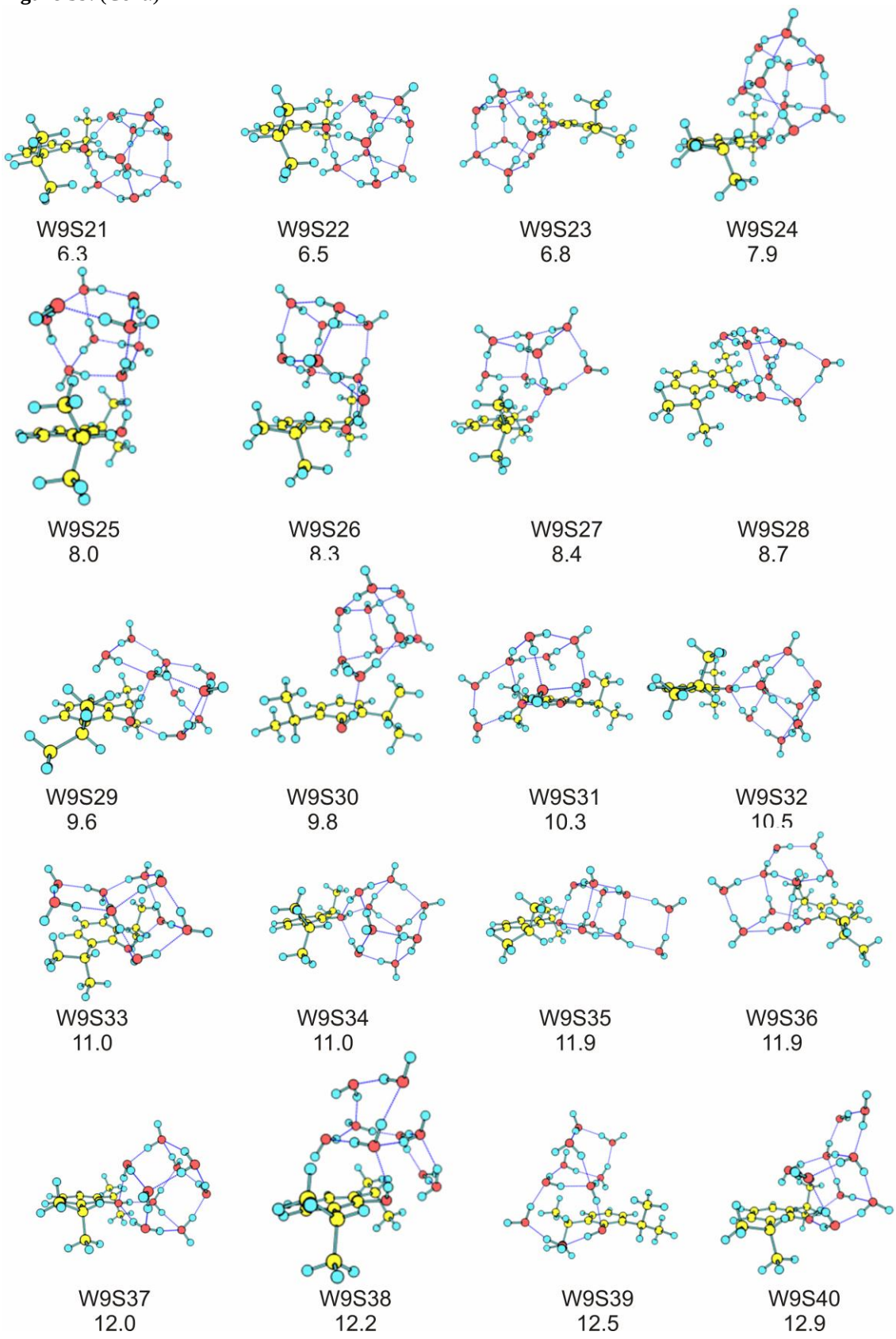


Figure S9. (Cont.)

