## 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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	1b•2M•2-BuOH•2H <sub>2</sub> O (A1)	1b•2O•2H₂O (A2)	10•2M•3H₂O (B1)	10•20•3H <sub>2</sub> O (B2)
formula	C <sub>35</sub> H <sub>42</sub> N <sub>2</sub> O <sub>11</sub>	C <sub>30</sub> H <sub>30</sub> N <sub>2</sub> O <sub>11</sub>	C <sub>33</sub> H <sub>38</sub> N <sub>2</sub> O <sub>11</sub>	C <sub>32</sub> H <sub>36</sub> N <sub>2</sub> O <sub>12</sub>
	$(C_{10}H_{12}O_{0})^{2^{-}} \cdot (C_{12}H_{16}N_{2})^{2^{+}} \cdot$	$(C_{10}H_{12}O_{0})^{2^{-}} \cdot (C_{12}H_{14}N_{2}O)^{2^{+}}$	$(C_{20}H_{10}O_{0})^{2^{-}} \cdot (C_{12}H_{10}N_{2})^{2^{+}} \cdot$	$(C_{20}H_{16}O_{8})^{2^{-}}$
moiety formula	C.H., O • 2H.O	• 2H-O	3H-O	$(C_{1}, H_{1}, N_{2}, O)^{2+} \cdot 3H_{2}O$
E\\/	666 71	504 56	638.65	(0 <sub>12</sub> 11 <sub>14</sub> 11 <sub>2</sub> 0) - 511 <sub>2</sub> 0
temperature (K)	273	150	100	150
crystal size (mm)	$0.80 \times 0.20 \times 0.03$	$0.50 \times 0.15 \times 0.05$	$0.16 \times 0.14 \times 0.02$	$0.21 \times 0.20 \times 0.06$
crystal system	monoclinic	monoclinic	monoclinic	monoclinic
space group	P2,	P2.	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 <sup>3</sup> )	1766.7(11)	1439.7(5)	1640.9(6)	1634.2(5)
Z	2	2	2	2
Dc (q/cm <sup>3</sup> )	1.253	1.372	1.293	1.302
$\mu$ (Mo <sub>ko</sub> ) (mm <sup>-1</sup> )	0.093	0.106	0.097	0.100
$\theta_{\min/\max}(^{\circ})$	1.63/25.00	1.68/24.99	1.68/25.00	1.67/24.99
$R1[F_0 > 2\sigma(F_0)]$	0.0776	0.0459	0.0369	0.0280
$WR2$ (all $E_0^2$ )	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 refins	10015	8149	3416	3938
independent refins	5775	3930	1956	2652
observed refins	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 <sub>2</sub> O (C2)	1p•2M (D1)	1p•2O•2(2-PenOH) (D2)
formula	2(1m)•2M•2-BuOH (C1) C <sub>28.5</sub> H <sub>30</sub> NO <sub>8.5</sub>	<b>1m•2O•2(2-BuOH)•H</b> <sub>2</sub> <b>O (C2)</b> C <sub>40</sub> H <sub>52</sub> N <sub>2</sub> O <sub>12</sub>	<b>1p•2M (D1)</b> C <sub>33</sub> H <sub>32</sub> N <sub>2</sub> O <sub>8</sub>	<b>1p•2O•2(2-PenOH) (D2)</b> C <sub>42</sub> H <sub>54</sub> N <sub>2</sub> O <sub>11</sub>
formula	2(1m)•2M•2-BuOH (C1) C <sub>28.5</sub> H <sub>30</sub> NO <sub>8.5</sub>	<b>1m+2O+2(2-BuOH)+H</b> <sub>2</sub> O (C2) $C_{40}H_{52}N_2O_{12}$	<b>1р•2М (D1)</b> С <sub>33</sub> Н <sub>32</sub> N <sub>2</sub> O <sub>8</sub>	<b>1p•20•2(2-PenOH) (D2)</b> C <sub>42</sub> H <sub>54</sub> N <sub>2</sub> O <sub>11</sub> (C H N O) <sup>2+</sup> •
formula moiety formula	<b>2(1m)·2M·2-BuOH (C1)</b> $C_{28.5}H_{30}NO_{8.5}$ $(C_{20}H_{17}O_8)^{-} \cdot 0.5(C_{13}H_{16}N_2)^{2+}$ $\cdot 0.5(C_{14}H_{16}O_2)$	<b>1m•20•2(2-BuOH)•H</b> <sub>2</sub> O (C2) $C_{40}H_{52}N_2O_{12}$ $(C_{20}H_{16}O_8)^{2^-} \cdot (C_{12}H_{14}N_2O)^{2^+}$ • 2(C_4H_4O) • HaO	$\frac{1p \cdot 2M (D1)}{C_{33}H_{32}N_2O_8}$ $(C_{20}H_{17}O_8)^{-} \cdot (C_{13}H_{15}N_2)^{+}$	<b>1p-2O-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_{12}H_{14}O)$
formula moiety formula	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}\textbf{H}_{30}\textbf{NO}_{8.5} \\ \hline \textbf{(C}_{20}\textbf{H}_{17}\textbf{O}_{8})^{-} \bullet 0.5(\textbf{C}_{13}\textbf{H}_{16}\textbf{N}_{2})^{2+} \\ \bullet 0.5(\textbf{C}_{4}\textbf{H}_{10}\textbf{O}) \\ \hline \textbf{522.54} \end{array}$	<b>1m-20-2(2-BuOH)-H<sub>2</sub>O (C2)</b> $C_{40}H_{52}N_2O_{12}$ $(C_{20}H_{16}O_8)^{2^-} \cdot (C_{12}H_{14}N_2O)^{2^+}$ $\cdot 2(C_4H_{10}O) \cdot H_2O$ 752.84	$\frac{1p \cdot 2M (D1)}{C_{33}H_{32}N_2O_8}$ $(C_{20}H_{17}O_8)^{-} \cdot (C_{13}H_{15}N_2)^{+}$	<b>1p-20-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ 762.87
formula moiety formula FW	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline C_{28.5}H_{30}NO_{8.5} \\ \hline (C_{20}H_{17}O_8)^{\bullet} \cdot 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ \hline 522.54 \\ 150 \end{array}$	<b>1m-20-2(2-BuOH)+H<sub>2</sub>O (C2)</b> $C_{40}H_{52}N_2O_{12}$ $(C_{20}H_{16}O_8)^{2^-} \cdot (C_{12}H_{14}N_2O)^{2^+}$ $\cdot 2(C_4H_{10}O) \cdot H_2O$ 752.84 150	$\frac{1p \cdot 2M (D1)}{C_{33}H_{32}N_2O_8}$ $(C_{20}H_{17}O_8)^{-} \cdot (C_{13}H_{15}N_2)^{+}$ 584.60	$\begin{array}{c} \textbf{1p-2O-2(2-PenOH) (D2)} \\ C_{42}H_{54}N_2O_{11} \\ (C_{12}H_{14}N_2O)^{2+} \bullet \\ 2(C_5H_{12}O) \\ 762.87 \\ 150 \end{array}$
formula moiety formula FW temperature (K) crystal size (mm)	$2(1m) \cdot 2M \cdot 2-BuOH (C1)$ $C_{28.5}H_{30}NO_{8.5}$ $(C_{20}H_{17}O_8)^{-} \cdot 0.5(C_{13}H_{16}N_2)^{2+}$ $\cdot 0.5(C_4H_{10}O)$ $522.54$ $150$ $0.12 \times 0.08 \times 0.08$	<b>1m-20-2(2-BuOH)+H<sub>2</sub>O (C2)</b> $C_{40}H_{52}N_2O_{12}$ $(C_{20}H_{16}O_8)^{2-} \cdot (C_{12}H_{14}N_2O)^{2+}$ $\cdot 2(C_4H_{10}O) \cdot H_2O$ 752.84 150 $0.28 \times 0.10 \times 0.02$	$\frac{1p \cdot 2M (D1)}{C_{33}H_{32}N_2O_8}$ $(C_{20}H_{17}O_8)^{-} \cdot (C_{13}H_{15}N_2)^{+}$ 584.60 200 0.18 × 0.03 × 0.01	<b>1p-2O-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ 762.87 150 $0.25 \times 0.05 \times 0.02$
