

Supporting Information.

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Molecular Dynamics and Interactions of Aqueous and Dichloromethane Solutions of Polyvinylpyrrolidone.

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A. Atom coordinates of optimized EP, H₂O, CH₂Cl₂, and EP/2H₂O calculated at the B3LYP/6-311++G(d,p) level of theory.

EP

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.614835	0.919194	0.004011
2	6	-0.339764	-1.408388	-0.341372
3	6	-1.734438	-1.210306	0.286457
4	6	-2.003106	0.292557	0.118569
5	1	-0.404805	-1.690701	-1.402360
6	1	0.241835	-2.178961	0.171014
7	1	-2.487835	-1.843842	-0.183338
8	1	-1.696606	-1.467613	1.347791
9	1	-2.545026	0.518318	-0.806122
10	1	-2.557992	0.746356	0.939817
11	7	0.283744	-0.096655	-0.200356
12	6	1.681738	0.146775	-0.523751
13	1	1.906374	-0.322918	-1.489851
14	1	1.784146	1.226391	-0.646727
15	6	2.649918	-0.358849	0.548361
16	1	3.681393	-0.149519	0.251540
17	1	2.461119	0.139139	1.502154
18	1	2.561510	-1.438189	0.700663
19	8	-0.345925	2.106529	0.058033
Rotational constants (GHz):		3.083520	1.754380	1.232585

H₂O

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	0.000000	0.000000	0.117009
2	1	0.000000	0.763592	-0.468036
3	1	0.000000	-0.763592	-0.468036
Rotational constants (GHz):		824.8385	430.0108	282.6550

CH₂Cl₂

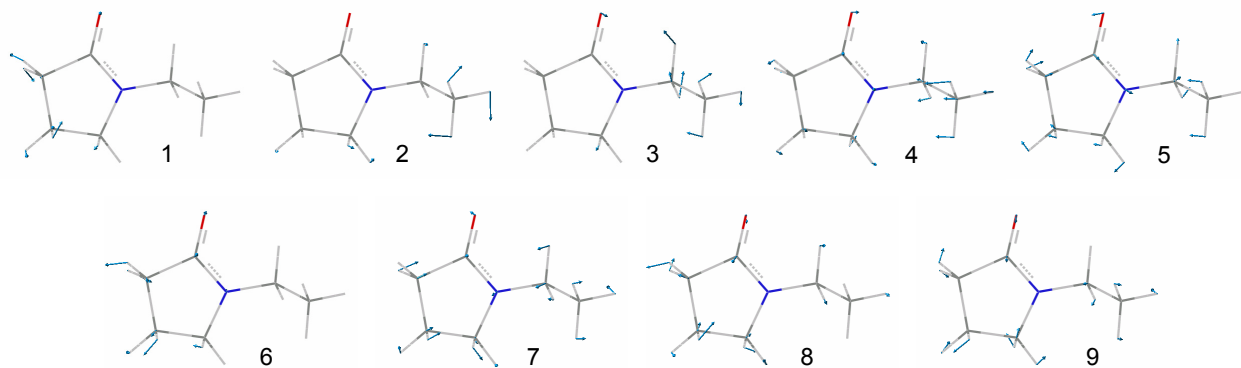
Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.768877
2	1	0.898972	0.000000	1.375154
3	1	-0.898972	0.000000	1.375154
4	17	0.000000	1.494827	-0.216576
5	17	0.000000	-1.494827	-0.216576
Rotational constants (GHz):		32.19576	3.200520	2.966806

EP/2H₂O

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.464065	-0.246234	-0.012210
2	6	0.984694	-2.099336	-0.032571
3	6	-0.451897	-2.654632	0.028313
4	6	-1.297971	-1.437106	0.430740
5	1	1.582473	-2.547815	-0.830559
6	1	1.521151	-2.247205	0.912479
7	1	-0.751826	-3.007836	-0.961088
8	1	-0.539188	-3.491223	0.721953
9	1	-2.291821	-1.397016	-0.015190
10	1	-1.430573	-1.360890	1.515652
11	7	0.787680	-0.670673	-0.292890
12	6	1.889419	0.210948	-0.675769
13	1	2.438128	-0.282560	-1.484705
14	1	1.451052	1.122646	-1.080536
15	6	2.831084	0.551469	0.481255
16	1	3.633713	1.198744	0.119982
17	1	2.298437	1.093320	1.264623
18	1	3.287570	-0.344368	0.911488
19	8	-0.862638	0.922553	-0.085605
20	1	-2.734543	1.051815	-0.064736
21	8	-3.694515	0.882607	-0.049630
22	1	-4.088265	1.586336	-0.572249
23	1	0.062800	2.539309	0.062001
24	8	0.677169	3.292952	0.117253
25	1	0.139423	4.045905	0.376421
Rotational constants (GHz):		1.0884949	0.9702714	0.5389498

B. Observed intramolecular vibrational modes of PVP and EP in H₂O and CH₂Cl₂ and calculated normal modes of gas phase EP from DFT calculations at the B3LYP/6-311++G(d,p) level of theory.

PVP		EP			
Observed (in H ₂ O)	Observed (in CH ₂ Cl ₂)	Observed (in H ₂ O)	Observed (in CH ₂ Cl ₂)	Calculated	Assignment
		135		150	1
		213		207	2
		327	~310	320	3
387	379	387	378	368	4
		495	498	500	5
555	553	573	566	566	6
605	609	616	613	612	7
648	654	655	654	655	8
746		743		743	9



C. Polarizability tensor elements α_{ij} of H₂O, CH₂Cl₂, and EP estimated by B3LYP/6-311++G(d,p) calculations. Unit is Å³.

	α_{xx}	α_{xy}	α_{yy}	α_{yx}	α_{yz}	α_{zz}
H ₂ O	0.984	0.000	1.186	0.000	0.000	0.980
CH ₂ Cl ₂	3.847	0.000	6.978	0.000	0.000	4.478
EP	13.002	-0.309	12.137	-0.241	0.277	9.356

D. Full author list of Reference 50.

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