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Supporting Information

A systematic study on ternary inclusion crystals consisting of dianilines and three positional isomers of ditoluoyl-L-tartaric acid

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Table S1. Crystallographic data of the inclusion crystals reported in this study and previous study.

	1b•2M•2-BuOH•2H_2O (A1)	**1b•2O•2H_2O (A2)**	**1o•2M•3H_2O (B1)**	**1o•2O•3H_2O (B2)**
formula	$C_{35}H_{42}N_2O_{11}$	$C_{30}H_{30}N_2O_{11}$	$C_{33}H_{38}N_2O_{11}$	$C_{32}H_{36}N_2O_{12}$
moiety formula	$(C_{18}H_{12}O_8)^{2-}$ • $(C_{13}H_{16}N_2)^{2+}$ • $C_4H_{10}O$ • $2H_2O$	$(C_{18}H_{12}O_8)^{2-}$ • $(C_{12}H_{14}N_2O)^{2+}$ • $2H_2O$	$(C_{20}H_{16}O_8)^{2-}$ • $(C_{13}H_{16}N_2)^{2+}$ • $3H_2O$	$(C_{20}H_{16}O_8)^{2-}$ • $(C_{12}H_{14}N_2O)^{2+}$ • $3H_2O$
FW	666.71	594.56	638.65	640.63
temperature (K)	273	150	100	150
crystal size (mm)	0.80 × 0.20 × 0.03	0.50 × 0.15 × 0.05	0.16 × 0.14 × 0.02	0.21 × 0.20 × 0.06
crystal system	monoclinic	monoclinic	monoclinic	monoclinic
space group	$P2_1$	$P2_1$	$C2$	$C2$
a (Å)	8.266(3)	13.029(3)	13.604(2)	13.524(2)
b (Å)	17.153(6)	9.107(2)	9.974(2)	9.9285(16)
c (Å)	12.824(5)	13.565(3)	13.840(3)	13.891(3)
α (°)	90	90	90	90
β (°)	103.670(9)	116.569(4)	119.099(4)	118.8166(19)
γ (°)	90	90	90	90
V (Å^3)	1766.7(11)	1439.7(5)	1640.9(6)	1634.2(5)
Z	2	2	2	2
Dc (g/cm^3)	1.253	1.372	1.293	1.302
μ ($Mo_{K\alpha}$) (mm^{-1})	0.093	0.106	0.097	0.100
$\theta_{min/max}$ (°)	1.63/25.00	1.68/24.99	1.68/25.00	1.67/24.99
*R*1 [$F_0 > 2\sigma(F_0)$]	0.0776	0.0459	0.0369	0.0280
*wR*2 (all F_0^2)	0.1951	0.1026	0.0972	0.0777
GOF	1.074	1.142	1.029	1.049
Flack parameter	-1.5(19)	0.0(10)	1.1(10)	1.2(3)
measured reflns	10015	8149	3416	3938
independent reflns	5775	3930	1956	2652
observed reflns	3924	3354	1845	2595
reflns used	5775	3930	1956	2652
parameters	455	428	234	234
CCDC number	827717	1414396	1414397	1414398
	2(1m)•2M•2-BuOH (C1)	**1m•2O•2(2-BuOH)•H_2O (C2)**	**1p•2M (D1)**	**1p•2O•2(2-PenOH) (D2)**
formula	$C_{28.5}H_{30}NO_{8.5}$	$C_{40}H_{52}N_2O_{12}$	$C_{33}H_{32}N_2O_8$	$C_{42}H_{54}N_2O_{11}$
moiety formula	$(C_{20}H_{17}O_8)^-$ • $0.5(C_{13}H_{16}N_2)^{2+}$ • $0.5(C_4H_{10}O)$	$(C_{20}H_{16}O_8)^{2-}$ • $(C_{12}H_{14}N_2O)^{2+}$ • $2(C_4H_{10}O)$ • H_2O	$(C_{20}H_{17}O_8)^-$ • $(C_{13}H_{15}N_2)^+$	$(C_{12}H_{14}N_2O)^{2+}$ • $2(C_5H_{12}O)$
FW	522.54	752.84	584.60	762.87
temperature (K)	150	150	200	150
crystal size (mm)	0.12 × 0.08 × 0.08	0.28 × 0.10 × 0.02	0.18 × 0.03 × 0.01	0.25 × 0.05 × 0.02
crystal system	monoclinic	orthorhombic	tetragonal	orthorhombic
space group	$C2$	$P2_12_12_1$	$I4_1$	$P2_12_12_1$
a (Å)	16.286(7)	7.7919(13)	28.639(5)	7.7836(8)
b (Å)	22.708(9)	21.208(4)	28.639(5)	22.234(2)
c (Å)	7.950(3)	24.416(4)	7.8757(15)	24.890(3)
α (°)	90	90	90	90
β (°)	115.707(5)	90	90	90
γ (°)	90	90	90	90
V (Å^3)	2649.2(19)	4034.7(12)	6460(3)	4307.5(8)
Z	4	4	8	4
Dc (g/cm^3)	1.310	1.239	1.202	1.176
μ ($Mo_{K\alpha}$)	0.097	0.091	0.087	0.085
$\theta_{min/max}$ (°)	1.65/25.00	1.27/25.00	1.005/25.00	1.23/25.00
*R*1 [$F_0 > 2\sigma(F_0)$]	0.0667	0.0853	0.0547	0.0719
*wR*2 (all F_0^2)	0.1704	0.2202	0.1313	0.1966
GOF	1.038	1.033	0.910	1.028
Flack parameter	-1.3(10)	1.0(10)	-2.6(10)	-0.8(7)
measured reflns	6331	18894	15524	20564
independent reflns	4317	7072	5607	7561
observed reflns	3460	4689	3031	5498
reflns used	4317	7072	5607	7561
parameters	349	454	396	523
CCDC number	1414399	1414400	1414401	1414403

