

Ultraviolet photodissociation action spectroscopy of quinolineH⁺ and isoquinolineH⁺

Electronic Supplementary Material

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1 m/z 77 structural elucidation mass spectra

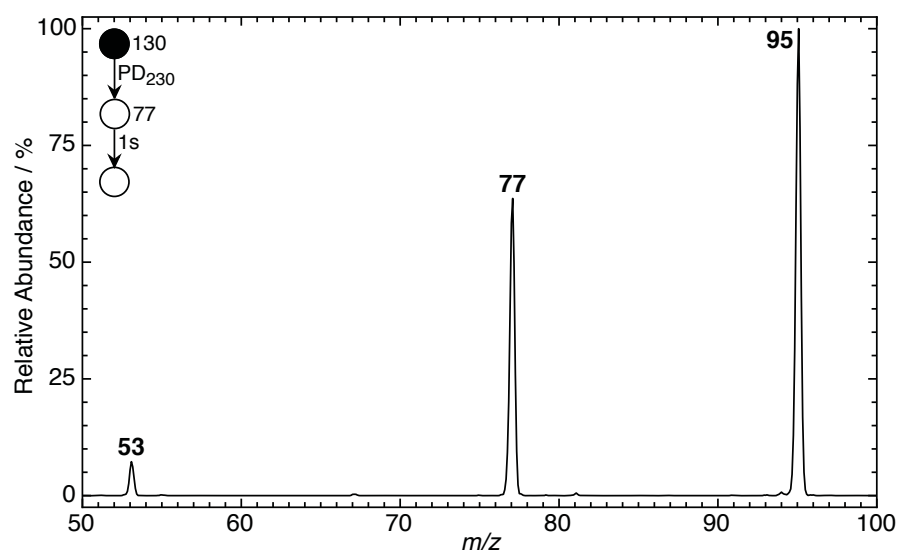


Figure S1: Mass spectrum recorded after mass-selecting a quinolineH⁺ (m/z 130) ion population, irradiating with a single 230 nm laser pulse and storing the m/z 77 photoproduct ions for 1 second.

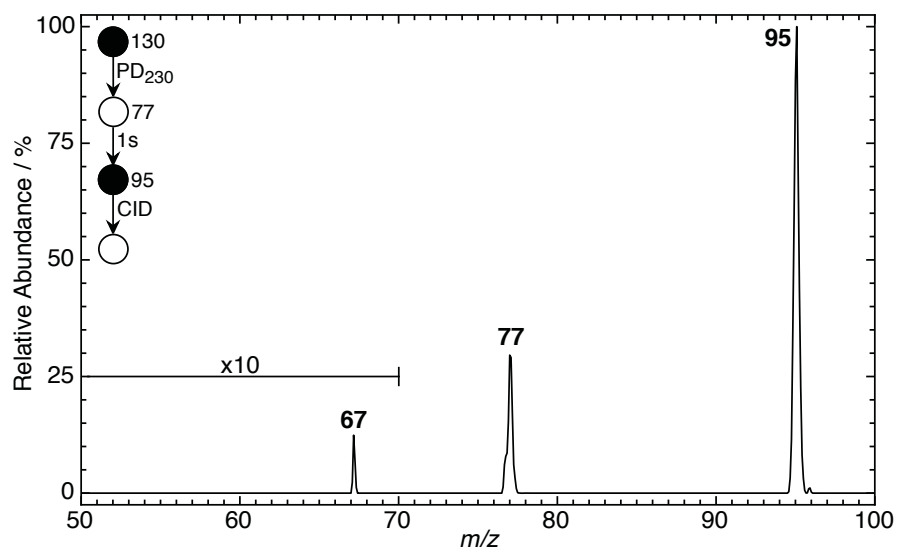
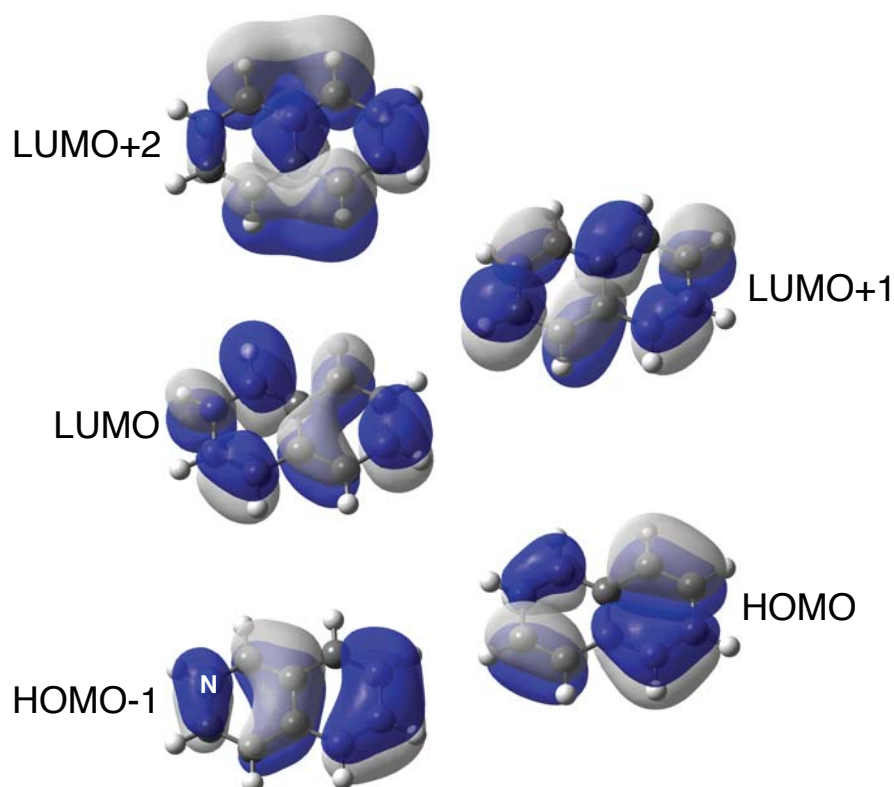


