# SUPPLEMENTARY INFORMATION

**TABLE S1** Crystal data and details of structure determination

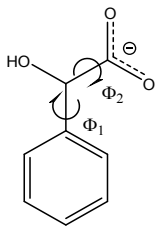
| Compound | HOM-2 | HET-2 | DOB-2 | HOM-4 | HET-4 | DOB-4 |
|---|---|---|---|---|---|---|
| Empirical formula | $C_{16}H_{24}ClNO_3$ | $C_{16}H_{24}ClNO_3$ | $C_{16}H_{24}ClNO_3$ | $C_{16}H_{24}ClNO_3$ | $C_{16}H_{24}ClNO_3$ | $C_{16}H_{24}ClNO_3$ |
| Formula weight | 313.81 | 313.81 | 313.81 | 313.81 | 313.81 | 313.81 |
| Temperature, K | 293(2) | 143(2) | 103(2) | 103(2) | 113(2) | 119(2) |
| Radiation and wavelength | Mo-Kα, λ =0.71075Å | Mo-Kα, λ =0.71075Å | Cu-Kα, λ =1.54178Å | Cu-Kα, λ =1.54178Å | Cu-Kα, λ =1.54178Å | Cu-Kα, λ =1.54178Å |
| Crystal system | orthorhombic | monoclinic | monoclinic | orthorhombic | monoclinic | monoclinic |
| Space group | $P2_12_12_1$ | $P2_1$ | $P2_1$ | $P2_12_12_1$ | $P2_1$ | $C2$ |
| a, Å | $a$ =6.8200(3)Å | $a$ =9.0572(9)Å | $a$ =9.6370(2)Å | $a$ =6.7938(3)Å | $a$ =10.4640(6)Å | $a$ =24.2266(8)Å |
| b, Å | $b$ =8.8363(3)Å | $b$ =29.711(3)Å | $b$ =25.3851(6)Å | $b$ =8.6704(3)Å | $b$ =10.4673(7)Å | $b$ =10.0661(8)Å |
| c, Å | $c$ =26.1400(11)Å | $c$ =12.6381(13)Å | $c$ =13.5859(3)Å | $c$ =27.7144(9)Å | $c$ =29.8915(16)Å | $c$ =13.3665(8)Å |
| α, deg | α =90° | α =90° | α =90° | α =90° | α =90° | α =90° |
| β, deg | β =90° | β =93.337(3)° | β =90.277(6)° | β =90° | β =96.843(3)° | β =92.5330(10)° |
| γ, deg | γ =90° | γ =90° | γ =90° | γ =90° | γ =90° | γ =90° |
| V, Å$^3$ | 1575.29(11)Å$^3$ | 3395.1(6)Å$^3$ | 3323.56(13)Å$^3$ | 1632.52(11)Å$^3$ | 3250.7(3)Å$^3$ | 3256.5(3)Å$^3$ |
| $Z'$ | 1 | 4 | 4 | 1 | 4 | 2 |
| $Z$ | 4 | 8 | 8 | 4 | 8 | 8 |
| Density (calculated) | 1.323 Mg/m$^3$ | 1.228 Mg/m$^3$ | 1.254 Mg/m$^3$ | 1.277 Mg/m$^3$ | 1.282 Mg/m$^3$ | 1.280 Mg/m$^3$ |
| KPI % | 70.4 | 65.2 | 66.1 | 68.0 | 68.6 | 67.9 |
| Absorption coefficient, μ | 0.252 mm$^{-1}$ | 0.234 mm$^{-1}$ | 2.113 mm$^{-1}$ | 2.151 mm$^{-1}$ | 2.161 mm$^{-1}$ | 2.157 mm$^{-1}$ |
| $F$(000) | 672 | 1344 | 1344 | 672 | 1344 | 1344 |
| Crystal colour | colorless | colorless | colorless | colorless | colorless | colorless |
| Crystal description | block | platelet | platelet | chunk | prism | platelet |
| Crystal size | 0.63 x 0.50 x 0.41 mm | 0.50 x 0.20 x 0.05 mm | 0.47 x 0.44 x 0.18 mm | 0.30 x 0.15 x 0.05 mm | 0.67 x 0.30 x 0.13 mm | 0.61 x 0.48 x 0.44 mm |
| Absorption correction | numerical | multi-scan | numerical | numerical | numerical | numerical |
| Max. and min. transmission | 0.974 0.985 | 0.298 1.000 | 0.973 0.992 | 0.5750 0.8212 | 0.373 0.841 | 0.882 0.964 |
| θ–range for data collection | 3.087 ≤ θ ≤ 27.471° | 3.023 ≤ θ ≤ 25.348° | 3.253 ≤ θ ≤ 68.238° | 6.710 ≤ θ ≤ 66.564° | 6.536 ≤ θ ≤ 50.435° | 3.310 ≤ θ ≤ 68.245° |
| Index ranges | $-8 \le h \le 8$;$-10 \le k \le 11$;$-33 \le l \le 33$ | $-10 \le h \le 10$;$-35 \le k \le 35$;$-15 \le l \le 15$ | $-11 \le h \le 11$;$-30 \le k \le 30$;$-16 \le l \le 16$ | $-6 \le h \le 8$;$-8 \le k \le 8$;$-32 \le l \le 28$ | $-10 \le h \le 10$;$-10 \le k \le 10$;$-5 \le l \le 29$ | $-29 \le h \le 29$;$-12 \le k \le 12$;$-14 \le l \le 15$ |
| Reflections collected | 50543 | 45929 | 25816 | 7677 | 6812 | 18879 |
| Completeness to 2θ | 0.998 | 0.998 | 0.989 | 0.880 | 0.995 | 0.970 |
| Absolute structure parameter | 0.041(10) | -0.02(7) | 0.189(14) | 0.05(4) | 0.035(11) | 0.099(9) |
| Friedel coverage | 0.718 | 0.958 | 0.751 | 0.568 | 0.868 | 0.846 |
| Friedel fraction max. | 0.999 | 0.996 | 0.779 | 0.719 | 0.997 | 0.927 |
| Friedel fraction full | 1.000 | 0.998 | 0.781 | 0.719 | 0.997 | 0.931 |
| Independent reflections | 50543 [$R$(int) = 0.0398] | 45929 [$R$(int) = 0.1811] | 25816 [$R$(int) = 0.0863] | 7677[$R$(int) = 0.0513] | 6812 [$R$(int) = 0.0982] | 5644 [$R$(int) = 0.0589] |
| Reflections $I>2\sigma(I)$ | 41935 | 5895 | 19821 | 5310 | 6308 | 5111 |
| Refinement method | full-matrix least-squares on $F2$ | full-matrix least-squares on $F2$ | full-matrix least-squares on $F2$ | full-matrix least-squares on $F2$ | full-matrix least-squares on $F2$ | full-matrix least-squares on $F2$ |
| Data / restraints / parameters | 50543 /0 /194 | 12376 /386 /972 | 25816 /235 /835 | 7677 /0 /194 | 6812 /602 /718 | 5644 /1 /413 |
| Goodness-of-fit on $F2$ | 0.990 | 1.018 | 1.023 | 1.130 | 1.132 | 1.080 |
| Final $R$ indices [$I>2\sigma(I)$] | $R1$ =0.0393, $wR2$ =0.0738 | $R1$ =0.0934, $wR2$ =0.1687 | $R1$ =0.1070, $wR2$ =0.2808 | $R1$ =0.0931, $wR2$ =0.1968 | $R1$ =0.0913, $wR2$ =0.1854 | $R1$ =0.0468, $wR2$ =0.1070 |
| R indices (all data) | $R1$ =0.0536, $wR2$ =0.0772 | $R1$ =0.1934, $wR2$ =0.2107 | $R1$ =0.1228, $wR2$ =0.3010 | $R1$ =0.1422, $wR2$ =0.2515 | $R1$ =0.0980, $wR2$ =0.1892 | $R1$ =0.0526, $wR2$ =0.1100 |
| Max. and mean shift/esd | 0.000;0.000 | 0.003;0.000 | 0.000;0.000 | 0.000;0.000 | 0.000;0.000 | 0.000;0.000 |
| Largest diff. peak and hole | 0.406;-0.278e.Å$^3$ | 0.481;-0.389e.Å$^3$ | 1.407;-0.567e.Å$^3$ | 0.834;-0.709e.Å$^3$ | 0.484;-0.521e.Å$^3$ | 0.277;-0.206e.Å$^3$ |

X-ray source and measurement temperature were based on availability. In some cases, the weight factors are high because of poor crystal quality.

