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Supporting Information

Z-Matrix 1S: Optimized Structure of H₃O⁺

o
h 1 ho2
h 1 ho3 2 hoh3
h 1 ho4 3 hoh4 2 dih4

ho2 0.981886
ho3 0.981903
hoh3 113.331
ho4 0.981884
hoh4 113.287
dih4 -130.934

Supporting InformationZ-Matrix 2S: Optimized Structure of $\text{H}^+(\text{H}_2\text{O})_2$

o						
o	1	oo2				
h	1	ho3	2	hoo3		
h	1	ho4	2	hoo4	3	dih4
h	2	ho5	1	hoo5	3	dih5
h	2	ho6	5	hoh6	1	dih6
h	2	ho7	5	hoh7	1	dih7
oo2		2.396776				
ho3		0.971019				
hoo3		116.149				
ho4		0.970418				
hoo4		122.359				
dih4		139.555				
ho5		1.199688				
hoo5		2.756				
dih5		-120.204				
ho6		0.971025				
hoh6		117.498				
dih6		60.632				
ho7		0.970424				
hoh7		119.767				
dih7		-161.562				

Supporting InformationZ-Matrix 3S: Optimized Structure of $H^+(H_2O)_3$

o					
o	1	oo2			
o	1	oo3	2	ooo3	
h	1	ho4	3	hoo4	2 dih4
h	1	ho5	3	hoo5	2 dih5
h	1	ho6	3	hoo6	2 dih6
h	2	ho7	1	hoo7	3 dih7
h	2	ho8	1	hoo8	3 dih8
h	3	ho9	1	hoo9	2 dih9
h	3	ho10	1	hoo10	2 dih10

oo2	2.472453
oo3	2.479576
ooo3	118.630
ho4	1.054557
hoo4	115.804
dih4	0.326
ho5	0.968835
hoo5	115.779
dih5	134.550
ho6	1.050407
hoo6	2.669
dih6	119.351
ho7	0.967465
hoo7	118.681
dih7	-113.104
ho8	0.966907
hoo8	125.174
dih8	30.987
ho9	0.967694
hoo9	117.872
dih9	117.629
ho10	0.967164
hoo10	124.956
dih10	-100.801

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Supporting InformationZ-Matrix 4S: Optimized Structure of $\text{H}^+(\text{H}_2\text{O})_4$

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o
o 1 oo2
o 1 oo3      2 ooo3
o 1 oo4      3 ooo4      2 dih4
h 3 ho5      1 hoo5      2 dih5
h 4 ho6      1 hoo6      2 dih6
h 2 ho7      1 hoo7      3 dih7
h 3 ho8      1 hoo8      2 dih8
h 3 ho9      1 hoo9      2 dih9
h 2 ho10     1 hoo10     3 dih10
h 2 ho11     1 hoo11     3 dih11
h 4 ho12     1 hoo12     2 dih12
h 4 ho13     1 hoo13     2 dih13

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oo2      2.545137
oo3      2.545150
ooo3     113.554
oo4      2.545741
ooo4     113.491
dih4     -131.590
ho5      1.525647
hoo5     1.683
dih5     -6.841
ho6      1.526425
hoo6     1.666
dih6     -139.856
ho7      1.525597
hoo7     1.671
dih7     -137.699
ho8      0.966919
hoo8     117.921
dih8     -117.083
ho9      0.966540
hoo9     123.379
dih9     20.362
ho10     0.966936
hoo10    117.948
dih10    111.609
ho11     0.966524
hoo11    123.376
dih11    -110.910
ho12     0.966606
hoo12    123.324
dih12    -111.176
ho13     0.966974
hoo13    117.926
dih13    111.461