Figure S2: Mass spectrum recorded following collisional activation of the m/z 95 ions formed from addition of water (18 Da) to the m/z 77 quinolineH⁺ photoproduct.

2 isoquinolineH⁺ molecular orbitals



3 Cartesian coordinates and normal modes

3.1 Cartesian coordinates

3.1.1 quinolineH⁺

	Atomic	Atomic	x	y	z
	Number	Symbol			
<u>S₀</u>	1	H	-1.26430600	-2.29235000	0.00000000
	14	N	-1.23454900	-1.27632600	0.00000000
	12	C	-2.38648100	-0.60756200	0.00000000
	1	H	-3.29775600	-1.20203900	0.00000000
	12	C	-2.38958100	0.78371800	0.00000000
	1	H	-3.33759100	1.31527000	0.00000000
	12	C	-1.18014400	1.45110200	0.00000000
	1	H	-1.15813300	2.54100800	0.00000000
	12	C	0.04044400	0.74265800	0.00000000
	12	C	1.30847000	1.38076000	0.00000000
	1	H	1.35140300	2.46874800	0.00000000
	12	C	2.45454700	0.62980700	0.00000000
	1	H	3.42787200	1.11712200	0.00000000
	12	C	2.38693900	-0.78504200	0.00000000
	1	H	3.30985000	-1.36325900	0.00000000
	12	C	1.17910400	-1.44057900	0.00000000
	1	H	1.13071200	-2.52905800	0.00000000
	12	C	0.00000000	-0.67505400	0.00000000

	Atomic Number	Atomic Symbol	x	y	z
<u>S₁</u>	1	H	0.33686154	0.00000000	-0.36121042
	14	N	0.34029535	0.00000000	0.65012113
	12	C	1.56323847	0.00000000	1.31252121
	1	H	2.44835522	0.00000000	0.68544045
	12	C	1.59124242	0.00000000	2.68168052
	1	H	2.55646682	0.00000000	3.18333299
	12	C	0.39715349	0.00000000	3.43263527
	1	H	0.41311863	0.00000000	4.51821477
	12	C	-0.83917714	0.00000000	2.72511128
	12	C	-2.09922999	0.00000000	3.37237715
	1	H	-2.12428269	0.00000000	4.46251985
	12	C	-3.33650412	0.00000000	2.65911424
	1	H	-4.27094906	0.00000000	3.21725562
	12	C	-3.32549622	0.00000000	1.28694683
	1	H	-4.24807635	0.00000000	0.71061319
	12	C	-2.07879054	0.00000000	0.61418103
	1	H	-2.06376452	0.00000000	-0.47640923
	12	C	-0.84891857	0.00000000	1.32555410