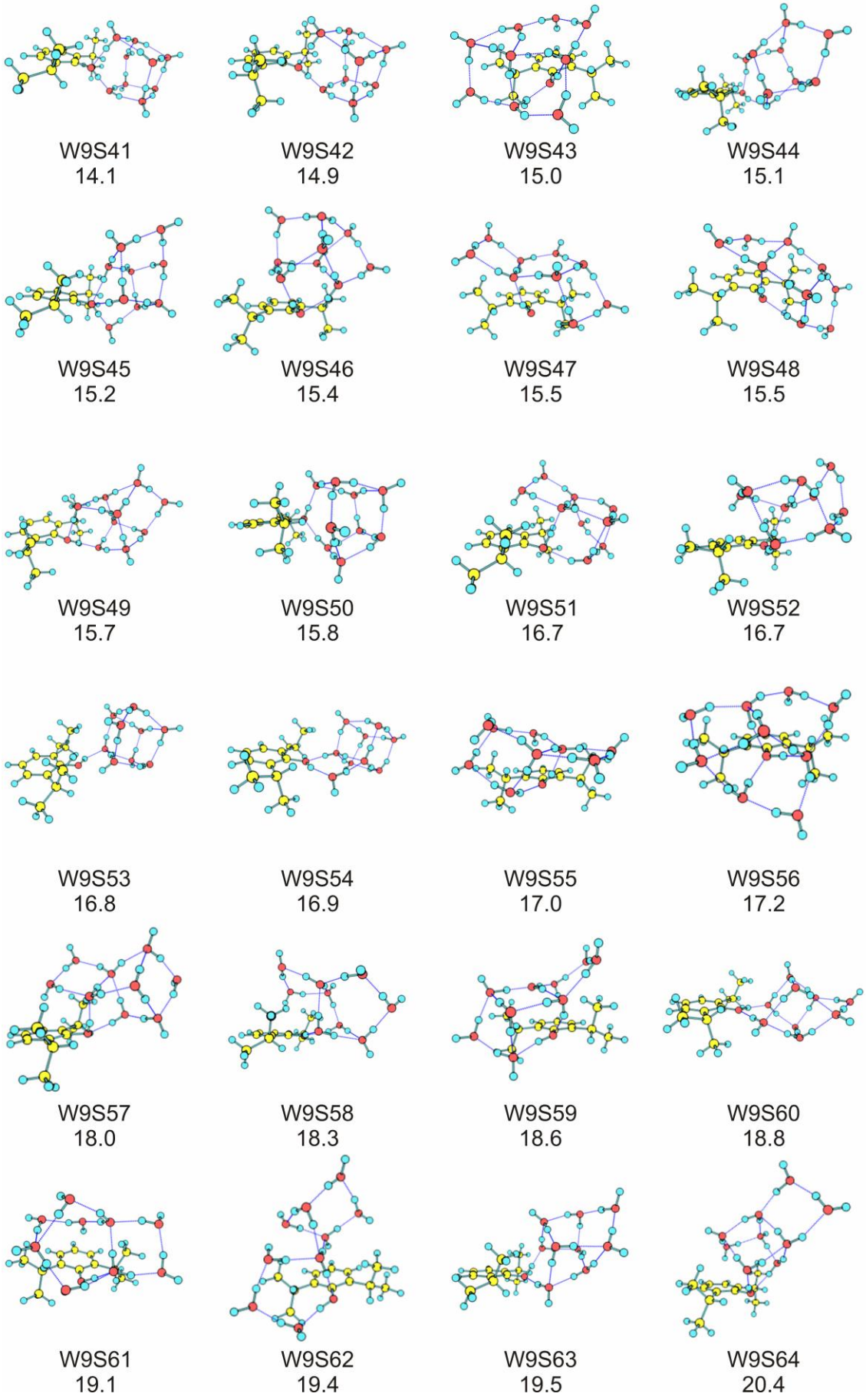


Figure S9. (Cont.)

