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# Supplementary Material

## Cocrystals and Salts of 3,5-bis(pyridinylmethylene)piperidin-4-one with Aromatic Poly-carboxylates and Resorcinols: Influence of Stacking Interactions on Solid-state Luminescence Properties

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CCDC numbers for crystal structures: 1875811-1875817.

**Contents**

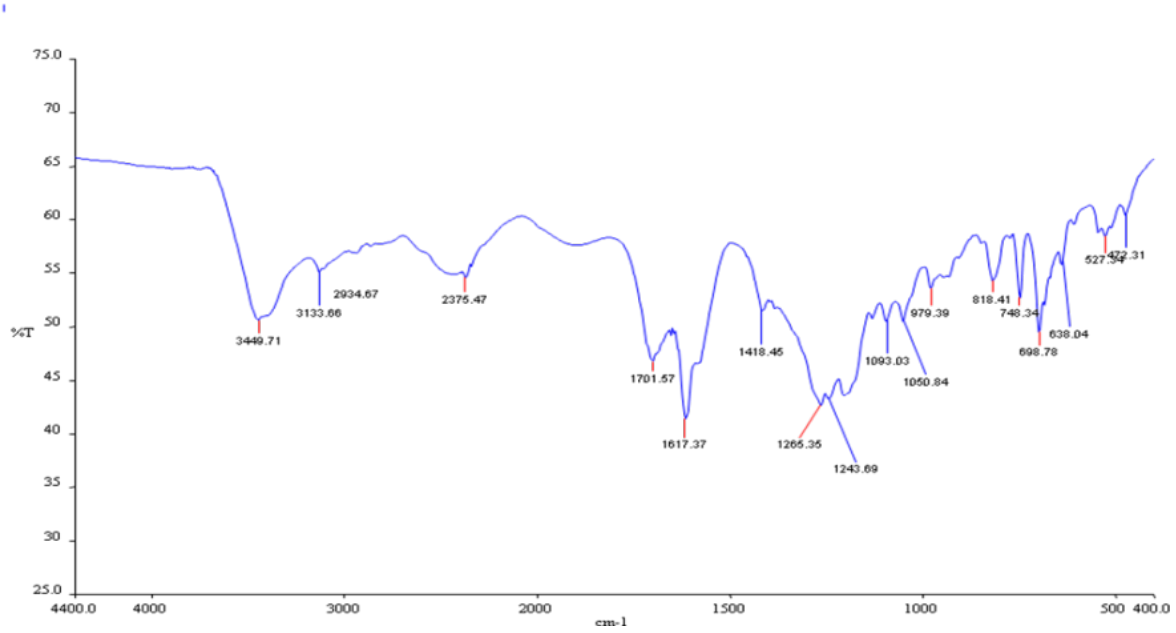


