

Study on the crystallization mechanism of CL-20 in different binary solvents: the theoretical- experimental method.

Table S1. Energy details of ϵ -cl-20-solvents interfacial models for each plane^a.

	(h k l)	E_{tot}	E_{sur}	E_{sol}	E_{int}	E_{att}^m	S%
Ethyl Acetate/ Dichloromethane	(1 1 0)	-20843.275	-19305.573	-1222.020	-315.682	-17.956	51.414
	(0 0 1)	-23566.820	-21699.381	-1420.813	-454.246	10.025	46.890
	(1 1 -1)	-23903.199	-21698.846	-1763.730	-440.623	-23.708	
	(0 1 1)	-23989.402	-21659.756	-1785.863	-543.782	24.801	
	(2 0 0)	-16028.374	-14479.605	-1266.492	-282.278	-63.846	
	(2 0 -1)	-16002.755	-14451.941	-1229.859	-320.956	-27.444	1.697
Aspect Ratio:			2.896	Relative Surface / Volume Ratio:			1.305
Ethyl Acetate/ Dibromomethane	(1 1 0)	-21118.113	-19308.142	-1486.273	-323.698	-16.210	58.920
	(0 0 1)	-23933.319	-21686.838	-1754.105	-492.375	18.404	19.685
	(1 1 -1)	-24308.127	-21701.739	-2152.834	-453.554	-21.674	14.497
	(0 1 1)	-24412.588	-21670.804	-2177.646	-564.138	29.398	
	(2 0 0)	-16346.420	-14483.281	-1542.541	-320.597	-59.617	
	(2 0 -1)	-16334.910	-14440.850	-1553.476	-340.583	-22.252	6.899
Aspect Ratio:			1.811	Relative Surface / Volume Ratio:			1.168
Ethyl Acetate/ Chloroform	(1 1 0)	-21792.762	-19301.462	-2186.585	-304.714	-20.345	36.234
	(0 0 1)	-23838.325	-21695.414	-1701.785	-441.126	7.142	58.371
	(1 1 -1)	-24163.167	-21705.294	-2025.439	-432.434	-24.997	
	(0 1 1)	-24292.370	-21664.187	-2066.844	-561.340	28.766	
	(2 0 0)	-16257.820	-14475.843	-1461.499	-320.478	-59.630	
	(2 0 -1)	-16260.622	-14452.771	-1473.729	-334.123	-23.961	5.395
Aspect Ratio:			4.161	Relative Surface / Volume Ratio:			1.404
Ethyl Acetate/ Tetrachloromethane	(1 1 0)	-21129.617	-19309.769	-1507.046	-312.802	-18.583	46.775
	(0 0 1)	-23939.164	-21696.648	-1782.139	-460.377	11.372	37.252
	(1 1 -1)	-24275.305	-21700.400	-2111.947	-462.957	-20.194	14.452
	(0 1 1)	-24442.829	-21673.554	-2198.823	-570.451	30.824	
	(2 0 0)	-16337.393	-14474.647	-1556.516	-306.229	-61.203	
	(2 0 -1)	-16331.166	-14450.759	-1559.718	-320.689	-27.515	1.521
Aspect Ratio:			2.594	Relative Surface / Volume Ratio:			1.209
Ethyl Acetate/ Dichloroethane	(1 1 0)	-21700.642	-19304.603	-2044.008	-352.032	-10.315	70.007
	(0 0 1)	-24599.920	-21683.210	-2417.940	-498.769	19.815	9.098
	(1 1 -1)	-25102.630	-21702.455	-2927.642	-472.533	-18.694	10.432
	(0 1 1)	-25249.975	-21669.712	-2972.167	-608.096	39.326	
	(2 0 0)	-16929.749	-14477.347	-2125.039	-327.363	-58.923	