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Supporting Information**Z-Matrix 5S: Optimized Structure of H⁺(H₂O)₅**

o				
o	1 oo2			
o	1 oo3	2 ooo3		
o	1 oo4	3 ooo4	2 dih4	
o	2 oo5	1 ooo5	3 dih5	
h	1 ho6	2 hoo6	5 dih6	
h	1 ho7	2 hoo7	5 dih7	
h	1 ho8	2 hoo8	5 dih8	
h	3 ho9	1 hoo9	2 dih9	
h	3 ho10	1 hoo10	2 dih10	
h	2 ho11	1 hoo11	3 dih11	
h	2 ho12	1 hoo12	3 dih12	
h	4 ho13	1 hoo13	2 dih13	
h	4 ho14	1 hoo14	2 dih14	
h	5 ho15	2 hoo15	1 dih15	
h	5 ho16	2 hoo16	1 dih16	
oo2	2.463402	oo3	2.581311	
ooo3	113.108	oo4	2.583563	
ooo4	111.691	dih4	-128.863	
oo5	2.644549	ooo5	116.075	
dih5	110.688	ho6	1.010427	
hoo6	110.893	dih6	109.890	
ho7	1.009784	hoo7	114.917	
dih7	-122.741	ho8	1.064397	
hoo8	2.043	dih8	-102.421	
ho9	0.966596	hoo9	117.657	
dih9	-118.950	ho10	0.966313	
hoo10	122.085			
dih10	15.609			
ho11	0.995531			
hoo11	116.964			
dih11	112.571			
ho12	0.965053			
hoo12	119.556			
dih12	-114.432			
ho13	0.966307			
hoo13	122.464			
dih13	-109.726			
ho14	0.966575			
hoo14	117.624			
dih14	115.285			
ho15	0.965333			
hoo15	125.393			
dih15	89.235			
ho16	0.965610			
hoo16	119.491			
dih16	-128.211			

Supporting InformationZ-Matrix 6S: Optimized Structure of NH_4^+

n						
h	1	hn2				
h	1	hn3	2	hnh3		
h	1	hn4	3	hnh4	2	dih4
h	1	hn5	4	hnh5	3	dih5

hn2	1.027503
hn3	1.027505
hnh3	109.455
hn4	1.027507
hnh4	109.486
dih4	120.013
hn5	1.027498
hnh5	109.485
dih5	-120.001

Supporting InformationZ-Matrix 7S: Optimized Structure of $\text{H}^+(\text{NH}_3)_2$

n					
n	1	nn2			
h	1	hn3	2	hnn3	
h	1	hn4	2	hnn4	3 dih4
h	1	hn5	2	hnn5	4 dih5
h	1	hn6	5	hnh6	2 dih6
h	2	hn7	1	hnn7	3 dih7
h	2	hn8	1	hnn8	3 dih8
h	2	hn9	1	hnn9	3 dih9

nn2	2.644036
hn3	1.022463
hnn3	110.937
hn4	1.022445
hnn4	110.989
dih4	119.986
hn5	1.022521
hnn5	110.974
dih5	120.027
hn6	1.194514
hnh6	110.976
dih6	0.021
hn7	1.021046
hnn7	112.165
dih7	173.541
hn8	1.021034
hnn8	112.290
dih8	53.504
hn9	1.021040
hnn9	112.155
dih9	-66.527

Supporting InformationZ-Matrix 8S: Optimized Structure of $\text{H}^+(\text{NH}_3)_3$

n				
n	1	nn2		
n	1	nn3	2	nnn3
h	3	hn4	1	hnn4
h	1	hn5	4	hnh5
h	1	hn6	4	hnh6
h	2	hn7	1	hnn7
h	2	hn8	1	hnn8
h	2	hn9	1	hnn9
h	2	hn10	1	hnn10
h	3	hn11	1	hnn11
h	3	hn12	1	hnn12
h	3	hn13	1	hnn13
			2	dih4
			3	dih5
			3	dih6
			3	dih7
			3	dih8
			3	dih9
			3	dih10
			2	dih11
			2	dih12
			2	dih13

nn2	2.781070
nn3	2.781075
nnn3	113.719
hn4	1.693583
hnn4	0.552
dih4	0.395
hn5	1.021309
hnh5	109.254
dih5	59.220
hn6	1.021312
hnh6	109.246
dih6	-58.421
hn7	1.693577
hnn7	0.552
dih7	0.333
hn8	1.019619
hnn8	111.759
dih8	173.000
hn9	1.019441
hnn9	113.240
dih9	53.304
hn10	1.019474
hnn10	113.053
dih10	-67.447
hn11	1.019440
hnn11	113.243
dih11	53.227
hn12	1.019474
hnn12	113.051
dih12	-67.525
hn13	1.019619
hnn13	111.758
dih13	172.924