**Figure S1**: IR spectrum of **4**.

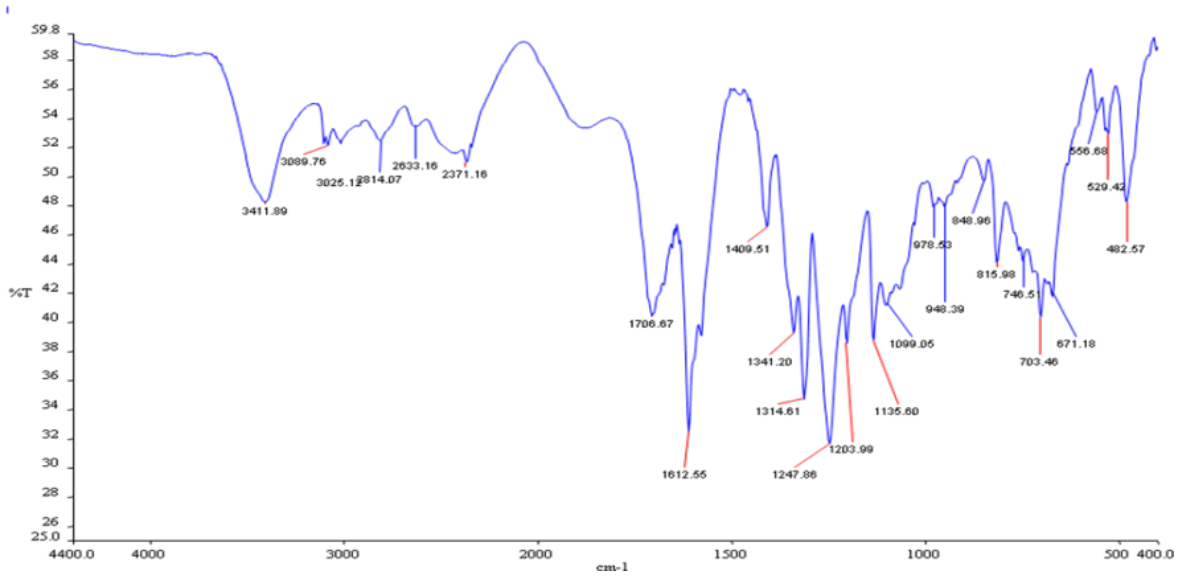


**Figure S2**: IR spectrum of **5**.

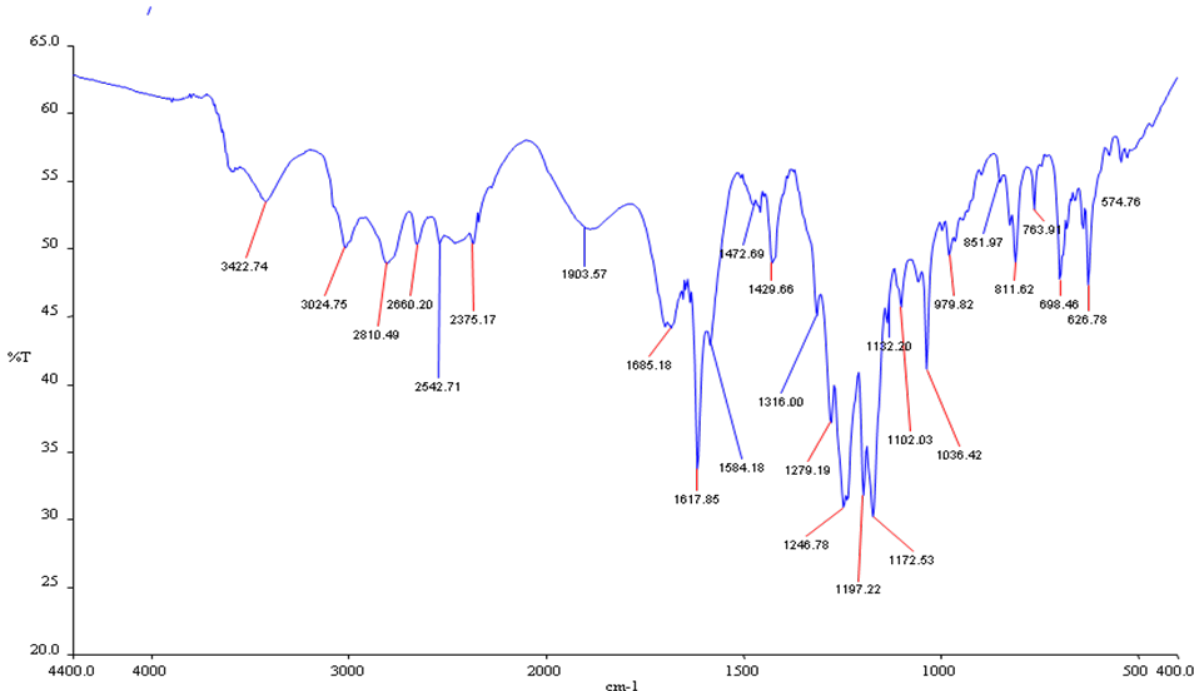


**Figure S3**: IR spectrum of **6**.

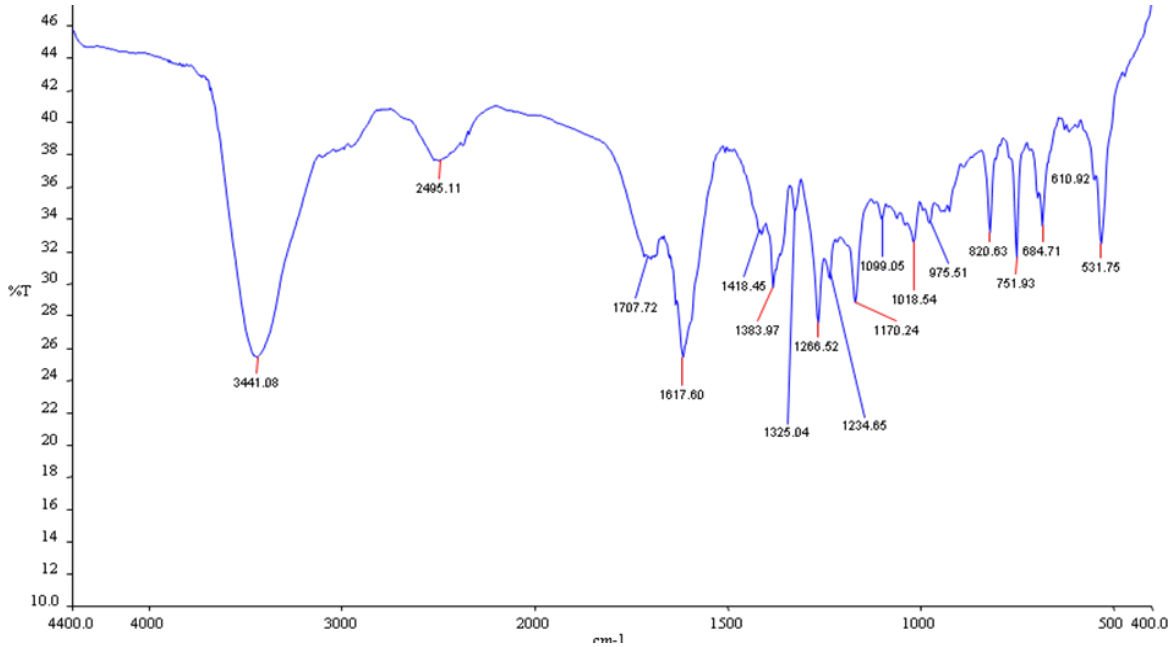


**Figure S4**: IR spectrum of **7**.

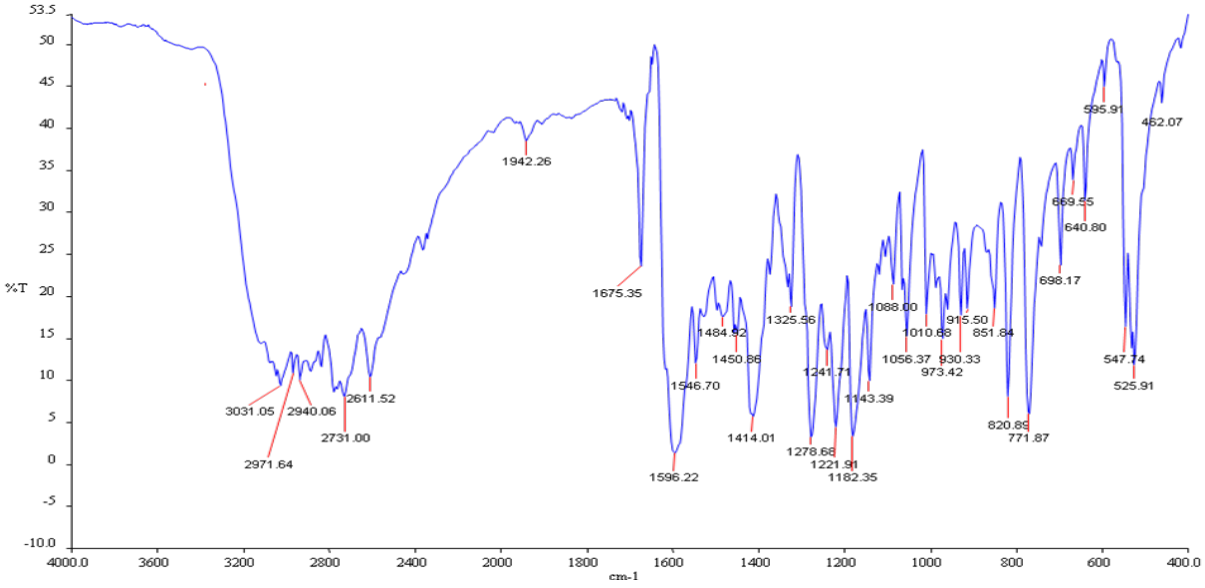


**Figure S5**: IR spectrum of **8**.

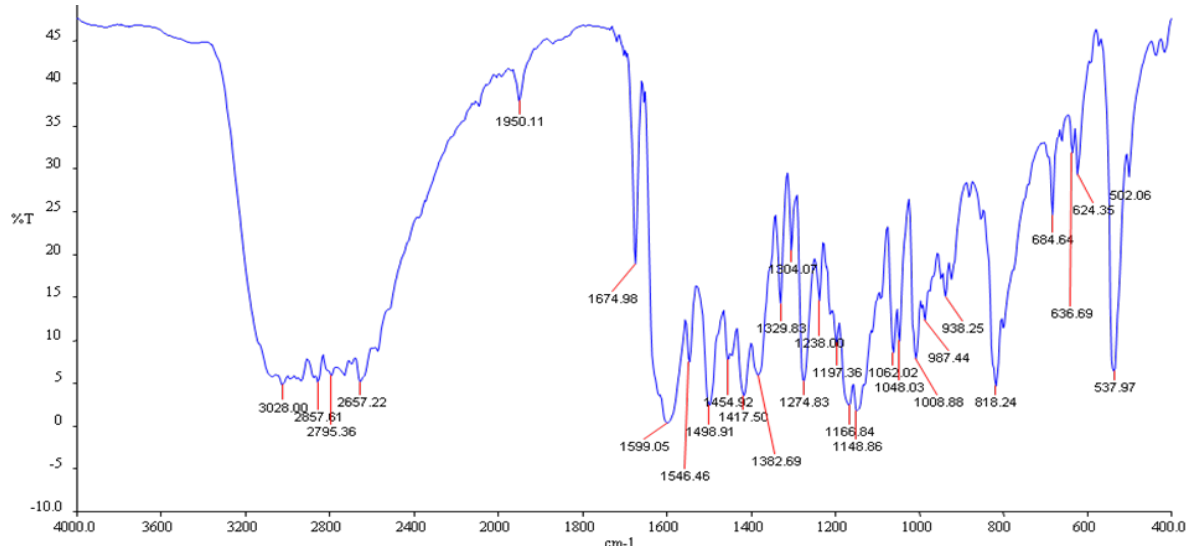


**Figure S6**: IR spectrum of **9**

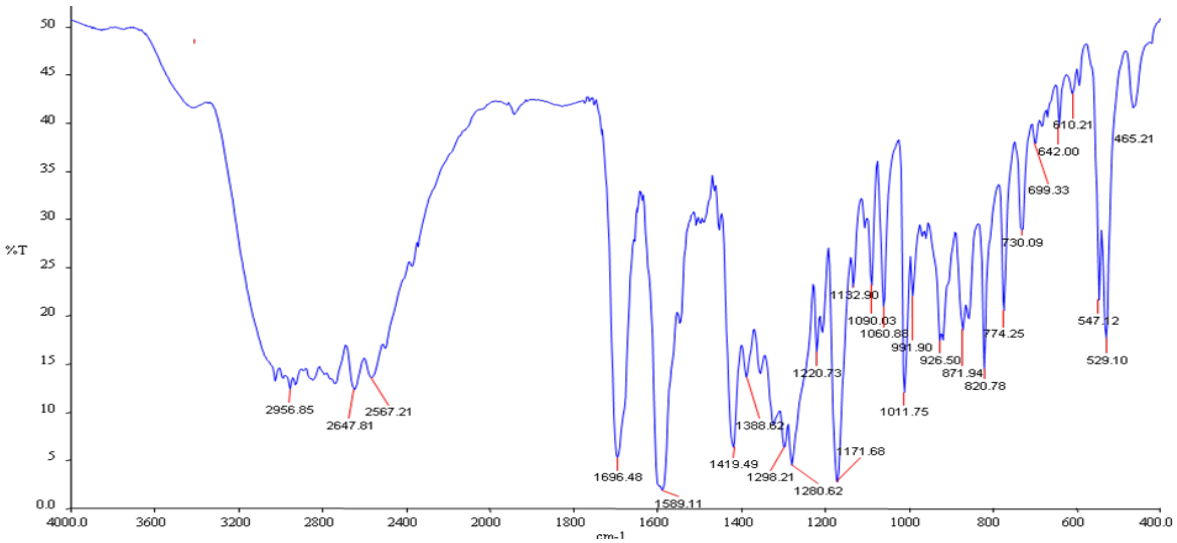


