Supplementary Information

Predicting the Solid–Liquid Phase Diagram of a Ternary System with Cocrystal Formation

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UV spectrophotometry

The calibration curve for catechol in acetonitrile was established prior to concentration analysis. Catechol was weighed and transferred into a volumetric flask, followed by the addition of acetonitrile. The mixture was shaken until the catechol dissolved completely, and the flask was filled to the mark with additional acetonitrile. Two stock solutions were prepared with concentrations of 7.2641×10^{-5} g/g solution and 6.1571×10^{-5} g/g solution. Thirteen diluted samples were prepared in triplicate from these stock solutions to construct the calibration curve. The resulting curve showed excellent accuracy, described by the equation:

$$\text{Absorbance} = 0.0163 \times C_{\text{catechol}}\ (\text{ppm}) + 0.0953$$

with a correlation coefficient (R^2) of 0.9963.

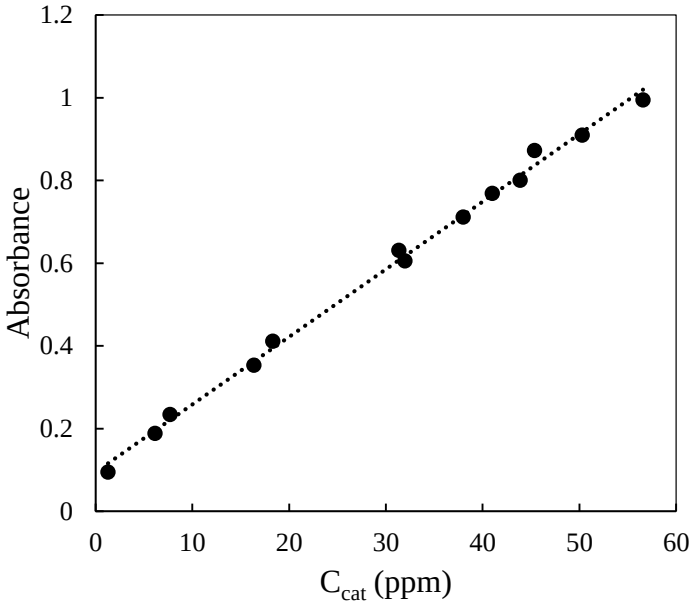

Figure S1. Calibration curve for catechol in acetonitrile, measured by UV spectroscopy.

Table S1. Measured solubility values using the variable-temperature method (n=3).

x_1	x_2	x_3	T/K	$\sigma(T)/K$
Catechol (2) + acetonitrile (3)*				
-	0.2639	0.7361	277.1	0.8662
-	0.3077	0.6923	284.7	0.5692
-	0.3902	0.6098	303.7	0.1414
-	0.4226	0.5774	313.3	0.3536
-	0.5051	0.4949	327.6	0.1768
-	0.5590	0.4410	333.6	0.7071
ChCl (1):catechol (2) C11 in acetonitrile (3)**				
0.0803	0.0803	0.8394	294.0	0.3711
0.1428	0.1428	0.7144	299.8	0.2646
0.2111	0.2111	0.5778	311.0	0.1461
0.2571	0.2571	0.4858	315.4	0.2646
0.3219	0.3219	0.3562	321.3	0.3055
ChCl (1):catechol (2) C12 in acetonitrile (3)**				
0.1169	0.2338	0.6493	289.8	0.1537
0.1387	0.2773	0.58405	296.8	1.6949
0.2226	0.4452	0.3322	308.2	0.5346
0.2921	0.5841	0.12385	320.1	0.2812
TMACl (1):catechol (2) C11 in acetonitrile (3)**				
0.0353	0.0353	0.9294	305.5	0.8485
0.0379	0.0379	0.9242	307.1	0.6089
0.0460	0.0460	0.9080	316.4	0.8372
0.0494	0.0494	0.9012	320.2	0.9452

* n=2, ** n=3 (n is number of experiments).

Table S2. Measured solubility values using the shake-flask method at 298.1 K*.

