

Table S1 Observed and measured lines of H₂O...⁷⁹Br³⁵Cl and H₂O...⁸¹Br³⁵Cl and H₂O...⁷⁹Br³⁷Cl.

J'_{K-1K+1}	←	J''_{K-1K+1}	F'	I'	←	F''	I''	H ₂ O... ⁷⁹ Br ³⁵ Cl		H ₂ O... ⁸¹ Br ³⁵ Cl		H ₂ O... ⁷⁹ Br ³⁷ Cl		H ₂ O... ⁸¹ Br ³⁷ Cl			
								ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a		
3 ₀₃	←	2 ₀₂	3	2	←	1	2	10143.6990	-3.1	-	-	-	-	-	-	-	
				3	4	←	1	2	10128.8856	-4.2	10119.2250	-4.3	-	-	-	-	-
			3	6	←	1	4	10143.3188	-1.2	10133.5403	-3.2	9894.3855	-2.0	9883.9563	-3.8	-	-
				3	6	←	3	6	9913.6817	12.3	9942.2632	12.8	-	-	-	-	-
			5	4	←	3	2	10134.2946	-4.2	10125.3096	-2.7	-	-	-	-	-	-
				5	6	←	3	4	10127.7205	-1.4	10119.0273	-1.1	-	-	9871.9337	-1.1	-
			5	6	←	5	6	9978.6164	7.2	-	-	-	-	-	-	-	-
				5	8	←	3	6	10139.5449	-1.1	10130.5473	-1.7	9890.7756	-	9881.2266	-1.8	-
			5	8	←	5	8	9982.0178	5.0	9997.5688	5.5	-	-	-	-	-	-
				7	4	←	5	2	10087.4661	2.0	10087.1225	2.2	-	-	-	-	-
			7	6	←	5	4	10079.4871	-	10079.0232	1.0	9832.1734	-2.0	9831.1180	2.1	-	-
				7	8	←	5	6	10078.6671	0.1	-	-	9831.3794	5.3	9830.4224	0.2	-
			7	10	←	5	8	10085.6858	3.5	10085.3234	0.1	9836.9654	-0.3	9835.9771	3.0	-	-
				9	6	←	7	4	10083.6500	-	10083.3021	-0.5	9835.3603	-0.6	9834.3376	2.6	-
			9	8	←	7	6	10081.9741	-0.2	10081.6339	1.8	9834.0334	-2.9	9833.0115	0.5	-	-
				9	10	←	7	8	-	-	10082.4304	0.8	9834.7825	-0.6	-	-	-
9	12	←	7	10	-	-	10083.9893	1.7	9836.0402	-1.8	9834.9603	2.8	-	-			
	3 ₁₂	←	2 ₁₁	3	2	←	1	2	10080.9090	1.6	-	-	-	-	-	-	
3					4	←	1	2	10069.4555	-0.8	10072.1405	0.3	-	-	-	-	
3				4	←	1	4	10069.0363	-0.5	10071.6642	1.8	-	-	-	-	-	
				3	6	←	1	4	10080.6151	-2.7	10083.1854	-2.0	9831.3093	1.3	9833.2711	-3.2	-
3				6	←	3	6	9972.4931	-10.4	9992.2760	-7.9	-	-	-	-	-	
				5	4	←	3	2	10134.1473	2.4	10126.6915	1.1	-	-	-	-	
5				4	←	3	4	10134.7709	1.2	10127.2465	-0.3	-	-	-	-	-	
				5	6	←	3	4	10130.4527	-3.0	10123.0517	1.5	-	-	9874.9822	1.9	-

[Continued]

^a $\Delta\nu = \nu_{\text{obs}} - \nu_{\text{calc}}$

Table S1 (Continued)

