

Article

Supplementary Materials

Figure S1. Powder diffraction diagram of **1** and fit using the derivative difference minimization (DDM) method (red line: experimental data; green line: DDM refinement).

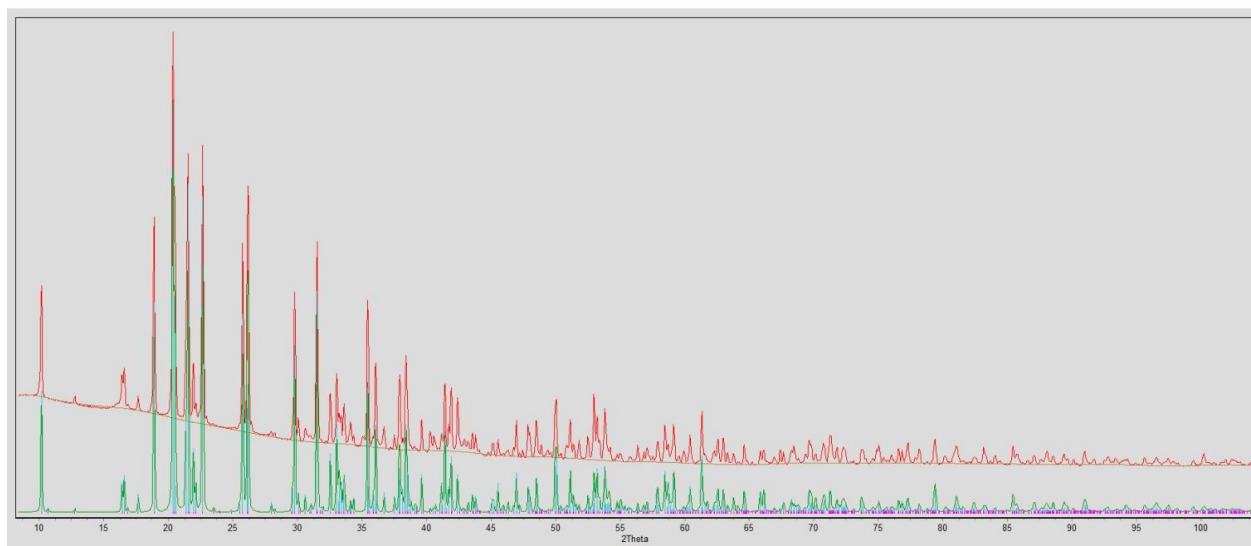


Figure S2. Powder diffraction diagram of **2** and fit using the DDM method (red line: experimental data; green line: DDM refinement).

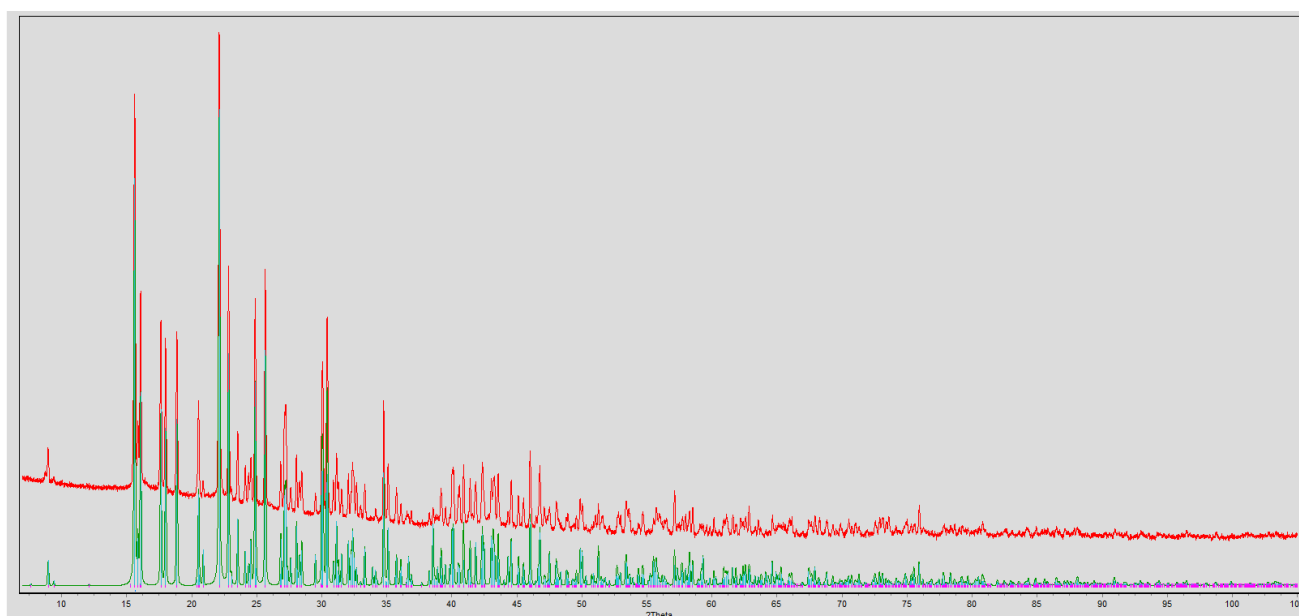


Table S1. Vibrational frequencies for *dpma*, **1** and **2** and their assignments.

