

Supporting Information

Tracking reactive water and hydrogen-bonding networks in photosynthetic oxygen evolution

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Table S1: Summary of assignments in the 3200-2000 cm^{-1} region of the S_2 -minus- S_1 RIFT-IR spectrum

Reference	PSII preparation*	Temperature, pH	Position	^{18}O -shift	Assignment
Noguchi ¹ , 2002	<i>Synechococcus elongatus</i>	283 K, pH 6.0	3000 cm^{-1}	N.D. ^a	Proton polarizability band, S_2 State
Barry ² , 2013	Spinach	263 and 283 K, pH 7.5	2880 cm^{-1}	N.D.	Protonated water cluster, S_2 state
Barry ³ , 2013	Spinach	263 K, pH 7.5	2880 cm^{-1}	N.D.	Protonated water cluster, S_2 state
Noguchi ⁴ , 2014	<i>T. elongatus</i> , Tris-washed (inactive in oxygen evolution)	250 K, pH 6.5	“Broad positive feature around 2800 cm^{-1} ”	N.D.	Protonated histidine in a putative YZ^{\bullet} -minus- YZ spectrum, but see ref; ⁷ proton polarizability band
	<i>T. elongatus</i>	N.S. ^b	“Around 3000 cm^{-1} ”	No	S_2 state
	Spinach	N.S.	“Around 3000 cm^{-1} ”	N.D.	S_2 state
Debus ⁵ , 2014	<i>Synechocystis</i> sp. PCC 6803	273 K, pH 6.0	“Centered at 3000 cm^{-1} ”	No	Proton polarizability band, S_2 state
Noguchi ⁶ , 2016	Spinach	283 K, pH 6.0	“Broad positive feature at 3200–2500 cm^{-1} ”	N.D.	OH bond of hydrogen bonded water, S_2 state
Barry ⁷ , 2016a	Spinach	190 K, pH 6.0 and 7.5	2900/2740 cm^{-1} , NaCl sensitive	Yes	Protonated water cluster, S_2 state
Barry ⁸ , 2016b	Spinach	263 and 283 K, pH 7.5	2830 cm^{-1} (at both temperatures)	Yes	Protonated water cluster, S_2 state
Noguchi ⁹ , 2017	Spinach	283 K, pH 6.0	Around 2900 cm^{-1} (positive) and 2700 cm^{-1} (negative)	N.D.	Protonated histidine, S_2 state

*Preparation used as isolated, unless noted

^a Not determined; ^b Not specified

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