Supporting Information**Z-Matrix 9S: Optimized Structure of H⁺(NH₃)₄**

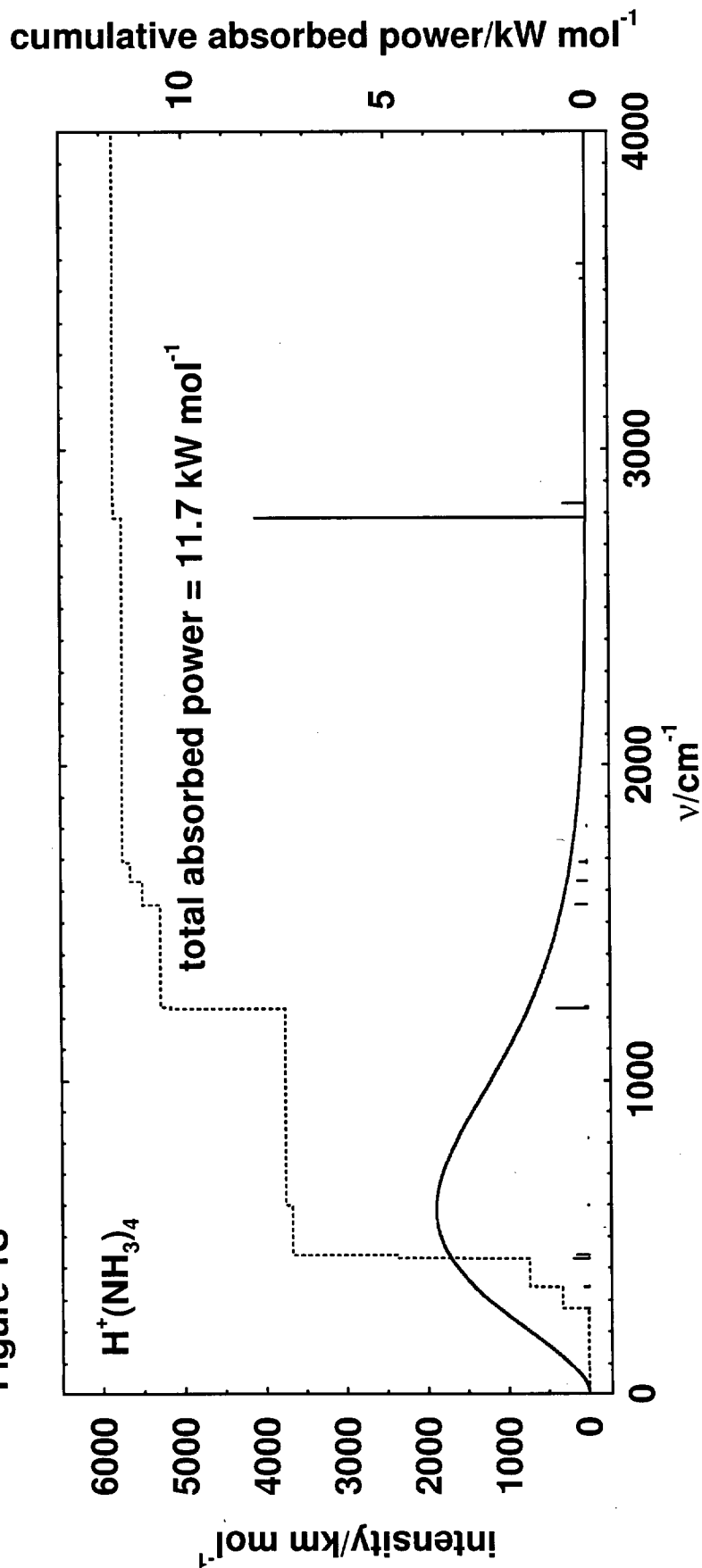
n				
n	1	nn2		
n	1	nn3	2	nnn3
n	1	nn4	3	nnn4
h	3	hn5	1	hnn5
h	2	hn6	1	hnn6
h	1	hn7	5	hnh7
h	4	hn8	1	hnn8
h	2	hn9	1	hnn9
h	2	hn10	1	hnn10
h	2	hn11	1	hnn11
h	4	hn12	1	hnn12
h	4	hn13	1	hnn13
h	4	hn14	1	hnn14
h	3	hn15	1	hnn15
h	3	hn16	1	hnn16
h	3	hn17	1	hnn17
nn2	2.860651		nn3	2.860905
nnn3	111.504		nn4	2.860946
nnn4	111.656		dih4	125.703
hn5	1.797458		hnn5	0.665
dih5	-62.252		hn6	1.797151
hnn6	0.639		dih6	66.384
hn7	1.020306		hnh7	108.354
dih7	0.622		hn8	1.797525
hnn8	0.678		dih8	63.115
hn9	1.018968		hnn9	112.213
dih9	-65.692		hn10	1.018916
hnn10	112.521		dih10	174.911
hn11	1.018859		hnn11	113.495
dih11	54.504		hn12	1.018960
hnn12	112.229			
dih12	-60.382			
hn13	1.018937			
hnn13	112.375			
dih13	-179.707			
hn14	1.018842			
hnn14	113.625			
dih14	59.890			
hn15	1.018858			
hnn15	113.668			
dih15	-62.318			
hn16	1.018978			
hnn16	112.240			
dih16	177.355			
hn17	1.018926			
hnn17	112.323			
dih17	58.101			