**Figure S7**: IR spectrum of **10**

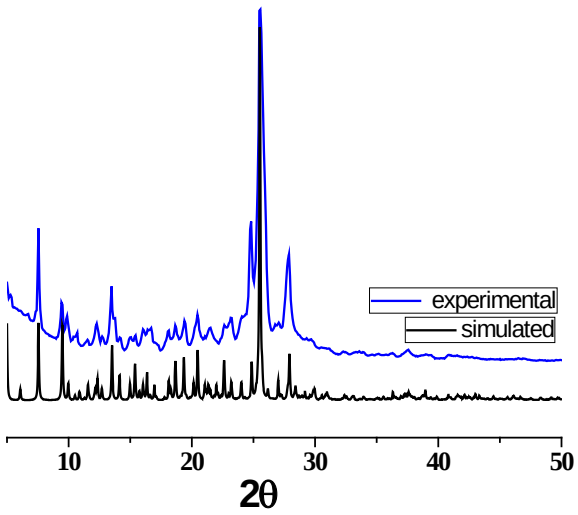


**Figure S8**: PXRD patterns of **4**.

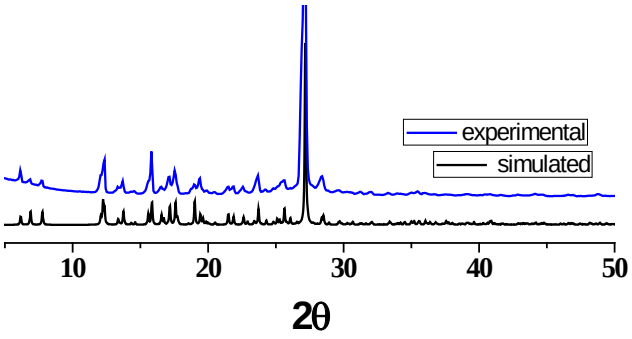


**Figure S9**: PXRD patterns of **5**.

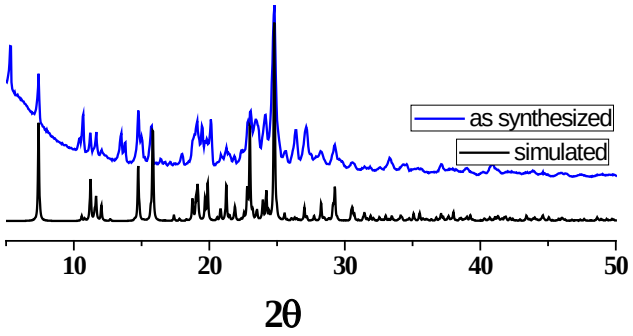


**Figure S10**: PXRD patterns of **6**.

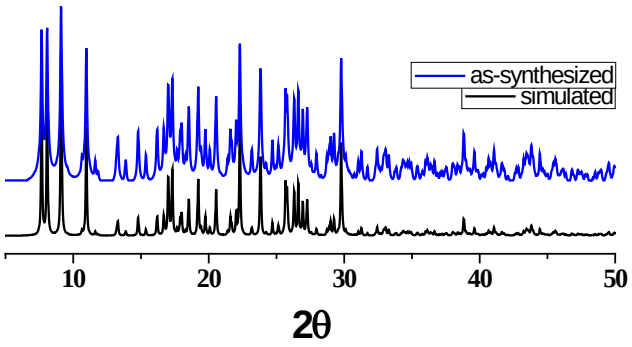


**Figure S11**: PXRD patterns of **7**.

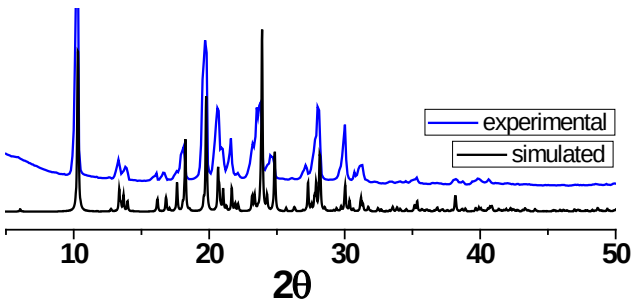


**Figure S12**: PXRD patterns of **8.**

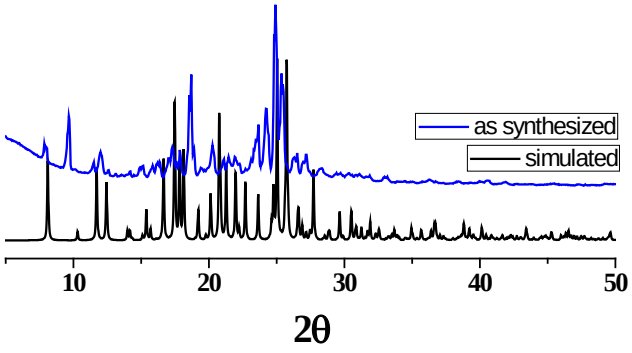