**TABLE S2** List of hydrogen bonds in the six isomeric structures

| **HOM-2** | | | | | **HOM-4** | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Donor—H...Acceptor** | **H...A** | **D...A** | **D-H...A** | **Symm. op.** | **Donor—H...Acceptor** | **H...A** | **D...A** | **D-H...A** | **Symm. op.** |
| N(1) --H(1A) ..O(2) | 1.95 | 2.822(3) | 167 | x,y,z | N(1) --H(1A) ..O(1) | 1.95 | 2.828(15) | 169 | 1+x,y,z |
| N(1) --H(1B) ..O(1) | 2.13 | 2.990(3) | 162 | 2-x,-1/2+y,1/2-z | N(1) --H(1B) ..O(1) | 2.01 | 2.885(17) | 167 | 1/2+x,1/2-y,2-z |
| N(1) --H(1C) ..O(2) | 2.19 | 2.962(3) | 145 | 1-x,-1/2+y,1/2-z | N(1) --H(1C) ..O(2) | 1.99 | 2.861(16) | 165 | x,y,z |
| O(3) --H(3) ..O(1) | 1.88 | 2.687(2) | 168 | 2-x,1/2+y,1/2-z | O(3) --H(3) ..O(2) | 2.02 | 2.782(15) | 154 | -1/2+x,3/2-y,2-z |
| | | | | | | | | | |
| **HET-2** | | | | | **HET-4** | | | | |
| **Donor—H...Acceptor** | **H...A** | **D...A** | **D-H...A** | **Symm. op.** | **Donor—H...Acceptor** | **H...A** | **D...A** | **D-H...A** | **Symm. op.** |
| N(1) --H(1A) ..O(5) | 1.86 | 2.726(10) | 165 | x,y,z | O3B --H3OB ..O2B | 2.21 | 2.739(14) | 113 | intra |
| N(1) --H(1B) ..O(7) | 1.98 | 2.836(9) | 161 | x,y,-1+z | O3B --H3OB ..O1B | 2.19 | 2.739(15) | 115 | -x,-1/2+y,1-z |
| N(1) --H(1C) ..O(2) | 2.21 | 2.877(11) | 131 | x,y,z | O3D --H3OD ..O2D | 2.29 | 2.931(14) | 120 | 1-x,1/2+y,-z |
| N(1) --H(1C) ..O(6) | 2.56 | 2.911(10) | 105 | -1+x,y,z | N1A --H1A1 ..O1B | 2.00 | 2.865(17) | 158 | -x,-1/2+y,1-z |
| N(2) --H(2A) ..O(2) | 1.86 | 2.730(10) | 164 | x,y,z | N1A --H1A2 ..O2A | 1.94 | 2.824(17) | 164 | x,y,z |
| N(2) --H(2B) ..O(10) | 1.87 | 2.730(9) | 163 | 1+x,y,z | N1A --H1A2 ..O3A | 2.44 | 2.976(16) | 118 | x,y,z |
| N(2) --H(2C) ..O(3) | 2.60 | 2.940(10) | 104 | 1+x,y,z | N1A --H1A3 ..O1A | 1.86 | 2.762(16) | 173 | 1-x,-1/2+y,1-z |
| N(2) --H(2C) ..O(5) | 2.21 | 2.878(10) | 131 | x,y,z | N1B --H1B1 ..O3B | 1.97 | 2.867(16) | 168 | 1+x,y,z |
| O(3) --H(3) ..O(1) | 2.23 | 2.699(9) | 116 | intra | N1B --H1B2 ..O2B | 1.92 | 2.815(15) | 168 | 1-x,-1/2+y,1-z |
| O(3) --H(3) ..O(10) | 2.15 | 2.813(9) | 139' | x,y,z | N1B --H1B3 ..O1A | 2.49 | 3.133(16) | 128 | x,y,z |
| N(3) --H(3A) ..O(8) | 2.14 | 2.869(10) | 138 | x,y,-1+z | N1B --H1B3 ..O2A | 1.91 | 2.809(16) | 168 | x,y,z |
| N(3) --H(3A) ..O(12) | 2.53 | 2.889(10) | 105 | x,y,z | N1C --H1C1 ..O2D | 1.96 | 2.842(16) | 163 | 1-x,1/2+y,-z |
| N(3) --H(3B) ..O(11) | 1.87 | 2.746(10) | 166 | 1+x,y,z | N1C --H1C2 ..O2C | 2.07 | 2.918(16) | 154 | x,y,z |
| N(3) --H(3C) ..O(1) | 1.99 | 2.843(9) | 160 | x,y,z | N1C --H1C2 ..O3C | 2.40 | 2.952(16) | 119 | x,y,z |
| N(4) --H(4A) ..O(9) | 2.52 | 2.929(10) | 109 | 1+x,y,z | N1C --H1C3 ..O1C | 1.88 | 2.771(15) | 166 | 2-x,1/2+y,-z |
| N(4) --H(4A) ..O(11) | 2.20 | 2.867(10) | 132 | 1+x,y,1+z | N1D --H1D1 ..O1C | 2.57 | 3.127(16) | 120 | -1+x,y,z |
| N(4) --H(4B) ..O(8) | 1.86 | 2.738(10) | 166 | x,y,z | N1D --H1D1 ..O2C | 1.97 | 2.871(16) | 174 | -1+x,y,z |
| N(4) --H(4C) ..O(4) | 1.97 | 2.825(9) | 160 | x,y,1+z | N1D --H1D2 ..O3D | 2.16 | 2.997(16) | 152 | x,y,z |
| O(6) --H(6A) ..O(4) | 2.26 | 2.716(9) | 115 | intra | N1D --H1D3 ..O1D | 1.83 | 2.741(15) | 174 | 1-x,1/2+y,-z |
| O(6) --H(6A) ..O(7) | 2.11 | 2.754(9) | 135 | 1+x,y,-1+z | O3C --H3OC ..O1D | 1.90 | 2.728(15) | 145 | x,y,z |
| O(9) --H(9) ..O(4) | 2.08 | 2.752(9) | 139 | -1+x,y,1+z | O3C --H3OC ..O3D | 2.49 | 3.279(15) | 140 | x,y,z |
| O(9) --H(9) ..O(7) | 2.31 | 2.748(9) | 114 | intra | O3A --H3OA ..O2B | 1.92 | 2.695(15) | 140 | x,y,z |
| O(12) --H(12) ..O(1) | 2.20 | 2.847(9) | 136 | x,y,z | | | | | |
| O(12) --H(12) ..O(10) | 2.19 | 2.664(9) | 117 | intra | | | | | |
| | | | | | | | | | |
| **DOB-2** | | | | | **DOB-4** | | | | |
| **Donor—H...Acceptor** | **H...A** | **D...A** | **D-H...A** | **Symm. op.** | **Donor—H...Acceptor** | **H...A** | **D...A** | **D-H...A** | **Symm. op.** |
| N1A --H1A1 ..O2A | 1.97 | 2.828(14) | 163 | 1+x,y,z | N1' --H1N' ..O1' | 1.85 | 2.856(5) | 165(4) | 1/2-x,-1/2+y,-z |
| N1A --H1A2 ..O1C | 1.95 | 2.835(13) | 176 | x,y,z | N1' --H1N' ..O3' | 2.37 | 2.932(5) | 114(4) | 1/2-x,-1/2+y,-z |
| N1A --H1A3 ..Cl1D | 2.79 | 3.342(11) | 121 | x,y,1+z | N1 --H1N ..O1 | 1.81 | 2.794(5) | 170(5) | 1/2-x,1/2+y,1-z |
| N1A --H1A3 ..O2D | 1.98 | 2.813(13) | 156' | x,y,1+z | O3 --H1O ..O1 | 1.98 | 2.708(4) | 167(7) | 1/2-x,-1/2+y,1-z |
| O3A --H3A ..O1C | 1.98 | 2.771(13) | 162 | x,y,z | N1' --H2N' ..O2 | 2.01 | 2.840(5) | 162(5) | x,y,z |
| O3B --H3B ..O1D | 2.09 | 2.677(12) | 128 | -1+x,y,z | N1 --H2N ..O2' | 1.91 | 2.778(5) | 161(4) | x,y,z |
| O3B --H3B ..O2D | 2.57 | 3.105(12) | 124 | -1+x,y,z | N1' --H3N' ..O2' | 1.92 | 2.844(5) | 171(4) | x,y,z |
| O3C --H3C ..O1A | 1.98 | 2.754(12) | 158 | 1+x,y,z | N1' --H3N' ..O3' | 2.60 | 2.932(5) | 102(3) | 1/2-x,-1/2+y,-z |
| O3D --H3D ..O1B | 1.83 | 2.640(13) | 169 | x,y,z | N1 --H3N ..O2 | 2.07 | 2.823(5) | 141(5) | x,y,z |
| N1B --H1B1 ..O1D | 2.00 | 2.867(14) | 165 | x,y,z | N1 --H3N ..O3 | 2.17 | 2.784(6) | 125(4) | 1/2-x,1/2+y,1-z |
| N1B --H1B2 ..O2B | 1.94 | 2.741(14) | 148 | x,y,z | O3' --H1O' ..O1' | 1.86 | 2.718(4) | 169(7) | 1/2-x,1/2+y,-z |
| N1B --H1B2 ..O3D | 2.39 | 2.826(13) | 110 | x,y,z | O3' --H1O' ..O2' | 2.59 | 3.097(4) | 118(6) | 1/2-x,1/2+y,-z |
| N1B --H1B3 ..O2C | 1.96 | 2.809(12) | 159 | x,y,z | | | | | |
| N1C --H1C1 ..O2C | 1.98 | 2.834(14) | 160 | x,y,z | | | | | |
| N1C --H1C1 ..O3A | 2.56 | 2.894(13) | 103 | x,y,z | | | | | |
| N1C --H1C2 ..O1A | 1.97 | 2.851(13) | 169 | x,y,z | | | | | |
| N1C --H1C2 ..O3A | 2.53 | 2.894(13) | 105 | x,y,z | | | | | |
| N1C --H1C3 ..O2B | 1.95 | 2.818(13) | 163 | x,y,z | | | | | |
| N1D --H1D1 ..O1B | 1.92 | 2.811(13) | 176 | x,y,z | | | | | |
| N1D --H1D1 ..O3B | 2.47 | 2.903(13) | 111 | x,y,z | | | | | |
| N1D --H1D2 ..O2D | 1.90 | 2.766(14) | 164 | -1+x,y,z | | | | | |
| N1D --H1D3 ..O2A | 1.99 | 2.839(13) | 158 | x,y,-1+z | | | | | |

