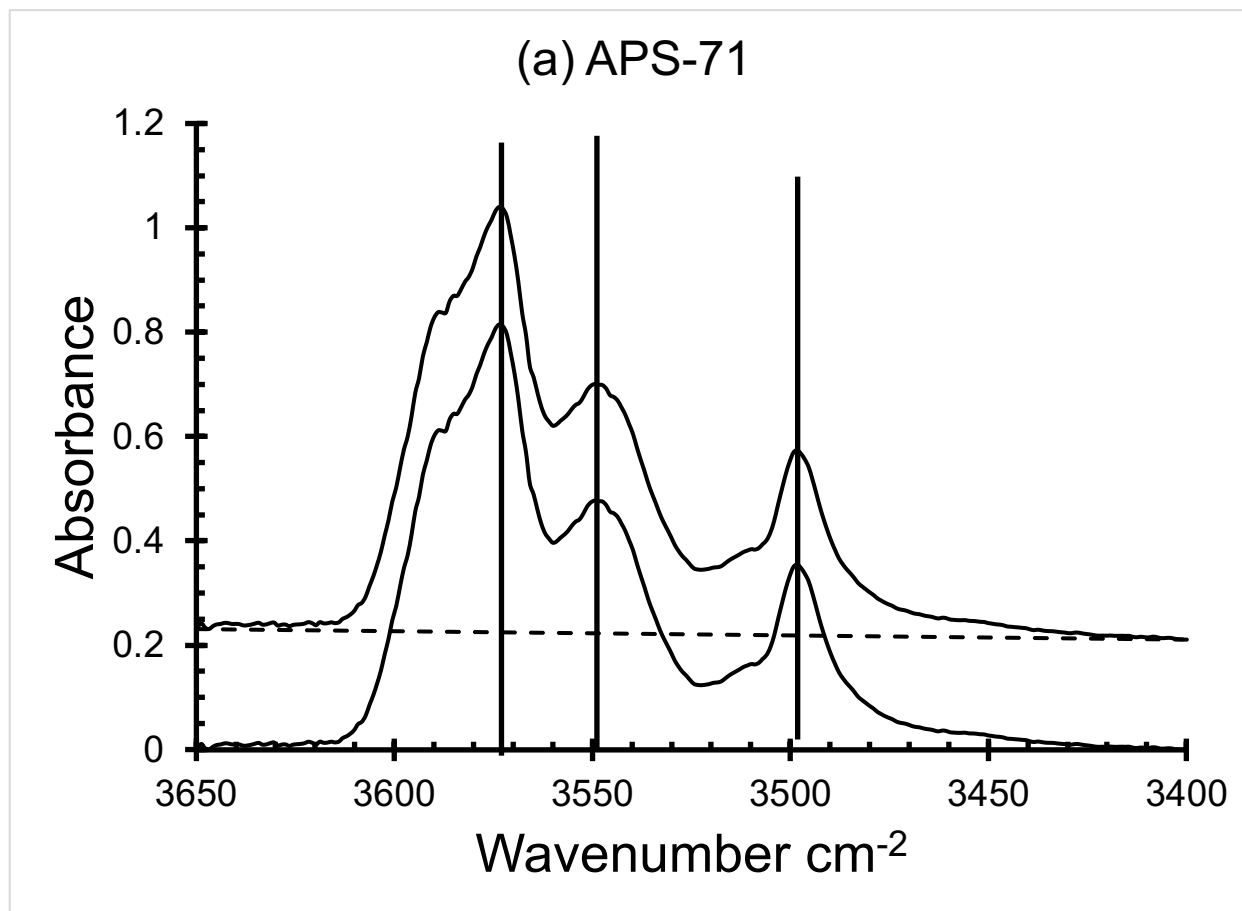
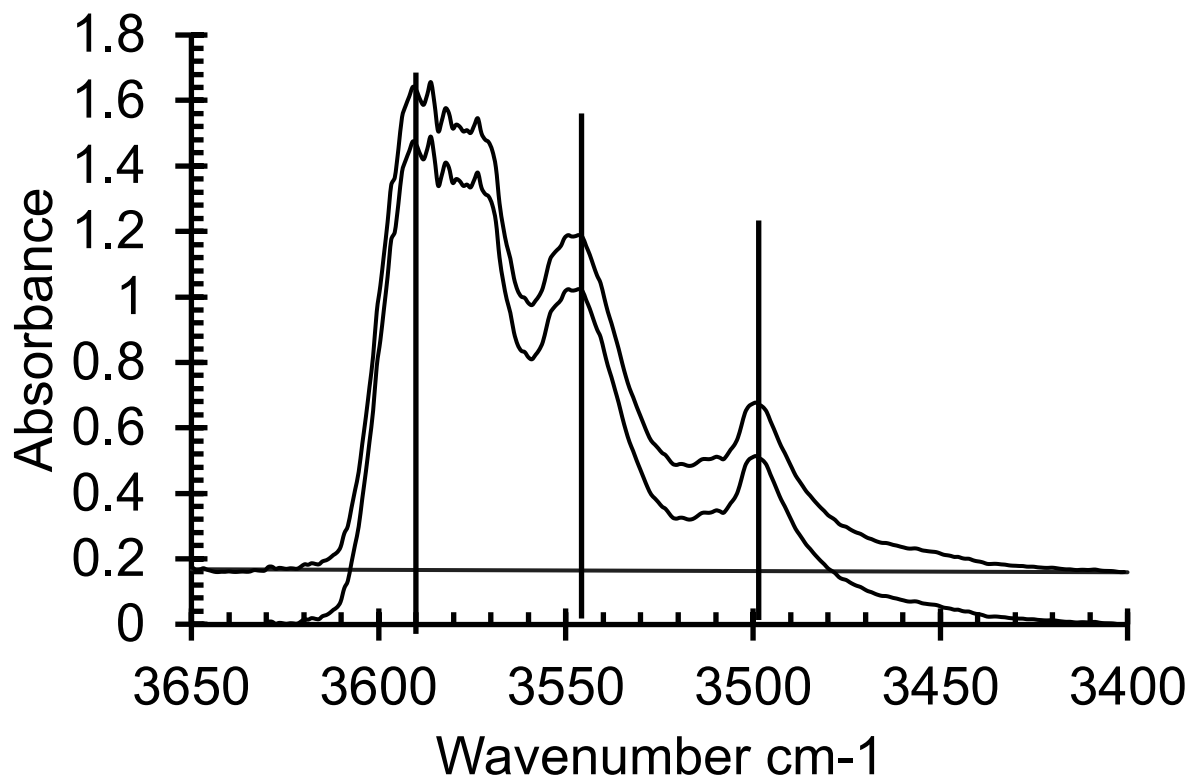