J'_{K-1K+1}	←	J''_{K-1K+1}	F'	I'	←	F''	I''	$\text{H}_2\text{O}\cdots^{79}\text{Br}^{35}\text{Cl}$		$\text{H}_2\text{O}\cdots^{81}\text{Br}^{35}\text{Cl}$		$\text{H}_2\text{O}\cdots^{79}\text{Br}^{37}\text{Cl}$		$\text{H}_2\text{O}\cdots^{81}\text{Br}^{37}\text{Cl}$				
								ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a			
3 ₁₂	←	2 ₁₁	5	8	←	3	6	10138.4025	2.0	10130.9327	0.1	9889.3825	2.5	9881.3289	3.5			
			5	8	←	5	8	10058.9440	-1.7	-	-	-	-	-	-			
			7	4	←	5	2	10140.5393	0.2	10133.4656	-2.2	-	-	-	-			
			7	6	←	5	4	10131.9591	-2.8	10124.9282	-2.2	9883.8595	7.9	9876.1974	-0.7			
			7	6	←	5	6	10134.0134	-7.4	10127.1428	-3.7	-	-	-	-			
			7	8	←	5	6	10129.6542	-1.2	10122.7938	-2.8	9881.9376	-2.7	9874.4013	0.5			
			7	8	←	7	8	10249.7833	4.5	10223.3854	5.9	-	-	-	-			
			7	10	←	5	8	10137.4376	1.3	10130.3937	1.7	9888.1512	-0.7	9880.4851	0.2			
			7	10	←	7	10	10250.2815	3.9	10223.8186	0.9	-	-	-	-			
			9	6	←	7	4	10083.8855	-0.2	10085.5598	-1.1	9834.4942	-0.7	9835.5136	-0.9			
			9	8	←	7	6	10077.9554	1.5	10079.6227	-0.6	9829.8103	-0.2	9830.8171	-1.0			
			9	10	←	7	8	10076.8081	1.6	10078.4222	0.1	9828.9334	-0.2	9829.9066	1.9			
			9	12	←	7	10	-	-	10084.4656	-0.5	9833.6729	2.4	9834.6658	-0.1			
			3 ₁₃	←	2 ₁₂	3	2	←	1	2	10061.0821	0.8	10063.6196	-3.1	-	-	-	-
						3	4	←	1	2	10049.5933	-6.2	10052.2265	0.5	-	-	-	-
3	4	←				1	4	10049.1893	4.2	10051.7578	3.4	-	-	-	-			
3	6	←				1	4	10060.7978	1.9	10063.3057	1.4	9812.4578	-3.4	-	-			
3	6	←				3	6	9950.7347	-8.2	9970.7734	-3.6	-	-	-	-			
5	4	←				3	2	10114.3380	1.0	10106.8175	-1.1	-	-	-	-			
5	4	←				3	4	10114.9568	2.0	10107.3715	2.6	-	-	-	-			
5	6	←				3	4	10110.6264	2.4	10103.1563	-0.1	9864.1761	-1.8	9856.0749	3.0			
5	8	←				3	6	10118.6006	1.5	10111.0678	1.6	9870.5578	4.4	9862.4321	0.1			
5	8	←				5	8	10037.7023	-5.2	10043.0771	-6.9	-	-	-	-			
7	4	←				5	2	10120.2271	-4.0	10113.1780	-0.5	-	-	-	-			
7	6	←				5	4	10111.6420	-0.7	10104.6329	-0.3	9864.5117	-3.8	9856.8856	-0.1			

[Continued]

^a $\Delta\nu = \nu_{\text{obs}} - \nu_{\text{calc}}$

Table S1 (Continued)