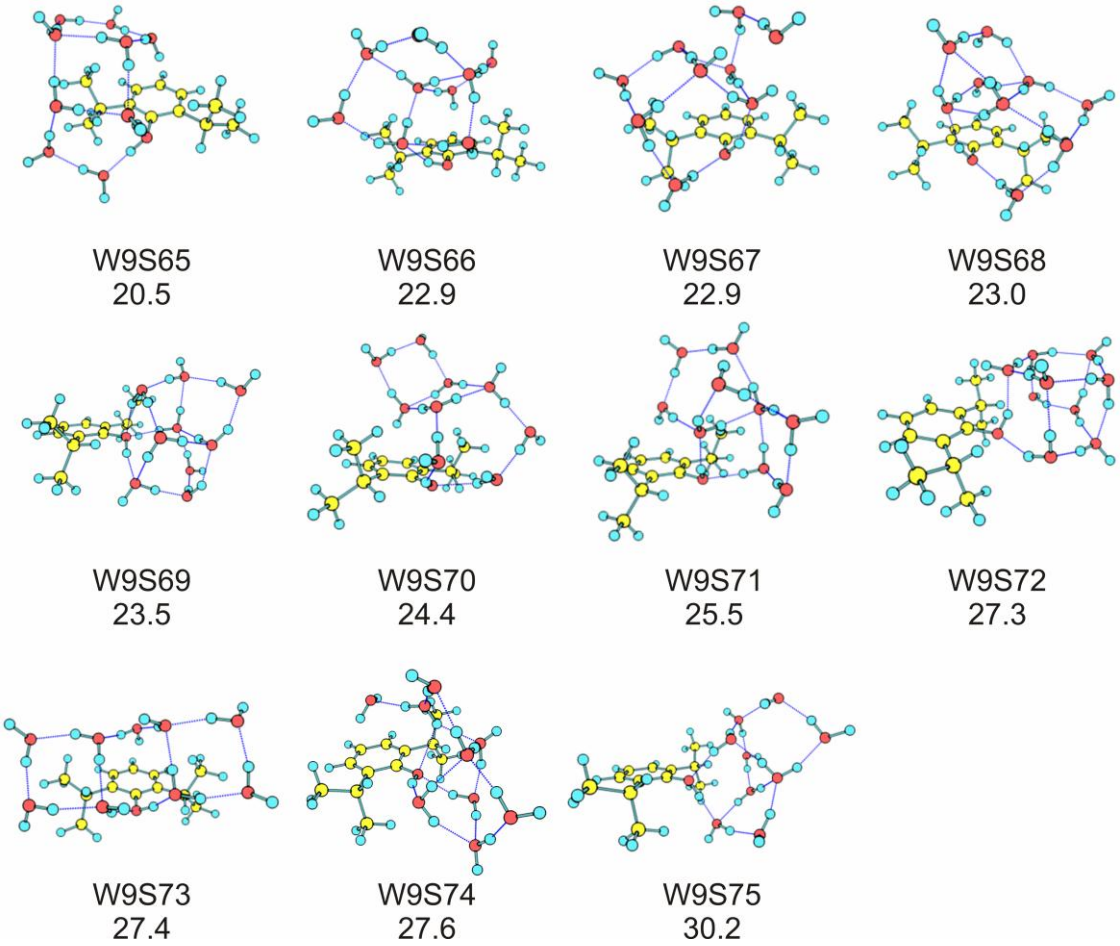


Figure S10. Experimental IDIRS in the fingerprint region for propofol$_1$(H_2O)$_9$ (upper trace) together with the predicted frequencies for the eight most stable calculated structures. A correction factor of 0.938 was employed.

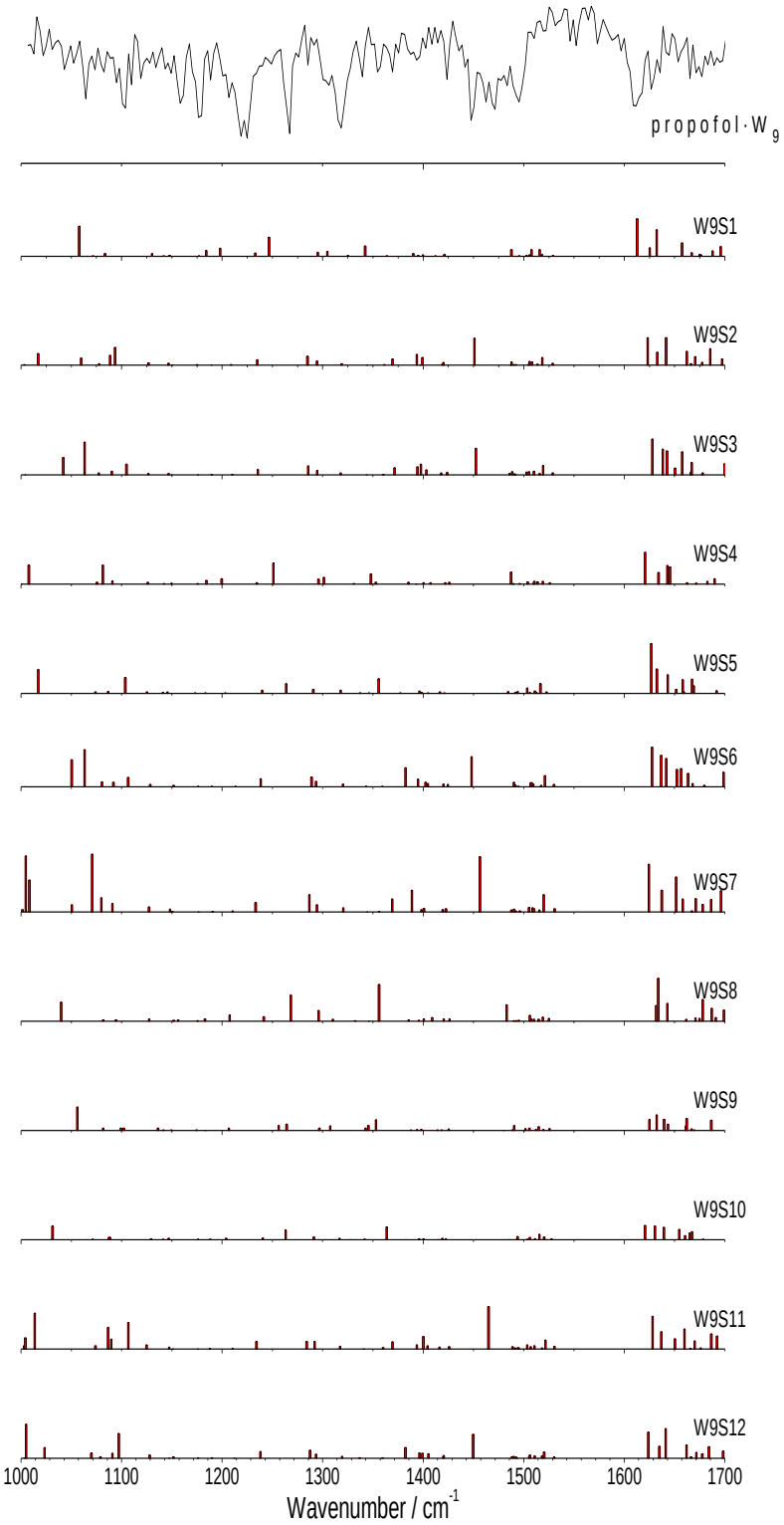


Figure S11. Experimental IDIRS for propofol$_1$(H_2O)$_9$ (upper trace) together with the predicted frequencies for each calculated structure. A correction factor of 0.938 was employed.