	Atomic Number	Atomic Symbol	x	y	z
<u>S₂</u>	1	H	0.34410398	0.00000000	-0.37591594
	14	N	0.34247348	0.00000000	0.63832703
	12	C	1.53009284	0.00000000	1.29727859
	1	H	2.42570030	0.00000000	0.68048503
	12	C	1.57169313	0.00000000	2.69801266
	1	H	2.54405351	0.00000000	3.18407271
	12	C	0.38878653	0.00000000	3.43663747
	1	H	0.40941220	0.00000000	4.52381604
	12	C	-0.86282505	0.00000000	2.75887491
	12	C	-2.10412145	0.00000000	3.41443455
	1	H	-2.12532142	0.00000000	4.50273715
	12	C	-3.29744500	0.00000000	2.69248465
	1	H	-4.25177850	0.00000000	3.21563009
	12	C	-3.28269516	0.00000000	1.26506039
	1	H	-4.22124847	0.00000000	0.71415892
	12	C	-2.06912472	0.00000000	0.57568798
	1	H	-2.05451586	0.00000000	-0.51375792
	12	C	-0.87569762	0.00000000	1.29197568

	Atomic Number	Atomic Symbol	x	y	z
<u>S₃</u>	1	H	1.21991000	2.35109800	0.00000000
	14	N	1.21406800	1.33625000	0.00000000
	12	C	2.38276200	0.67755300	0.00000000
	1	H	3.28517800	1.28499800	0.00000000
	12	C	2.41997300	-0.74568800	0.00000000
	1	H	3.38858100	-1.23897600	0.00000000
	12	C	1.24138400	-1.45694200	0.00000000
	1	H	1.24356300	-2.54494900	0.00000000
	12	C	-0.00394400	-0.75096900	0.00000000
	12	C	-1.27895800	-1.41055400	0.00000000
	1	H	-1.30169000	-2.50047700	0.00000000
	12	C	-2.47310400	-0.69140600	0.00000000
	1	H	-3.42560700	-1.21620000	0.00000000
	12	C	-2.44450600	0.73933600	0.00000000
	1	H	-3.37501400	1.30340400	0.00000000
	12	C	-1.23103800	1.41264200	0.00000000
	1	H	-1.20881000	2.50321800	0.00000000
	12	C	0.00000000	0.67671600	0.00000000

3.1.2 isoquinolineH⁺

	Atomic Number	Atomic Symbol	x	y	z
<u>S₀</u>	1	H	-1.39618400	2.37834900	0.00000000
	1	H	-3.26406500	1.01922600	0.00000000
	12	C	-2.34307700	-0.81829900	0.00000000
	1	H	-3.30905500	-1.31510100	0.00000000
	12	C	-1.14742200	-1.46682100	0.00000000
	1	H	-1.13067800	-2.55467000	0.00000000
	12	C	0.06835000	-0.73154300	0.00000000
	12	C	1.33719600	-1.35154700	0.00000000
	1	H	1.40291100	-2.43819300	0.00000000
	12	C	2.47374700	-0.57930500	0.00000000
	1	H	3.45130600	-1.06015400	0.00000000
	12	C	2.40403300	0.83728800	0.00000000
	1	H	3.32476400	1.41814100	0.00000000
	12	C	1.19110300	1.47130900	0.00000000
	1	H	1.12720600	2.55853900	0.00000000
	12	C	0.00000000	0.69624300	0.00000000
	12	C	-1.26231400	1.29791500	0.00000000
	12	N	-2.36227100	0.55177400	0.00000000

	Atomic Number	Atomic Symbol	x	y	z
<u>S₁</u>	1	H	-1.38987420	-2.42688606	0.00000000
	1	H	-3.32223697	-1.04415102	0.00000000
	12	C	-2.38148957	0.77205454	0.00000000
	1	H	-3.34057174	1.28600636	0.00000000
	12	C	-1.18366082	1.45274315	0.00000000
	1	H	-1.18769696	2.53921472	0.00000000
	12	C	0.03894785	0.71652446	0.00000000
	12	C	1.30723001	1.35983122	0.00000000
	1	H	1.33727031	2.44952958	0.00000000
	12	C	2.51761165	0.63223122	0.00000000
	1	H	3.47205949	1.15332683	0.00000000
	12	C	2.45374945	-0.74564287	0.00000000
	1	H	3.36258333	-1.34573489	0.00000000
	12	C	1.19494537	-1.41092077	0.00000000
	1	H	1.17960472	-2.50116445	0.00000000
	12	C	-0.02492922	-0.69906117	0.00000000
	12	C	-1.26878847	-1.34973285	0.00000000
	14	N	-2.42395423	-0.57924398	0.00000000