J'_{K-1K+1}	←	J''_{K-1K+1}	F'	I'	←	F''	I''	$\text{H}_2\text{O}\cdots^{79}\text{Br}^{35}\text{Cl}$		$\text{H}_2\text{O}\cdots^{81}\text{Br}^{35}\text{Cl}$		$\text{H}_2\text{O}\cdots^{79}\text{Br}^{37}\text{Cl}$		$\text{H}_2\text{O}\cdots^{81}\text{Br}^{37}\text{Cl}$		
								ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	
3 ₁₃	←	2 ₁₂	7	6	←	5	6	10113.7101	2.4	-	-	-	-	-	-	-
			7	8	←	5	6	10109.3291	0.4	10102.4893	-1.0	9862.5956	-3.8	9855.0815	-1.3	-
			7	8	←	7	8	10231.4081	5.0	10204.7076	2.5	-	-	-	-	-
			7	10	←	5	8	10117.1246	-1.6	10110.1017	0.8	9868.8222	3.4	9861.1737	-1.1	-
			7	10	←	7	10	10231.8970	-1.3	10205.1459	2.3	-	-	-	-	-
			9	6	←	7	4	10063.5581	-0.3	10065.2532	-2.4	9815.1449	-2.8	9816.1890	-4.1	-
			9	8	←	7	6	10057.6244	0.2	10059.3159	-0.1	9810.4623	-0.2	9811.4934	-2.5	-
			9	10	←	7	8	10056.4802	0.5	10058.1174	-0.5	9809.5926	5.3	9810.5836	-0.8	-
			9	12	←	7	10	10062.5025	1.5	10064.1672	2.1	9814.3238	-2.1	9815.3476	0.2	-
			4 ₀₄	←	3 ₀₃	5	4	←	3	2	13471.0945	-4.5	-	-	-	-
5	6	←				3	4	13475.2361	0.8	13469.3783	-1.6	-	-	-	-	-
5	8	←				3	6	13479.4905	-0.8	13473.6025 ^b	-	-	-	-	-	-
7	6	←				5	4	-	-	13467.9317	-0.4	-	-	-	-	-
7	8	←				5	6	13473.4402	-3.0	13467.8211	0.4	-	-	-	-	-
7	10	←				5	8	13478.3003	0.5	-	-	13147.0167	0.9	13140.4927	-2.1	-
9	6	←				7	4	13452.2552	-5.5	-	-	-	-	-	-	-
9	8	←				7	6	13448.9519	2.0	-	-	-	-	-	-	-
9	10	←				7	8	13449.6215	-4.9	-	-	-	-	-	-	-
9	12	←				7	10	13452.7373	-0.3	13451.0622	-3.5	13121.5583	-1.9	-	-	-
11	10	←				9	8	13450.3920 ^b	-	-	-	-	-	-	-	-
11	12	←	9	10	13451.3215	0.8	13449.6155	-4.1	13120.4707	5.6	13117.9020	-1.4	-			
11	14	←	9	12	13452.1176	4.0	13450.3920 ^b	-	13121.0993	-1.0	13118.5330	0.2	-			
4 ₁₃	←	3 ₁₂	5	4	←	3	2	13463.5637	6.6	13461.4342	-3.0	-	-	-	-	
			5	6	←	3	4	13465.8778	-1.2	13463.7234	-1.2	-	-	-	-	
			5	8	←	3	6	13470.7583	2.0	13468.6195	2.8	13138.7217	0.4	13135.7376	2.8	
			7	4	←	5	2	13494.4341	-6.3	13488.3198	-0.9	-	-	-	-	

[Continued]

^a $\Delta\nu = \nu_{\text{obs}} - \nu_{\text{calc}}$
^b Line not included in fit

Table S1 (Continued)