**Table S3** ϕ1 and ϕ2 torsion angles of different stereoisomers of mandelic adic for comparison




| | $\Phi_1$ | $\Phi_2$ |
|---|---|---|
| **BOBQOA** | -31° | 56° |
| | -80° | 58° |
| **FEGHAA** | 32° | -60° |
| | 79° | -59° |
| **DLMAND02** | -38° | 59° |
| | -81° | 60° |
| **DLMAND03** | -72° | 77° |

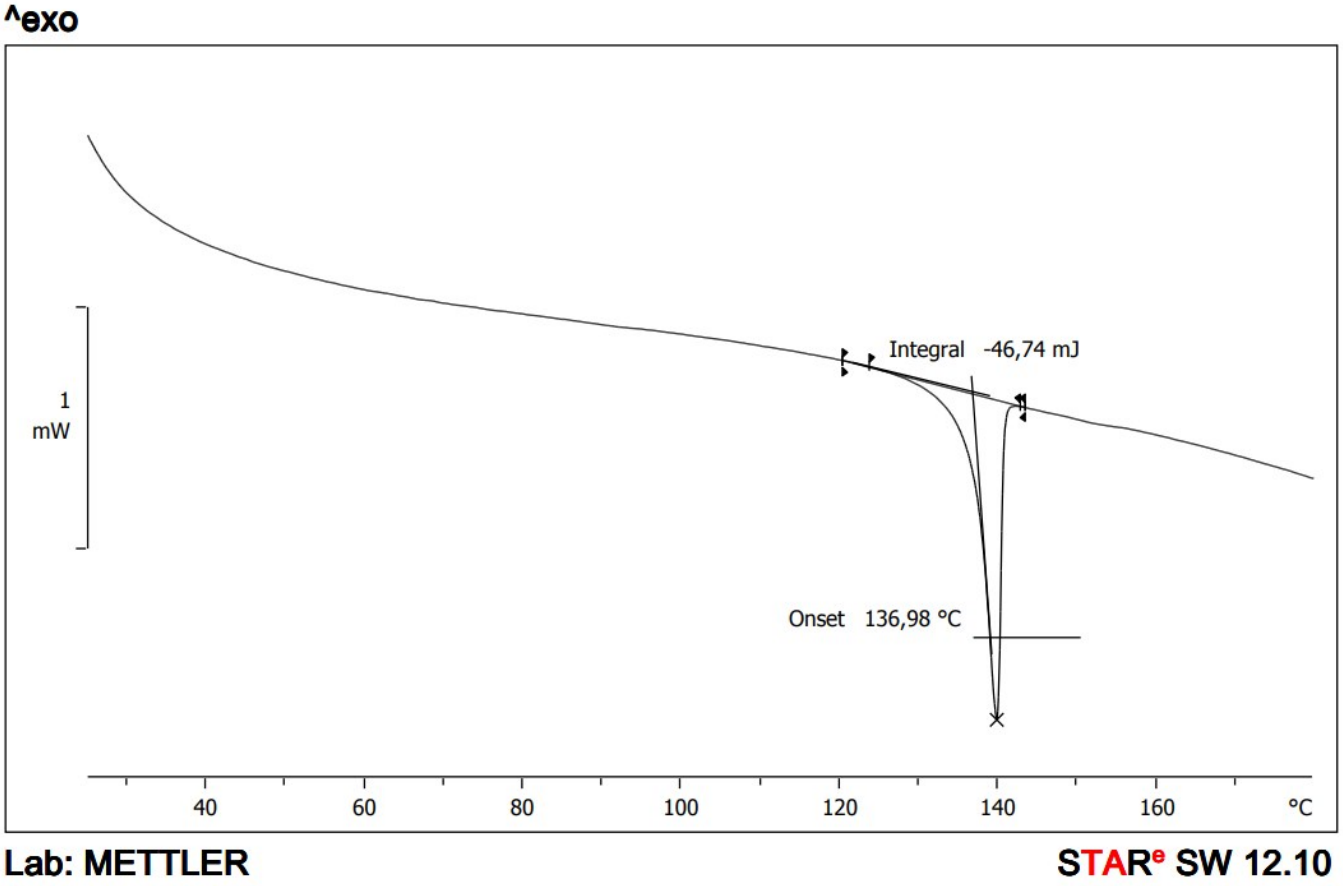



**Figure S1** DSC curve of **HOM-2**

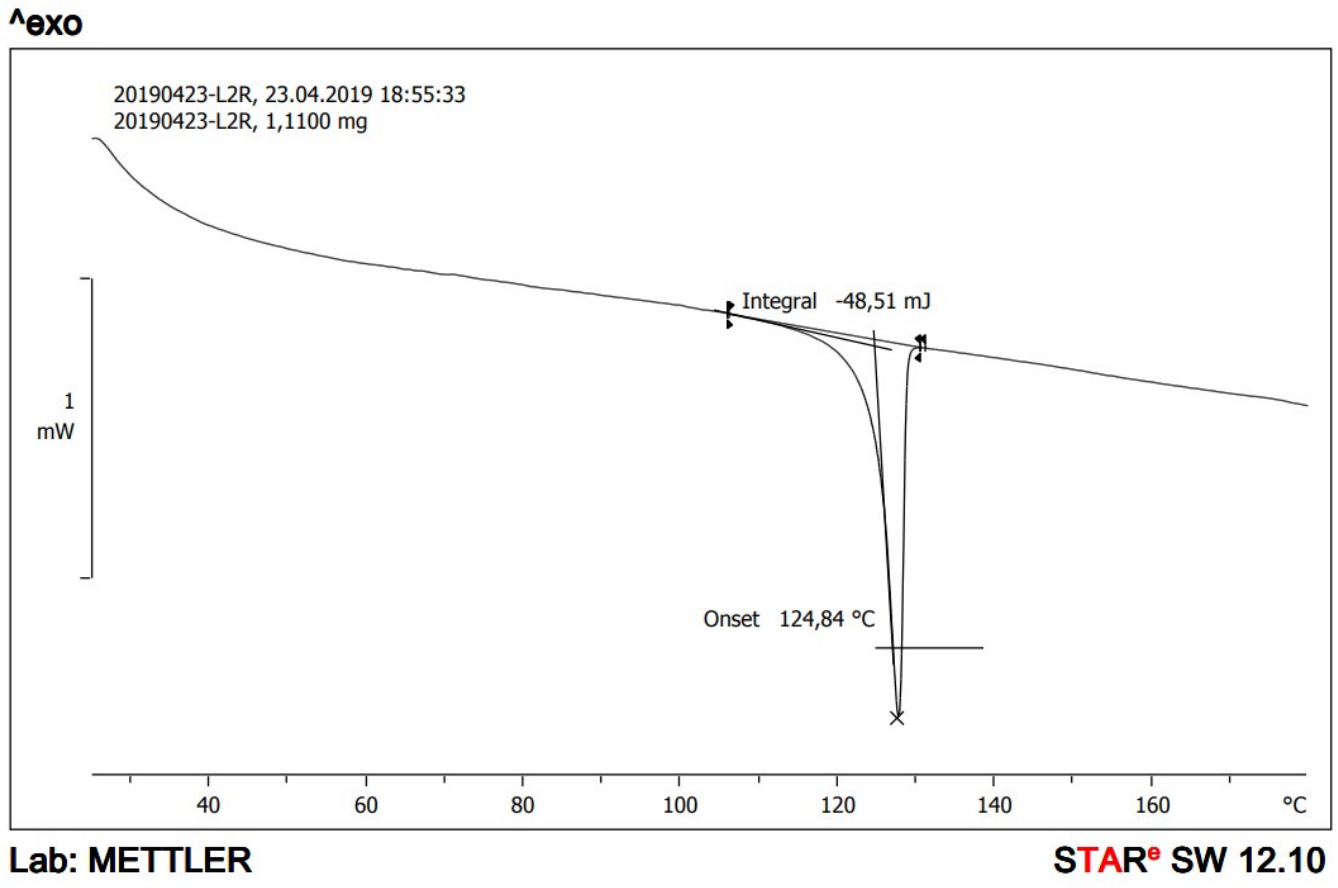



**Figure S2** DSC curve of **HET-2**

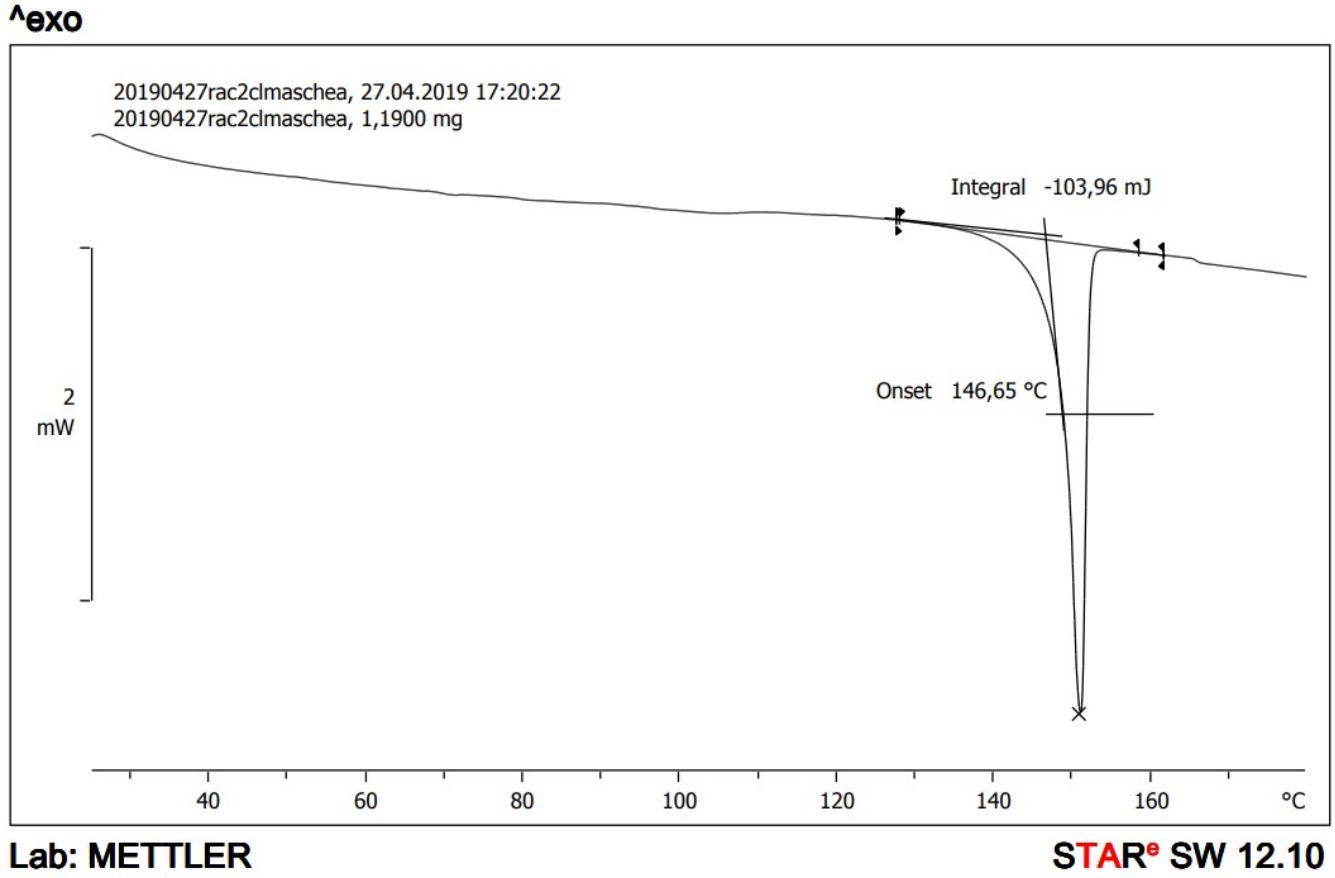



**Figure S3** DSC curve of **DOB-2**

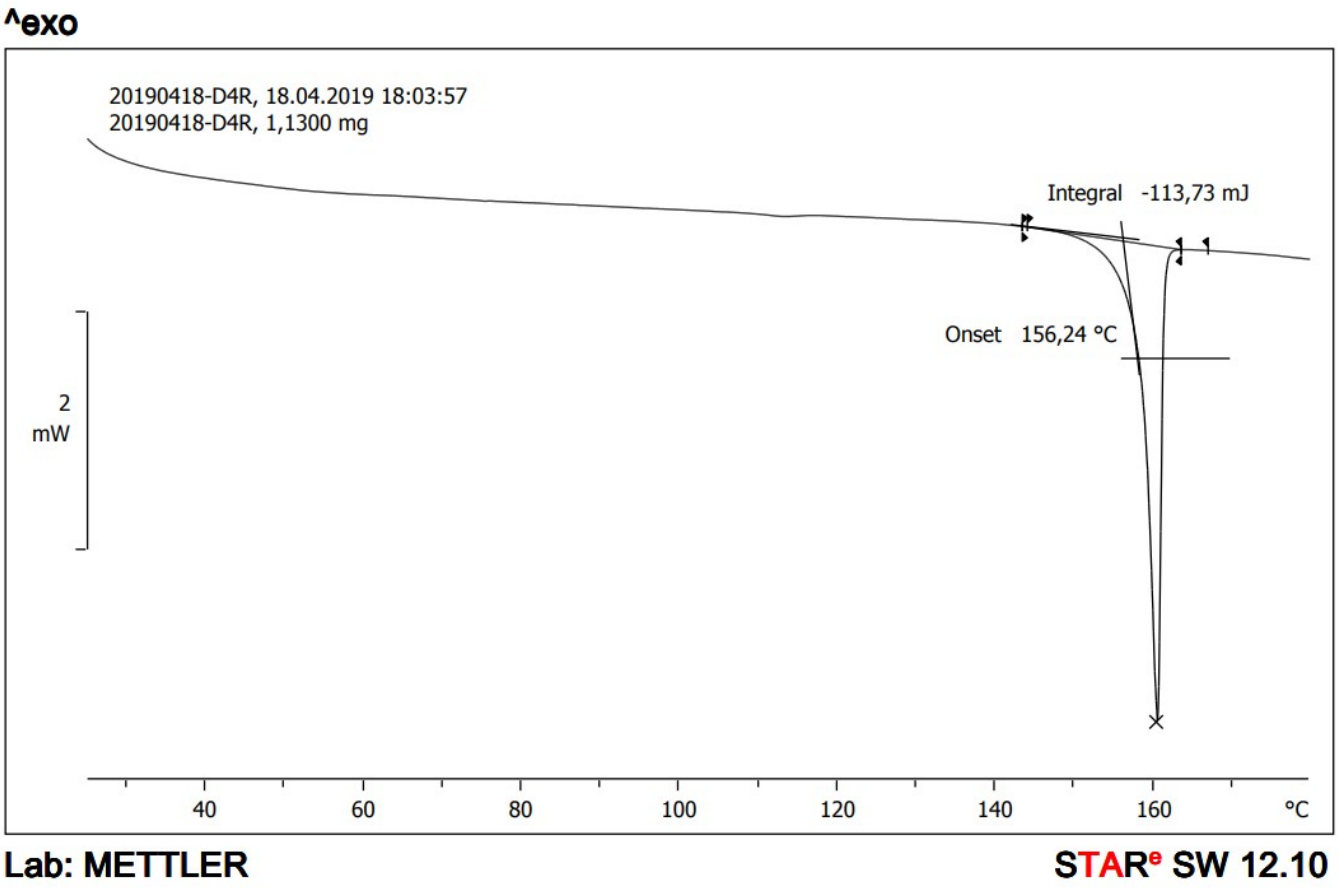



