Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Microsolvation of 2-azetidinone: a model for the peptide group-water interactions.

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ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. Observed and calculated frequencies (MHz) for the parent species of the 1:1a complex of 2-azetidinone···H_2O

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	*obs.*	*obs.-cal.*	J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	*obs.*	*obs.-cal.*
2	0	2	1	0	1	1	1	7658.986	0.003	4	1	4	3	1	3	3	3	14309.286	0.000
						3	2	7660.062	-0.001							5	4	14311.153	-0.001
						2	1	7660.202	0.002							4	3	14311.300	-0.001
						1	0	7660.593	-0.004							4	4	14312.758	0.001
						2	2	7660.846	0.001	4	1	3	3	1	2	3	2	16328.117	-0.001
2	1	2	1	1	1	1	1	7193.020	0.000							5	4	16328.182	0.003
						3	2	7194.173	0.006							4	3	16328.294	-0.003
						2	1	7194.894	0.001	4	2	3	3	2	2	3	2	15370.855	0.003
						2	2	7195.370	-0.001							3	3	15370.855	0.003
2	1	1	1	1	0	1	0	8207.861	-0.002							5	4	15370.934	0.001
						2	2	8208.753	0.002							4	3	15371.249	0.000
						3	2	8209.264	0.001							4	4	15371.249	0.000
						2	1	8209.874	-0.001	4	2	2	3	2	1	3	2	15771.958	0.004
						1	1	8210.672	0.000							5	4	15772.009	-0.002
3	0	3	2	0	2	2	2	11386.516	-0.003	4	3	2	3	3	1	5	4	15480.748	-0.001
						4	3	11387.635	0.001							4	3	15481.348	0.000
						2	1	11387.734	-0.001	4	3	1	3	3	0	5	4	15493.600	0.000
						3	2	11387.800	0.001	5	1	5	4	1	4	6	5	17824.178	0.002
						3	3	11388.581	-0.001							4	3	17824.241	0.001
3	1	3	2	1	2	2	2	10764.595	-0.002							5	4	17824.286	-0.001
						4	3	10766.313	0.003	1	1	1	0	0	0	0	1	8216.875	0.000
						3	3	10767.768	0.001							2	1	8217.592	0.000
3	1	2	2	1	1	3	3	12286.335	0.000							1	1	8218.068	-0.002
						2	1	12286.487	0.005	2	1	2	1	0	1	1	1	11559.623	0.004
						4	3	12286.654	-0.001							3	2	11560.935	0.002
						3	2	12286.848	0.001							1	0	11561.231	-0.001
						2	2	12287.279	-0.001							2	1	11561.490	-0.002
3	2	2	2	2	1	2	1	11552.185	-0.002							2	2	11562.138	0.001
						4	3	11552.571	0.000	3	0	3	2	1	2	2	2	7485.224	-0.004
						3	3	11552.571	0.000							3	2	7486.511	0.003
						3	2	11553.260	-0.004							4	3	7486.764	0.000
						2	2	11553.260	-0.004							2	1	7487.102	0.002
3	2	1	2	2	0	2	1	11717.244	-0.005	3	1	3	2	0	2	2	2	14665.886	-0.002
						4	3	11717.605	0.003							4	3	14667.179	-0.001
						3	2	11718.154	0.001							3	2	14667.852	-0.002
4	0	4	3	0	3	5	4	15002.268	0.001							3	3	14668.637	0.001
						3	2	15002.302	-0.003	4	0	4	3	1	3	3	3	11720.971	0.001
						4	3	15002.462	0.001							4	3	11722.407	0.000
																5	4	11722.719	-0.001
																3	2	11722.933	-0.002
																4	4	11723.859	-0.003

Table S2. Observed and calculated frequencies (MHz) for the ^{13}C species of the 1:1a complex of 2-azetidinone···H_2O