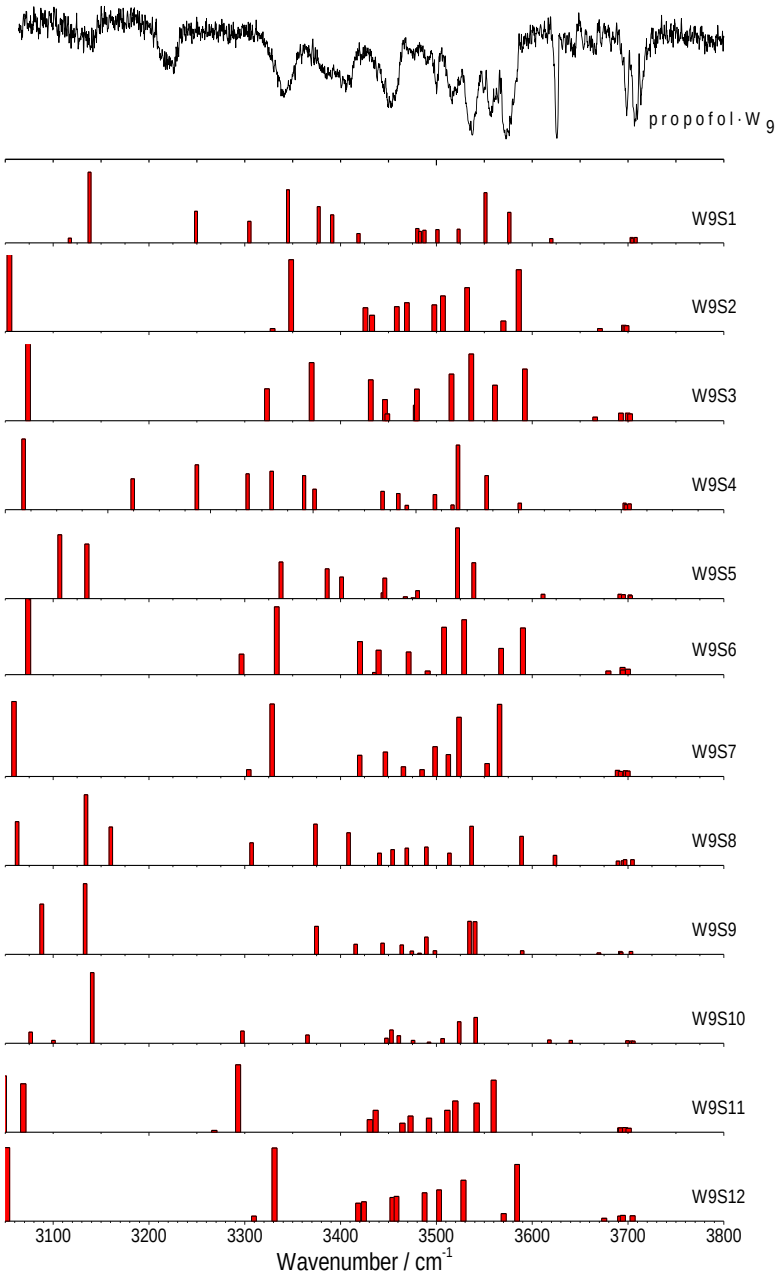


Figure S11. (Cont.)