**Figure S4** DSC curve of **HOM-4**

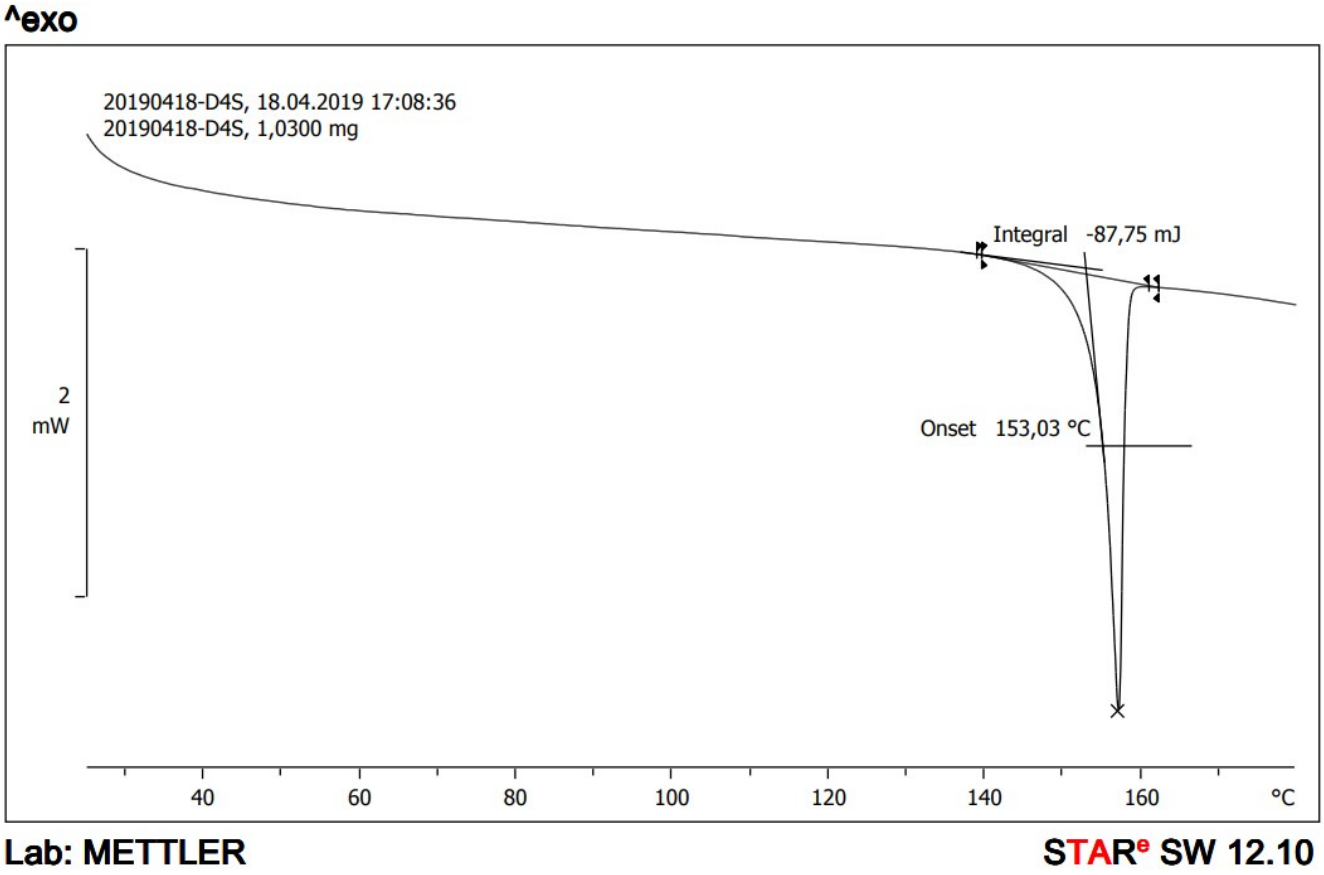



**Figure S5** DSC curve of **HET-2**

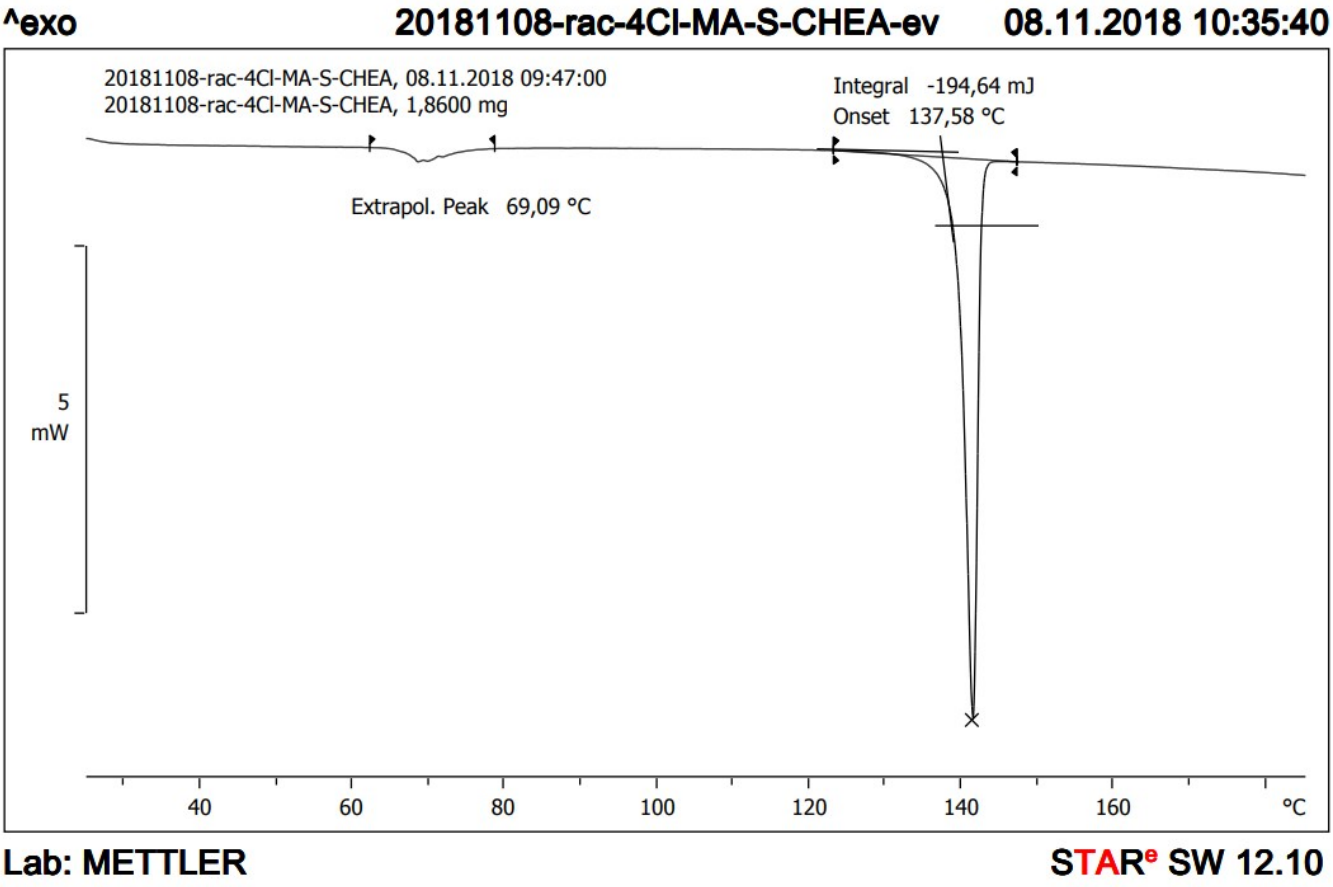



**Figure S6** DSC curve of **DOB-4**

The solid-liquid phase diagrams of the **HOM-4** and **HET-4** and of the **HOM-2** and **HET-2** diastereomeric salt pairs have been calculated on the basis of the DSC data (Figures S1-S6) by the simplified Schröder-van Laar and the Prigogine-Defay equations[34–37]. At the 0.5 mole fraction an independent solid phase is formed, called the double salt (**DOB-2** and **DOB-4** in our case) (Figures S7-S8). **DOB-2** has higher melting point than the diastereomeric salts however, the melting point of the **DOB-4** is lower than that of the diastereomers. In case of the salts of 2-chloromandelic acid, at 0.15 molar fraction and at 110.5°C a eutectic can be observed for the **HET-2** – **DOB-2** mixture and at 0.85 molar fraction and 117.7°C there is another eutectic for the **DOB-2** – **HOM-2** mixture. Similarly, in the case of the salts of 4-chloromandelic acid, the first eutectic is at 0.35 molar fraction and 131.4°C for the **HET-4** – **DOB-4** mixture and a second one is at 0.65 molar fraction and 134.2°C for the **DOB-4** – **HOM-4** mixture.