Supporting Information**Z-Matrix 10S: Optimized Structure of H⁺(NH₃)₅**

n				
n	1 nn2			
n	1 nn3	2 nnn3		
n	1 nn4	3 nnn4	2 dih4	
n	1 nn5	4 nnn5	3 dih5	
h	1 hn6	5 hnn6	4 dih6	
h	4 hn7	1 hnn7	2 dih7	
h	2 hn8	1 hnn8	3 dih8	
h	1 hn9	6 hnh9	5 dih9	
h	4 hn10	1 hnn10	2 dih10	
h	4 hn11	1 hnn11	2 dih11	
h	4 hn12	1 hnn12	2 dih12	
h	3 hn13	1 hnn13	2 dih13	
h	3 hn14	1 hnn14	2 dih14	
h	3 hn15	1 hnn15	2 dih15	
h	5 hn16	1 hnn16	2 dih16	
h	5 hn17	1 hnn17	2 dih17	
h	5 hn18	1 hnn18	2 dih18	
h	2 hn19	1 hnn19	3 dih19	
h	2 hn20	1 hnn20	3 dih20	
h	2 hn21	1 hnn21	3 dih21	
nn2	2.925090	nn3	2.925138	
nnn3	109.380	nn4	2.925814	
nnn4	109.213	dih4	-120.075	
nn5	2.926361	nnn5	109.275	
dih5	119.796	hn6	1.051090	
hnn6	0.167	dih6	166.211	
hn7	1.874685	hnn7	0.118	
dih7	26.799	hn8	1.873924	
hnn8	0.100	dih8	146.844	
hn9	1.051218	hnh9	109.473	
dih9	133.502	hn10	1.018537	
hnn10	112.903	dih10	54.772	
hn11	1.018572	hnn11	112.726	
dih11	-65.274	hn12	1.018524	
hnn12	112.612	dih12	174.808	
hn13	1.018527	hnn13	112.876	
dih13	59.217	hn14	1.018550	
hnn14	112.841	dih14	-60.937	
hn15	1.018501	hnn15	112.514	
dih15	179.133	hn16	1.018498	
hnn16	112.891			
dih16	169.886			
hn17	1.018508			
hnn17	112.726			
dih17	49.786			
hn18	1.018512			
hnn18	112.601			
dih18	-70.035			
hn19	1.018495			
hnn19	112.542			
dih19	-68.108			
hn20	1.018524			
hnn20	112.911			
dih20	171.885			
hn21	1.018447			
hnn21	112.747			
dih21	51.764			