formula moiety formula FW temperature (K) crystal size (mm) crystal system	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}\textbf{H}_{30}\textbf{NO}_{8.5} \\ (\textbf{C}_{20}\textbf{H}_{17}\textbf{O}_{8})^{-} \bullet 0.5(\textbf{C}_{13}\textbf{H}_{16}\textbf{N}_{2})^{2+} \\ \bullet 0.5(\textbf{C}_{4}\textbf{H}_{10}\textbf{O}) \\ \hline \textbf{522.54} \\ \textbf{150} \\ 0.12 \times 0.08 \times 0.08 \\ \textbf{monoclinic} \end{array}$	$\begin{array}{c} \textbf{1m-2O-2(2-BuOH)-H}_2O\ (C2)\\ \hline C_{40}H_{52}N_2O_{12}\\ (C_{20}H_{16}O_8)^{2^-} \cdot (C_{12}H_{14}N_2O)^{2^+}\\ \cdot 2(C_4H_{10}O) \cdot H_2O\\ \hline 752.84\\ 150\\ 0.28 \times 0.10 \times 0.02\\ orthorhombic \end{array}$	$\begin{array}{c} \textbf{1p-2M (D1)} \\ C_{33}H_{32}N_2O_8 \\ (C_{20}H_{17}O_8)^{-} \cdot (C_{13}H_{15}N_2)^{+} \\ 584.60 \\ 200 \\ 0.18 \times 0.03 \times 0.01 \\ tetragonal \end{array}$	$\begin{array}{c} \textbf{1p-2O-2(2-PenOH) (D2)} \\ \hline C_{42}H_{54}N_2O_{11} \\ \hline (C_{12}H_{14}N_2O)^{2+} \bullet \\ 2(C_5H_{12}O) \\ \hline 762.87 \\ \hline 150 \\ \hline 0.25 \times 0.05 \times 0.02 \\ \hline \text{orthorhombic} \end{array}$
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}\textbf{H}_{30}\textbf{NO}_{8.5} \\ (\textbf{C}_{20}\textbf{H}_{17}\textbf{O}_{8})^{-} \bullet 0.5(\textbf{C}_{13}\textbf{H}_{16}\textbf{N}_{2})^{2+} \\ \bullet 0.5(\textbf{C}_{4}\textbf{H}_{10}\textbf{O}) \\ \hline \textbf{522.54} \\ \textbf{150} \\ 0.12 \times 0.08 \times 0.08 \\ \textbf{monoclinic} \\ \textbf{C2} \end{array}$	$\frac{1 \text{m} \cdot 20 \cdot 2(2 \cdot BuOH) \cdot H_2 O (C2)}{C_{40} H_{52} N_2 O_{12}}$ $(C_{20} H_{16} O_8)^{2-} \cdot (C_{12} H_{14} N_2 O)^{2+}$ $\cdot 2(C_4 H_{10} O) \cdot H_2 O$ $752.84$ $150$ $0.28 \times 0.10 \times 0.02$ orthorhombic $P_{2-2,2} A$	$\begin{array}{c} \textbf{1p-2M (D1)} \\ C_{33}H_{32}N_2O_8 \\ (C_{20}H_{17}O_8)^{-} \cdot (C_{13}H_{15}N_2)^{+} \\ 584.60 \\ 200 \\ 0.18 \times 0.03 \times 0.01 \\ tetragonal \\ 14_4 \end{array}$	$\begin{array}{c} \textbf{1p-20-2(2-PenOH) (D2)} \\ \hline C_{42}H_{54}N_2O_{11} \\ \hline (C_{12}H_{14}N_2O)^{2+} \\ 2(C_5H_{12}O) \\ \hline 762.87 \\ \hline 150 \\ 0.25 \times 0.05 \times 0.02 \\ \hline orthorhombic \\ \hline P_{2,2,2,4} \end{array}$
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å)	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}\textbf{H}_{30}\textbf{NO}_{8.5} \\ (\textbf{C}_{20}\textbf{H}_{17}\textbf{O}_{8})^{-} \bullet 0.5(\textbf{C}_{13}\textbf{H}_{16}\textbf{N}_{2})^{2+} \\ \bullet 0.5(\textbf{C}_{4}\textbf{H}_{10}\textbf{O}) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ \text{monoclinic} \\ \hline \textbf{C2} \\ 16.286(7) \\ \end{array}$	<b>1m-20-2(2-BuOH)+H</b> <sub>2</sub> O (C2) $C_{40}H_{52}N_2O_{12}$ $(C_{20}H_{16}O_8)^{2-} \cdot (C_{12}H_{14}N_2O)^{2+}$ $\cdot 2(C_4H_{10}O) \cdot H_2O$ 752.84 150 $0.28 \times 0.10 \times 0.02$ orthorhombic $P_{2_12_12_1}$ 7 7019(13)	<b>1p-2M (D1)</b> $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60 200 0.18 × 0.03 × 0.01 tetragonal <i>I</i> 4 <sub>1</sub> 28.639(5)	<b>1p-2O-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ 762.87           150 $0.25 \times 0.05 \times 0.02$ orthorhombic $P2_{12}I_{2}I$ 7           7           7
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å)	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ (C_{20}H_{17}O_8)^{-} \bullet 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ monoclinic \\ \hline \textbf{C2} \\ 16.286(7) \\ 22.708(9) \end{array}$	$\frac{1 \text{m} \cdot 20 \cdot 2(2 \cdot BuOH) \cdot H_2 O (C2)}{C_{40} \text{H}_{52} \text{N}_2 \text{O}_{12}}$ $(C_{20} \text{H}_{16} \text{O}_8)^{2^-} \cdot (C_{12} \text{H}_{14} \text{N}_2 \text{O})^{2^+}$ $\cdot 2(C_4 \text{H}_{10} \text{O}) \cdot \text{H}_2 \text{O}$ $752.84$ $150$ $0.28 \times 0.10 \times 0.02$ orthorhombic $P2_1 2_1 2_1$ $7.7919(13)$ $21.208(4)$	1p•2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $I4_1$ 28.639(5)           28.639(5)	<b>1p-2O-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ 762.87           150 $0.25 \times 0.05 \times 0.02$ orthorhombic $P2_{12}1_{21}$ 7.7836(8)           22 234(2)