**Figure S13**: PXRD patterns of **9**.

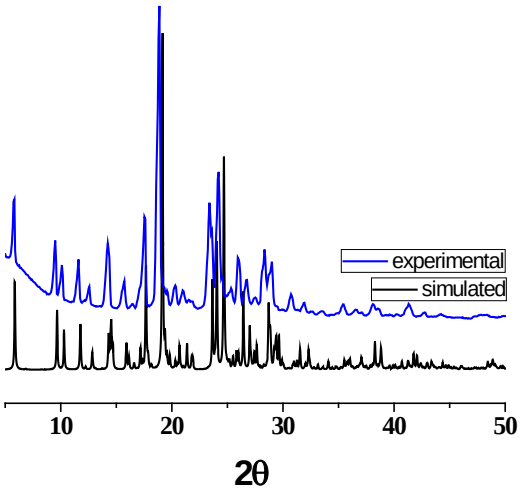


**Figure S14**: PXRD patterns of **10**.

**Table S1. Hydrogen Bonding Parameters in the Crystal Structures of 4-10**

| Complexes | Interaction | H···A (Å) | D···A (Å) | D–H···A (°) |
|---|---|---|---|---|
| **4** | O-H···O | 1.80 | 2.580(7) | 159 |
| | | 2.06 | 2.623(11) | 126 |
| | | 1.90 | 2.640(13) | 149 |
| | | 1.85 | 2.627(5) | 158 |