Table S2. Hydrogen bond metrics of the inclusion crystals (**A2**, **B1**, and **B2**)

Compound name	D-H…A	D-H / Å	H-A / Å	D-A / Å	∠D-H…A / °
1b•2O•2H_2O (A2)					
	N1-H3…O9	1.162	1.707	2.811	156.42
	N1-H5…O6	0.847	1.92	2.722	157.69
	N1-H4…O11	0.907	2.56	2.91	103.59
	N2-H8…O8	0.822	2.171	2.883	144.88
	N2-H9…O7	1.054	1.622	2.671	172.55
	N2-H10…O4	1.007	1.858	2.737	143.94
	O8-H2…O7	0.837	2.046	2.811	151.81
	O8-H1…O4	0.930	2.042	2.951	165.17
	O11-H15…O9	0.973	1.897	2.782	149.94
	O11-H16…O6	0.828	2.128	2.861	147.51
1o•2M•3H_2O (B1)					
	N1-H4…O5	0.882	1.905	2.749	159.78
	N1-H5…O2	0.891	1.878	2.757	168.69
	N1-H6…O3	1.019	1.733	2.728	164.36
	O2-H1…O6	0.851	1.816	2.649	165.93
	O6-H2…O3	0.813	1.994	2.758	156.11
	O6-H3…O5	0.858	1.922	2.759	165.06
1o•2O•3H_2O (B2)					
	N1-H13…O2	0.861	1.938	2.758	158.72
	N1-H14…O5	0.948	1.796	2.725	165.5
	N1-H15…O1	0.921	1.843	2.752	168.39
	O1-H16…O7	0.943	1.701	2.641	173.69
	O7-H17…O2	0.887	1.885	2.750	164.65
	O7-H18…O5	0.930	1.842	2.747	163.66

Table S3. Hydrogen bond metrics of the inclusion crystals (**C1**, **C2**, **D1**, and **D2**)

Compound name	D-H…A	D-H / Å	H-A / Å	D-A / Å	∠D-H…A / °
2(1m)•2M•2-BuOH (C1)					
	N1-H37…O7	1.059	1.601	2.635	164.04
	N1-H38…O5	0.846	2.014	2.848	168.45
	N1-H39…O3	0.948	1.833	2.778	174.21
	O4-H1…O4	0.840	1.745	2.475	143.98
	O6-H36…O6	0.840	1.632	2.420	155.16
1m•2O•2(2-BuOH)•H_2O (C2)					
	N1-H1…O6	1.057	1.771	2.828	179.21
	N1-H2…O4	0.882	1.941	2.737	149.39
	N1-H3…O10	0.846	1.997	2.797	157.26
	N2-H4…O11	0.908	1.811	2.716	174.68
	N2-H5…O4	0.911	1.844	2.753	176.54
	N2-H6…O10	0.91	2.15	2.806	128.32
1p•2M (D1)					
	N1-H11…O7	0.91	2.081	2.924	153.58
	N1-H12…O8	0.91	1.957	2.801	153.58
	N2-H18…O5	0.91	2.059	2.943	163.2
	N2-H19…O6	0.91	1.99	2.78	144.28
	O4-H12…O3	0.839	1.605	2.431	167.23
	N1-H10…N2	0.909	1.823	2.702	161.95
	N2-H20…N1	0.908	1.81	2.702	166.69
1p•2O•2(2-PenOH) (D2)					
	N1-H2…O1	0.995	1.793	2.703	150.31
	N1-H3…O8	0.932	1.9	2.803	162.58
	N1-H4…O10	0.98	1.885	2.735	143.43
	N2-H7…O1	1.032	1.683	2.712	174.79
	N2-H8…O10	1.033	1.972	2.82	137.38
	N2-H9…O11	1.033	1.702	2.719	167.25
	O8-H1…O6	1.049	1.764	2.792	165.73