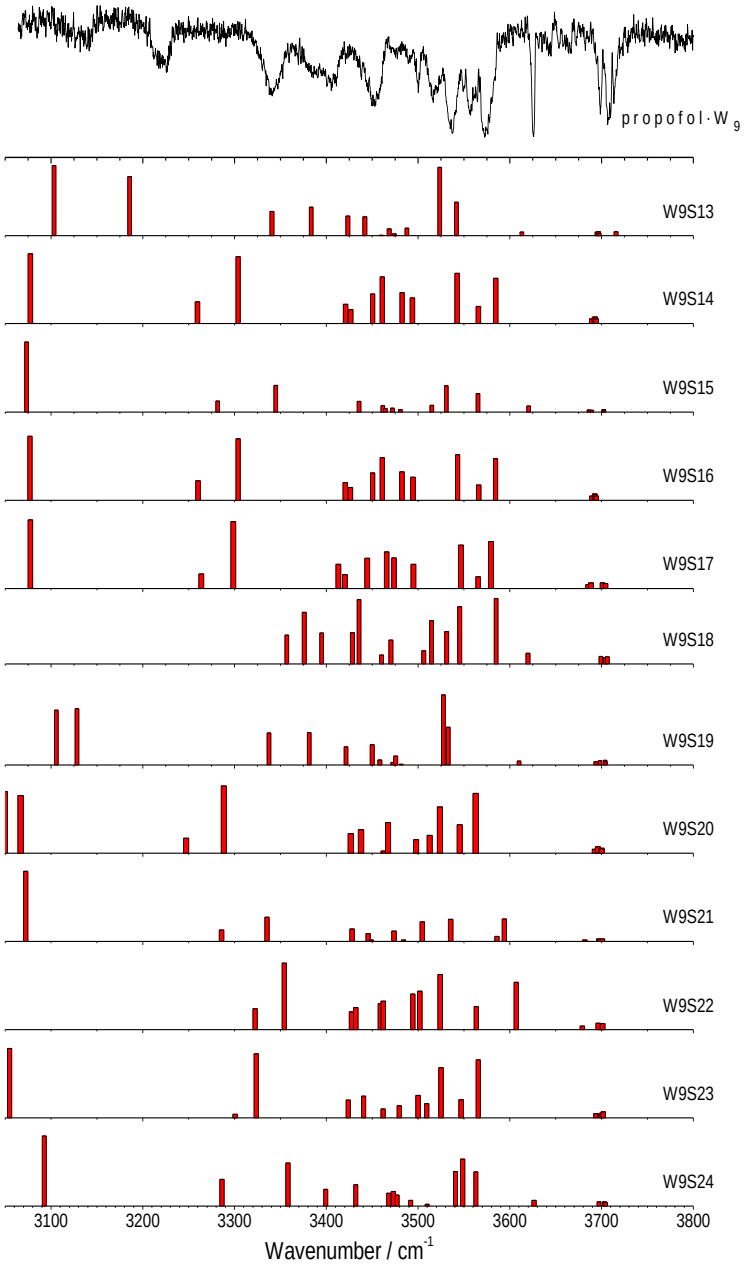


Figure S11. (Cont.)

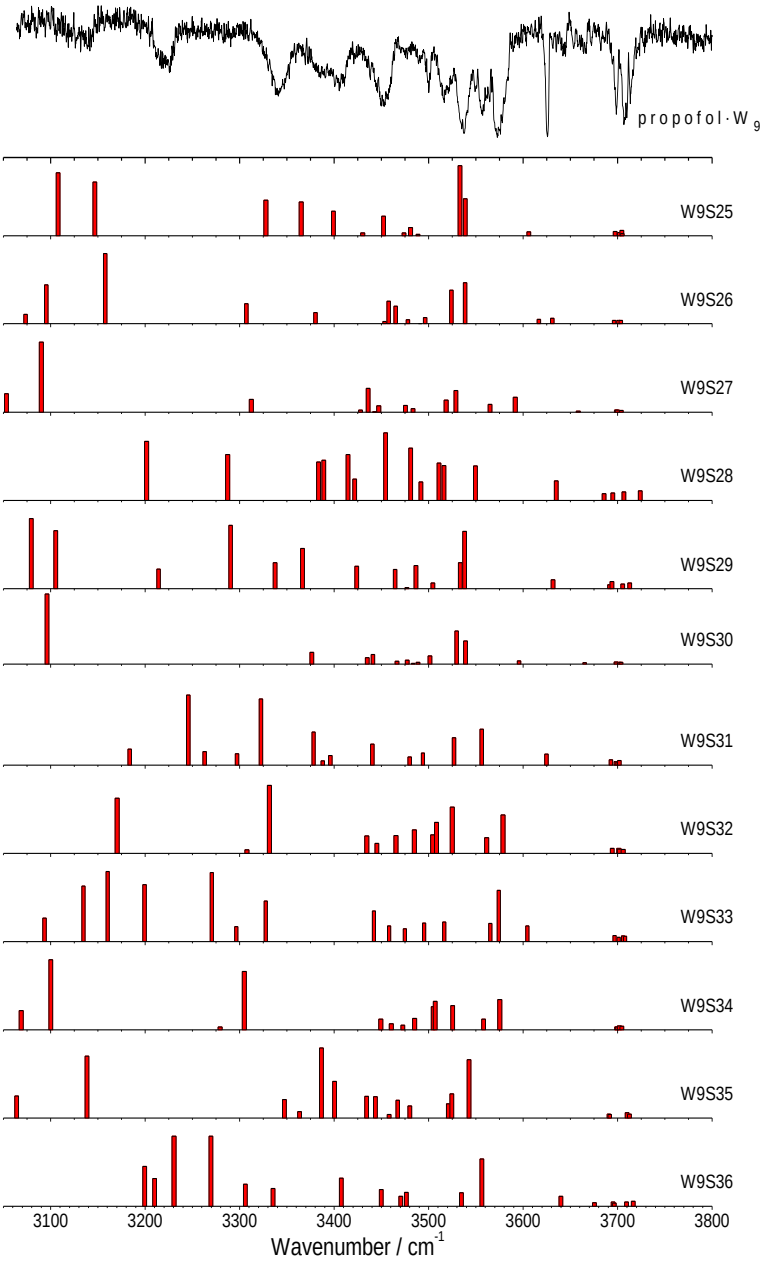


Figure S11. (Cont.)