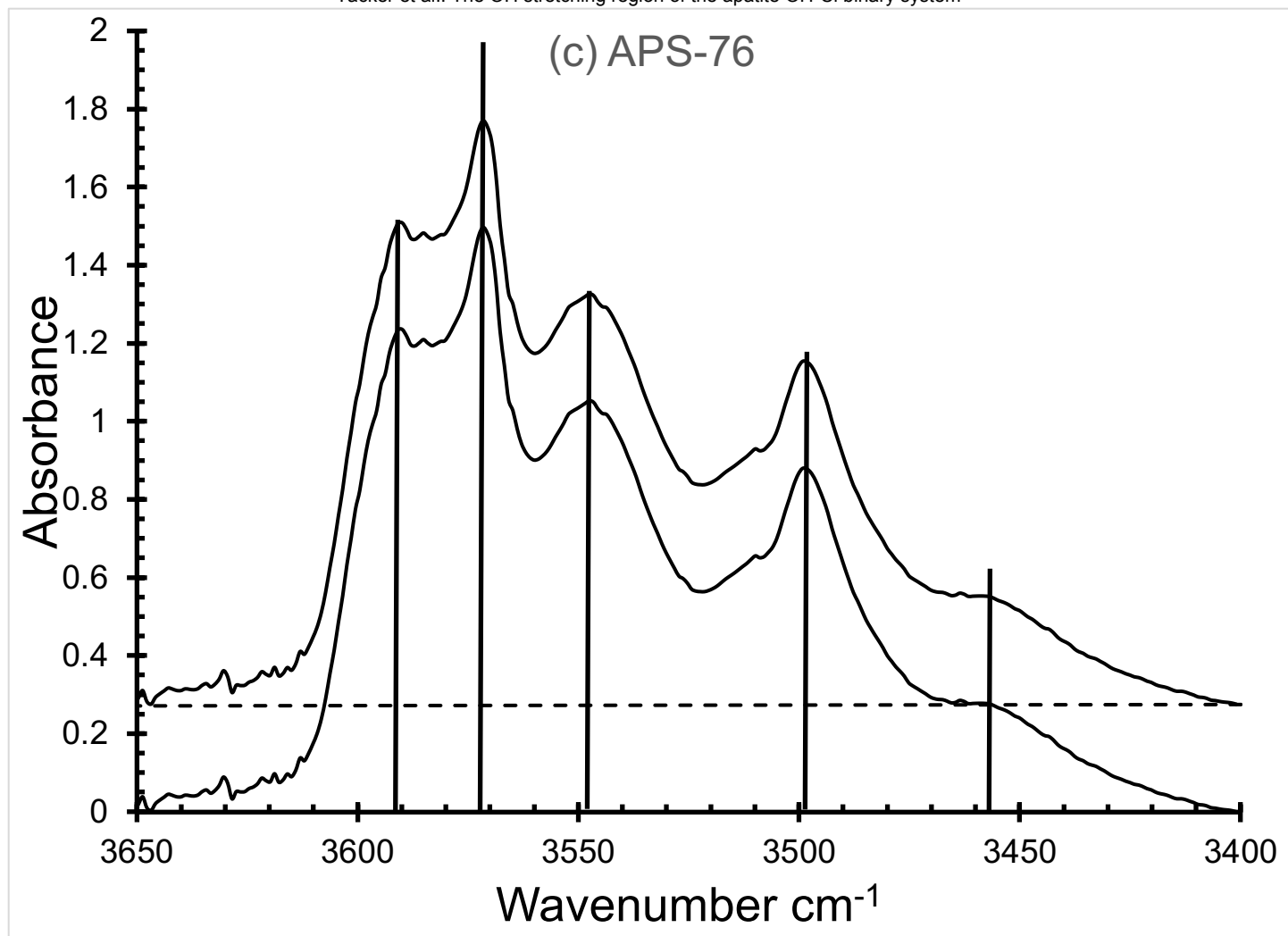
Supplemental material

Figure 1- A comment was made in review that background correction changes the position of the peak maximum. The following graphs demonstrate that, for these spectra, linear background correction does not change the maxima. Upper spectrum is baseline corrected, where the minimum value for the entire spectrum is used to lower the baseline to zero. The dotted line shows the linear background correction used. The lower spectrum is background corrected prior to peak fitting. Vertical lines are used on topographically distinct elements of the spectrum to show that the peak maxima do not shift with background correction. (a) APS-71, (b) APS-72, (c) APS-76, (d) APS-78, (e) APS-80, (f) APS-82, (g) APS-83.