Solid	x_1	x_2	x_3	Precipitate	$\sigma(x_2)$	$\sigma(x_1)$
ChCl (1) + catechol (2) + acetonitrile (3)						
Catechol	0.0000	0.3641	0.6359	Catechol	0.0028	-
C12+catechol (Invariant 1)	0.0711	0.4937	0.4351	C12+catechol	0.0016	0.0069
C12+catechol	0.1038	0.4182	0.4780	C12	0.0011	0.0007
C12+catechol	0.1065	0.3262	0.5673	C12	0.0088	0.0061
C12	0.1549	0.2787	0.5664	C12	0.0009	0.0043
C12+C11	0.1476	0.2534	0.5990	C12+C11	0.0061	0.0025
C11	0.1393	0.1348	0.7259	C11	0.0020	0.0036
C11+ChCl	0.0525	0.0558	0.7049	ChCl	0.0024	0.0051
C11+ChCl (Invariant 2)	0.1338	0.1414	0.8917	C11+ChCl	0.0029	0.0024
ChCl	0.0013	0.0000	0.9987	ChCl	-	3.36×10^{-5}
TMACl (1) + catechol (2) + acetonitrile (3)						
C12+catechol	0.1011	0.4904	0.4085	C12+catechol		
C12+catechol (Invariant 1)	0.078	0.31	0.612	C12	0.0003	0,0006
C12	0.0712	0.2001	0.7287	C12	0.0072	0.0188
C12+C11	0.0663	0.1847	0.7491	C12+C11	0.0032	0.0061
C11	0.0513	0.0533	0.9148	C11	0.0011	0.0012
C11+TMACl (Invariant 2)	0.0597	0.0528	0.9179	C11+TMACl	0.0020	0.0013
TMACl	0.001896	0	0.9981	TMACl	-	9.79×10^{-5}