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å)	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ \hline (\textbf{C}_{20}H_{17}O_8)^{-} \bullet 0.5(\textbf{C}_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(\textbf{C}_4H_{10}\textbf{O}) \\ \hline \textbf{522.54} \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ \hline \textbf{monoclinic} \\ \hline \textbf{C2} \\ \hline \textbf{16.286(7)} \\ \textbf{22.708(9)} \\ \hline \textbf{7.950(3)} \end{array}$	$\frac{1 \text{m} \cdot 20 \cdot 2(2 \cdot BuOH) \cdot H_2 O (C2)}{C_{40} H_{52} N_2 O_{12}}$ $(C_{20} H_{16} O_8)^{2^-} \cdot (C_{12} H_{14} N_2 O)^{2^+}$ $\cdot 2(C_4 H_{10} O) \cdot H_2 O$ $752.84$ $150$ $0.28 \times 0.10 \times 0.02$ orthorhombic $P2_1 2_1 2_1$ $7.7919(13)$ $21.208(4)$ $24.416(4)$	1p•2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal           14_1           28.639(5)           28.639(5)           28.639(5)           7.8757(15)	<b>1p-2O-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ 762.87           150 $0.25 \times 0.05 \times 0.02$ orthorhombic $P2_12_12_1$ 7.7836(8)           22.234(2)           24.890(3)
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) c (Å) α (°)	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ (C_{20}H_{17}O_8)^{-} \bullet 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ monoclinic \\ C2 \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \end{array}$	$\begin{array}{c} \textbf{1m-20-2(2-BuOH)+H}_2O\ (C2)\\ \hline \textbf{C}_{40}\textbf{H}_{52}\textbf{N}_2O_{12}\\ \hline \textbf{(C}_{20}\textbf{H}_{16}O_8)^{2^-} \cdot \textbf{(C}_{12}\textbf{H}_{14}\textbf{N}_2O)^{2^+}\\ \cdot 2(\textbf{C}_4\textbf{H}_{10}O) \cdot \textbf{H}_2O\\ \hline \textbf{752.84}\\ \textbf{150}\\ 0.28\times0.10\times0.02\\ orthorhombic\\ P2_12_12_1\\ \textbf{7.7919}(13)\\ \textbf{21.208}(4)\\ \textbf{24.416}(4)\\ \textbf{90} \end{array}$	1p•2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $I4_1$ 28.639(5)           28.639(5)           28.639(5)           90	$\begin{array}{c} \textbf{1p-20-2(2-PenOH) (D2)} \\ \hline C_{42}H_{54}N_2O_{11} \\ \hline (C_{12}H_{14}N_2O)^{2+} \bullet \\ 2(C_5H_{12}O) \\ \hline 762.87 \\ 150 \\ 0.25 \times 0.05 \times 0.02 \\ orthorhombic \\ \hline P_{21}2_{12} \\ 7.7836(8) \\ 22.234(2) \\ 24.890(3) \\ 90 \end{array}$
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) c (Å) α (°) β (°)	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ \hline (C_{20}H_{17}O_8)^{-} \bullet 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ \hline \textbf{monoclinic} \\ \hline \textbf{C2} \\ 16.286(7) \\ 22.708(9) \\ \hline \textbf{7.950(3)} \\ \textbf{90} \\ 115.707(5) \end{array}$	$\frac{1 \text{m} \cdot 20 \cdot 2(2 \cdot BuOH) \cdot H_2 O (C2)}{C_{40} H_{52} N_2 O_{12}}$ $(C_{20} H_{16} O_8)^{2-} \cdot (C_{12} H_{14} N_2 O)^{2+}$ $\cdot 2(C_4 H_{10} O) \cdot H_2 O$ $752.84$ $150$ $0.28 \times 0.10 \times 0.02$ orthorhombic $P2_1 2_1 2_1$ $7.7919(13)$ $21.208(4)$ $24.416(4)$ $90$ $90$	1p•2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal           14_1           28.639(5)           28.639(5)           28.639(5)           90	$\begin{array}{c} \textbf{1p-20-2(2-PenOH) (D2)} \\ \hline C_{42}H_{54}N_2O_{11} \\ \hline (C_{12}H_{14}N_2O)^{2+} \bullet \\ 2(C_5H_{12}O) \\ \hline 762.87 \\ 150 \\ 0.25 \times 0.05 \times 0.02 \\ \hline orthorhombic \\ P2_{1}2_{1}2_{1} \\ \hline 7.7836(8) \\ 22.234(2) \\ 24.890(3) \\ 90 \\ 90 \end{array}$
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) $\alpha$ (°) $\beta$ (°) $\gamma$ (°)	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ (C_{20}H_{17}O_8)^{-} \bullet 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ monoclinic \\ \hline \textbf{C2} \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ \end{array}$	$\begin{array}{c} \textbf{1m-2O-2(2-BuOH)-H}_2O\ (C2)\\ \hline \textbf{C}_{40}\textbf{H}_{52}\textbf{N}_2O_{12}\\ \hline \textbf{(C}_{20}\textbf{H}_{16}O_8)^{2^-} \cdot \textbf{(C}_{12}\textbf{H}_{14}\textbf{N}_2O)^{2^+}\\ \cdot 2(\textbf{C}_4\textbf{H}_{10}O) \cdot \textbf{H}_2O\\ \hline \textbf{752.84}\\ \textbf{150}\\ 0.28\times0.10\times0.02\\ \hline \textbf{orthorhombic}\\ P2_12_12_1\\ \textbf{7.7919}(13)\\ \textbf{21.208}(4)\\ \textbf{24.416}(4)\\ \textbf{90}\\ \textbf{90}\\ \textbf{90}\\ \textbf{90}\\ \textbf{90} \end{array}$	1p•2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           90           90	$\begin{array}{c} \textbf{1p-20-2(2-PenOH) (D2)} \\ \hline C_{42}H_{54}N_2O_{11} \\ \hline (C_{12}H_{14}N_2O)^{2+} \bullet \\ 2(C_5H_{12}O) \\ \hline 762.87 \\ 150 \\ 0.25 \times 0.05 \times 0.02 \\ \hline 0.25 \times 0.02 \\ \hline 0.2$