	Atomic Number	Atomic Symbol	x	y	z
<u>S₂</u>	1	H	-1.39575460	-2.41183863	0.00000000
	1	H	-3.27832599	-1.06442285	0.00000000
	12	C	-2.39586260	0.78276475	0.00000000
	1	H	-3.36927068	1.262119	0.00000000
	12	C	-1.17805534	1.4697093	0.00000000
	1	H	-1.18537832	2.55702315	0.00000000
	12	C	0.02956541	0.76240179	0.00000000
	12	C	1.29768668	1.38671963	0.00000000
	1	H	1.35609970	2.4745669	0.00000000
	12	C	2.48186674	0.62886186	0.00000000
	1	H	3.44067766	1.14511498	0.00000000
	12	C	2.44494615	-0.78788615	0.00000000
	1	H	3.36967456	-1.35932588	0.00000000
	12	C	1.20680965	-1.43913517	0.00000000
	1	H	1.16761715	-2.52792562	0.00000000
	12	C	0.00018747	-0.70370812	0.00000000
	12	C	-1.26797168	-1.33268735	0.00000000
	13	N	-2.38371194	-0.58342761	0.00000000

	Atomic Number	Atomic Symbol	x	y	z
$\underline{\mathbf{S}_3}$	1	H	-1.39644238	2.41135958	0.00000000
	1	H	-3.28264660	1.04007105	0.00000000
	12	C	-2.36522554	-0.82337731	0.00000000
	1	H	-3.33608362	-1.30798110	0.00000000
	12	C	-1.16483561	-1.48665819	0.00000000
	1	H	-1.15608911	-2.57396874	0.00000000
	12	C	0.04993391	-0.75352364	0.00000000
	12	C	1.34107408	-1.36152832	0.00000000
	1	H	1.42016205	-2.44856742	0.00000000
	12	C	2.50521847	-0.58791381	0.00000000
	1	H	3.47692905	-1.08079800	0.00000000
	12	C	2.43750612	0.85330318	0.00000000
	1	H	3.35593899	1.43658141	0.00000000
	12	C	1.21490569	1.46776791	0.00000000
	1	H	1.13962957	2.55527229	0.00000000
	12	C	0.00000000	0.68374363	0.00100000
	12	C	-1.27888201	1.32998540	0.00000000
	13	N	-2.37993838	0.57674825	0.00000000

3.2 Dominant normal modes in FC simulations

3.2.1 quinolineH⁺

	ν_{31}		
	x	y	z
Frequency	512.6395		
Reduced mass	2.1174		
Force constant	1.1013		
Atom #	x	y	z
1	0.02	-0.16	0.00
2	-0.13	-0.15	0.00
3	-0.07	-0.16	0.00
4	-0.19	0.00	0.00
5	0.26	-0.13	0.00
6	0.32	-0.01	0.00
<u>S₁</u> 7	0.21	-0.07	0.00
8	0.08	-0.08	0.00
9	0.19	0.01	0.00
10	0.19	0.15	0.00
11	0.06	0.16	0.00
12	0.11	0.14	0.00
13	0.25	-0.09	0.00
14	-0.27	0.15	0.00
15	-0.38	-0.01	0.00
16	-0.27	0.10	0.00
17	-0.16	0.10	0.00
18	-0.19	0.00	0.00

3.2.2 isoquinolineH⁺

<u>S₀</u>		ν_{31}		
	Frequency	526.1339		
	Reduced mass	6.7793		
	Force constant	1.1057		
	Atom #	<i>x</i>	<i>y</i>	<i>z</i>
	1	0.12	0.16	0.00
	2	0.09	-0.09	0.00
	3	0.32	0.08	0.00
	4	0.33	0.06	0.00
	5	0.24	-0.01	0.00
	6	0.23	-0.01	0.00
	7	0.10	0.00	0.00
	8	-0.05	-0.19	0.00
	9	-0.15	-0.2 0	0.00
	10	-0.19	-0.08	0.00
	11	-0.09	0.12	0.00
	12	-0.36	-0.08	0.00
	13	-0.34	-0.12	0.00
	14	-0.24	0.06	0.00
	15	-0.22	0.06	0.00
	16	-0.07	0.01	0.00
	17	0.06	0.15	0.00
	18	0.17	0.06	0.00