								$^{13}C_{c=o}$/ $^{12}C_{c=o}$		$^{13}C_{\alpha}$ / $^{12}C_{\alpha}$		$^{13}C_{\beta}$ / $^{12}C_{\beta}$	
J'	***K'$_{-1}$***	***K'$_{+1}$***	***J''***	***K''$_{-1}$***	***K''$_{+1}$***	***F'***	***F''***	***obs.***	***obs.-cal.***	***obs.***	***obs.-cal.[a]***	***Obs.***	***obs.-cal.[a]***
2	0	2	1	0	1	3	2	7654.248	0.002	7561.437	0.000	7566.334	0.000
						2	1	7654.387	0.003	7561.574	0.001	7566.469	-0.002
						1	0	-	-	-	-	7566.866	-0.002
3	0	3	2	0	2	4	3	11377.908	-0.001	11244.121	0.002	11247.751	0.000
						3	2	11378.074	-0.002	11244.285	0.003	11247.918	0.000
3	1	3	2	1	2	4	3	10756.039	-0.001	10633.605	-0.006	10633.179	0.001
						3	2	10756.293	0.001	10633.866	0.004	-	-
3	1	2	2	1	1	2	1	-	-	-	-	12137.924	-0.005
						4	3	12280.201	0.001	12120.282	-0.002	12138.104	0.002
						3	2	12280.391	-0.001	-	-	12138.297	0.004
4	0	4	3	0	3	5	4	14987.679	0.001	14818.346	0.000	14817.081	0.002
						3	2	-	-	-	-	14817.116	0.000
						4	3	14987.873	0.000	14818.535	-0.002	14817.272	-0.002

Table S3. Observed and calculated frequencies (MHz) for the ^{18}O species of the 1:1a complex of 2-azetidinone···H_2O

$^{18}O_B/^{16}O_B$																			
J'	***K'$_{-1}$***	***K'$_{+1}$***	***J''***	***K''$_{-1}$***	***K''$_{+1}$***	***F'***	***F''***	***obs.***	***obs.-cal.***	***J'***	***K'$_{-1}$***	***K'$_{+1}$***	***J''***	***K''$_{-1}$***	***K''$_{+1}$***	***F'***	***F''***	***obs.***	***obs.-cal.***
2	0	2	1	0	1	3	2	7278.043	0.000	4	0	4	3	0	3	5	4	14293.48	0.002
						2	1	7278.174	0.003							3	2	14293.513	-0.004
						1	0	7278.576	-0.005							4	3	14293.659	0.001
						2	2	-	-							4	4	-	-
3	0	3	2	0	2	2	2	-	-	4	1	4	3	1	3	5	4	13637.202	0.001
						4	3	10832.894	0.001							3	2	13637.3	0.001
						2	1	10833	0.002							4	3	13637.344	0.000
						3	2	10833.043	-0.003	4	1	3	3	1	2	3	2	15474.239	0.001
						3	3	-	-							5	4	15474.297	0.000
3	1	3	2	1	2	2	2	-	-							4	3	15474.409	0.000
						4	3	10255.154	0.000	1	1	1	0	0	0	0	1	8096.76	-0.003
						2	1	10255.311	-0.003							2	1	8097.48	0.000
						3	2	10255.404	0.001							1	1	8097.959	0.002
						3	3	-	-	2	1	2	1	0	1	3	2	11291.86	0.002
3	1	2	2	1	1	3	3	-	-							1	0	11292.152	-0.005
						2	1	11638.405	0.001							2	1	11292.42	0.004
						4	3	11638.576	0.000										
						3	2	11638.763	-0.002										
						2	2	-	-										

Table S4. Observed and calculated frequencies (MHz) for the monodeuterated species of the 1:1a complex of 2-azetidinone···H_2O