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) $\alpha$ (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> )	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ \hline (C_{20}H_{17}O_8)^{-} \bullet 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ \hline \textbf{monoclinic} \\ \hline \textbf{C2} \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ 2649.2(19) \\ \end{array}$	$\frac{1 \text{m} \cdot 20 \cdot 2(2 - \text{BuOH}) \cdot \text{H}_2 \text{O} (\text{C2})}{\text{C}_{40} \text{H}_{52} \text{N}_2 \text{O}_{12}}$ $(\text{C}_{20} \text{H}_{16} \text{O}_8)^{2^-} \cdot (\text{C}_{12} \text{H}_{14} \text{N}_2 \text{O})^{2^+}$ $\cdot 2(\text{C}_4 \text{H}_{10} \text{O}) \cdot \text{H}_2 \text{O}$ $752.84$ $150$ $0.28 \times 0.10 \times 0.02$ orthorhombic $P2_1 2_1 2_1$ $7.7919(13)$ $21.208(4)$ $24.416(4)$ $90$ $90$ $90$ $90$ $4034.7(12)$	1p•2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           90           90           90           90           6460(3)	<b>1p-2O-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ 762.87           150 $0.25 \times 0.05 \times 0.02$ orthorhombic $P2_{12}1_{21}$ 7.7836(8)           22.234(2)           24.890(3)           90           90           90           90           90           90           90           90           90
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) $\alpha$ (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> ) Z	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ (C_{20}H_{17}O_8)^- \bullet 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ monoclinic \\ \hline \textbf{C2} \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ 2649.2(19) \\ 4 \end{array}$	$\frac{1 \text{m} \cdot 20 \cdot 2(2 \cdot BuOH) \cdot H_2 O (C2)}{C_{40} H_{52} N_2 O_{12}}$ $(C_{20} H_{16} O_8)^{2-} \cdot (C_{12} H_{14} N_2 O)^{2+}$ $\cdot 2(C_4 H_{10} O) \cdot H_2 O$ $752.84$ $150$ $0.28 \times 0.10 \times 0.02$ orthorhombic $P2_1 2_1 2_1$ $7.7919(13)$ $21.208(4)$ $24.416(4)$ $90$ $90$ $90$ $4034.7(12)$ $4$	1p•2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           7.8757(15)           90           90           90           6460(3)           8	$\begin{array}{c} \textbf{1p-20-2(2-PenOH) (D2)} \\ \hline C_{42}H_{54}N_2O_{11} \\ \hline (C_{12}H_{14}N_2O)^{2+} \bullet \\ 2(C_5H_{12}O) \\ \hline 762.87 \\ 150 \\ 0.25 \times 0.05 \times 0.02 \\ \hline orthorhombic \\ \hline P_{21}2_{12}2_{1} \\ \hline 7.7836(8) \\ 22.234(2) \\ 24.890(3) \\ 90 \\ 90 \\ 90 \\ 90 \\ 90 \\ 4307.5(8) \\ 4 \end{array}$
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) $\alpha$ (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> ) Z Dc (g/cm <sup>3</sup> )	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ \hline (C_{20}H_{17}O_8)^- \bullet 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ \hline monoclinic \\ \hline \textbf{C2} \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ 2649.2(19) \\ 4 \\ 1.310 \\ \end{array}$	$\frac{1 \text{m} \cdot 20 \cdot 2(2 - \text{BuOH}) \cdot \text{H}_2 \text{O} (\text{C2})}{\text{C}_{40} \text{H}_{52} \text{N}_2 \text{O}_{12}}$ $(\text{C}_{20} \text{H}_{16} \text{O}_8)^{2^-} \cdot (\text{C}_{12} \text{H}_{14} \text{N}_2 \text{O})^{2^+}$ $\cdot 2(\text{C}_4 \text{H}_{10} \text{O}) \cdot \text{H}_2 \text{O}$ $752.84$ $150$ $0.28 \times 0.10 \times 0.02$ orthorhombic $P2_1 2_1 2_1$ $7.7919(13)$ $21.208(4)$ $24.416(4)$ $90$ $90$ $90$ $4034.7(12)$ $4$ $1.239$	1p•2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           7.8757(15)           90           90           6460(3)           8           1.202	<b>1p-2O-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ 762.87           150 $0.25 \times 0.05 \times 0.02$ orthorhombic $P2_{12}1_{21}$ 7.7836(8)           22.234(2)           24.890(3)           90           90           4           1.176
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a $(Å)$ b $(Å)$ c $(Å)$ a $(°)$ $\beta$ $(°)$ $\gamma$ $(°)$ V $(Å^3)$ Z Dc $(g/cm^3)$ $\mu$ $(Mo_{K_2})$	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ \hline (C_{20}H_{17}O_8)^- \bullet 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ \hline monoclinic \\ \hline \textbf{C2} \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ 2649.2(19) \\ 4 \\ 1.310 \\ 0.097 \\ \end{array}$	$\frac{1 \text{m} \cdot 20 \cdot 2(2 - \text{BuOH}) \cdot \text{H}_2 \text{O} (\text{C2})}{\text{C}_{40} \text{H}_{52} \text{N}_2 \text{O}_{12}}$ $(\text{C}_{20} \text{H}_{16} \text{O}_8)^{2^-} \cdot (\text{C}_{12} \text{H}_{14} \text{N}_2 \text{O})^{2^+}$ $\cdot 2(\text{C}_4 \text{H}_{10} \text{O}) \cdot \text{H}_2 \text{O}$ $752.84$ $150$ $0.28 \times 0.10 \times 0.02$ orthorhombic $P2_1 2_1 2_1$ $7.7919(13)$ $21.208(4)$ $24.416(4)$ $90$ $90$ $90$ $4034.7(12)$ $4$ $1.239$ $0.091$	1p•2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           7.8757(15)           90           90           6460(3)           8           1.202           0.087	<b>1p-20-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ 762.87           150 $0.25 \times 0.05 \times 0.02$ orthorhombic $P2_{12}_{12}_{1}$ 7.7836(8)           22.234(2)           24.890(3)           90           90           4           1.176           0.085