	(2 0 -1)	-16920.703	-14426.474	-2127.571	-366.659	-15.902	10.464
	Aspect Ratio:	2.111		Relative Surface / Volume Ratio:			1.205
	(1 1 0)	-20854.045	-19310.684	-1201.861	-341.500	-12.333	53.116
Ethyl Acetate/ Tetrachloroethane	(0 0 1)	-23624.288	-21692.100	-1468.550	-463.638	12.089	26.014
	(1 1 -1)	-23846.231	-21705.890	-1680.886	-459.454	-20.745	
	(0 1 1)	-24014.178	-21678.091	-1742.939	-593.148	35.950	
	(2 0 0)	-16080.015	-14484.327	-1247.806	-347.882	-56.606	
	(2 0 -1)	-16079.323	-14445.956	-1252.468	-380.899	-11.587	20.870
	Aspect Ratio:	1.862		Relative Surface / Volume Ratio:			1.919
	(1 1 0)	-20582.261	-19303.978	-958.961	-319.322	-8.752	53.985
Ethyl Acetate/ n-Pentane	(0 0 1)	-23271.463	-21691.696	-1147.776	-431.991	5.134	46.015
	(1 1 -1)	-23491.268	-21698.154	-1368.098	-425.017	-24.265	
	(0 1 1)	-23578.955	-21663.378	-1410.778	-504.799	17.174	
	(2 0 0)	-15785.708	-14477.995	-986.346	-321.367	-59.532	
	(2 0 -1)	-15778.694	-14452.587	-1029.541	-296.567	-33.896	
	Aspect Ratio:	3.228		Relative Surface / Volume Ratio:			1.317
	(1 1 0)	-20722.931	-19309.521	-1092.035	-321.375	-16.716	20.194
Ethyl Acetate/ n-Hexane	(0 0 1)	-23420.994	-21687.415	-1336.536	-397.043	-2.546	74.549
	(1 1 -1)	-23714.585	-21706.056	-1567.357	-441.172	-23.622	
	(0 1 1)	-23791.903	-21669.248	-1636.786	-485.870	11.721	5.257
	(2 0 0)	-15931.961	-14480.724	-1168.001	-283.237	-63.740	
	(2 0 -1)	-15867.108	-14430.550	-1164.420	-272.138	-40.359	
	Aspect Ratio:	10.689		Relative Surface / Volume Ratio:			1.912
	(1 1 0)	-20803.167	-19300.022	-1207.482	-295.663	-22.317	28.493
Ethyl Acetate/ n-Heptane	(0 0 1)	-23513.277	-21690.218	-1447.058	-376.001	-7.170	50.237
	(1 1 -1)	-23835.113	-21705.478	-1717.569	-412.066	-28.202	
	(0 1 1)	-23937.881	-21669.198	-1772.517	-496.166	14.047	20.769
	(2 0 0)	-16020.802	-14489.038	-1251.139	-280.625	-64.028	
	(2 0 -1)	-15991.876	-14440.000	-1256.019	-295.857	-34.084	0.501
	Aspect Ratio:	5.030		Relative Surface / Volume Ratio:			1.422
	(1 1 0)	-21434.020	-19312.350	-1812.578	-309.092	-19.392	25.870
Ethyl Acetate/ Cyclohexane	(0 0 1)	-24296.434	-21690.883	-2176.974	-428.576	4.384	64.967
	(1 1 -1)	-24692.870	-21700.885	-2549.151	-442.833	-23.361	
	(0 1 1)	-24883.833	-21668.508	-2721.115	-494.210	13.605	8.896
	(2 0 0)	-16658.822	-14479.440	-1894.400	-284.981	-63.547	
	(2 0 -1)	-16655.221	-14437.565	-1902.611	-315.044	-29.008	0.268
	Aspect Ratio:	7.062		Relative Surface / Volume Ratio:			1.618
	(1 1 0)	-18364.679	-19311.730	1257.363	-310.312	-19.126	51.750
Ethyl Acetate/	(0 0 1)	-20495.216	-21687.390	1540.594	-348.421	-13.231	34.772
	(1 1 -1)	-20382.010	-21701.788	1752.195	-432.417	-25.000	2.229

	(0 1 1)	-20303.989	-21678.351	1895.030	-520.668	19.581	9.293
	(2 0 0)	-13515.816	-14482.284	1244.446	-277.977	-64.320	
	(2 0 -1)	-13501.043	-14452.768	1261.715	-309.990	-30.345	1.956
	Aspect Ratio:	2.393		Relative Surface / Volume Ratio:		1.216	
	(1 1 0)	-19512.847	-19305.029	105.024	-312.842	-18.575	53.084
	(0 0 1)	-21861.564	-21691.943	163.366	-332.988	-16.623	21.799
Ethyl Acetate/ Toluene	(1 1 -1)	-21914.857	-21703.659	180.754	-391.952	-31.368	
	(0 1 1)	-21952.105	-21673.431	240.525	-519.198	19.249	19.593
	(2 0 0)	-14646.875	-14476.385	94.093	-264.583	-65.798	
	(2 0 -1)	-15239.312	-14445.840	-472.656	-320.815	-27.482	5.523
	Aspect Ratio:	1.809		Relative Surface / Volume Ratio:		1.167	
	(1 1 0)	-19349.713	-19310.048	286.175	-325.841	-15.743	36.999
	(0 0 1)	-21731.431	-21683.615	381.868	-429.683	4.627	62.979
Ethyl Acetate/ Bromoben zene	(1 1 -1)	-21752.315	-21700.552	385.000	-436.763	-24.316	
	(0 1 1)	-21767.458	-21673.467	466.226	-560.218	28.513	
	(2 0 0)	-14516.585	-14483.184	287.757	-321.158	-59.555	
	(2 0 -1)	-14481.274	-14446.165	292.990	-328.099	-25.555	0.022
	Aspect Ratio:	3.296		Relative Surface / Volume Ratio:		1.332	

^{2a}Energy unit is in kcal·mol⁻¹