								D_a/H_a		D_b/H_b		D_c/H_c	
J'	***K'$_{-1}$***	***K'$_{+1}$***	***J''***	***K''$_{-1}$***	***K''$_{+1}$***	***F'***	***F''***	***obs.***	***obs.-cal***	***obs.***	***obs.-cal***	***Obs.***	***obs.-cal***
2	0	2	1	0	1	3	2	7633.116	-0.002	7527.277	-0.001	7324.7286	0.00313
						2	1	7633.259	-0.001	7527.413	0.001	7324.8524	-0.00144
						1	0	7633.648	-0.001	-	-	7325.2658	0.00189
						2	2	7633.908	0.003	7528.056	-0.001	7325.4999	0.00045
3	0	3	2	0	2	2	2	11337.798	-0.001	11194.755	-0.002	10900.9311	-0.00305
						4	3	11338.923	0.000	11195.865	0.000	10902.0345	0.00173
						2	1	-	-	11195.967	-0.002	10902.126	-0.01206
						3	2	11339.096	-0.001	11196.023	-0.002	10902.1878	0.00142
						3	3	11339.890	0.005	11196.805	0.000	10902.9597	-0.00066
3	1	3	2	1	2	2	2	10710.540	-0.003	10588.712	-0.003	-	-
						4	3	10712.259	0.002	10590.427	-0.001	10320.7755	0.00203
						2	1	10712.417	0.000	-	-	10320.9327	-0.00103
						3	2	10712.509	-0.002	10590.674	-0.005	10321.0233	0.00054
						3	3	10713.716	0.002	10591.887	0.004	10322.227	0.00023
3	1	2	2	1	1	3	3	12265.601	0.003	12058.511	0.003	11713.3099	0.00513
						2	1	12265.745	0.001	12058.663	0.005	11713.4559	-0.00103
						4	3	12265.911	-0.006	12058.829	-0.001	11713.6275	-0.00091
						3	2	12266.109	-0.001	12059.016	-0.005	11713.8157	-0.00131
						2	2	12266.543	0.002	-	-	-	-
4	0	4	3	0	3	5	4	14923.895	0.002	14758.983	0.001	14384.1376	0.00247
						3	2						
						4	3	14924.092	-0.004	14759.172	0.001	14384.3165	0.00042
						4	4	-	-	-	-	14385.2455	0.00183
4	1	4	3	1	3	5	4	-	-	14079.707	0.000	-	-
						3	2	-	-	14079.812	0.008	-	-
						4	3	-	-	14079.848	-0.003	-	-

Table S5. Observed and calculated frequencies (MHz) for the parent species of the 1:1b complex of 2-azetidinone···H_2O

J'	*K'$_{-1}$*	*K'$_{+1}$*	*J''*	*K''$_{-1}$*	*K''$_{+1}$*	*F'*	*F''*	*obs.*	*obs.-cal.*	*J'*	*K'$_{-1}$*	*K'$_{+1}$*	*J''*	*K''$_{-1}$*	*K''$_{+1}$*	*F'*	*F''*	*obs.*	*obs.-cal.*
2	0	2	1	0	1	1	1	7151.964	0.003	3	2	1	2	2	0	2	1	10881.373	0.000
						3	2	7152.790	-0.001							4	3	10881.635	-0.001
						2	1	7152.912	0.000							3	2	10882.026	-0.002
						1	0	7153.190	0.002	4	0	4	3	1	3	4	3	10317.865	0.001
						2	2	7153.403	0.001							3	2	10318.660	-0.001
2	1	1	1	1	0	3	2	7608.966	0.001							3	3	14088.325	-0.001
						2	1	7609.407	0.000							5	4	14089.333	-0.001
3	0	3	2	0	2	2	2	10659.375	-0.001							3	2	14089.361	0.004
						4	3	10660.254	0.000							4	3	14089.519	-0.001
						2	1	10660.331	0.004	4	1	4	3	1	3	5	4	13452.112	-0.001
						3	2	10660.408	0.001							3	2	13452.216	-0.001
						3	3	10661.018	0.000							4	3	13452.240	-0.001
3	1	3	2	1	2	2	2	10109.851	-0.002							4	4	13453.718	0.001
						4	3	10111.636	0.001	4	1	3	3	1	2	3	2	15158.097	0.001
						3	3	10113.108	-0.003							4	3	15158.264	0.000
3	1	2	2	1	1	3	3	11394.689	-0.002	4	2	3	3	2	2	3	2	14339.467	0.000
						2	1	11395.093	0.000							5	4	14339.530	0.000
						4	3	11395.292	-0.001							4	3	14339.772	-0.002
						3	2	11395.430	-0.001	4	2	2	3	2	1	5	4	14611.033	0.002
						2	2	11396.243	-0.001							4	3	14611.101	-0.001
3	2	2	2	2	1	2	1	10770.742	-0.001	5	1	5	4	1	4	6	5	16769.952	0.001
						4	3	10771.039	0.005	2	1	2	1	0	1	3	2	11472.356	0.000
						3	2	10771.562	0.002							2	1	11473.131	0.000
										3	1	3	2	0	2	4	3	14431.201	0.001
																3	2	14432.061	-0.002