	ν_{31}			ν_{30}		
	Frequency	506.2389		1072.7510		
	Reduced mass	6.8889		2.0146		
	Force constant	1.0402		1.3660		
Atom #	x	y	z	x	y	z
1	0.13	0.15	0.00	-0.31	-0.09	0.00
2	0.07	-0.07	0.00	0.02	-0.10	0.00
3	0.32	0.06	0.00	0.06	0.09	0.00
4	0.34	0.04	0.00	0.03	0.15	0.00
5	0.24	-0.01	0.00	-0.03	0.01	0.00
6	0.2	-0.01	0.00	-0.34	0.02	0.00
7	0.13	-0.01	0.00	0.01	-0.02	0.00
8	-0.02	-0.20	0.00	0.06	0.06	0.00
9	-0.12	-0.20	0.00	0.41	0.07	0.00
10	-0.17	-0.09	0.00	-0.10	0.10	0.00
11	-0.05	0.13	0.00	0.00	0.30	0.00
12	-0.38	-0.08	0.00	-0.12	-0.08	0.00
13	-0.37	-0.10	0.00	-0.07	-0.2	0.00
14	-0.25	0.07	0.00	0.10	-0.08	0.00
15	-0.21	0.07	0.00	0.58	-0.09	0.00
16	-0.09	0.02	0.00	0.01	0.04	0.00
17	0.04	0.14	0.00	-0.06	-0.06	0.00
18	0.15	0.08	0.00	0.04	-0.05	0.00

S₁

3.3 Calculated normal mode frequencies

3.3.1 quinolineH⁺

<u>S₀</u>				<u>S₁</u>			
Label	Freq. / cm ⁻¹	Label	Freq. / cm ⁻¹	Label	Freq. / cm ⁻¹	Label	Freq. / cm ⁻¹
ν_1 (a')	3573.3508	ν_{25} (a')	1092.3760	ν_1 (a')	3633.9228	ν_{25} (a')	1079.2274
ν_2 (a')	3258.4461	ν_{26} (a')	1053.3654	ν_2 (a')	3278.3564	ν_{26} (a')	1044.8179
ν_3 (a')	3246.4491	ν_{27} (a')	960.2950	ν_3 (a')	3256.6898	ν_{27} (a')	938.5256
ν_4 (a')	3241.2669	ν_{28} (a')	825.9803	ν_4 (a')	3251.4195	ν_{28} (a')	812.1457
ν_5 (a')	3230.7546	ν_{29} (a')	787.2642	ν_5 (a')	3242.2875	ν_{29} (a')	783.9691
ν_6 (a')	3221.7043	ν_{30} (a')	630.8466	ν_6 (a')	3238.6671	ν_{30} (a')	600.4611
ν_7 (a')	3219.9410	ν_{31} (a')	530.3478	ν_7 (a')	3222.0985	ν_{31} (a')	512.6395
ν_8 (a')	3211.0979	ν_{32} (a')	527.2880	ν_8 (a')	3214.3556	ν_{32} (a')	507.2788
ν_9 (a')	1717.4471	ν_{33} (a')	375.6749	ν_9 (a')	1677.6790	ν_{33} (a')	368.5141
ν_{10} (a')	1676.6702	ν_{34} (a'')	1057.6550	ν_{10} (a')	1638.1481	ν_{34} (a'')	1028.3811
ν_{11} (a')	1663.6327	ν_{35} (a'')	1045.9031	ν_{11} (a')	1581.7551	ν_{35} (a'')	984.7365
ν_{12} (a')	1619.0205	ν_{36} (a'')	1018.2138	ν_{12} (a')	1548.5208	ν_{36} (a'')	967.3339
ν_{13} (a')	1527.1764	ν_{37} (a'')	1008.4842	ν_{13} (a')	1515.0954	ν_{37} (a'')	933.7807
ν_{14} (a')	1510.7153	ν_{38} (a'')	919.1977	ν_{14} (a')	1446.7760	ν_{38} (a'')	777.0812
ν_{15} (a')	1446.9264	ν_{39} (a'')	853.7368	ν_{15} (a')	1428.1348	ν_{39} (a'')	748.3533
ν_{16} (a')	1439.0424	ν_{40} (a'')	822.1356	ν_{16} (a')	1423.3911	ν_{40} (a'')	735.3702
ν_{17} (a')	1418.9105	ν_{41} (a'')	810.6516	ν_{17} (a')	1389.4583	ν_{41} (a'')	687.0341
ν_{18} (a')	1330.8382	ν_{42} (a'')	749.7148	ν_{18} (a')	1313.0641	ν_{42} (a'')	552.2840
ν_{19} (a')	1297.5638	ν_{43} (a'')	634.6853	ν_{19} (a')	1288.2475	ν_{43} (a'')	516.0032
ν_{20} (a')	1257.5115	ν_{44} (a'')	495.8468	ν_{20} (a')	1245.7896	ν_{44} (a'')	447.6766
ν_{21} (a')	1243.1653	ν_{45} (a'')	483.8157	ν_{21} (a')	1207.3007	ν_{45} (a'')	403.7084
ν_{22} (a')	1187.8215	ν_{46} (a'')	392.0895	ν_{22} (a')	1192.2968	ν_{46} (a'')	286.1900
ν_{23} (a')	1178.0932	ν_{47} (a'')	191.8412	ν_{23} (a')	1107.9085	ν_{47} (a'')	166.6438
ν_{24} (a')	1164.2525	ν_{48} (a'')	181.3755	ν_{24} (a')	1100.5944	ν_{48} (a'')	154.2465