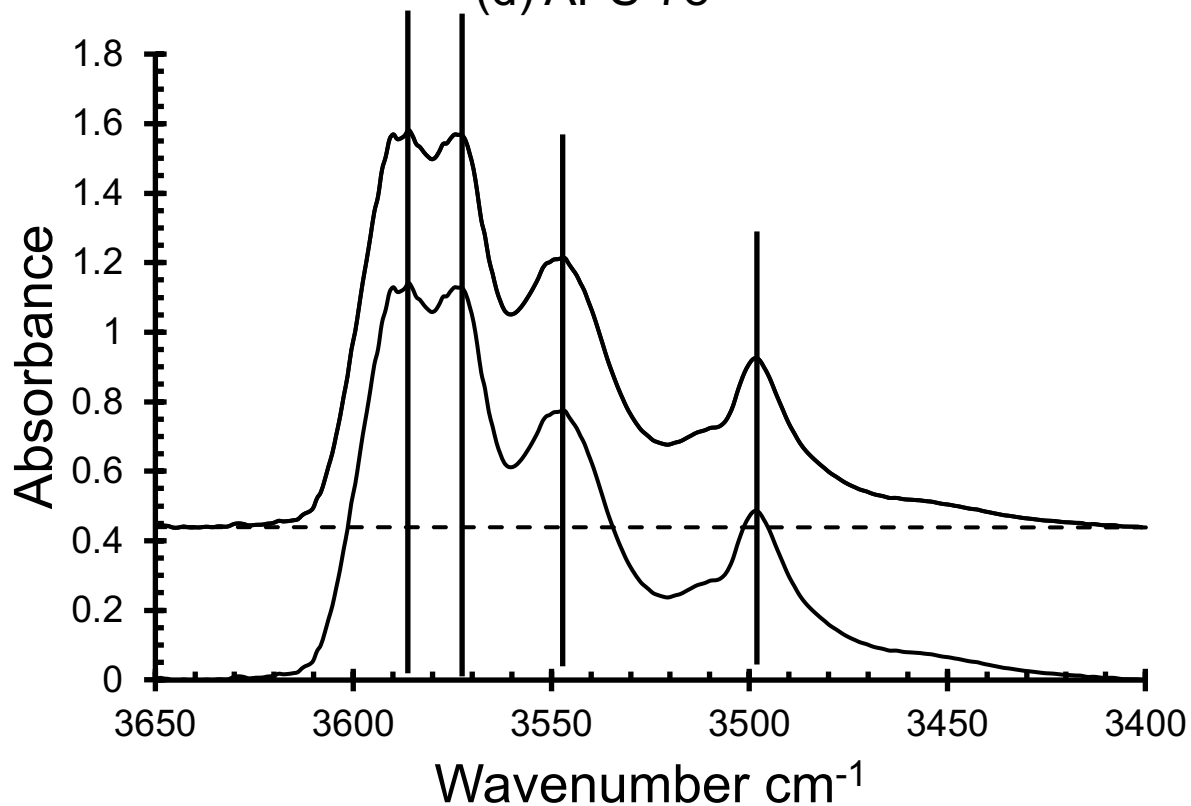


(b) APS-72

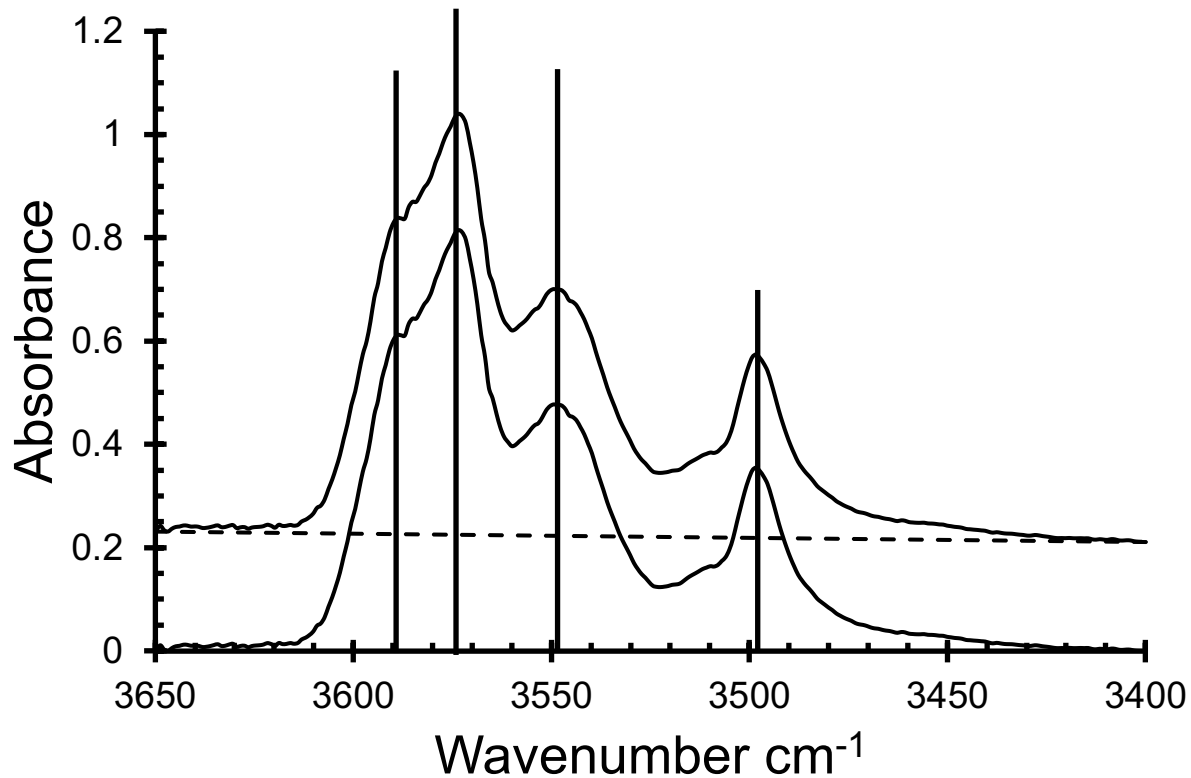


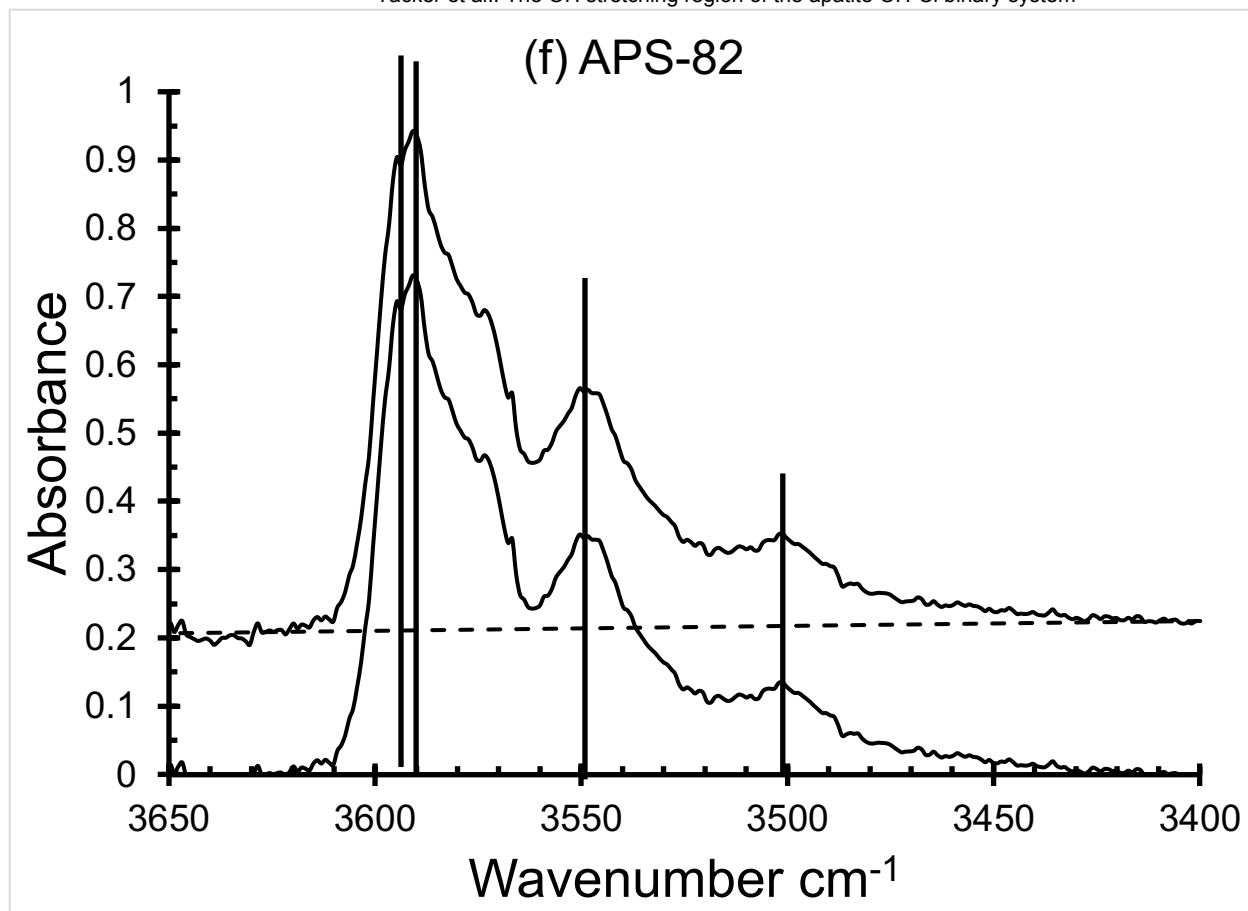


(d) APS-78



(e) APS-80





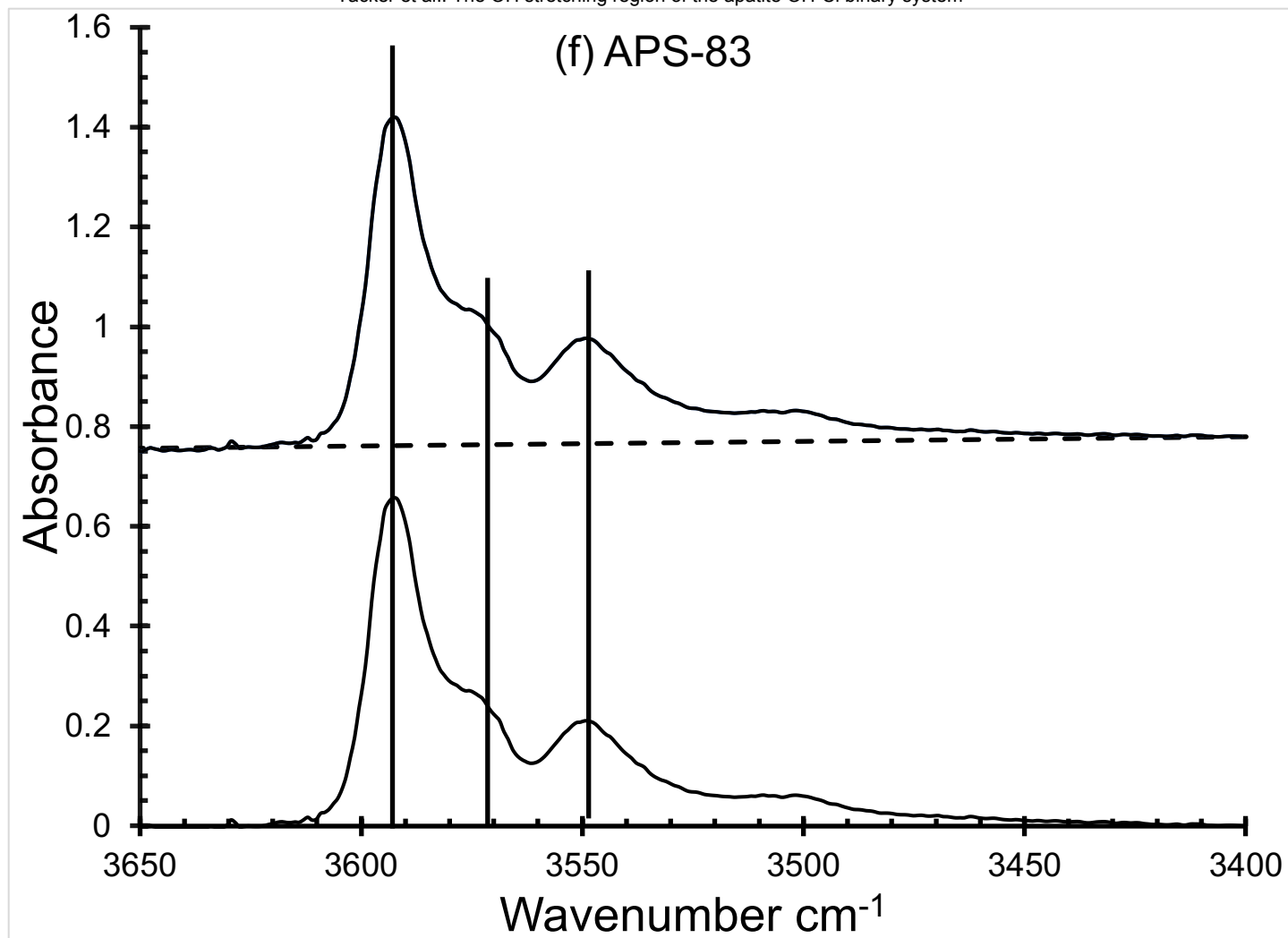


Table 1. Results of spectroscopy and peakfitting for 3573, 3548, and 3498 cm⁻¹ peaks, combined with anionic pairs assigned to that peak. O(H)-O distances with an * superscript are actually too close for assignment to the 3498 cm⁻¹ peak. They would exhibit strong hydrogen bonding, leading to a peak at much lower wavenumbers, which is not observed.

Structural group	Experiment	Peak maximum	Proton donor	Proton "acceptor"	Distance Å	1σ error
Group 1	APS-71 A	3574	OH	OH	3.4234	0.0001