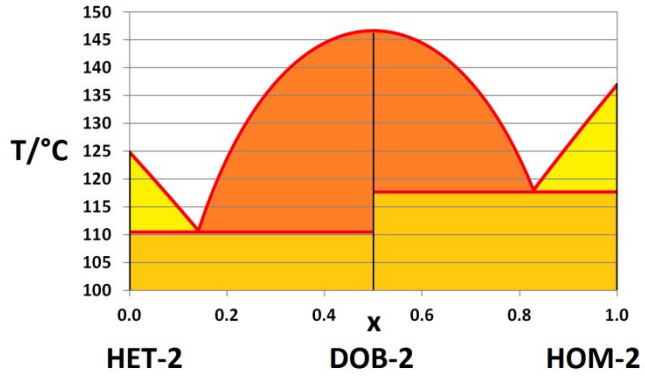



**Figure S7** Calculated solid-liquid phase diagram of **2**

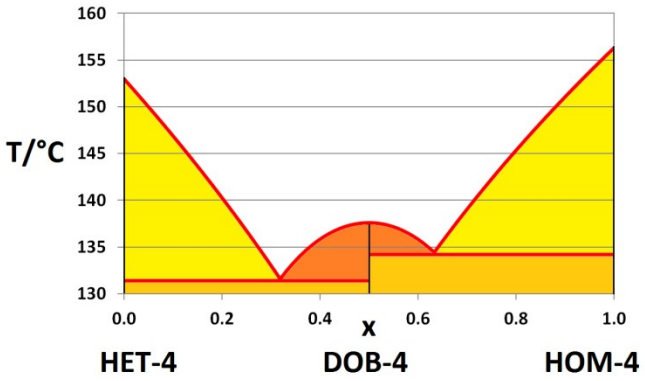



**Figure S8** Calculated solid-liquid phase diagram of **4**

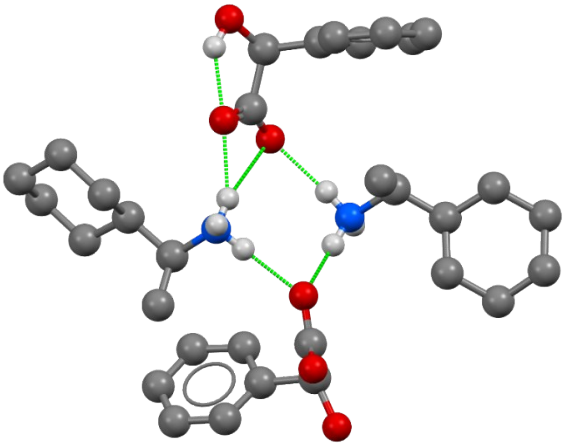


**FIGURE S9** Graph set analysis of QEMZIS, $R_4^2(8)$ and $R_2^1(4)$ rings and intramolecular hydrogen bond of the hydroxyl group (hydrogens not involved in the hydrogen bond network are omitted for clarity)

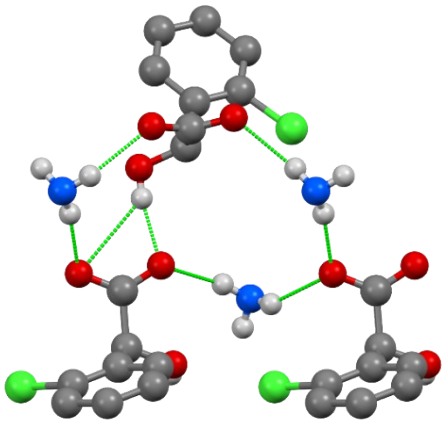


**FIGURE S10** Graph set analysis of **HOM-2**, $R_5^3(13)$, $R_3^2(9)$ and small $R_2^1(4)$ rings in the structure (hydrogens not involved in the hydrogen bond network and amine skeletons are omitted for clarity)

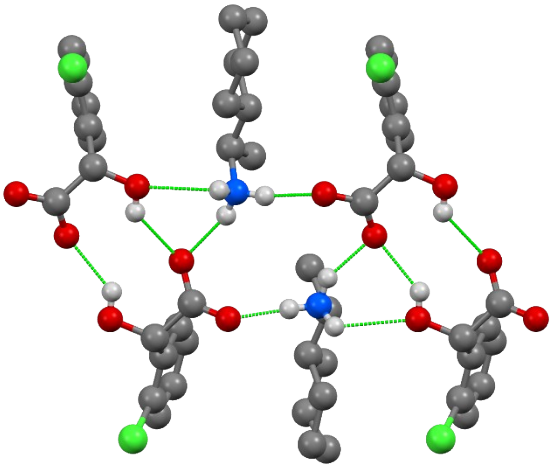


**FIGURE S11** Symmetric $R_4^4(12)$ and $R_2^2(10)$ rings in **HET-2**, $R_2^3(6)$ rings (hydrogens not involved in the hydrogen bond network are omitted for clarity)

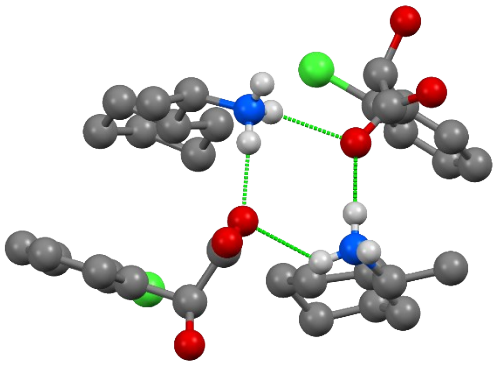


**FIGURE S12** $R_4^2(8)$ rings in **HET-2** (hydrogens not involved in the hydrogen bond network are omitted for clarity)

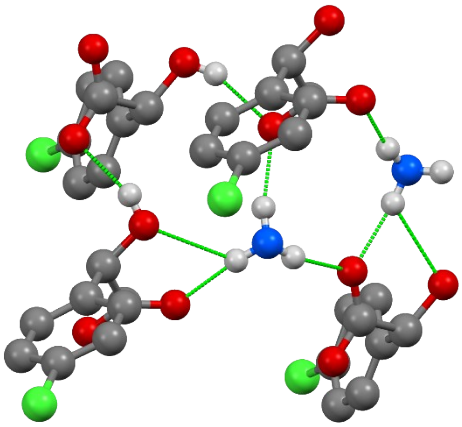


**FIGURE S13** $R_4^3(10)$, $R_4^3(11)$ and $R_1^2(5)$ rings in **HOM-4** (hydrogens not involved in the hydrogen bond network and amine skeletons are omitted for clarity)

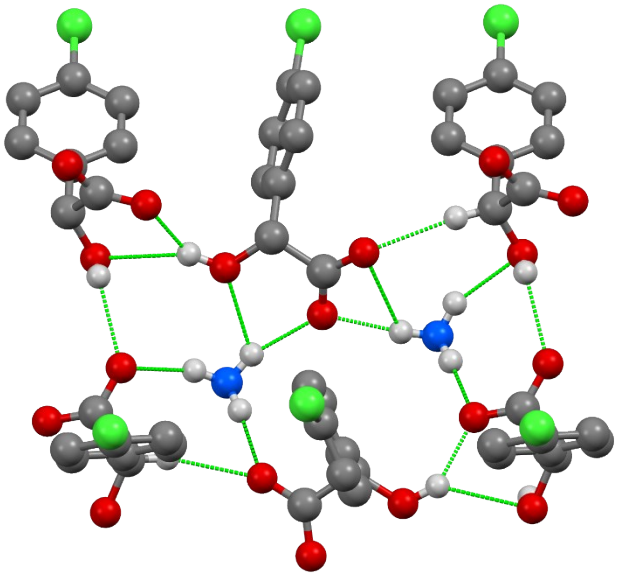


**FIGURE S14** $R_5^3(13)$, $R_3^2(7)$, $R_3^2(8)$, $R_3^3(8)$, $R_4^3(8)$, $R_2^1(4)$ and $R_1^2(5)$ rings in **HET-4** (hydrogens not involved in the hydrogen bond network and amine skeletons are omitted for clarity)