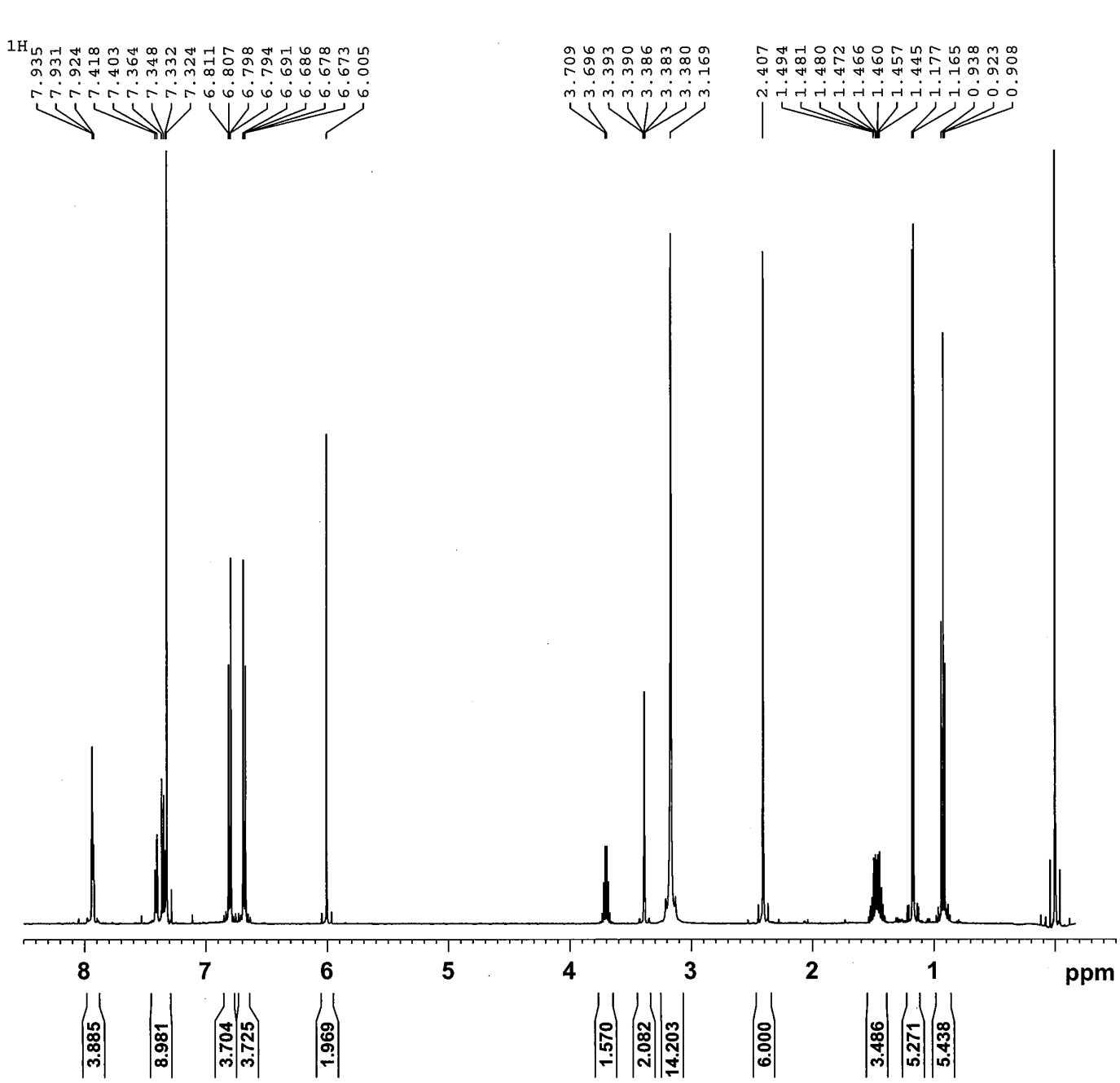

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Figure S1. ^{1}H NMR spectrum of **1m**·**2O** salt obtained from a 2-butanol solution.