<i>dpma</i>			<i>dpma</i> HClO ₄ (1)		<i>dpma</i> HClO ₄ • <i>dpma</i> (2)		Assignment ^a
B3LYP [cm ⁻¹]	IR ^b [cm ⁻¹]	Raman ^b [cm ⁻¹]	IR ^b [cm ⁻¹]	Raman ^b [cm ⁻¹]	IR ^b [cm ⁻¹]	Raman ^b [cm ⁻¹]	
287	–	282 m	–	290 w	–	293 w	τ(CPCN)
312	–	306 w	–	312 w	–	325 m	τ(NH ₂)/τ(NH ₃)
352	–	353 m	–	385 w	–	364 w, 376 w	δ(PCN), δ(OPC)
429	–	400 m, 440 w	–	461 m	–	459 m	δ(CPC), δ(OPC)
–	–	–	618 s	623 m	622 s	625 w	δ(OCIO)
628, 685, 715	648 w, 716 w	652 s, 714 w	654 w, 725 w	655 s, 728 w	658 w, 670 w, 723 m	661 m, 671 s, 726 m	ν(PC)
780	735 m, 762 s	738 w, 771 w	766 w, 783 m	771 w, 788 w	753 m, 785 w	756 w, 787 w	δ(CH ₃), δ(CH ₂)
858, 878	857 s, 889 vs	–	853 m	–	863 m	–	δ(CH ₃)
906	898 vs	–	882 s	–	885 s	–	δ(NH ₂)/δ(NH ₃)
924, 954	915 m, 934 s	905 w, 938 w	912 m, 941 s	932 vs	916 m, 939 s	913 w, 936 vs	δ(CH ₃)
–	–	–	1015 s, 1046 vs	1016 w	984 m	985 w, 1024 w	ν(ClO ₄)
1086	1097 m	1067 w	1073 vs	1084 w	1077 vs	1076 w	ν(CN), δ(NH ₂)/ δ(NH ₃)
1119	1147 vs	1138 m, 1149 m	1142 m	1107 w, 1160 w	1143 vs	1124 w, 1157 m	δ(CH ₂), δ(NH ₂)/ δ(NH ₃)
1222	1288 s	–	–	1265 w	–	–	ν(PO)
1302	1298 m, 1308 m	–	1306 m	–	1296 m	1309 w	δ(CH ₂)
1322, 1336	–	–	1315 m, 1343 w	1311 w	1313 m, 1348 w	1334 w, 1358 w	δ(CH ₃)
1389	1385 w	–	1405 w	1402 w	–	1407 w	δ(CH ₂), δ(NH ₂)/ δ(NH ₃)
1452, 1460, 1463	1418 w, 1425 w	1413 m, 1448 w	1412 w, 1429 w	1426 w	1426 w, 1437 w	1418 w, 1428 w, 1439 w	δ(CH ₃), δ(CH ₂)
1466, 1467	1472 w, 1503 w	–	1500 m	1514 w	–	–	δ(CH ₃)
–	–	–	1557 w	1548 w	1564 w	–	–

Table S1. Cont.

<i>dpma</i>			<i>dpmaHClO₄</i> (1)		<i>dpmaHClO₄•dpma</i> (2)		Assignment ^a
B3LYP [cm ⁻¹]	IR ^b [cm ⁻¹]	Raman ^b [cm ⁻¹]	IR ^b [cm ⁻¹]	Raman ^b [cm ⁻¹]	IR ^b [cm ⁻¹]	Raman ^b [cm ⁻¹]	
1672	1634 w	–	1638 m	1619 w	1622 w	–	δ(NH ₂)/δ(NH ₃)
–	–	–	2573 w, 2695 w	–	2025 w, 2038 w, 2172 w, 2185 w, 2199 w, 2648 m	–	ν(H ₂ O)
3025	2808 w	2825 w	2810 w	–	2794 m	2806 w	ν ^s (CH ₂)
3036, 3039	2873 m, 2913 m	2876 m, 2913 vs	2927 m, 2947 m	2930 s, 2947 m	2829 m, 2916 m	2828 w, 2853 w, 2921 s, 2961 w	ν ^s (CH ₃)
3,071	2977 m	2982 s	2993 m	2997 m	2997 m	2992 m	ν ^{as} (CH ₂)
3114, 3118, 3121, 3122	–	3025 w	3008 m, 3112 m, 3175 m	–	3192 m	3198 w	ν ^{as} (CH ₃)
3,472	3174 s	3177 w	3215 m	–	3267 s	3261 w	ν ^s (NH ₂)/ν ^s (NH ₃)
3546	3296 s	3310 w	3536 w	–	3348 s	3351 w, 3398 w	ν ^{as} (NH ₂)/ν ^{as} (NH ₃)

^a Vibrational modes: ν, stretching; δ, deformation (all kinds of); τ, torsion; ^b Relative intensities: w, weak; m, medium; s, strong; vs, very strong.