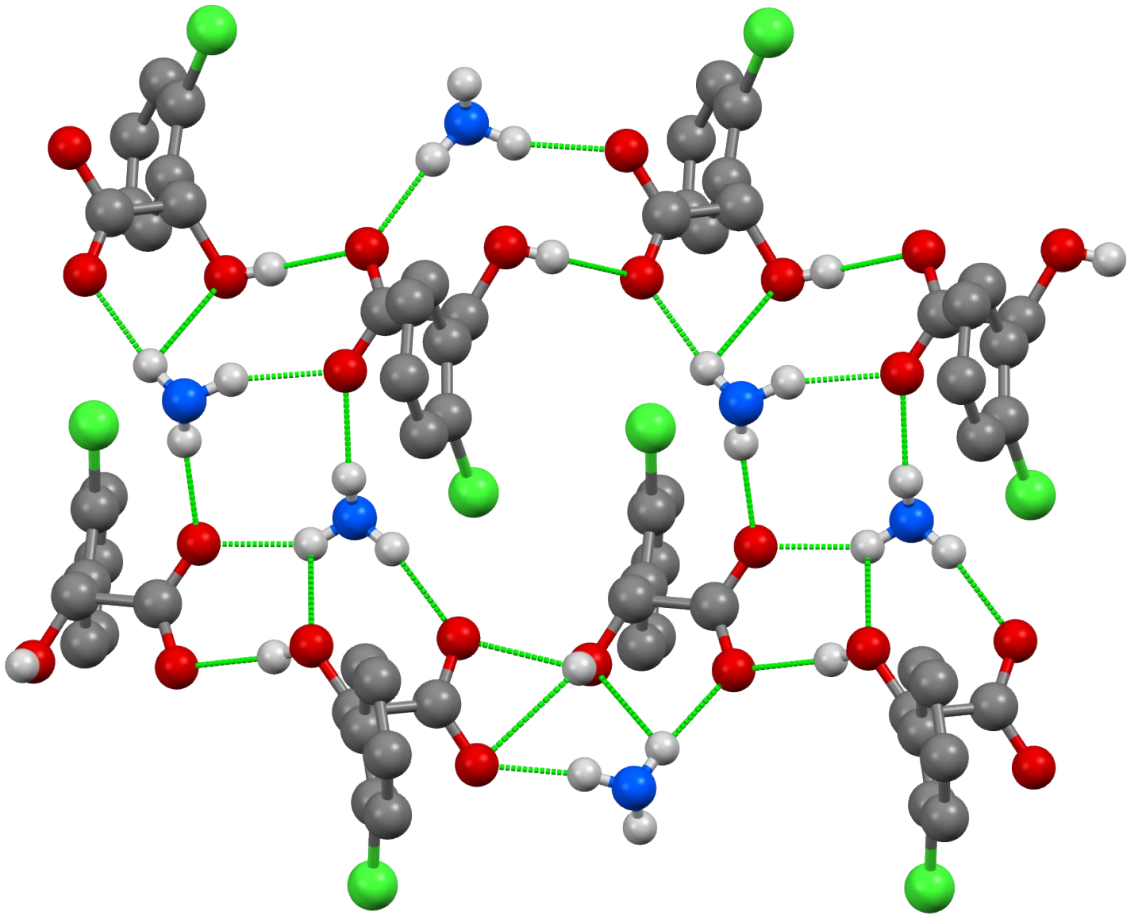


**FIGURE S15** Large $R_6^4(18)$ rings (center) and $R_4^2(8)$, $R_1^2(5)$, $R_2^3(6)$ and $R_2^1(4)$ rings in the **DOB-2** structure (hydrogens not involved in the hydrogen bond network and amine skeletons are omitted for clarity)

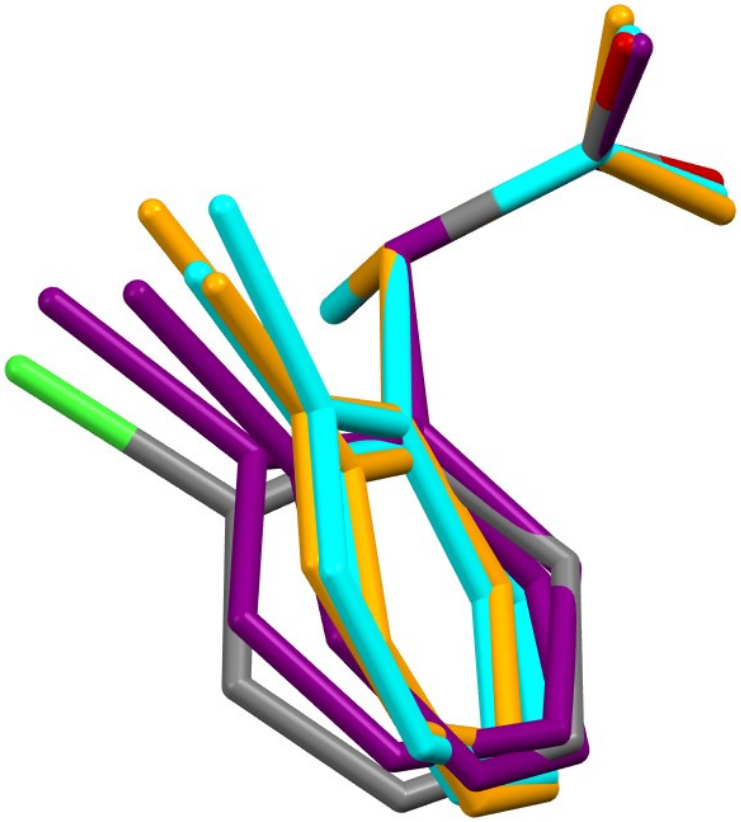


**FIGURE S16** Overlaid structure of the four crystallographically unrelated anions in **HET-2** for comparison, the molecules are overlaid so that the bonds of the asymmetric carbon atom overlapped

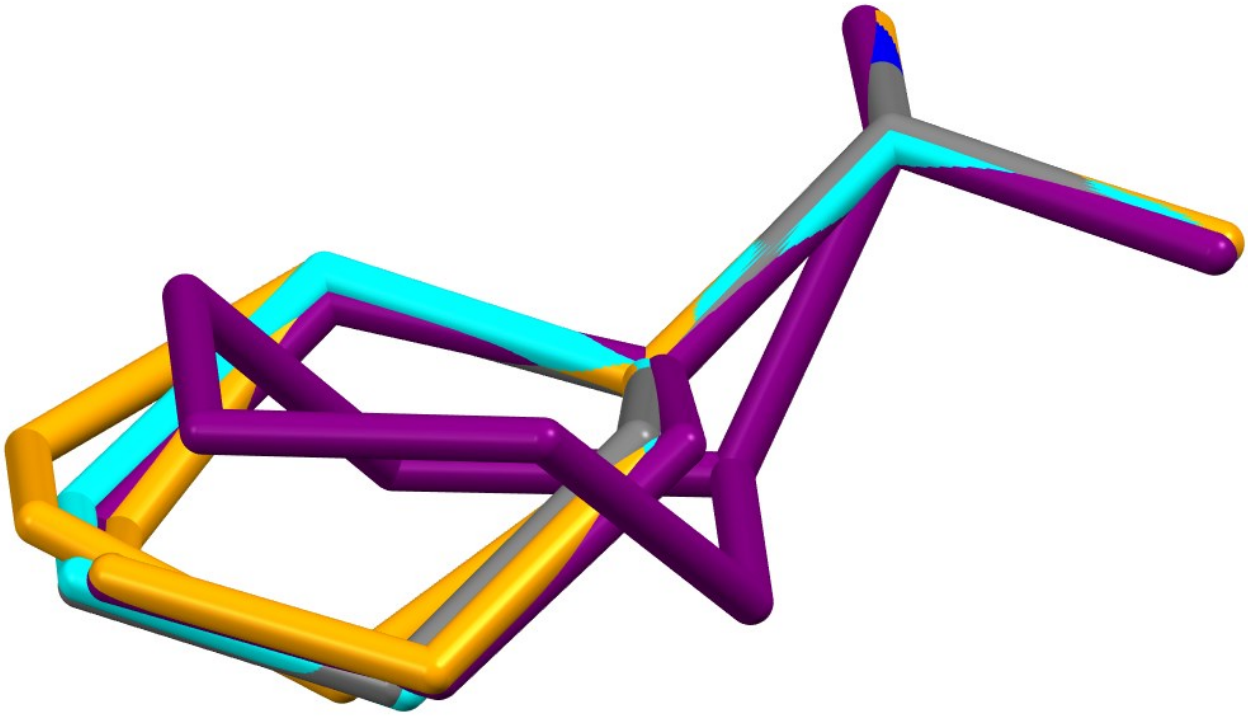


**FIGURE S17** Overlaid structure of the four crystallographically unrelated cations in **HET-2** for comparison, the molecules are overlaid so that the bonds of the asymmetric carbon atom overlapped