J'_{K-1K+1}	←	J''_{K-1K+1}	F'	I'	←	F''	I''	$\text{H}_2\text{O}\cdots^{79}\text{Br}^{35}\text{Cl}$		$\text{H}_2\text{O}\cdots^{81}\text{Br}^{35}\text{Cl}$		$\text{H}_2\text{O}\cdots^{79}\text{Br}^{37}\text{Cl}$		$\text{H}_2\text{O}\cdots^{81}\text{Br}^{37}\text{Cl}$	
								ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a
4 ₁₃	←	3 ₁₂	7	6	←	5	4	13489.1351	-1.4	13483.0451	-1.6	-	-	-	-
			7	8	←	5	6	13488.5332	-0.2	13482.4541	3.2	13157.6759	-5.9	13150.7466	0.8
			7	10	←	5	8	13493.6795	2.2	13487.5217	2.6	13161.7937	4.3	13154.8169	0.6
			9	6	←	7	4	13482.2935	-3.5	13478.0981	-5.6	-	-	-	-
			9	8	←	7	6	13477.7481	0.4	13473.5610 ^b	-	13146.7395	1.2	13141.7201	-0.1
			9	10	←	7	8	13477.6664	1.4	13473.5971	9.2	13146.5984	-3.2	13141.6362	-5.2
			9	12	←	7	10	13481.9169	2.9	13477.7481	-0.7	13150.0010	1.7	13144.9909	1.2
			11	8	←	9	6	13459.7100	-3.8	13459.0346	1.5	13127.9142	-6.6	13126.3771	1.1
			11	10	←	9	8	13456.8634	3.6	13456.1590	-0.5	13125.6791	-1.6	13124.1178	-3.0
			11	12	←	9	10	13457.0149	1.4	13456.3076	1.6	13125.8039	-0.9	-	-
			11	14	←	9	12	13459.7991	3.9	13459.0904	-0.1	13128.0034	3.3	13126.4404	0.4
4 ₁₄	←	3 ₁₃	5	6	←	3	4	13439.0785	7.9	13436.8993	1.7	-	-	-	-
			5	8	←	3	6	13443.9601	2.9	13441.7985	0.9	13113.2278	2.0	13110.2215	-
			7	4	←	5	2	-	-	13461.5012	-3.7	-	-	-	-
			7	6	←	5	4	13462.3276	-1.0	13456.2157	-4.3	-	-	-	-
			7	8	←	5	6	13461.7271	1.8	13455.6259	1.6	13132.1844	1.4	13125.2264	-2.9
			7	10	←	5	8	13466.8804	-1.1	13460.7068	2.7	13136.3000	3.4	13129.3093	3.6
			7	10	←	7	10	13387.4579	-4.9	13393.6825	-4.7	-	-	-	-
			9	6	←	7	4	13455.2645	-1.7	13451.1056 ^b	-	-	-	-	-
			9	8	←	7	6	13450.7475 ^b	-	13446.5417 ^b	-	13121.0115	1.6	-	-
			9	10	←	7	8	13450.6175 ^b	-	13446.5722 ^b	-	13120.8715	-0.1	13115.9302	-4.1
			9	12	←	7	10	13454.8803	-2.8	13450.7476 ^b	-	13124.2563	-16.6	13119.2916	5.2
11	8	←	9	6	13432.6745	0.2	13432.0181	4.5	13102.1898	1.9	13100.6674	-			
11	10	←	9	8	13429.8205	1.3	13429.1405	1.1	13099.9505	2.9	13098.4171	5.0			
11	12	←	9	10	13429.9749	-	13429.2887	1.0	13100.0751	2.5	13098.5306	-1.5			
11	14	←	9	12	13432.7589	0.4	13432.0747	0.9	13102.2735	4.7	13100.7325	-0.5			

^a $\Delta\nu = \nu_{\text{obs}} - \nu_{\text{calc}}$

^b Line not included in fit

Table S2 Observed and measured lines of $\text{D}_2\text{O}\cdots^{79}\text{Br}^{35}\text{Cl}$ and $\text{D}_2\text{O}\cdots^{81}\text{Br}^{35}\text{Cl}$ and $\text{HDO}\cdots^{79}\text{Br}^{35}\text{Cl}$ and $\text{HDO}\cdots^{81}\text{Br}^{35}\text{Cl}$.