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) $\alpha$ (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> ) Z Dc (g/cm <sup>3</sup> ) $\mu$ (Mo <sub>Ka</sub> ) $\theta$ min/max (°)	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ \hline (C_{20}H_{17}O_8)^- \bullet 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ \hline \textbf{monoclinic} \\ \hline \textbf{C2} \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ 2649.2(19) \\ 4 \\ 1.310 \\ 0.097 \\ 1.65/25.00 \\ \end{array}$	$\begin{array}{c} \textbf{1m-2O-2(2-BuOH)-H}_2O\ (C2)\\ \hline \textbf{C}_{40}\textbf{H}_{52}\textbf{N}_2O_{12}\\ \hline \textbf{(C}_{20}\textbf{H}_{16}O_8)^{2^-} \cdot \textbf{(C}_{12}\textbf{H}_{14}\textbf{N}_2O)^{2^+}\\ \bullet\ 2(\textbf{C}_4\textbf{H}_{10}O) \bullet\ \textbf{H}_2O\\ \hline \textbf{752.84}\\ 150\\ 0.28\times0.10\times0.02\\ orthorhombic\\ P2_12_12_1\\ \hline \textbf{7.7919}(13)\\ 21.208(4)\\ 24.416(4)\\ 90\\ 90\\ 90\\ 90\\ 90\\ 4034.7(12)\\ 4\\ 1.239\\ 0.091\\ 1.27/25.00\\ \end{array}$	Ip•2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $I4_1$ 28.639(5)           28.639(5)           28.639(5)           90           90           9460(3)           8           1.202           0.087           1.005/25.00	$\begin{array}{c} \textbf{1p-20-2(2-PenOH) (D2)} \\ \hline C_{42}H_{54}N_2O_{11} \\ \hline (C_{12}H_{14}N_2O)^{2+} \bullet \\ 2(C_5H_{12}O) \\ \hline 762.87 \\ \hline 150 \\ 0.25 \times 0.05 \times 0.02 \\ \hline orthorhombic \\ \hline P_{21}2_{12} \\ \hline 7.7836(8) \\ 22.234(2) \\ 24.890(3) \\ 90 \\ 90 \\ 90 \\ 90 \\ 90 \\ 90 \\ 90 \\ 9$
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) a (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> ) Z Dc (g/cm <sup>3</sup> ) $\mu$ (Mo <sub>Ka</sub> ) $\theta_{min/max}$ (°) R1 [ $F_0 > 2\sigma(F_0)$ ]	$\begin{array}{c} 2(1m) \cdot 2M \cdot 2 \cdot BuOH (C1) \\ \hline 2_{28.5}H_{30}NO_{8.5} \\ (C_{20}H_{17}O_8)^{-} \cdot 0.5(C_{13}H_{16}N_2)^{2+} \\ \cdot 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ monoclinic \\ \hline C2 \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ 2649.2(19) \\ 4 \\ 1.310 \\ 0.097 \\ 1.65/25.00 \\ 0.0667 \\ \end{array}$	$\begin{array}{c} \mbox{1m*2O*2(2-BuOH)*H}_2O (C2) \\ \mbox{C}_{40}\mbox{H}_{52}\mbox{N}_2O_{12} \\ \mbox{(}C_{20}\mbox{H}_{16}\mbox{O}_8\mbox{)}^{2^+} \cdot (\mbox{C}_{12}\mbox{H}_{14}\mbox{N}_2O\mbox{)}^{2^+} \\ \cdot 2(\mbox{C}_4\mbox{H}_{10}\mbox{O}) \cdot \mbox{H}_2O \\ \mbox{752.84} \\ \mbox{150} \\ \mbox{0.28} \times 0.10 \times 0.02 \\ \mbox{orthorhombic} \\ \mbox{P}_{21}\mbox{2}_1\mbox{2}_1 \\ \mbox{Orthorhombic} \\ \mbox{P}_{21}\mbox{2}_1\mbox{2}_1\mbox{2}_1 \\ \mbox{Orthorhombic} \\ \mbox{P}_{21}\mbox{2}_1\mbox{2}_1 \\ \mbox{Orthorhombic} \\ \mbox{P}_{21}\mbox{2}_1\mbox{2}_1 \\ \mbox{Orthorhombic} \\ \mbox{P}_{21}\mbox{2}_1\mbox{2}_1\mbox{2}_1\mbox{2}_1\mbox{2}_1 \\ \mbox{Orthorhombic} \\ \mbox{P}_{21}\mbox{2}_1\mbox{2}_$	Ip•2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $I4_1$ 28.639(5)           28.639(5)           28.639(5)           90           91           92           93	$1p \cdot 20 \cdot 2(2 \cdot PenOH) (D2)$ $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ $762.87$ $150$ $0.25 \times 0.05 \times 0.02$ orthorhombic $P2_{12}1_{21}$ $7.7836(8)$ $22.234(2)$ $24.890(3)$ $90$ <
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) a (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> ) Z Dc (g/cm <sup>3</sup> ) $\mu$ (Mo <sub>Ka</sub> ) $\theta_{min/max}$ (°) R1 [ $F_0 > 2\sigma(F_0)$ ] wR2 (all $F_0^2$ )	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ \hline (C_{20}H_{17}O_8)^{-} \bullet 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ \hline monoclinic \\ \hline \textbf{C2} \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ 2649.2(19) \\ 4 \\ 1.310 \\ 0.097 \\ 1.65/25.00 \\ 0.0667 \\ 0.1704 \\ \end{array}$	$\begin{array}{c} \medskip \\ \hline \medskip \\ $	1p-2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           90           91           92           <	$\begin{array}{c} \textbf{1p-20-2(2-PenOH) (D2)} \\ \hline C_{42}H_{54}N_2O_{11} \\ \hline (C_{12}H_{14}N_2O)^{2+} \bullet \\ 2(C_5H_{12}O) \\ \hline 762.87 \\ 150 \\ 0.25 \times 0.05 \times 0.02 \\ 0 \\ 0.25 \times 0.05 \times 0.02 \\ 0 \\ 0.25 \times 0.05 \times 0.02 \\ 0 \\ 0.25 \times 0.05 \times 0.02 \\ 0.25 \times 0.05 \\ 0.05 \times 0.02 \\ 0.05 \times 0.02 \\ 0.07 \\ 150 \\ 0.085 \\ 1.23/25.00 \\ 0.0719 \\ 0.1966 \\ \end{array}$