Table S6. Observed and calculated frequencies (MHz) for the ^{18}O species of the 1:1b complex of 2-azetidinone···H_2O

$^{18}O_B/^{16}O_B$																			
J'	*K'$_{-1}$*	*K'$_{+1}$*	*J''*	*K''$_{-1}$*	*K''$_{+1}$*	*F'*	*F''*	*obs.*	*obs.-cal.*	*J'*	*K'$_{-1}$*	*K'$_{+1}$*	*J''*	*K''$_{-1}$*	*K''$_{+1}$*	*F'*	*F''*	*obs.*	*obs.-cal.*
2	0	2	1	0	1	3	2	6782.553	0.000	4	0	4	3	0	3	5	4	13388.117	0.000
						2	1	6782.669	0.004							3	2	13388.141	0.000
						1	0	6782.952	-0.003							4	3	13388.288	0.001
3	0	3	2	0	2	4	3	10117.626	0.000	4	1	4	3	1	3	5	4	12791.170	0.002
						2	1	10117.699	-0.001							3	2	12791.267	-0.005
						3	2	10117.765	0.000							4	3	12791.294	0.002
3	1	3	2	1	2	4	3	9611.883	0.001	4	1	3	3	1	2	3	2	14338.237	0.001
						3	2	9612.089	-0.001							5	4	14338.315	0.002
3	1	2	2	1	1	2	1	10775.074	-0.001							4	3	14338.394	-0.003
						4	3	10775.275	0.000										
						3	2	10775.410	0.000										

Table S7. Observed and calculated frequencies (MHz) for the monodeuterated species of the 1:1b complex of 2-azetidinone···H_2O

								D_a/H_a		D_b/H_b		D_c/H_c	
J'	***K'$_{-1}$***	***K'$_{+1}$***	***J''***	***K''$_{-1}$***	***K''$_{+1}$***	***F'***	***F''***	***obs.***	***obs.-cal.***	***obs.***	***obs.-cal.***	***obs.***	***obs.-cal.***
2	0	2	1	0	1	3	2	7008.263	-0.004	7035.434	-0.005	6849.123	-0.001
3	0	3	2	0	2	4	3	10443.623	-0.001	10488.969	-0.001	10215.989	-0.001
						3	2	10443.776	-0.002	10489.114	-0.004	-	-
3	1	3	2	1	2	4	3	9903.847	0.000	9954.763	0.002	9703.974	-0.001
						3	2	9904.059	0.002	9954.971	0.001	9704.185	0.002
3	1	2	2	1	1	2	1	-	-	-	-	10883.734	0.000
						4	3	11169.410	0.002	11196.720	0.003	10883.934	0.000
						3	2	11169.546	0.000	-	-	10884.069	0.000
4	0	4	3	0	3	5	4	13800.877	0.001	13869.218	-0.003	13516.636	0.002
						4	3	13801.066	0.001	13869.407	0.006	13516.805	-0.001

Table S8. Observed and calculated frequencies (MHz) for the parect species of the 2-azetidinone···$(H_2O)_2$ complex.