J'_{K-1K+1}	\leftarrow	J''_{K-1K+1}	F'	I'	\leftarrow	F''	I''	$\text{D}_2\text{O}\cdots^{79}\text{Br}^{35}\text{Cl}$		$\text{D}_2\text{O}\cdots^{81}\text{Br}^{35}\text{Cl}$		$\text{HDO}\cdots^{79}\text{Br}^{35}\text{Cl}$		$\text{HDO}\cdots^{81}\text{Br}^{35}\text{Cl}$	
								ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a
3 ₀₃	\leftarrow	2 ₀₂	2	2	\leftarrow	2	2	9421.4671	1.0	9412.9845	-0.5	9765.2007	1.8	9756.2022	0.5
			2	2	\leftarrow	2	2	-	-	-	-	-	9563.3706	9.4	
			4	2	\leftarrow	4	2	9406.6881	-2.7	9398.2343	3.0	9750.4081	1.1	9741.4339	-0.1
			4	2	\leftarrow	4	2	9406.1489	8.5	9397.5626	1.7	9749.8553	2.7	9740.7659	6.3
			4	2	\leftarrow	4	2	-	-	-	-	9519.1255	1.5	-	-
			4	2	\leftarrow	4	2	-	-	-	-	9520.0519	1.8	-	-
			6	2	\leftarrow	6	2	9421.0890	0.0	9412.5184	-1.8	9764.8212	1.9	9755.7287	-5.7
			6	2	\leftarrow	6	2	9191.0933	-1.9	-	-	9535.0165	-0.3	9564.3402	-4.1
			2	2	\leftarrow	2	2	-	-	-	-	9768.9491	-1.0	9760.9353 ^b	-
			2	2	\leftarrow	2	2	-	-	-	-	9606.3948	0.2	9622.7686	-1.0
			4	2	\leftarrow	4	2	9411.8549	-1.9	9404.1505	0.2	9755.6945	1.1	9747.4302	-2.8
			4	2	\leftarrow	4	2	9410.8907	3.0	9403.3378	-0.7	9754.7546	-3.7	9746.6485	-1.3
			4	2	\leftarrow	4	2	-	-	-	-	9600.8046	-0.1	9616.8071	-3.6
			6	2	\leftarrow	6	2	9405.2327	2.6	9397.8256	1.6	9749.0880	-4.2	9741.1317	3.4
			6	2	\leftarrow	6	2	-	-	-	-	9750.0176	-0.7	9741.9063	2.0
			6	2	\leftarrow	6	2	-	-	-	-	9600.2474	-3.7	9616.5400	-2.6
			8	2	\leftarrow	8	2	9417.0851	-0.1	9409.3724	1.8	9760.9344	3.9	9752.6603	-0.8
			8	2	\leftarrow	8	2	9260.0070	-2.6	9276.7005	-0.7	9603.6443	2.5	9619.8522	2.6
			4	2	\leftarrow	4	2	9365.1532	-1.8	9366.0446	1.9	9708.9315	0.9	9709.2851	-1.4
			4	2	\leftarrow	4	2	-	-	-	-	9716.5976	0.2	9716.8668	0.9
6	2	\leftarrow	6	2	9357.1972	0.4	9357.9634	2.5	9700.9683	4.2	9701.1946	-2.7			
6	2	\leftarrow	6	2	-	-	-	-	9706.0737	-2.9	-	-			
6	2	\leftarrow	6	2	-	-	-	-	9932.2286	-0.5	-	-			

[Continued]

^a $\Delta\nu = \nu_{\text{obs}} - \nu_{\text{calc}}$

^b Line not included in fit

Table S2 (Continued)