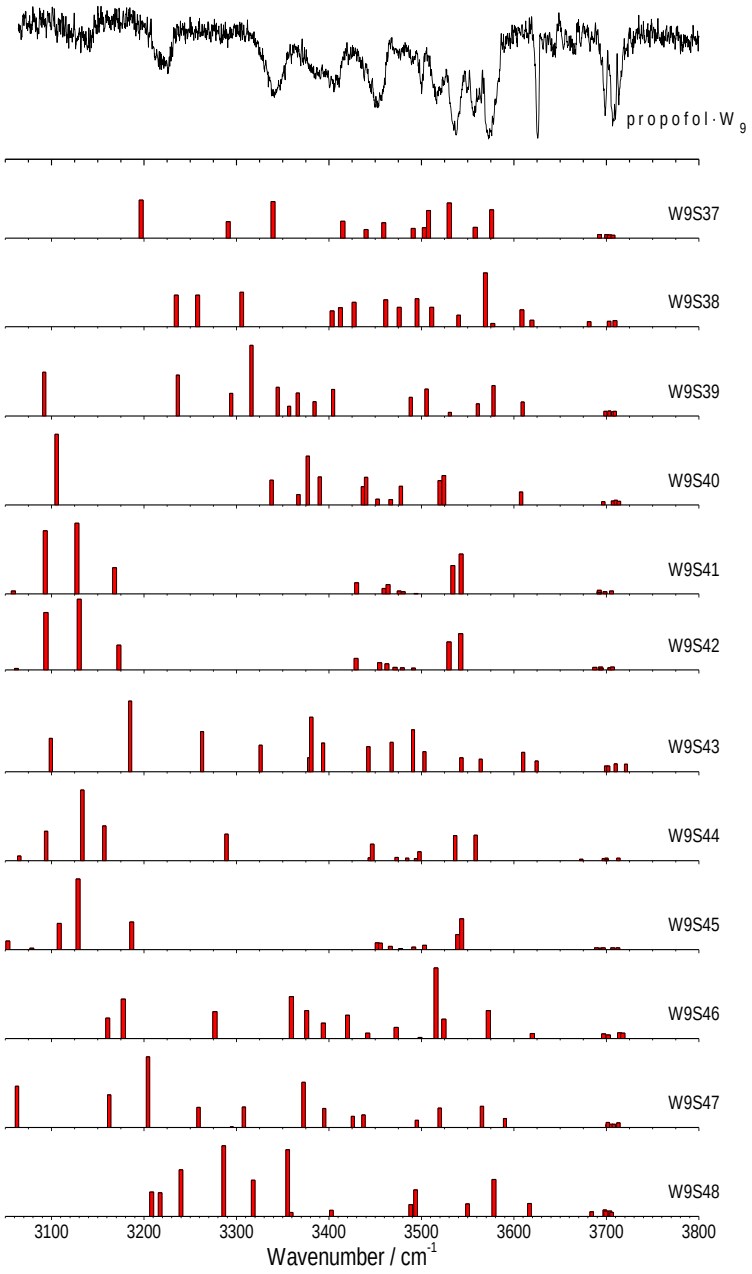
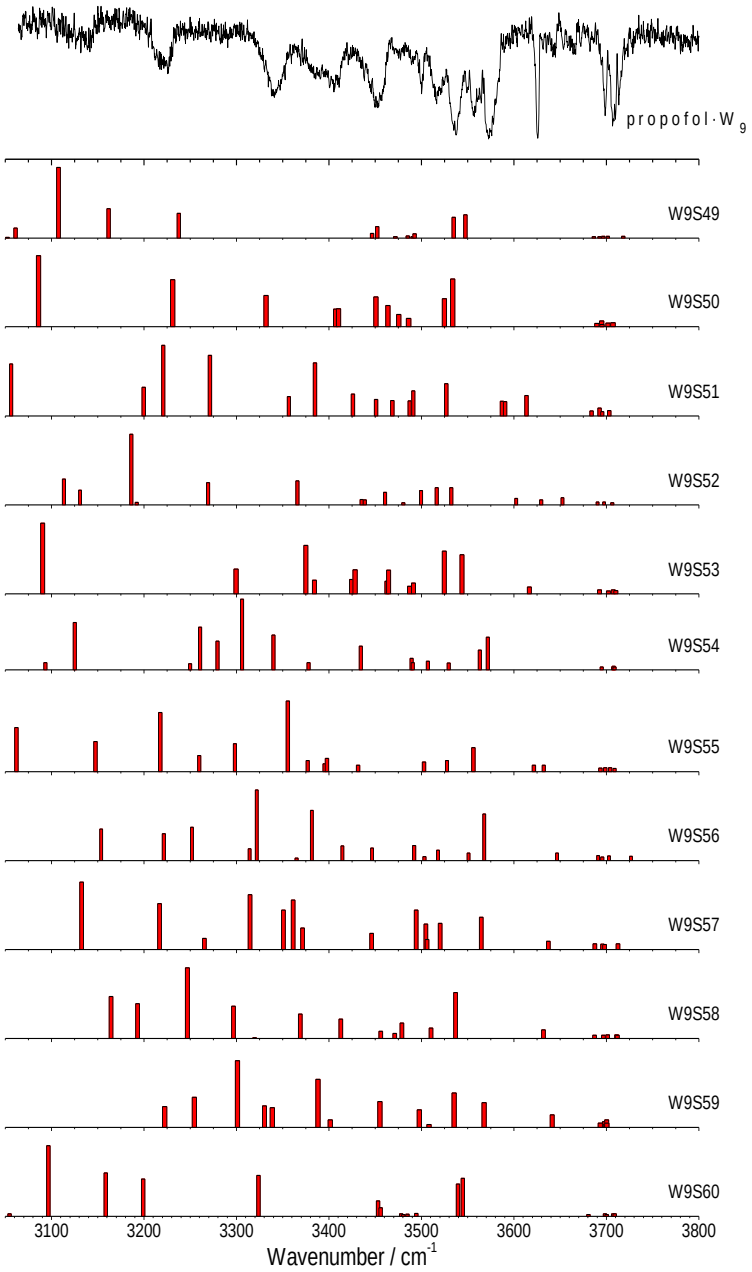


Figure S11. (Cont.)