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) a (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> ) Z Dc (g/cm <sup>3</sup> ) $\mu$ (Mo <sub>Ka</sub> ) $\theta_{min/max}$ (°) R1 [ $F_0 > 2\sigma(F_0)$ ] $wR2$ (all $F_0^2$ ) GOF	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ \hline (C_{20}H_{17}O_8)^{-} \bullet 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ \hline monoclinic \\ \hline \textbf{C2} \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ 2649.2(19) \\ 4 \\ 1.310 \\ 0.097 \\ 1.65/25.00 \\ 0.0667 \\ 0.1704 \\ 1.038 \\ \end{array}$	$\begin{array}{c} \hline \mathbf{1m} \mathbf{*20} \mathbf{*2(2-BuOH)} \mathbf{*H}_2 O (\mathbf{C2}) \\ \hline \mathbf{C}_{40} \mathbf{H}_{52} \mathbf{N}_2 O_{12} \\ \hline (\mathbf{C}_{20} \mathbf{H}_{16} \mathbf{O}_8)^{2^-} \mathbf{*} (\mathbf{C}_{12} \mathbf{H}_{14} \mathbf{N}_2 \mathbf{O})^{2^+} \\ \mathbf{*2(C_4} \mathbf{H}_{10} \mathbf{O}) \mathbf{*H}_2 \mathbf{O} \\ \hline 752.84 \\ \hline 150 \\ 0.28 \times 0.10 \times 0.02 \\ orthorhombic \\ \hline P2_1 2_1 2_1 \\ 7.7919 (13) \\ 21.208 (4) \\ 24.416 (4) \\ 90 \\ 90 \\ 90 \\ 90 \\ 90 \\ 90 \\ 4034.7 (12) \\ 4 \\ 1.239 \\ 0.091 \\ 1.27 / 25.00 \\ 0.0853 \\ 0.2202 \\ 1.033 \\ \end{array}$	1p-2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           90           91	<b>1p-2O-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ 762.87           150 $0.25 \times 0.05 \times 0.02$ orthorhombic $P2_{12}1_{21}$ 7.7836(8)           22.234(2)           24.890(3)           90<
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) a (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> ) Z Dc (g/cm <sup>3</sup> ) $\mu$ (Mo <sub>Ka</sub> ) $\theta_{min/max}$ (°) R1 [ $F_0 > 2\sigma(F_0)$ ] $wR2$ (all $F_0^2$ ) GOF Flack parameter	$\begin{array}{c} 2(1m) \cdot 2M \cdot 2 \cdot BuOH (C1) \\ \hline 2_{28.5}H_{30}NO_{8.5} \\ (C_{20}H_{17}O_8)^{-} \cdot 0.5(C_{13}H_{16}N_2)^{2+} \\ \cdot 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ monoclinic \\ \hline C2 \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ 2649.2(19) \\ 4 \\ 1.310 \\ 0.097 \\ 1.65/25.00 \\ 0.0667 \\ 0.1704 \\ 1.038 \\ -1.3(10) \\ \end{array}$	$\begin{array}{c} \hline \mathbf{1m} \mathbf{*20} \mathbf{*2(2-BuOH)} \mathbf{*H}_2 O (\mathbf{C2}) \\ \hline \mathbf{C}_{40} \mathbf{H}_{52} \mathbf{N}_2 O_{12} \\ \hline (\mathbf{C}_{20} \mathbf{H}_{16} \mathbf{O}_8)^{2^+} \mathbf{\cdot} (\mathbf{C}_{12} \mathbf{H}_{14} \mathbf{N}_2 \mathbf{O})^{2^+} \\ \mathbf{*2(C_4} \mathbf{H}_{10} \mathbf{O}) \mathbf{*H}_2 \mathbf{O} \\ \hline 752.84 \\ 150 \\ \hline 0.28 \times 0.10 \times 0.02 \\ \hline 0.760 \mathbf{r} \mathbf{thorhombic} \\ \hline \mathbf{P}_{2,1} 2_{1} \mathbf{C} \\ \hline 7.7919 (13) \\ 21.208 (4) \\ 24.416 (4) \\ 90 \\ 90 \\ 90 \\ 90 \\ 90 \\ 4034.7 (12) \\ 4 \\ 1.239 \\ 0.091 \\ 1.27 / 25.00 \\ 0.0853 \\ 0.2202 \\ 1.033 \\ 1.0 (10) \\ \end{array}$	1p-2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           7.8757(15)           90           91           1.202           0.087           1.005/25.00           0.0547           0.1313           0.910           -2.6(10)	$\begin{array}{c} \textbf{1p-20-2(2-PenOH) (D2)} \\ \hline C_{42}H_{54}N_2O_{11} \\ \hline (C_{12}H_{14}N_2O)^{2+} \bullet \\ 2(C_5H_{12}O) \\ 762.87 \\ 150 \\ 0.25 \times 0.05 \times 0.02 \\ 0.762.87 \\ 150 \\ 0.25 \times 0.05 \times 0.02 \\ 0.762.87 \\ 150 \\ 0.25 \times 0.05 \times 0.02 \\ 0.071 \\ 0.085 \\ 1.23/25.00 \\ 0.0719 \\ 0.1966 \\ 1.028 \\ -0.8(7) \\ \end{array}$
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) a (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> ) Z Dc (g/cm <sup>3</sup> ) $\mu$ (Mo <sub>Ka</sub> ) $\theta_{min/max}$ (°) R1 [ $F_0 > 2\sigma(F_0)$ ] wR2 (all $F_0^2$ ) GOF Flack parameter measured refins	$\begin{array}{c} 2(1m) \cdot 2M \cdot 2 \cdot BuOH (C1) \\ \hline 2_{28.5}H_{30}NO_{8.5} \\ (C_{20}H_{17}O_8)^{-} \cdot 0.5(C_{13}H_{16}N_2)^{2+} \\ \cdot 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ monoclinic \\ \hline C2 \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ 2649.2(19) \\ 4 \\ 1.310 \\ 0.097 \\ 1.65/25.00 \\ 0.0667 \\ 0.1704 \\ 1.038 \\ -1.3(10) \\ 6331 \\ \end{array}$	$\begin{tabular}{ c c c c c } \hline $\mathbf{1m}$-2O$-2(2-BuOH)$+$H_2O$ (C2) \\ \hline $C_{40}$H_{52}$N_2O_{12}$ \\ \hline $(C_{20}$H_{16}O_8$)^{2-}$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$	1p-2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           28.639(5)           90           91           1.202           0.087           1.005/25.00           0.0547           0.1313           0.910           -2.6(10)           15524	<b>1p-2O-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ 762.87           150 $0.25 \times 0.05 \times 0.02$ orthorhombic $P2_{12}1_{21}$ 7.7836(8)           22.234(2)           24.890(3)           90           91           92           90           90           90           90           90           90           91           92           93<
