

Supplementary Material for Parker REMPI of water:

Table S1 Selected line list for REMPI transitions of HDO.

C ¹ B ₁ state			X ¹ A ₁ state			Branch $\Delta K_a \Delta J K_a'', K_c''(J'')$	Energy (cm ⁻¹)	Line strength S
J'	K _a '	K _c '	J''	K _a ''	K _c ''			
2	2	1	0	0	0	sS0,0(0)	80787.02	0.4000
2	1	1	0	0	0	rS0,0(0)	80746.51	0.0653
1	0	1	1	1	0	pQ1,0(1)	80668.51	0.0588
1	1	1	1	1	0	qQ1,0(1)	80682.02	0.3600
2	2	1	1	1	0	rR1,0(1)	80754.59	0.0327
2	1	1	1	1	0	qR1,0(1)	80714.08	0.2000
3	0	3	1	1	0	pS1,0(1)	80736.75	0.0258
3	2	1	1	1	0	rS1,0(1)	80797.40	0.0787
3	1	3	1	1	0	qS1,0(1)	80745.90	0.0302
3	3	1	1	1	0	sS1,0(1)	80869.26	0.6098
1	1	0	1	0	1	rQ0,1(1)	80701.12	0.0588
2	0	2	1	0	1	qR0,1(1)	80712.99	0.0032
2	2	0	1	0	1	sR0,1(1)	80771.77	0.7968
2	1	2	1	0	1	rR0,1(1)	80724.58	0.0327
3	2	2	1	0	1	sS0,1(1)	80813.18	0.4000
3	1	2	1	0	1	rS0,1(1)	80775.74	0.1044
3	3	0	1	0	1	tS0,1(1)	80886.23	0.0001
1	1	0	1	1	1	qQ1,1(1)	80686.85	0.3600
2	0	2	1	1	1	pR1,1(1)	80698.73	0.0905
2	2	0	1	1	1	rR1,1(1)	80757.51	0.0401
2	1	2	1	1	1	qR1,1(1)	80710.31	0.2000

3	2	2	1	1	1	rSI,1(1)	80798.92	0.0653
3	1	2	1	1	1	qSI,1(1)	80761.48	0.0525
3	3	0	1	1	1	sSI,1(1)	80871.97	0.5875
1	0	1	2	0	2	qP0,2(2)	80654.84	0.0044
1	0	1	2	2	0	oP2,0(2)	80591.85	0.7956
1	1	1	2	0	2	rP0,2(2)	80668.34	0.0893
1	1	1	2	2	0	pP2,0(2)	80605.35	0.0414
2	2	1	2	0	2	sQ0,2(2)	80740.92	0.5683
2	2	1	2	2	0	qQ2,0(2)	80677.92	0.0031
2	1	1	2	0	2	rQ0,2(2)	80700.41	0.0296
2	1	1	2	2	0	pQ2,0(2)	80637.41	0.0638
3	0	3	2	0	2	qR0,2(2)	80723.08	0.0293
3	2	1	2	0	2	sR0,2(2)	80783.73	0.9663
3	0	3	2	2	0	oR2,0(2)	80660.09	0.1861
3	2	1	2	2	0	qR2,0(2)	80720.73	0.0183
3	1	3	2	0	2	rR0,2(2)	80732.23	0.0731
3	3	1	2	0	2	tR0,2(2)	80855.59	0.0009
3	1	3	2	2	0	pR2,0(2)	80669.24	0.0369
3	3	1	2	2	0	rR2,0(2)	80792.60	0.0850
4	2	3	2	0	2	sS0,2(2)	80837.90	0.4289
4	4	1	2	0	2	uS0,2(2)	81013.21	0.0028
4	2	3	2	2	0	qS2,0(2)	80774.91	0.0003
4	4	1	2	2	0	sS2,0(2)	80950.22	0.9966
4	1	3	2	0	2	rS0,2(2)	80804.42	0.1337

4	3	1	2	0	2	tS0,2(2)	80911.66	0.0001
4	1	3	2	2	0	pS2,0(2)	80741.43	0.0126
4	3	1	2	2	0	rS2,0(2)	80848.67	0.0869
1	0	1	2	1	2	pP1,2(2)	80642.92	0.0327
1	1	1	2	1	2	qP1,2(2)	80656.42	0.2000
2	2	1	2	1	2	rQ1,2(2)	80728.99	0.0700
2	1	1	2	1	2	qQ1,2(2)	80688.49	0.4286
3	0	3	2	1	2	pR1,2(2)	80711.16	0.1281
3	2	1	2	1	2	rR1,2(2)	80771.80	0.0025
3	1	3	2	1	2	qR1,2(2)	80720.31	0.3264
3	3	1	2	1	2	sR1,2(2)	80843.67	0.4736
4	2	3	2	1	2	rS1,2(2)	80825.98	0.0932
4	4	1	2	1	2	tS1,2(2)	81001.29	0.0001
4	1	3	2	1	2	qS1,2(2)	80792.50	0.1042
4	3	1	2	1	2	sS1,2(2)	80899.74	0.4672
0	0	0	2	2	1	oO2,1(2)	80578.31	0.4000
1	1	0	2	2	1	pP2,1(2)	80607.85	0.0327
2	0	2	2	2	1	oQ2,1(2)	80619.72	0.5691
2	2	0	2	2	1	qQ2,1(2)	80678.51	0.0023
2	1	2	2	2	1	pQ2,1(2)	80631.31	0.0700
3	1	2	2	2	1	pR2,1(2)	80682.47	0.0443
3	3	0	2	2	1	rR2,1(2)	80792.96	0.0864
4	0	4	2	2	1	oS2,1(2)	80713.74	0.0253
4	2	2	2	2	1	qS2,1(2)	80778.63	0.0050