Supporting Information:

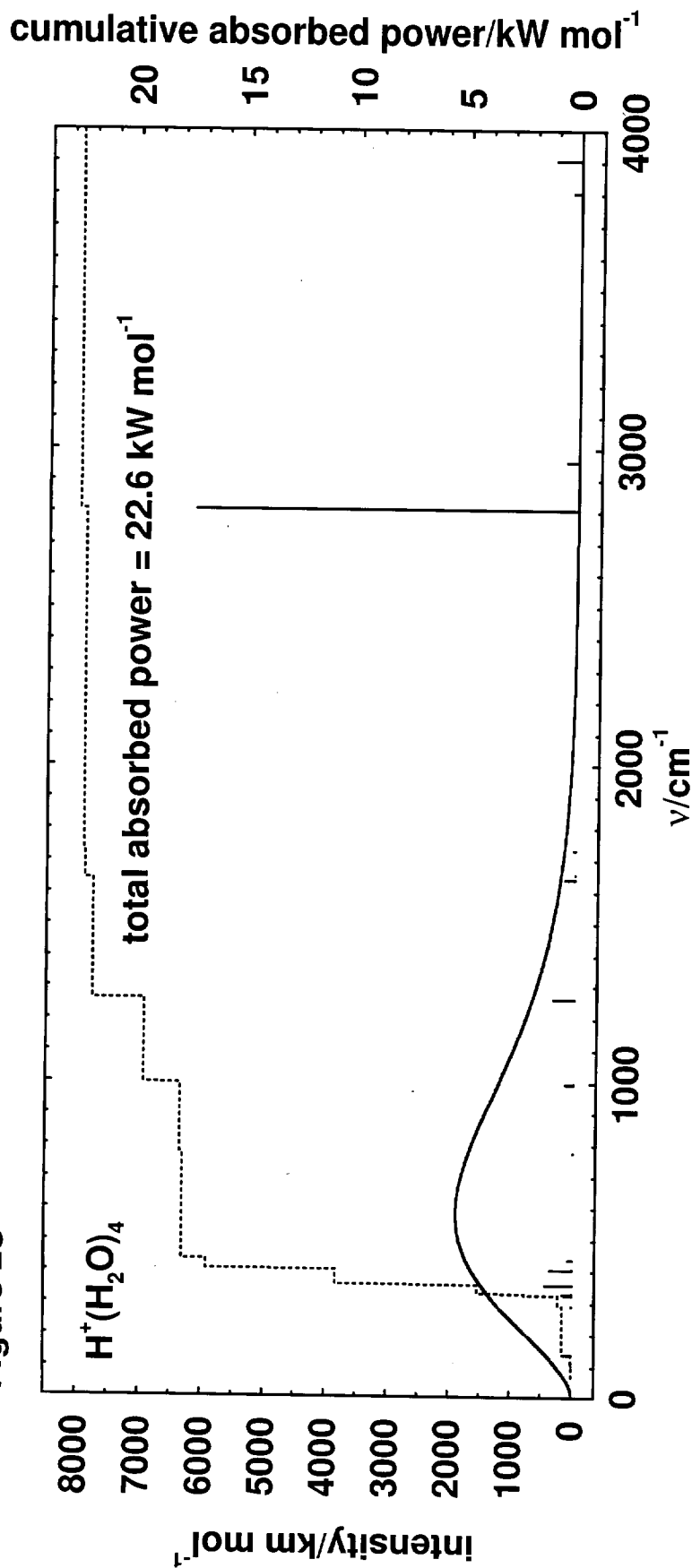
Figure 1S



Calculated IR spectrum of $\text{H}^+(\text{NH}_3)_4$ superimposed over the 300 K Planck distribution function. Intensities for vibrations within 3 cm^{-1} were summed into one peak. The dotted line represents the cumulative absorbed power in kW/mol.

