Electronic Supporting Information

Microsolvation of H_2O^+, H_3O^+, and $CH_3OH_2^+$ by He in a cryogenic ion trap: Structure of solvation shells

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Table S1. NBO charge distribution on the He atoms in X^+He_n clusters evaluated at the CCSD(T)/aug-cc-pVTZ level (in e).

n	H_2O^+	H_3O^+	$CH_3OH_2^+$
0 [a]	0.54504	0.58759	0.56127
1 (H)	0.00913	0.00524	0.00278
1 (p)	0.00120		
2 (2H)	0.00866	0.00494	0.00273
	0.00866	0.00494	0.00273
2 (2p)	0.00120		
	0.00120		
3	0.00843	0.00478	
	0.00843	0.00478	
	0.00098	0.00478	
4	0.00821	0.00460	
	0.00821	0.00452	
	0.00097	0.00472	
	0.00097	0.00037	
5	0.00795	0.00439	
	0.00795	0.00437	
	0.00104	0.00443	
	0.00104	0.00037	
	0.00027	0.00037	
6		0.00432	
		0.00432	
		0.00432	
		0.00034	
		0.00034	
		0.00034	

[a] Partial charge on the equivalent OH protons.

Table S2. Scaled vibrational OH stretch and bend frequencies of $H_2O^+He_n$ calculated at the CCSD/aug-cc-pVTZ level (in cm^{-1}).[a]

n	ν_1	ν_3	ν_2
0	3210.7 (115) *3212.86*	3261.0 (447) *3259.04*	1408.5 (166) *1408.4*
1 (H)	3184.8 (308) *3198.0* [b]	3253.0 (412) *3253.9* [b]	1412.1 (152)
1 (p)	3214.9 (112)	3265.3 (437)	1411.2 (162)
2 (2H)	3189.7 (177)	3220.3 (701)	1415.4 (139)
2 (2p)	3219.2 (108)	3269.5 (426)	1413.7 (158)
3	3194.8 (172)	3225.3 (682)	1418.3 (137)
4	3200.0 (167)	3230.2 (663)	1420.8 (134)
5	3204.5 (162)	3233.5 (644)	1417.7 (146)

[a] IR intensities in km/mol are listed in parentheses. Scaling factor of 0.9442 and 0.9492 for $\nu_{1/3}$ and ν_2. Experimental values are listed in italics. [b] B tunnelling component of K_a = 0-0 subband.

Table S3. Scaled vibrational OH stretch frequencies of $H_3O^+He_n$ calculated at the CCSD/aug-cc-pVTZ level (in cm^{-1}).[a]

n	ν_1	$\nu_3(1)$	$\nu_3(2)$
0	3438.7 (32) *3440*	3529.1 (459) *3528*	3529.1 (459) *3528*
1	3433.7 (75)	3512.2 (548)	3535.1 (451)
2	3433.0 (63)	3504.2 (644)	3530.7 (484)
3	3434.3 (43)	3511.4 (630)	3511.5 (630)
4	3437.1 (42)	3513.9 (615)	3514.6 (624)
5	3439.7 (41)	3516.4 (607)	3517.6 (610)
6	3436.2 (40)	3512.6 (601)	3512.6 (601)

[a] IR intensities in km/mol are listed in parentheses. Scaling factor of 0.9505. Experimental values (averaged tunnelling components) are listed in italics. The ν_3 mode has two components, which are degenerate for n=3 and 6.

Table S4. Scaled vibrational OH stretch frequencies of $CH_3OH_2^+He_n$ calculated at the CCSD/aug-cc-pVTZ level (in cm^{-1}).[a]

n	ν_{OH}^s	ν_{OH}^a
0	3510.0 (198)	3584.9 (320)
1	3508.3 (236) *3504*	3581.2 (370) *3571*
2	3508.4 (252)	3577.1 (439)

[a] IR intensities in km/mol are listed in parentheses. Scaling factor of 0.9505. Experimental values are listed in italics.