J'	*K'*$_{-1}$	*K'*$_{+1}$	*J''*	*K''*$_{-1}$	*K''*$_{+1}$	*F'*	*F''*	*obs.*	*obs.-cal.*	*J'*	*K'*$_{-1}$	*K'*$_{+1}$	*J''*	*K''*$_{-1}$	*K''*$_{+1}$	*F'*	*F''*	*obs.*	*obs.-cal*
3	0	3	2	0	2	4	3	6876.645	0.000	5	1	4	4	1	3	4	3	12504.053	0.001
						2	1	6876.710	-0.003							6	5	12504.094	-0.001
						3	2	6876.876	0.001							5	4	12504.252	0.000
3	1	3	2	1	2	4	3	6468.076	0.000	5	2	4	4	2	3	4	3	11693.438	-0.002
						2	1	6468.220	-0.001							6	5	11693.464	0.002
						3	2	6468.308	-0.002							5	4	11693.649	0.002
3	1	2	2	1	1	3	3	7640.579	-0.001	5	2	3	4	2	2	6	5	12564.143	0.004
						2	1	7640.743	0.000	5	3	3	4	3	2	4	3	11957.843	0.006
						4	3	7640.915	0.001							6	5	11957.900	-0.002
						3	2	7641.096	0.000							5	4	11958.145	0.001
						2	2	7641.547	-0.001	6	0	6	5	0	5	7	6	12879.070	-0.001
3	2	2	2	2	1	2	1	7088.626	0.002							5	4	12879.092	0.002
3	2	1	2	2	0	2	1	7301.123	-0.003							6	5	12879.249	0.000
						4	3	7301.397	-0.007	6	1	6	5	1	5	7	6	12676.604	0.002
						3	2	7301.773	-0.003							5	4	12676.639	-0.002
4	0	4	3	0	3	3	3	8957.083	-0.001							6	5	12676.703	0.000
						5	4	8958.345	0.000	6	1	5	5	1	4	5	4	14785.394	0.006
						3	2	8958.368	-0.001							7	6	14785.420	-0.002
						4	3	8958.594	0.000							6	5	14785.610	-0.001
						4	4	8959.545	-0.001	6	2	5	5	2	4	5	4	13934.733	-0.002
4	1	4	3	1	3	3	3	8568.737	-0.001							7	6	13934.743	0.000
						5	4	8570.449	0.001							6	5	13934.891	0.000
						3	2	8570.533	-0.001	6	2	4	5	2	3	6	5	15221.244	-0.003
						4	3	8570.598	-0.001							7	6	15221.261	0.000
						4	4	8571.929	0.000	6	3	4	5	3	3	5	4	14363.502	-0.006
4	1	3	3	1	2	3	2	10111.911	0.002							7	6	14363.534	-0.001
						5	4	10111.978	0.000							6	5	14363.678	-0.002
						4	3	10112.120	0.001	6	4	2	5	4	1	5	4	14372.319	0.006
						3	3	10112.362	0.001							7	6	14372.367	-0.001
4	2	3	3	2	2	3	2	9409.110	-0.002							6	5	14372.597	-0.001
						5	4	9409.187	0.003	4	0	4	3	1	3	4	3	7805.090	-0.002
						4	3	9409.468	0.002							5	4	7805.220	0.000
5	0	5	4	0	4	6	5	10941.603	0.000							3	2	7805.379	0.001
						4	3	10941.627	0.006	4	1	4	3	0	3	5	4	9723.577	0.004
						5	4	10941.830	0.001							4	3	9724.106	0.005
5	1	5	4	1	4	4	4	10637.074	-0.002	5	0	5	4	1	4	5	4	10176.324	0.002
						6	5	10638.882	0.000							6	5	10176.376	0.001
						4	3	10638.940	0.003	5	1	5	4	0	4	4	3	11404.091	-0.002
						5	4	10639.001	0.000							6	5	11404.116	0.006
						5	5	10640.481	0.000							5	4	11404.490	-0.017

Table S9. Observed and calculated frequencies (MHz) for the ^{18}O species of the of 2-azetidinone···$(H_2O)_2$ complex.