| | O-H···N | 1.85 | 2.624(7) | 158 |
| | | 1.82 | 2.616(7) | 162 |
| | N-H···N | 2.40 | 3.120(7) | 138 |
| | N-H···O | 2.53 | 3.202(7) | 133 |
| | | 1.83 | 2.707(6) | 170 |
| | | 1.95 | 2.766(6) | 151 |
| | | 2.38 | 3.028(6) | 129 |
| | | 1.80 | 2.691(6) | 174 |
| | | 2.55 | 3.1886) | 129 |
| | C-H···O | 2.22 | 3.127(8) | 164 |
| | | 2.19 | 3.094(9) | 164 |
| | | 2.27 | 3.076(7) | 144 |
| | | 2.55 | 3.418(14) | 155 |
| | | 2.46 | 3.358(8) | 162 |
| | | 2.44 | 3.282(7) | 146 |
| **5** | O-H···N | 1.74 | 2.561(3) | 176 |
| | | 1.87 | 2.690(3) | 180 |
| | N-H···O | 1.97 | 2.795(3) | 154 |
| | | 2.02 | 2.868(3) | 158 |
| | | 2.43 | 2.899(3) | 113 |
| | O-H···O | 1.74 | 2.555(3) | 172 |
| | C-H···O | 2.29 | 3.171(3) | 159 |
| | | 2.41 | 2.748(3) | 101 |
| | | 2.36 | 2.754(3) | 105 |
| | | 2.54 | 3.368(3) | 149 |
| | | 2.36 | 2.754(3) | 106 |
| | C-H···N | 2.58 | 3.461(4) | 158 |
| | | 2.62 | 3.363(4) | 137 |