Group 1	APS-71 B	3574	OH	OH	3.4234	0.0001
Group 1	APS-71 C	3574	OH	OH	3.4234	0.0001
Group 1	APS-72 A	3574	OH	OH	3.4097	0.0002
Group 1	APS-80 A	3573	OH	OH	3.4318	0.0001
Group 1	APS-80 B	3573	OH	OH	3.4318	0.0001
Group 1	APS-80 C	3573	OH	OH	3.4318	0.0001
Group 1	APS-80 D	3573	OH	OH	3.4318	0.0001
Group 1	APS-80 E	3573	OH	OH	3.4318	0.0001
Group 1	APS-80 F	3573	OH	OH	3.4318	0.0001
Group 1	APS-71 A	3574	ClOH-OH	ClOH-OH	3.4234	0.0087
Group 1	APS-71 B	3574	ClOH-OH	ClOH-OH	3.4234	0.0087
Group 1	APS-71 C	3574	ClOH-OH	ClOH-OH	3.4234	0.0087
Group 1	APS-72 A	3574	ClOH-OH	ClOH-OH	3.4097	0.0096
Group 1	APS-80 A	3573	ClOH-OH	ClOH-OH	3.4318	0.0126
Group 1	APS-80 B	3573	ClOH-OH	ClOH-OH	3.4318	0.0126
Group 1	APS-80 C	3573	ClOH-OH	ClOH-OH	3.4318	0.0126
Group 1	APS-80 D	3573	ClOH-OH	ClOH-OH	3.4318	0.0126
Group 1	APS-80 E	3573	ClOH-OH	ClOH-OH	3.4318	0.0126

Group 1	APS-80 F	3573	ClOH-OH	ClOH-OH	3.4318	0.0126
Group 2	APS-76 A	3574	OH	OH	3.4409	0.0136
Group 2	APS-76 B	3574	OH	OH	3.4409	0.0136
Group 2	APS-76 C	3571	OH	OH	3.4409	0.0136
Group 2	APS-76 D	3574	OH	OH	3.4409	0.0136
Group 2	APS-76 A	3574	ClOH-OH	ClOH-OH	3.4409	0.0487
Group 2	APS-76 B	3574	ClOH-OH	ClOH-OH	3.4409	0.0487
Group 2	APS-76 C	3571	ClOH-OH	ClOH-OH	3.4409	0.0487
Group 2	APS-76 D	3574	ClOH-OH	ClOH-OH	3.4409	0.0487
Group 3	APS-78 A	3575	OH	OH	3.4014	0.0385