<u>S₂</u>				<u>S₃</u>			
Label	Freq. / cm ⁻¹	Label	Freq. / cm ⁻¹	Label	Freq. / cm ⁻¹	Label	Freq. / cm ⁻¹
ν_1 (a')	3597.1417	ν_{25} (a')	1050.4434	ν_1 (a')	3594.3765	ν_{25} (a')	1032.2402
ν_2 (a')	3261.8747	ν_{26} (a')	1011.8244	ν_2 (a')	3258.0887	ν_{26} (a')	996.4563
ν_3 (a')	3251.3978	ν_{27} (a')	946.2243	ν_3 (a')	3252.2185	ν_{27} (a')	929.2043
ν_4 (a')	3248.4271	ν_{28} (a')	810.9461	ν_4 (a')	3249.9946	ν_{29} (a')	789.3728
ν_5 (a')	3240.1188	ν_{29} (a')	740.7672	ν_5 (a')	3239.8388	ν_{28} (a')	754.1632
ν_6 (a')	3239.2873	ν_{30} (a')	604.7024	ν_6 (a')	3237.1837	ν_{30} (a')	610.4133
ν_7 (a')	3227.3960	ν_{31} (a')	530.2010	ν_7 (a')	3219.9787	ν_{31} (a')	501.0905
ν_8 (a')	3214.2763	ν_{32} (a')	514.2506	ν_8 (a')	3208.3940	ν_{32} (a')	459.5765
ν_9 (a')	1831.7280	ν_{33} (a')	376.6316	ν_9 (a')	1684.0501	ν_{33} (a')	345.5554
ν_{10} (a')	1625.9606	ν_{34} (a'')	987.3393	ν_{10} (a')	1639.1482	ν_{34} (a'')	958.3192
ν_{11} (a')	1600.4351	ν_{35} (a'')	951.2694	ν_{11} (a')	1571.7661	ν_{35} (a'')	948.9814
ν_{12} (a')	1540.3491	ν_{36} (a'')	939.1144	ν_{12} (a')	1535.5996	ν_{36} (a'')	937.7775
ν_{13} (a')	1527.8593	ν_{37} (a'')	876.7374	ν_{13} (a')	1520.4933	ν_{37} (a'')	873.6224
ν_{14} (a')	1502.3354	ν_{38} (a'')	835.6330	ν_{14} (a')	1472.4319	ν_{38} (a'')	800.1161
ν_{15} (a')	1477.9273	ν_{39} (a'')	774.0416	ν_{15} (a')	1458.0833	ν_{39} (a'')	728.9121
ν_{16} (a')	1419.2360	ν_{40} (a'')	737.9451	ν_{16} (a')	1407.4087	ν_{40} (a'')	670.9420
ν_{17} (a')	1405.2284	ν_{41} (a'')	709.3844	ν_{17} (a')	1395.8263	ν_{41} (a'')	650.7461
ν_{18} (a')	1302.2754	ν_{42} (a'')	634.5627	ν_{18} (a')	1282.1959	ν_{42} (a'')	572.5530
ν_{19} (a')	1293.7592	ν_{43} (a'')	452.3388	ν_{19} (a')	1267.8704	ν_{43} (a'')	408.1170
ν_{20} (a')	1252.3639	ν_{44} (a'')	421.8283	ν_{20} (a')	1239.3120	ν_{44} (a'')	363.1653
ν_{21} (a')	1200.1013	ν_{45} (a'')	406.9719	ν_{21} (a')	1217.4448	ν_{45} (a'')	323.5739
ν_{22} (a')	1188.0462	ν_{46} (a'')	280.1137	ν_{22} (a')	1184.5746	ν_{46} (a'')	293.5818
ν_{23} (a')	1163.6903	ν_{47} (a'')	157.2690	ν_{23} (a')	1150.6802	ν_{47} (a'')	134.1332
ν_{24} (a')	1142.7423	ν_{48} (a'')	129.2463	ν_{24} (a')	1139.7658	ν_{48} (a'')	114.1647