Table-S1 continued

| | | | | |
|---|---|---|---|---|
| **6** | O-H···N | 1.80 | 2.615(3) | 170 |
| | O-H···O | 1.93 | 2.742(3) | 170 |
| | | 2.04 | 2.852(4) | 171 |
| | N-H···O | 2.50(3) | 2.911(3) | 107.3(19) |
| | | 2.01(3) | 2.876(3) | 155(2) |
| | N-H···N | 1.84(3) | 2.771(3) | 167(2) |
| | C-H···O | 2.48 | 3.373(3) | 161 |
| | | 2.33 | 2.727(3) | 106 |
| | | 2.38 | 3.237(3) | 153 |
| | | 2.44 | 3.364(3) | 175 |
| | | 2.50 | 3.471(4) | 175 |
| | | 2.54 | 2.900(3) | 103 |
| **7** | O-H···O | 1.24 | 2.471(2) | 180 |
| | | 1.94 | 2.735(5) | 162 |
| | O-H···N | 1.46(2) | 2.605(3) | 170(3) |
| | N-H···O | 1.77(2) | 2.679(2) | 162(3) |
| | C-H···N | 2.45 | 3.348(4) | 153 |
| | C-H···O | 2.51 | 3.302(3) | 138 |
| | | 2.57 | 3.359(5) | 138 |
| | | 2.52 | 3.468(2) | 164 |
| | | 2.58 | 3.447(3) | 156 |
| | | 2.40 | 3.267(3) | 156 |
| | | 2.37 | 2.737(3) | 103 |
| | | 2.45 | 3.348(3) | 153 |
| | | 2.33 | 2.729(3) | 106 |
| | | 2.38 | 3.241(3) | 155 |
| **8** | O-H···N | 1.85(2) | 2.869(3) | 176.8(11) |
| | | 1.85(2) | 2.776(3) | 173.3(16) |
| | C-H···N | 2.60 | 3.323(3) | 135 |
| | C-H···O | 2.33 | 2.735(3) | 106 |
| | | 2.33 | 2.733(2) | 106 |
| **9** | O-H···N | 1.93 | 2.748(2) | 176 |
| | | 2.00 | 2.8155(19) | 174 |
| | C-H···O | 2.43 | 3.362(2) | 164 |
| | | 2.34 | 2.736(2) | 105 |
| | | 2.33 | 2.733(2) | 106 |
| **10** | O-H···O | 1.87 | 2.6917(18) | 176 |
| | | 1.80 | 2.6212(18) | 176 |
| | O-H···N | 2.03 | 2.846(2) | 177 |
| | | 2.02 | 2.840(2) | 173 |
| | | 1.88 | 2.687(2) | 170 |
| | | 1.92 | 2.733(2) | 170 |
| | C-H···O | 2.41 | 3.337(2) | 161 |
| | | 2.53 | 3.167(2) | 123 |
| | | 2.51 | 3.360(2) | 146 |
| | | 2.32 | 2.734(2) | 107 |
| | | 2.35 | 2.741(2) | 105 |
| | | 2.54 | 3.239(2) | 130 |
| | | 2.32 | 2.728(2) | 106 |

**Table S2: p*K*a and Δp*K*a values**

| Ketones | Co-formers | p$K_a$ | | Δp$K_a$ | Complexes | Prediction | Complexes obtained |
|---|---|---|---|---|---|---|---|
| | | $pK_a(BH^+)$ | $pK_a(A)$ | | | | |
| **1** | $H_2$TMA | 6.36 | 3.14 | +3.22 | **4** | salt | salt |
| | $H_2$PDC | | 3.38 | +2.98 | **5** | salt | salt |
| | $H_2$SIP | | -2.88 | +9.24 | **6** | salt | salt |
| **3** | $H_2$TMA | 3.93 | 3.14 | +0.79 | **7** | Partial transfer of proton | Salt, exhibited mixed ionic hydrogen bonds |
| | DHBA | | 3.61 | +0.32 | **10** | Partial transfer of proton | Co-crystal |