J'_{K-1K+1}	←	J''_{K-1K+1}	F'	I'	←	F''	I''	$\text{D}_2\text{O}\cdots^{79}\text{Br}^{35}\text{Cl}$		$\text{D}_2\text{O}\cdots^{81}\text{Br}^{35}\text{Cl}$		$\text{HDO}\cdots^{79}\text{Br}^{35}\text{Cl}$		$\text{HDO}\cdots^{81}\text{Br}^{35}\text{Cl}$	
								ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a
3 ₀₃	←	2 ₀₂	8	2	←	8	2	9356.3771	-2.9	9357.3303	0.8	9700.1466	0.9	9700.5639	-0.8
			8	2	←	8	2	-	-	-	-	9692.6205	-3.6	-	-
			8	2	←	8	2	-	-	-	-	9933.9791	1.2	9897.3497	-0.8
			10	2	←	10	2	9363.3837	1.5	9364.2539	0.1	9707.1527	-0.9	-	-
			10	2	←	10	2	9584.8748	-6.0	9548.5587	-1.8	9928.5974	-0.1	-	-
			6	2	←	6	2	-	-	9362.2486	1.7	9705.1285	-4.8	-	-
			6	2	←	6	2	-	-	-	-	9724.3742	-0.3	-	-
			8	2	←	8	2	9359.7024	2.4	9360.5846	5.2	9703.4610	1.3	9703.8110	0.6
			8	2	←	8	2	9367.3842	3.9	-	-	9711.1363	-3.0	9711.4263	0.9
			10	2	←	10	2	9360.5846	-0.9	9361.3827	-0.8	9704.3422	0.4	9704.6139	2.7
			10	2	←	10	2	9340.6871	0.1	-	-	9684.4329	1.0	9684.6428	-3.5
			12	2	←	12	2	9362.1566	1.4	9362.9366	-1.0	9705.9147	0.9	9706.1692	2.1
3 ₁₂	←	2 ₁₁	8	2	←	8	2	9422.3541	8.6	9416.1188	-1.8	-	-	-	-
			8	2	←	8	2	9413.5261	-11.4	9407.9305	-11.7	-	-	-	-
			10	2	←	10	2	9421.3461	-10.5	9415.5634	-6.0	-	-	-	-
			6	2	←	6	2	9367.9295	-0.2	9370.8182	-1.4	-	-	-	-
			8	2	←	8	2	9362.0214	3.6	9364.8984	0.3	-	-	-	-
			10	2	←	10	2	9360.8807	-2.7	9363.7039	-5.1	-	-	-	-
3 ₁₃	←	2 ₁₂	12	2	←	12	2	9366.8837	3.6	9369.7395	4.0	-	-	-	-
			8	2	←	8	2	9390.1444	7.2	9383.8578	4.7	-	-	-	-
			8	2	←	8	2	9380.8139	2.1	9375.2374	0.2	-	-	-	-
			10	2	←	10	2	9388.6485	5.4	9382.8807	4.5	-	-	-	-
			6	2	←	6	2	9335.1961	-7.3	9338.1142	-1.1	-	-	-	-
			8	2	←	8	2	9329.2898	-0.1	9332.1919	-0.6	-	-	-	-
10	2	←	10	2	9328.1598	1.9	9331.0041	-2.0	-	-	-	-			
12	2	←	12	2	9334.1531	-4.4	9337.0381	2.8	-	-	-	-			

[Continued]

^a $\Delta\nu = \nu_{\text{obs}} - \nu_{\text{calc}}$

Table S2 (Continued)