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) a (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> ) Z Dc (g/cm <sup>3</sup> ) $\mu$ (Mo <sub>Ka</sub> ) $\theta_{min/max}$ (°) R1 [ $F_0 > 2\sigma(F_0)$ ] wR2 (all $F_0^2$ ) GOF Flack parameter measured reflns independent reflns	$\begin{array}{c} 2(1m) \cdot 2M \cdot 2 \cdot BuOH (C1) \\ \hline C_{28.5}H_{30}NO_{8.5} \\ (C_{20}H_{17}O_8)^{-} \cdot 0.5(C_{13}H_{16}N_2)^{2+} \\ \cdot 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ monoclinic \\ \hline C2 \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ 2649.2(19) \\ 4 \\ 1.310 \\ 0.097 \\ 1.65/25.00 \\ 0.0667 \\ 0.1704 \\ 1.038 \\ -1.3(10) \\ 6331 \\ 4317 \\ \end{array}$	$\begin{array}{c} \medskip \\ \med$	1p-2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           28.639(5)           7.8757(15)           90           90           6460(3)           8           1.202           0.087           1.005/25.00           0.0547           0.1313           0.910           -2.6(10)           15524           5607	$\begin{array}{c} \textbf{1p-20-2(2-PenOH) (D2)} \\ \hline C_{42}H_{54}N_2O_{11} \\ \hline (C_{12}H_{14}N_2O)^{2+} \bullet \\ 2(C_5H_{12}O) \\ \hline 762.87 \\ 150 \\ 0.25 \times 0.05 \times 0.02 \\ \hline 0.25 \times 0.05 \times 0.02 \\ \hline 0.767 \\ 0.25 \times 0.05 \times 0.02 \\ \hline 0.0719 \\ \hline 0.1966 \\ 1.028 \\ -0.8(7) \\ 20564 \\ \hline 7561 \\ \hline 0.0719 \\ \hline 0.0719 \\ \hline 0.0751 \\ \hline $
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) a (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> ) Z Dc (g/cm <sup>3</sup> ) $\mu$ (Mo <sub>Ka</sub> ) $\theta_{min/max}$ (°) R1 [ $F_0 > 2\sigma(F_0)$ ] wR2 (all $F_0^2$ ) GOF Flack parameter measured refins independent refins observed refins	$\begin{array}{ c c c c c } \hline 2(1m) \cdot 2M \cdot 2 \cdot BuOH (C1) \\ \hline C_{28.5}H_{30}NO_{8.5} \\ \hline (C_{20}H_{17}O_8)^{-} \cdot 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ \hline 522.54 \\ \hline 150 \\ \hline 0.12 \times 0.08 \times 0.08 \\ \hline monoclinic \\ \hline C2 \\ \hline 16.286(7) \\ \hline 22.708(9) \\ \hline 7.950(3) \\ 90 \\ \hline 115.707(5) \\ 90 \\ \hline 2649.2(19) \\ 4 \\ \hline 1.310 \\ \hline 0.097 \\ \hline 1.65/25.00 \\ \hline 0.0667 \\ \hline 0.1704 \\ \hline 1.038 \\ -1.3(10) \\ \hline 6331 \\ \hline 4317 \\ \hline 3460 \\ \hline \end{array}$	$\begin{array}{c} \medskip \\ \hline \begin{tabular}{lllllllllllllllllllllllllllllllllll$	1p-2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           28.639(5)           7.8757(15)           90           90           6460(3)           8           1.202           0.087           1.005/25.00           0.0547           0.1313           0.910           -2.6(10)           15524           5607           3031	$\begin{array}{c} \textbf{1p-20-2(2-PenOH) (D2)} \\ \hline C_{42}H_{54}N_2O_{11} \\ \hline (C_{12}H_{14}N_2O)^{2+} \bullet \\ 2(C_5H_{12}O) \\ \hline 762.87 \\ 150 \\ 0.25 \times 0.05 \times 0.02 \\ \hline 0rthorhombic \\ \hline P_{21}2_{12} \\ 0.25 \times 0.05 \times 0.02 \\ \hline 0rthorhombic \\ \hline P_{21}2_{12} \\ 1.7836(8) \\ 22.234(2) \\ 24.890(3) \\ 90 \\ 90 \\ 90 \\ 90 \\ 90 \\ 90 \\ 90 \\ 9$
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) a (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> ) Z Dc (g/cm <sup>3</sup> ) $\mu$ (Mo <sub>Ka</sub> ) $\theta_{min/max}$ (°) R1 [ $F_0 > 2\sigma(F_0)$ ] wR2 (all $F_0^2$ ) GOF Flack parameter measured refins independent refins observed refins refins used	$\begin{array}{ c c c c c } \hline 2(1m) \cdot 2M \cdot 2 \cdot BuOH (C1) \\ \hline C_{28.5}H_{30}NO_{8.5} \\ \hline (C_{20}H_{17}O_8)^{-} \cdot 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ \hline 522.54 \\ \hline 150 \\ \hline 0.12 \times 0.08 \times 0.08 \\ \hline monoclinic \\ \hline C2 \\ \hline 16.286(7) \\ \hline 22.708(9) \\ \hline 7.950(3) \\ 90 \\ \hline 115.707(5) \\ 90 \\ \hline 2649.2(19) \\ \hline 4 \\ \hline 1.310 \\ \hline 0.097 \\ \hline 1.65/25.00 \\ \hline 0.0667 \\ \hline 0.1704 \\ \hline 1.038 \\ -1.3(10) \\ \hline 6331 \\ \hline 4317 \\ \hline 3460 \\ \hline 4317 \\ \hline \end{array}$	$\begin{array}{c} \medskip \\ \hline \begin{tabular}{lllllllllllllllllllllllllllllllllll$	1p-2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           28.639(5)           7.8757(15)           90           90           6460(3)           8           1.202           0.087           1.005/25.00           0.0547           0.1313           0.910           -2.6(10)           15524           5607           3031           5607	<b>1p-2O-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ 762.87           150 $0.25 \times 0.05 \times 0.02$ orthorhombic $P2_{12}_{12}_{1}$ 7.7836(8)           22.234(2)           24.890(3)           90           91           92           93           94           1.176           0.0719           0.1966           1.028           -0.8(7)           20564