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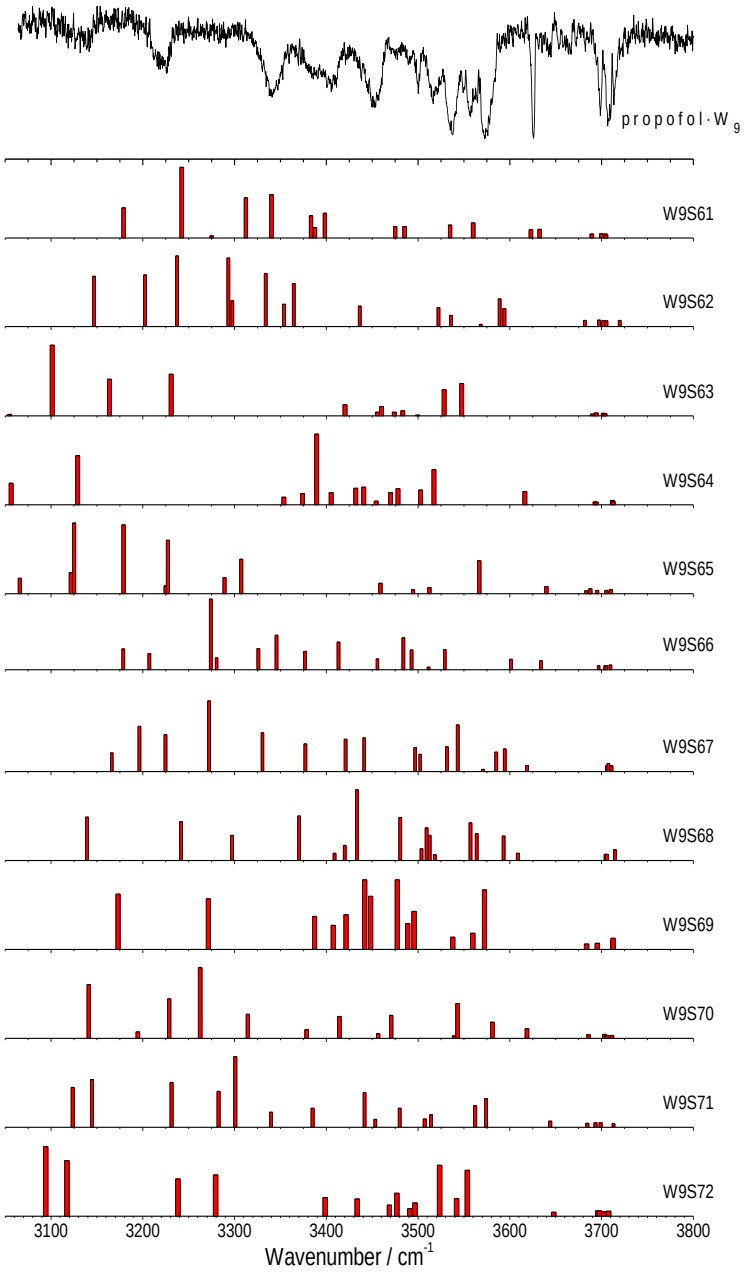
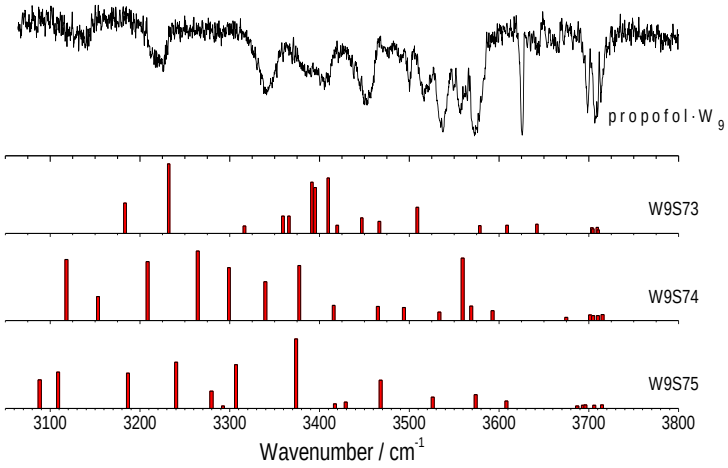
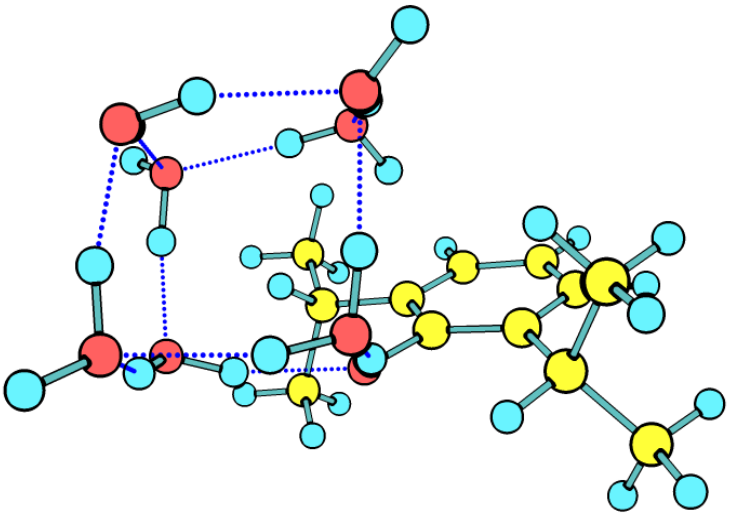