3.3.2 isoquinolineH⁺

S₀				S₁			
Label	Freq. / cm ⁻¹	Label	Freq. / cm ⁻¹	Label	Freq. / cm ⁻¹	Label	Freq. / cm ⁻¹
ν_1 (a')	3586.1481	ν_{25} (a')	1066.5795	ν_1 (a')	3636.7686	ν_{25} (a')	1072.7510
ν_2 (a')	3267.6184	ν_{26} (a')	1050.0877	ν_2 (a')	3280.4756	ν_{26} (a')	1036.7309
ν_3 (a')	3240.7494	ν_{27} (a')	969.0596	ν_3 (a')	3255.4708	ν_{27} (a')	946.0153
ν_4 (a')	3239.5912	ν_{28} (a')	819.3493	ν_4 (a')	3250.9100	ν_{28} (a')	809.9744
ν_5 (a')	3237.6580	ν_{29} (a')	793.2986	ν_5 (a')	3243.2060	ν_{29} (a')	782.9217
ν_6 (a')	3230.7270	ν_{30} (a')	646.2467	ν_6 (a')	3234.3989	ν_{30} (a')	611.6382
ν_7 (a')	3220.0488	ν_{31} (a')	526.1339	ν_7 (a')	3220.4034	ν_{31} (a')	506.2389
ν_8 (a')	3216.3205	ν_{32} (a')	514.3028	ν_8 (a')	3216.7221	ν_{32} (a')	500.3212
ν_9 (a')	1706.9904	ν_{33} (a')	372.2766	ν_9 (a')	1666.2286	ν_{33} (a')	363.3662
ν_{10} (a')	1687.3835	ν_{34} (a'')	1062.4450	ν_{10} (a')	1619.0702	ν_{34} (a'')	1022.6297
ν_{11} (a')	1659.0443	ν_{35} (a'')	1024.5099	ν_{11} (a')	1565.7944	ν_{35} (a'')	981.6976
ν_{12} (a')	1609.2617	ν_{36} (a'')	1007.3294	ν_{12} (a')	1560.7973	ν_{36} (a'')	976.6393
ν_{13} (a')	1543.2599	ν_{37} (a'')	990.3441	ν_{13} (a')	1500.9185	ν_{37} (a'')	926.5891
ν_{14} (a')	1504.6912	ν_{38} (a'')	933.1426	ν_{14} (a')	1483.8561	ν_{38} (a'')	787.6494
ν_{15} (a')	1461.6650	ν_{39} (a'')	866.7987	ν_{15} (a')	1438.9279	ν_{39} (a'')	751.3256
ν_{16} (a')	1443.9972	ν_{40} (a'')	826.3943	ν_{16} (a')	1423.3736	ν_{40} (a'')	732.2681
ν_{17} (a')	1421.5167	ν_{41} (a'')	801.3491	ν_{17} (a')	1400.7893	ν_{41} (a'')	658.9849
ν_{18} (a')	1313.6111	ν_{42} (a'')	757.0410	ν_{18} (a')	1295.1933	ν_{42} (a'')	600.3496
ν_{19} (a')	1305.0327	ν_{43} (a'')	644.5982	ν_{19} (a')	1267.2609	ν_{43} (a'')	481.8391
ν_{20} (a')	1281.5898	ν_{44} (a'')	498.0600	ν_{20} (a')	1249.9349	ν_{44} (a'')	441.6474
ν_{21} (a')	1243.4936	ν_{45} (a'')	479.3649	ν_{21} (a')	1243.0349	ν_{45} (a'')	389.4258
ν_{22} (a')	1201.1108	ν_{46} (a'')	405.1339	ν_{22} (a')	1187.8118	ν_{46} (a'')	301.4382
ν_{23} (a')	1187.6616	ν_{47} (a'')	187.7186	ν_{23} (a')	1150.0623	ν_{47} (a'')	169.7097
ν_{24} (a')	1176.2998	ν_{48} (a'')	176.5170	ν_{24} (a')	1110.0644	ν_{48} (a'')	151.8884