								$^{18}O_A/^{16}O_A$		$^{18}O_B/^{16}O_B$	
J'	***K'$_{-1}$***	***K'$_{+1}$***	***J''***	***K''$_{-1}$***	***K''$_{+1}$***	***F'***	***F''***	***obs.***	***obs.-cal.***	***Obs.***	***obs.-cal.***
4	0	4	3	0	3	5	4	8700.937	0.000	-	-
						3	2	8700.963	0.001	-	-
						4	3	8701.180	-0.001	-	-
4	1	4	3	1	3	5	4	8317.713	0.000	8342.721	-0.001
						3	2	8317.798	0.000	8342.805	0.000
						4	3	8317.860	0.000	8342.870	0.000
4	1	3	3	1	2	3	2	9786.284	-0.001	9858.668	-0.002
						5	4	9786.351	0.000	9858.738	-0.003
						4	3	9786.490	0.001	9858.881	-0.002
5	0	5	4	0	4	6	5	10635.327	-0.001	10643.093	-0.001
						4	3	10635.344	0.001	10643.113	0.003
						5	4	10635.551	-0.001	10643.320	-0.002
5	1	5	4	1	4	6	5	10328.836	-0.001	10354.265	-0.001
						5	4	10328.953	-0.001	10354.384	0.000
						4	3	-	-	12185.817	0.003
5	1	4	4	1	3	4	3	12111.015	0.001	-	-
						6	5	12111.054	0.000	12185.859	0.001
						5	4	12111.204	-0.001	12186.021	0.002
6	0	6	5	0	5	7	6	12521.520	-0.001	12526.150	-0.001
						5	4	12521.541	0.002	12526.171	0.000
						6	5	12521.700	-0.001	12526.330	0.000
5	0	5	4	1	4	5	4	9832.936	-0.003	9924.896	0.002
						6	5	9833.012	0.004	9924.946	0.002
						4	3	9833.101	0.000	9925.031	-0.002
5	1	5	4	0	4	4	3	11131.131	-0.004	11072.395	-0.003
						6	5	11131.161	0.005	11072.421	0.005
						5	4	11131.567	0.000	11072.810	-0.002

Table S10. Observed and calculated frequencies (MHz) for the monodeuterated species of the of 2-azetidinone···$(H_2O)_2$ complex.

								D_a/H_a		D_b/H_b		D_c/H_c		D_d/H_d		D_e/H_e	
J'	***K'$_{-1}$***	***K'$_{+1}$***	***J''***	***K''$_{-1}$***	***K''$_{+1}$***	***F'***	***F''***	***obs.***	***obs.-cal.***	***obs.***	***obs.-cal.***	***obs.***	***obs.-cal.***	***obs.***	***obs.-cal.***	***obs.***	***obs.-cal.***
3	0	3	2	0	2	4	3	-	-	6820.800	0.004	6718.825	-0.001	6784.290	0.003	6731.740	-0.001
4	0	4	3	0	3	5	4	8936.058	-0.001	8883.468	0.001	8757.790	0.001	8844.035	-0.005	8764.934	-0.001
						4	3	8936.307	-0.004	-	-	8758.034	-0.003	8844.283	-0.003	8765.190	0.003
4	1	4	3	1	3	5	4	8552.464	-0.001	8500.010	-0.005	8376.762	0.001	8457.371	0.000	8389.717	-0.001
						3	2	-	-	-	-	8376.845	-0.002	8457.452	-0.004	-	-
						4	3	-	-	-	-	8376.910	0.000	8457.520	0.000	8389.872	0.003
4	1	3	3	1	2	3	2	-	-	-	-	9866.983	0.000			9908.532	-0.001
						5	4	10105.277	-0.002	10034.921	0.001	9867.050	0.000	9962.184	0.003	9908.602	0.000
						4	3	10105.424	0.000	10035.064	0.000	9867.191	0.001	9962.320	-0.001	9908.745	-0.002
5	0	5	4	0	4	6	5	10910.318	-0.003	10848.489	0.000	10700.845	0.000	10806.730	-0.002	10702.090	-0.002
						4	3	-	-	-	-	-	-	10806.749	0.000	-	-
						5	4	10910.545	-0.001	10848.713	-0.001	10701.069	-0.001	10806.956	-0.001	10702.317	-0.001
5	1	5	4	1	4	6	5	10614.628	0.004	10550.679	0.001	10400.283	0.001	10500.691	0.002	10412.851	0.000
						5	4	10614.740	-0.003	10550.800	0.003	10400.400	0.000	10500.806	-0.001	10412.969	-0.001
5	1	4	4	1	3	6	5	12490.626	-0.003	12406.776	0.001			-	-	-	-
						5	4	12490.794	0.005	12406.931	-0.002	12205.986	0.000	-	-	12248.027	0.003
6	0	6	5	0	5	7	6	12840.881	0.002	12768.857	0.000	12597.604	0.001	12722.033	0.003	12596.500	0.000
						6	5	12841.060	0.004	12769.033	-0.001	12597.783	0.001	12722.212	0.003	12596.676	0.000