Group 3	APS-78 A	3574	OH	OH	3.4014	0.0385
Group 3	APS-78 A	3573	OH	OH	3.4014	0.0385
Group 3	APS-78 A	3576	OH	OH	3.4014	0.0385
Group 3	APS-78 A	3576	OH	OH	3.4014	0.0385
Group 3	APS-78 A	3575	OH	OH	3.4014	0.0385
Group 3	APS-82 A	3573	OH	OH	3.3993	0.0385
Group 3	APS-82 B	3576	OH	OH	3.3993	0.0385
Group 3	APS-82 C	3576	OH	OH	3.3993	0.0385
Group 3	APS-83 A	3576	OH	OH	3.3972	0.048
Group 3	APS-83 B	3576	OH	OH	3.3972	0.048
Group 3	APS-83 C	3573	OH	OH	3.3972	0.048
Group 3	APS-83 D	3576	OH	OH	3.3972	0.048
Group 1	APS-71 A	3548	ClOH-OH	Cl _b	3.891	0.009
Group 1	APS-71 B	3548	ClOH-OH	Cl _b	3.891	0.009
Group 1	APS-71 C	3548	ClOH-OH	Cl _b	3.891	0.009
Group 1	APS-71 A	3548	OH _a	ClOH-Cl	3.9937	0.0062