$\underline{\mathbf{S}}_2$				$\underline{\mathbf{S}}_3$			
Label	Freq. / cm^{-1}	Label	Freq. / cm^{-1}	Label	Freq. / cm^{-1}	Label	Freq. / cm^{-1}
$\nu_1 (a')$	3587.7200	$\nu_{25} (a')$	1048.7769	$\nu_1 (a')$	3599.4294	$\nu_{25} (a')$	979.8772
$\nu_2 (a')$	3278.8715	$\nu_{26} (a')$	1005.6269	$\nu_2 (a')$	3278.9313	$\nu_{26} (a')$	963.1069
$\nu_3 (a')$	3258.3004	$\nu_{27} (a')$	952.2421	$\nu_3 (a')$	3247.7568	$\nu_{27} (a')$	929.6831
$\nu_4 (a')$	3253.9242	$\nu_{28} (a')$	803.1497	$\nu_4 (a')$	3245.9423	$\nu_{28} (a')$	770.8580
$\nu_5 (a')$	3243.5325	$\nu_{29} (a')$	752.1170	$\nu_5 (a')$	3241.3505	$\nu_{29} (a')$	762.9461
$\nu_6 (a')$	3237.2718	$\nu_{30} (a')$	627.0522	$\nu_6 (a')$	3232.1077	$\nu_{30} (a')$	616.7299
$\nu_7 (a')$	3222.7880	$\nu_{31} (a')$	516.3441	$\nu_7 (a')$	3219.2037	$\nu_{31} (a')$	508.1180
$\nu_8 (a')$	3219.3610	$\nu_{32} (a')$	492.8486	$\nu_8 (a')$	3214.0501	$\nu_{32} (a')$	446.5289
$\nu_9 (a')$	1718.6072	$\nu_{33} (a')$	362.5870	$\nu_9 (a')$	1916.5129	$\nu_{33} (a')$	347.7360
$\nu_{10} (a')$	1658.7682	$\nu_{34} (a'')$	986.5805	$\nu_{10} (a')$	1596.3215	$\nu_{34} (a'')$	982.7460
$\nu_{11} (a')$	1586.7244	$\nu_{35} (a'')$	949.5495	$\nu_{11} (a')$	1557.5895	$\nu_{35} (a'')$	950.2702
$\nu_{12} (a')$	1539.8425	$\nu_{36} (a'')$	903.5806	$\nu_{12} (a')$	1539.9818	$\nu_{36} (a'')$	890.2445
$\nu_{13} (a')$	1499.3365	$\nu_{37} (a'')$	867.6524	$\nu_{13} (a')$	1482.3894	$\nu_{37} (a'')$	811.5904
$\nu_{14} (a')$	1484.6710	$\nu_{38} (a'')$	839.6390	$\nu_{14} (a')$	1442.4613	$\nu_{38} (a'')$	790.6414
$\nu_{15} (a')$	1437.9542	$\nu_{39} (a'')$	776.0501	$\nu_{15} (a')$	1433.7462	$\nu_{39} (a'')$	723.1111
$\nu_{16} (a')$	1420.6893	$\nu_{40} (a'')$	737.3131	$\nu_{16} (a')$	1392.3700	$\nu_{40} (a'')$	719.6567
$\nu_{17} (a')$	1391.5973	$\nu_{41} (a'')$	703.0013	$\nu_{17} (a')$	1355.4506	$\nu_{41} (a'')$	657.1093
$\nu_{18} (a')$	1297.5614	$\nu_{42} (a'')$	688.6062	$\nu_{18} (a')$	1275.8849	$\nu_{42} (a'')$	564.4138
$\nu_{19} (a')$	1278.4249	$\nu_{43} (a'')$	493.6547	$\nu_{19} (a')$	1251.9587	$\nu_{43} (a'')$	415.4329
$\nu_{20} (a')$	1270.4482	$\nu_{44} (a'')$	423.0527	$\nu_{20} (a')$	1240.5259	$\nu_{44} (a'')$	338.2444
$\nu_{21} (a')$	1232.2660	$\nu_{45} (a'')$	383.7337	$\nu_{21} (a')$	1225.4087	$\nu_{45} (a'')$	291.4487
$\nu_{22} (a')$	1190.2016	$\nu_{46} (a'')$	334.5943	$\nu_{22} (a')$	1189.3692	$\nu_{46} (a'')$	249.1265
$\nu_{23} (a')$	1147.2716	$\nu_{47} (a'')$	172.3539	$\nu_{23} (a')$	1158.6847	$\nu_{47} (a'')$	138.0402
$\nu_{24} (a')$	1111.7838	$\nu_{48} (a'')$	129.1915	$\nu_{24} (a')$	1151.3603	$\nu_{48} (a'')$	62.9935