Figure S11. (Cont.)



Structures assigned to the experimental conformers in xyz format. An image of the structure is also shown to assist in identification.



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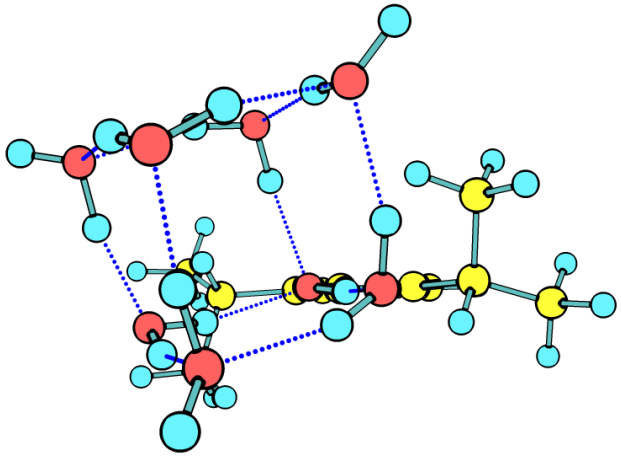

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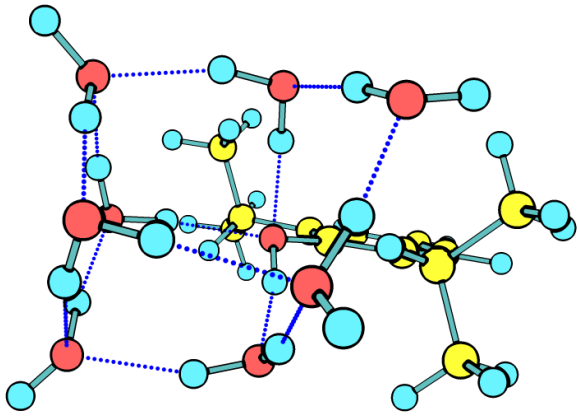

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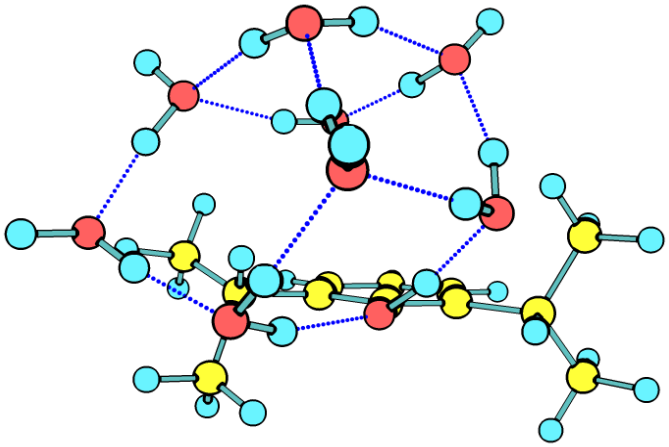

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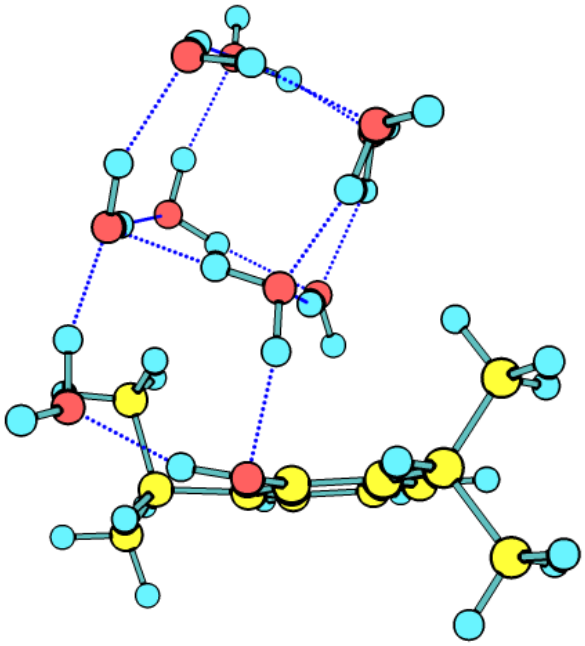

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