* n=3

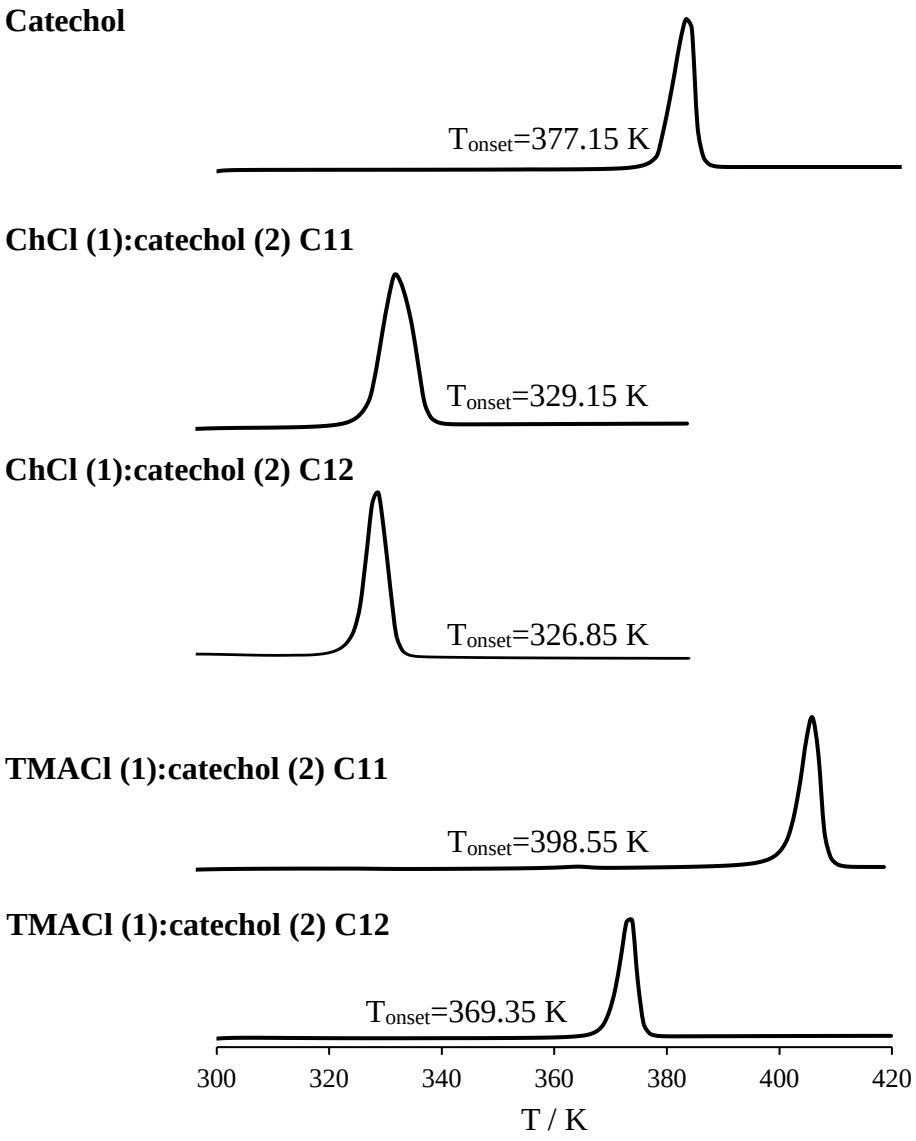

Figure S2. Differential scanning calorimetry curve of cocrystals and pure components.

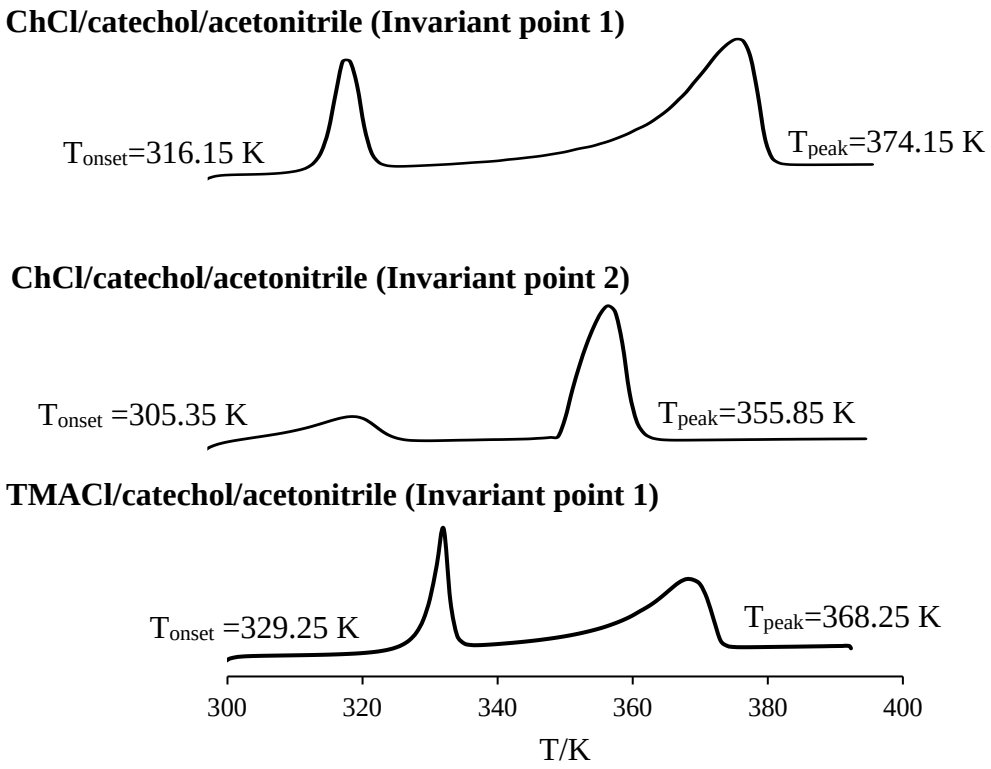

Figure S3. Differential scanning calorimetry curve of solid phase at equilibrium