formula moiety formula FW temperature (K) crystal size (mm) crystal system space group a (Å) b (Å) c (Å) $\alpha$ (°) $\beta$ (°) $\gamma$ (°) V (Å <sup>3</sup> ) Z Dc (g/cm <sup>3</sup> ) $\mu$ (Mo <sub>Ka</sub> ) $\theta_{min/max}$ (°) R1 [ $F_0 > 2\sigma(F_0)$ ] $wR2$ (all $F_0^2$ ) GOF Flack parameter measured refins independent refins observed refins refins used parameters	$\begin{array}{c} \textbf{2(1m)-2M-2-BuOH (C1)} \\ \hline \textbf{C}_{28.5}H_{30}NO_{8.5} \\ \hline (C_{20}H_{17}O_8)^- \bullet 0.5(C_{13}H_{16}N_2)^{2+} \\ \bullet 0.5(C_4H_{10}O) \\ 522.54 \\ 150 \\ 0.12 \times 0.08 \times 0.08 \\ \hline monoclinic \\ \hline \textbf{C2} \\ 16.286(7) \\ 22.708(9) \\ 7.950(3) \\ 90 \\ 115.707(5) \\ 90 \\ 2649.2(19) \\ 4 \\ 1.310 \\ 0.097 \\ 1.65/25.00 \\ 0.0667 \\ 0.1704 \\ 1.038 \\ -1.3(10) \\ 6331 \\ 4317 \\ 3460 \\ 4317 \\ 349 \\ \hline \textbf{N}_{11} \\ \textbf{C}_{11} \\ \textbf{C}_$	Im-20-2(2-BuOH)+H <sub>2</sub> O (C2) $C_{40}H_{52}N_2O_{12}$ $(C_{20}H_{16}O_8)^{2^-} \cdot (C_{12}H_{14}N_2O)^{2^+}$ $\cdot 2(C_4H_{10}O) \cdot H_2O$ 752.84           150           0.28 × 0.10 × 0.02           orthorhombic $P2_12_12_1$ 7.7919(13)           21.208(4)           24.416(4)           90           90           4034.7(12)           4           1.239           0.091           1.27/25.00           0.0853           0.2202           1.033           1.0(10)           18894           7072           4689           7072           454	Ip•2M (D1) $C_{33}H_{32}N_2O_8$ $(C_{20}H_{17}O_8)^- \cdot (C_{13}H_{15}N_2)^+$ 584.60           200           0.18 × 0.03 × 0.01           tetragonal $l4_1$ 28.639(5)           28.639(5)           28.639(5)           7.8757(15)           90           90           6460(3)           8           1.202           0.087           1.005/25.00           0.0547           0.1313           0.910           -2.6(10)           15524           5607           3031           5607           396	<b>1p-2O-2(2-PenOH) (D2)</b> $C_{42}H_{54}N_2O_{11}$ $(C_{12}H_{14}N_2O)^{2+} \cdot$ $2(C_5H_{12}O)$ 762.87           150 $0.25 \times 0.05 \times 0.02$ orthorhombic $P2_{12}_{12}_{1}$ 7.7836(8)           22.234(2)           24.890(3)           90           91           92           93           94           1.176           0.0719           0.1966           1.028           -0.8(7)           20564

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

Compound name	D-HA	D-H/Å	H-A/Å	D-A/Å	∠D-H…A/°
1b•2O•2H <sub>2</sub> O (A2)					
	N1-H3O9	1.162	1.707	2.811	156.42
	N1-H5O6	0.847	1.92	2.722	157.69
	N1-H4O11	0.907	2.56	2.91	103.59
	N2-H8O8	0.822	2.171	2.883	144.88
	N2-H9O7	1.054	1.622	2.671	172.55
	N2-H10O4	1.007	1.858	2.737	143.94
	O8-H2O7	0.837	2.046	2.811	151.81
	O8-H1O4	0.930	2.042	2.951	165.17
	O11-H15O9	0.973	1.897	2.782	149.94
	O11-H16O6	0.828	2.128	2.861	147.51
10•2M•3H <sub>2</sub> O (B1)					
	N1-H4O5	0.882	1.905	2.749	159.78
	N1-H5O2	0.891	1.878	2.757	168.69
	N1-H6O3	1.019	1.733	2.728	164.36
	O2-H1O6	0.851	1.816	2.649	165.93
	O6-H2O3	0.813	1.994	2.758	156.11
	O6-H3O5	0.858	1.922	2.759	165.06
10•20•3H <sub>2</sub> O (B2)					
	N1-H13O2	0.861	1.938	2.758	158.72
	N1-H14O5	0.948	1.796	2.725	165.5
	N1-H15O1	0.921	1.843	2.752	168.39
	O1-H16O7	0.943	1.701	2.641	173.69
	O7-H17O2	0.887	1.885	2.750	164.65
	O7-H18O5	0.930	1.842	2.747	163.66

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

Compound name	D-HA	D-H/Å	H-A/Å	D-A/Å	∠D-H…A/°
2(1m)•2M•2-BuOH (C1)					
	N1-H3707	1.059	1.601	2.635	164.04
	N1-H38O5	0.846	2.014	2.848	168.45
	N1-H39O3	0.948	1.833	2.778	174.21
	O4-H1O4	0.840	1.745	2.475	143.98
	O6-H36O6	0.840	1.632	2.420	155.16
1m•2O•2(2-BuOH)•H <sub>2</sub> O (C2)					
	N1-H1O6	1.057	1.771	2.828	179.21
	N1-H2O4	0.882	1.941	2.737	149.39
	N1-H3O10	0.846	1.997	2.797	157.26
	N2-H4011	0.908	1.811	2.716	174.68
	N2-H5O4	0.911	1.844	2.753	176.54
	N2-H6O10	0.91	2.15	2.806	128.32
1p•2M (D1)					
	N1-H1107	0.91	2.081	2.924	153.58
	N1-H12O8	0.91	1.957	2.801	153.58
	N2-H18O5	0.91	2.059	2.943	163.2
	N2-H19O6	0.91	1.99	2.78	144.28
	O4-H12O3	0.839	1.605	2.431	167.23
	N1-H10N2	0.909	1.823	2.702	161.95
	N2-H20N1	0.908	1.81	2.702	166.69
1p•2O•2(2-PenOH) (D2)					
	N1-H2O1	0.995	1.793	2.703	150.31
	N1-H3O8	0.932	1.9	2.803	162.58
	N1-H4O10	0.98	1.885	2.735	143.43
	N2-H7O1	1.032	1.683	2.712	174.79
	N2-H8O10	1.033	1.972	2.82	137.38
	N2-H9O11	1.033	1.702	2.719	167.25
	O8-H1O6	1.049	1.764	2.792	165.73

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



Figure S1. <sup>1</sup>H NMR spectrum of  $1m \cdot 2O$  salt obtained from a 2-butanol solution.



Figure S2. <sup>1</sup>H NMR spectrum of  $1p \cdot 2O$  salt obtained from a 2-pentanol solution.