Supporting Information:

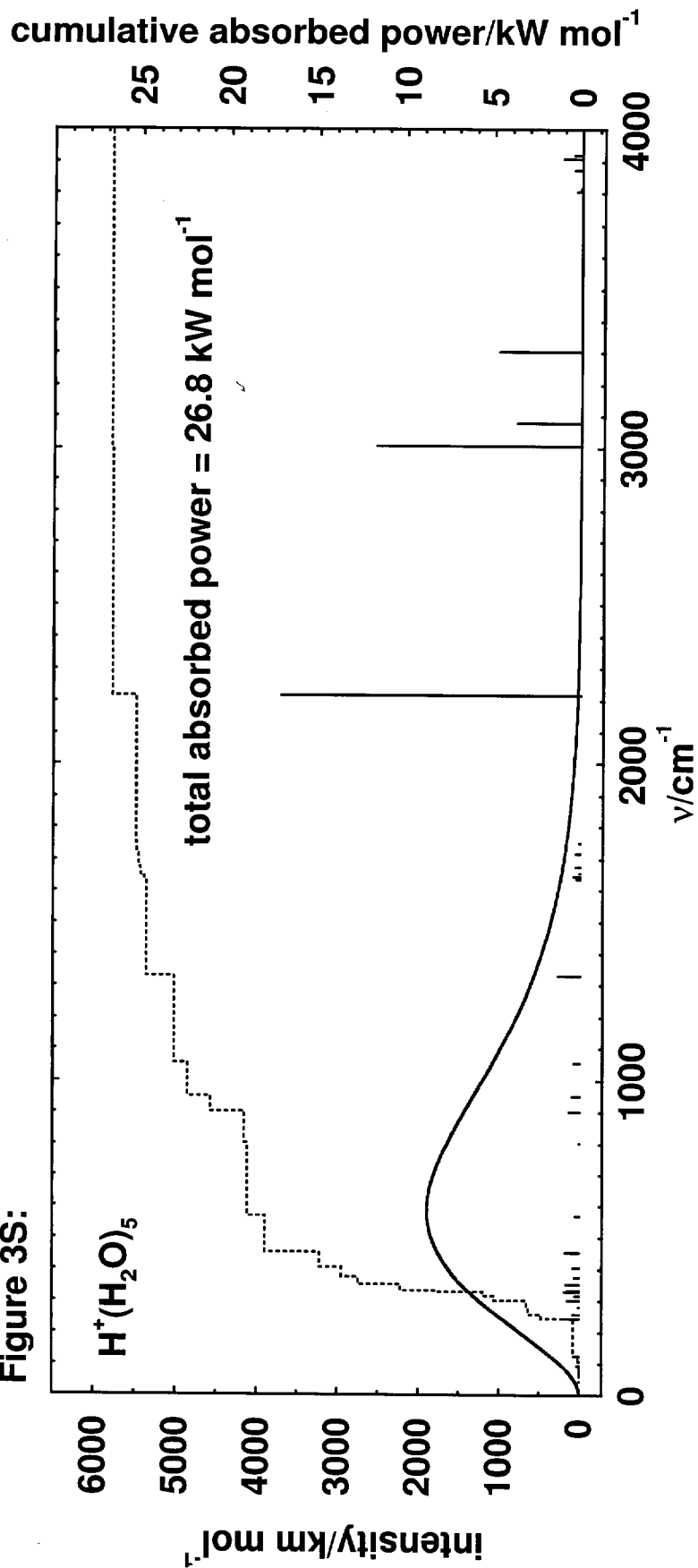
Figure 2S



Calculated IR spectrum of $\text{H}^+(\text{H}_2\text{O})_4$ superimposed over the 300 K Planck distribution function. Intensities for vibrations within 3 cm^{-1} were summed into one peak. The dotted line represents the cumulative absorbed power in kW/mol .

Supporting Information:

Figure 3S:



Calculated IR spectrum of $\text{H}^+(\text{H}_2\text{O})_5$ superimposed over the 300 K Planck distribution function. Intensities for vibrations within 3 cm^{-1} were summed into one peak. The dotted line represents the cumulative absorbed power in kW/mol .