Group 1	APS-71 B	3548	OH _a	ClOH-Cl	3.9937	0.0062
Group 1	APS-71 C	3548	OH _a	ClOH-Cl	3.9937	0.0062
Group 1	APS-72 A	3548	ClOH-OH	Cl _b	3.9109	0.0076
Group 1	APS-72 A	3548	OH _a	ClOH-Cl	4.0521	0.0068
Group 1	APS-80 A	3548	ClOH-OH	Cl _b	3.8814	0.01637
Group 1	APS-80 B	3547	ClOH-OH	Cl _b	3.8814	0.01637
Group 1	APS-80 C	3548	ClOH-OH	Cl _b	3.8814	0.01637
Group 1	APS-80 D	3548	ClOH-OH	Cl _b	3.8814	0.01637
Group 1	APS-80 E	3547	ClOH-OH	Cl _b	3.8814	0.01637
Group 1	APS-80 F	3547	ClOH-OH	Cl _b	3.8814	0.01637
Group 1	APS-80 A	3548	OH _a	ClOH-Cl	3.9363	0.0089
Group 1	APS-80 B	3547	OH _a	ClOH-Cl	3.9363	0.0089
Group 1	APS-80 C	3548	OH _a	ClOH-Cl	3.9363	0.0089
Group 1	APS-80 D	3548	OH _a	ClOH-Cl	3.9363	0.0089
Group 1	APS-80 E	3547	OH _a	ClOH-Cl	3.9363	0.0089
Group 1	APS-80 F	3547	OH _a	ClOH-Cl	3.9363	0.0089
Group 2	APS-76 A	3547	ClOH-OH	Cl _b	3.9295	0.0959
Group 2	APS-76 B	3547	ClOH-OH	Cl _b	3.9295	0.0959
Group 2	APS-76 C	3543	ClOH-OH	Cl _b	3.9295	0.0959
Group 2	APS-76 D	3547	ClOH-OH	Cl _b	3.9295	0.0959
Group 3	APS-78 A	3548	OH	Cl _b	3.925	0.030
Group 3	APS-78 A	3547	OH	Cl _b	3.925	0.030
Group 3	APS-78 A	3548	OH	Cl _b	3.925	0.030
Group 3	APS-78 A	3549	OH	Cl _b	3.925	0.030
Group 3	APS-78 A	3549	OH	Cl _b	3.925	0.030
Group 3	APS-78 A	3549	OH	Cl _b	3.925	0.030

Group 3	APS-82 A	3547	OH	Cl _b	3.8956	0.034
Group 3	APS-82 B	3548	OH	Cl _b	3.8956	0.034
Group 3	APS-82 C	3548	OH	Cl _b	3.8956	0.034
Group 3	APS-83 A	3549	OH	Cl _b	3.9408	0.0396
Group 3	APS-83 B	3549	OH	Cl _b	3.9408	0.0396
Group 3	APS-83 C	3548	OH	Cl _b	3.9408	0.0396
Group 3	APS-83 D	3548	OH	Cl _b	3.9408	0.0396
Group 1	APS-71 A	3497	ClOH-OH	OH _a	2.853	0.0062
Group 1	APS-71 B	3497	ClOH-OH	OH _a	2.853	0.0062
Group 1	APS-71 C	3497	ClOH-OH	OH _a	2.853	0.0062
Group 1	APS-72 A	3498	ClOH-OH	OH _a	2.767	0.0068
Group 1	APS-80 A	3497	ClOH-OH	OH _a	2.927	0.0089
Group 1	APS-80 B	3497	ClOH-OH	OH _a	2.927	0.0089
Group 1	APS-80 C	3497	ClOH-OH	OH _a	2.927	0.0089
Group 1	APS-80 D	3497	ClOH-OH	OH _a	2.927	0.0089
Group 1	APS-80 E	3497	ClOH-OH	OH _a	2.927	0.0089
Group 1	APS-80 F	3495	ClOH-OH	OH _a	2.927	0.0089
Group 2	APS-76 A		OH	ClOH-OH	2.453*	0.0357
Group 2	APS-76 B		OH	ClOH-OH	2.453*	0.0357
Group 2	APS-76 C		OH	ClOH-OH	2.453*	0.0357
Group 2	APS-76 D		OH	ClOH-OH	2.453*	0.0357
Group 2	APS-76 A	3499	OH	OH	2.7857	0.0136
Group 2	APS-76 B	3499	OH	OH	2.7857	0.0136
Group 2	APS-76 C	3496	OH	OH	2.7857	0.0136
Group 2	APS-76 D	3499	OH	OH	2.7857	0.0136
Group 3	APS-78 A		OH	OH	2.490*	0.038