J'_{K-1K+1}	←	J''_{K-1K+1}	F'	I'	←	F''	I''	$\text{D}_2\text{O}\dots^{79}\text{Br}^{35}\text{Cl}$		$\text{D}_2\text{O}\dots^{81}\text{Br}^{35}\text{Cl}$		$\text{HDO}\dots^{79}\text{Br}^{35}\text{Cl}$		$\text{HDO}\dots^{81}\text{Br}^{35}\text{Cl}$	
								ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a
4 ₀₄	←	3 ₀₃	4	3	←	4	3	12508.0373	-0.3	12503.8134	0.2	12966.3932	-0.7	12961.4620	0.1
			6	3	←	6	3	-	-	12507.9483	0.2	12970.5171	-3.4	12965.6039	-0.1
			6	3	←	6	3	-	-	-	-	-	-	12950.6315	2.3
			8	3	←	8	3	12516.4168	2.5	12512.1760	0.8	12974.7759	-1.4	12969.8290	-0.6
			6	3	←	6	3	12510.4166	-1.8	12506.4615	-0.6	-	-	12964.1383	2.2
			8	3	←	8	3	12510.3015	1.7	12506.3415	-3.2	12968.6955	-1.5	12964.0185	-3.2
			10	3	←	10	3	12515.1570	-1.7	12511.1141	-4.5	12973.5563	2.1	12968.8034	9.2
			10	3	←	10	3	-	-	12423.5634	-2.5	12870.0399	-2.5	12881.1451	-4.9
			6	3	←	6	3	12489.1927	-1.2	12489.1274	-4.3	12947.5567	1.0	-	-
			8	3	←	8	3	12485.8905	-0.7	-	-	12944.2451	-4.2	12943.4647	0.8
			10	3	←	10	3	12486.5588	-8.2	12486.6012	8.4	12944.9312	5.9	12944.2451	3.6
			12	3	←	12	3	12489.6755	2.8	12489.6410	-3.5	12948.0325	-0.9	12947.2968	1.7
			8	3	←	8	3	12488.2594	-4.2	-	-	-	-	12945.8864 ^b	-
			10	3	←	10	3	12487.3069	-1.0	12487.2500	0.2	12945.6620	0.1	12944.8890	-5.2
			12	3	←	12	3	12488.2740	2.9	-	-	-	-	12945.8483	-5.7
			4 ₁₃	←	3 ₁₂	14	3	←	14	3	12489.0679	6.1	12488.9895	-1.0	12947.4188
10	3	←				10	3	12538.9893	-1.5	12534.4893	7.7	-	-	-	-
10	3	←				10	3	12522.9684	2.6	12520.5505	7.6	-	-	-	-
12	3	←				12	3	12527.2198	-0.1	12524.7090	0.9	-	-	-	-
10	3	←				10	3	12502.2351	4.2	12503.1704	6.0	-	-	-	-
12	3	←				12	3	12502.3861	-0.8	12503.3098	-3.1	-	-	-	-
4 ₁₄	←	3 ₁₃	14	3	←	14	3	12505.1629	2.4	12506.0881	-2.6	-	-	-	-
			8	3	←	8	3	12472.6744	2.6	-	-	-	-	-	-
			8	3	←	8	3	12490.5141	-0.4	-	-	-	-	-	-
			10	3	←	10	3	-	-	12491.1339	-1.8	-	-	-	-

[Continued]

^a $\Delta\nu = \nu_{\text{obs}} - \nu_{\text{calc}}$

^b Line not included in fit

Table S2 (Continued)

J'_{K-1K+1}	\leftarrow	J''_{K-1K+1}	F'	I'	\leftarrow	F''	I''	$\text{D}_2\text{O}\cdots^{79}\text{Br}^{35}\text{Cl}$		$\text{D}_2\text{O}\cdots^{81}\text{Br}^{35}\text{Cl}$		$\text{HDO}\cdots^{79}\text{Br}^{35}\text{Cl}$		$\text{HDO}\cdots^{81}\text{Br}^{35}\text{Cl}$	
								ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a	ν_{obs} (MHz)	$\Delta\nu$ (kHz) ^a
4 ₁₄	\leftarrow	3 ₁₃	8	3	\leftarrow	8	3	12479.4869	0.8	-	-	-	-	-	-
			10	3	\leftarrow	10	3	12479.3936	-2.8	12476.9939	1.4	-	-	-	-
			12	3	\leftarrow	12	3	12483.6581	1.6	12481.1664	2.3	-	-	-	-
			8	3	\leftarrow	8	3	12461.5056	-0.5	-	-	-	-	-	-
			10	3	\leftarrow	10	3	12458.6563	-4.5	12459.6117	-3.1	-	-	-	-
			12	3	\leftarrow	12	3	12458.8166	-1.3	12459.7605	-3.8	-	-	-	-
			14	3	\leftarrow	14	3	12461.5938	0.8	12462.5420	-1.5	-	-	-	-

^a $\Delta\nu = \nu_{obs} - \nu_{calc}$