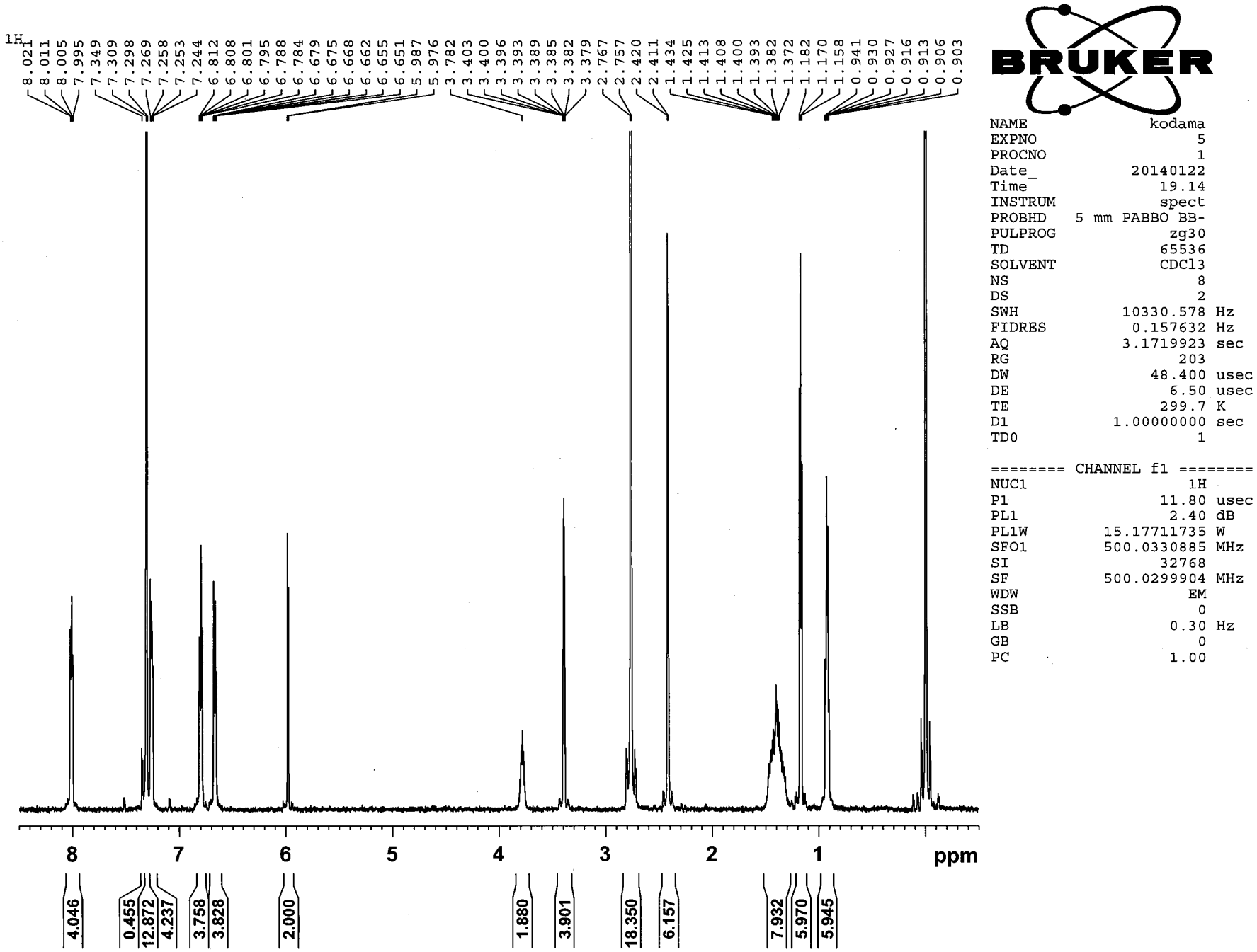

Figure S2. ^{1}H NMR spectrum of **1p**·**2O** salt obtained from a 2-pentanol solution.