4	4	0	2	2	1	sS2,I(2)	80950.56	0.9982
4	1	4	2	2	1	pS2,I(2)	80720.38	0.0079
4	3	2	2	2	1	rS2,I(2)	80848.90	0.0854
0	0	0	2	1	1	pOI,I(2)	80620.98	0.0653
1	1	0	2	1	1	qPI,I(2)	80650.51	0.2000
2	0	2	2	1	1	pQI,I(2)	80662.39	0.0286
2	2	0	2	1	1	rQI,I(2)	80721.17	0.0647
2	1	2	2	1	1	qQI,I(2)	80673.98	0.4286
3	1	2	2	1	1	qRI,I(2)	80725.14	0.2711
3	3	0	2	1	1	sRI,I(2)	80835.63	0.5289
4	0	4	2	1	1	pSI,I(2)	80756.41	0.0385
4	2	2	2	1	1	rSI,I(2)	80821.30	0.1293
4	4	0	2	1	1	tSI,I(2)	80993.23	0.0001
4	1	4	2	1	1	qSI,I(2)	80763.05	0.0482
4	3	2	2	1	1	sSI,I(2)	80891.57	0.5232

Table S2 Transitions in the 2+1 REMPI spectrum of H₂O with narrow linewidths suitable for state-selective probes of nascent molecules.

J'	Ka'	Kc'	<Ja'2>	<Jb'2>	<Jc'2>	Linewidth (cm ⁻¹)
0	0	0	0	0	0	1.317(89)
1	0	1	0	1	1	1.309(61)
1	1	0	1	1	0	2.170(127)
1	1	1	1	0	1	2.924(54)
2	0	2	0	2.580	3.367	1.752(48)
2	1	1	1	4	1	2.556(300)
2	1	2	1	1	4	2.347(265)
2	2	1	4	1	1	4.812(126)
2	2	0	3.949	1.413	0.638	6.031(66)
3	2	2	4	4	4	5.576(154)

Table S3 Transitions in the 2+1 REMPI spectrum of HDO with narrow linewidths suitable for state-selective probes of nascent molecules.

J'	Ka'	Kc'	<Ja'2>	<Jb'2>	<Jc'2>	Linewidth (cm ⁻¹)
1	0	1	0	1	1	0.950(146)
1	1	1	1	0	1	1.518(86)
1	1	0	1	1	0	1.597(240)
2	0	2	0.016	2.777	3.208	1.030(100)
2	1	2	1	1	4	1.433(80)
2	1	1	1	4	1	1.606(69)
2	2	0	3.9848	1.2238	0.792	3.696(138)
2	2	1	4	1	1	3.430(91)
3	1	3	1.011	8.347	2.642	2.036(236)
3	1	2	1.011	8.347	2.642	1.980(339)
3	2	2	4	4	4	3.991(199)

Table S4 Transitions in the 2+1 REMPI spectrum of D₂O with narrow linewidths suitable for state-selective probes of nascent molecules.

J'	K_a'	K_c'	$\langle J_a'^2 \rangle$	$\langle J_b'^2 \rangle$	$\langle J_c'^2 \rangle$	Linewidth (cm ⁻¹)
0	0	0	0	0	0	0.743(139)
1	0	1	0	1	1	0.901(60)
1	1	1	1	0	1	0.979(89)
1	1	0	1	1	0	0.801(25)
2	0	2	0.031	2.681	3.288	0.662(101)
2	1	2	1	1	4	1.197(148)
2	1	1	1	4	1	0.958(184)
2	2	1	4	1	1	1.809(50)
2	2	0	3.969	1.319	0.712	1.814(80)
3	0	3	0.142	4.497	7.361	0.972(101)
3	1	3	1.017	2.32	8.663	2.064(452)
3	1	2	1.023	8.272	2.705	1.679(782)
3	2	2	4	4	4	1.683(75)
3	3	0	8.977	1.728	1.295	4.837(247)
4	1	3	1.105	13.479	5.416	2.328(366)
4	2	2	3.669	11.753	4.579	3.900(1140)
4	2	3	4.024	7.749	8.226	2.229(229)