Group 3	APS-78 A	OH	OH	2.490*	0.038
Group 3	APS-78 A	OH	OH	2.490*	0.038
Group 3	APS-78 A	OH	OH	2.490*	0.038
Group 3	APS-78 A	OH	OH	2.490*	0.038
Group 3	APS-78 A	OH	OH	2.490*	0.038
Group 3	APS-82 A	OH	OH	2.461*	0.038
Group 3	APS-82 B	OH	OH	2.461*	0.038
Group 3	APS-82 C	OH	OH	2.461*	0.038
Group 3	APS-83 A	OH	OH	2.487*	0.048
Group 3	APS-83 B	OH	OH	2.487*	0.048
Group 3	APS-83 C	OH	OH	2.487*	0.048
Group 3	APS-83 D	OH	OH	2.487*	0.048

Table 2. Pairings assigned to the 3593 cm⁻¹ peak. The radii of the chlorine and OH atoms are those of Shannon (1976), r_{OH}= 1.20Å, r_{Cl}=1.67 Å. The variable d is the interatomic distance.

Structural group	Experiment	Peak maximum	OH position	Neighboring chlorine	Distance Å	1 σ error	d/(r _{Cl} +r _{OH})	(d+2σ)/ (r _{Cl} +r _{OH})
Group 1	APS-71 A	3591	OH _a	ClOH-Cl	2.8531	0.0062	0.99	1.00
Group 1	APS-71 B	3591	OH _a	ClOH-Cl	2.8531	0.0062	0.99	1.00
Group 1	APS-71 C	3591	OH _a	ClOH-Cl	2.8531	0.0062	0.99	1.00
Group 1	APS-72 A	3592	OH _a	ClOH-Cl	2.7673	0.0068	0.96	0.97
Group 1	APS-80 A	3590	OH	Cl _b	2.8537	0.0396	0.99	1.02
Group 1	APS-80 B	3592	OH	Cl _b	2.8537	0.0396	0.99	1.02
Group 1	APS-80 C	3590	OH	Cl _b	2.8537	0.0396	0.99	1.02
Group 1	APS-80 D	3591	OH	Cl _b	2.8537	0.0396	0.99	1.02

Group 1	APS-80 E	3591	OH	Cl _b	2.8537	0.0396	0.99	1.02
Group 1	APS-80 F	3592	OH	Cl _b	2.8537	0.0396	0.99	1.02
Group 2	APS-76 A	3592	OH	ClOH-Cl	3.1078	0.0357	1.08	1.11
Group 2	APS-76 B	3592	OH	ClOH-Cl	3.1078	0.0357	1.08	1.11
Group 2	APS-76 C	3589	OH	ClOH-Cl	3.1078	0.0357	1.08	1.11
Group 2	APS-76 D	3593	OH	ClOH-Cl	3.1078	0.0357	1.08	1.11
Group 3	APS-78 A	3592	OH	Cl _b	2.8776	0.0304	1.00	1.02
Group 3	APS-78 A	3591	OH	Cl _b	2.8776	0.0304	1.00	1.02
Group 3	APS-78 A	3591	OH	Cl _b	2.8776	0.0304	1.00	1.02
Group 3	APS-78 A	3593	OH	Cl _b	2.8776	0.0304	1.00	1.02
Group 3	APS-78 A	3593	OH	Cl _b	2.8776	0.0304	1.00	1.02
Group 3	APS-78 A	3592	OH	Cl _b	2.8776	0.0304	1.00	1.02
Group 3	APS-82 A	3592	OH	Cl _b	2.903	0.034	1.01	1.04
Group 3	APS-82 B	3593	OH	Cl _b	2.903	0.034	1.01	1.04
Group 3	APS-82 C	3593	OH	Cl _b	2.903	0.034	1.01	1.04
Group 3	APS-83 A	3593	OH	Cl _b	2.8537	0.0396	0.99	1.02
Group 3	APS-83 B	3593	OH	Cl _b	2.8537	0.0396	0.99	1.02
Group 3	APS-83 C	3590	OH	Cl _b	2.8537	0.0396	0.99	1.02
Group 3	APS-83 D	3593	OH	Cl _b	2.8537	0.0396	0.99	1.02