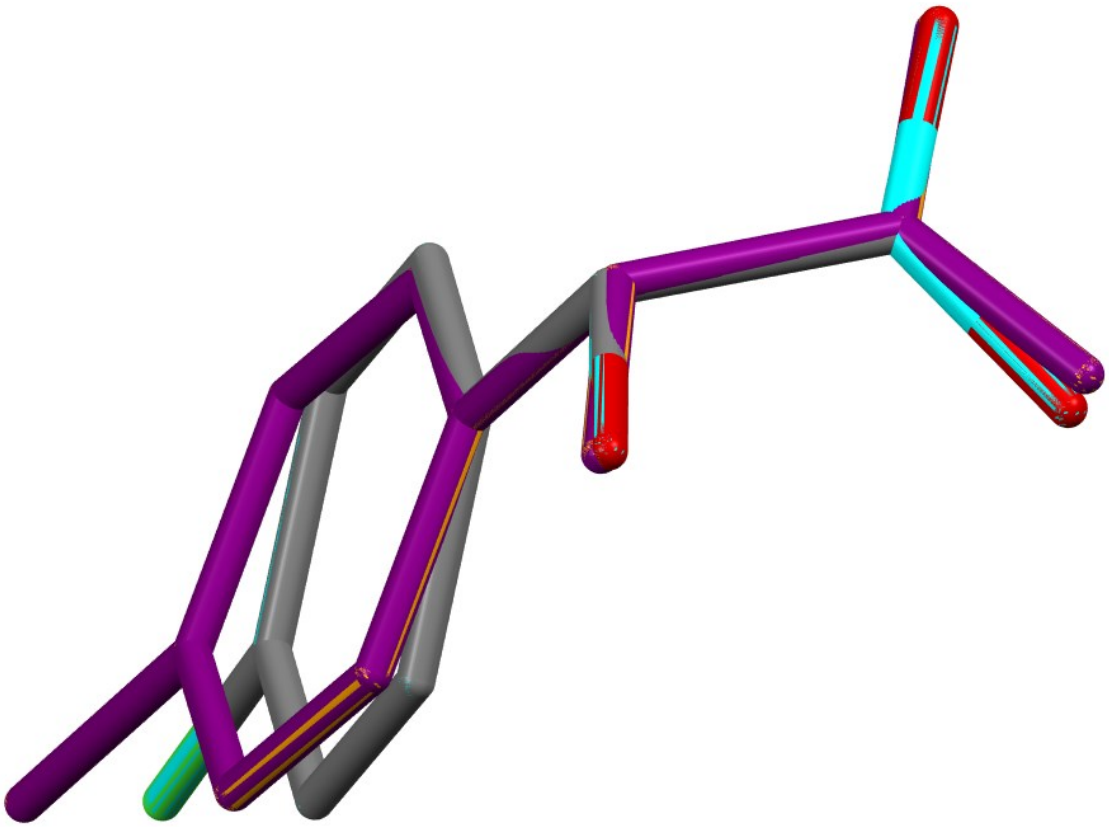


**FIGURE S18** Overlaid structure of the four crystallographically unrelated anions in **HET-4** for comparison, the molecules are overlaid so that the bonds of the asymmetric carbon atom overlapped

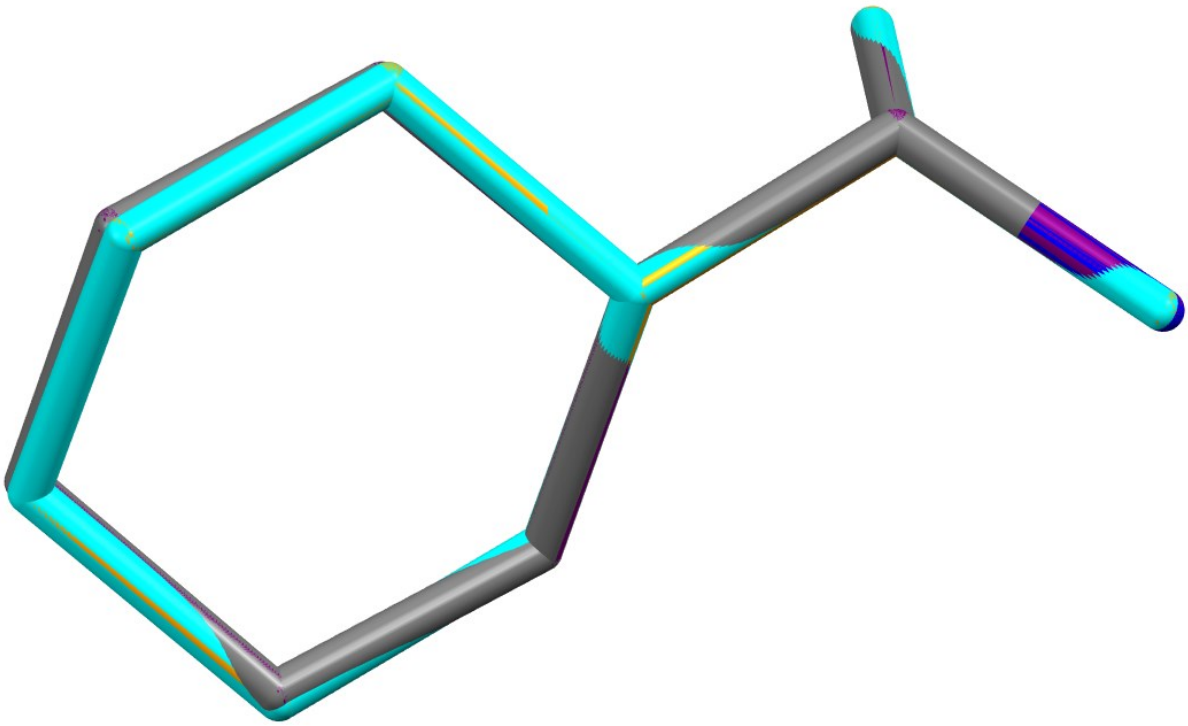


**FIGURE S19** Overlaid structure of the four crystallographically unrelated cations in **HET-4** for comparison, the molecules are overlaid so that the bonds of the asymmetric carbon atom overlapped

**Table S3** Properties of the Hirshfeld surfaces of the different ionpairs in the salts

| | HET4-1 | HET4-2 | HET4-3 | HET4-4 | HOM4 | HET2-1 | HET2-2 | HET2-3 | HET2-4 | HOM-2 |
|---|---|---|---|---|---|---|---|---|---|---|
| **Volume** | 397,24 | 400,30 | 401,47 | 401,19 | 401,52 | 421,08 | 407,82 | 418,74 | 424,87 | 387,86 |
| **Area** | 326,90 | 368,68 | 372,46 | 354,72 | 333,66 | 322,79 | 330,91 | 337,13 | 327,53 | 319,51 |
| **Globularity** | 0,799 | 0,712 | 0,707 | 0,742 | 0,789 | 0,842 | 0,804 | 0,803 | 0,834 | 0,805 |
| **Asphericity** | 0,066 | 0,375 | 0,446 | 0,102 | 0,112 | 0,049 | 0,022 | 0,052 | 0,023 | 0,021 |

| | DOB4-all | DOB4-1 | DOB4-2 | DOB2-all | DOB2-1 | DOB2-2 |
|---|---|---|---|---|---|---|
| **Volume** | 805,52 | 404,88 | 396,52 | 823,78 | 411,20 | 408,94 |
| **Area** | 575,83 | 338,79 | 327,91 | 590,28 | 335,58 | 337,16 |
| **Globularity** | 0,727 | 0,781 | 0,796 | 0,72 | 0,797 | 0,79 |
| **Asphericity** | 0,075 | 0,065 | 0,091 | 0,148 | 0,028 | 0,049 |

**Table S4** Percentage of the total Hirshfeld surface area for the short interactions of the different atom types

| | HET4-1 | HET4-2 | HET4-3 | HET4-4 | HOM4 | HET2-1 | HET2-2 | HET2-3 | HET2-4 | HOM-2 |
|---|---|---|---|---|---|---|---|---|---|---|
| **H** | 75,8 | 74,0 | 72,8 | 74,6 | 75,3 | 79,0 | 76,6 | 77,6 | 78,5 | 76,9 |
| **C** | 4,8 | 7,8 | 7,7 | 6,6 | 5,0 | 5,1 | 4,5 | 5,6 | 4,2 | 5,0 |
| **O** | 10,7 | 8,7 | 10,6 | 9,3 | 11,0 | 10,2 | 10,5 | 10,2 | 10,2 | 10,9 |
| **N** | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 |
| **Cl** | 8,6 | 9,5 | 8,8 | 9,5 | 8,7 | 5,7 | 8,4 | 6,7 | 7,1 | 7,3 |

| | DOB4-all | DOB4-1 | DOB4-2 | DOB2-all | DOB2-1 | DOB2-2 |
|---|---|---|---|---|---|---|
| **H** | 75,9 | 75,5 | 75,7 | 79,7 | 77,6 | 77,0 |
| **C** | 4,8 | 4,5 | 4,6 | 4,8 | 4,6 | 4,6 |
| **O** | 9,2 | 11,1 | 11,0 | 9,2 | 10,4 | 10,7 |
| **N** | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 |
| **Cl** | 10,2 | 8,8 | 8,8 | 6,3 | 7,4 | 7,7 |