New coordination compounds of Cu\textsuperscript{II} with Schiff base ligands – crystal structure, thermal and spectral investigations.

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**Table S1.** List of chosen mono- and polynuclear Schiff base complexes of Cu\textsuperscript{II} found in the CSD search [1]

| Complex (CSD refcodes) | Cu–N (Å) | Cu–O\textsubscript{phen} (Å) | Cu–O\textsubscript{hydr} (Å) | Cu–O\textsubscript{methoxy} (Å) | Ref. |
|------------------------|----------|--------------------------|--------------------------|----------------------------|-----|
| [Cu\textsubscript{2}(L)(O\textsubscript{2}CMe)] \cdot (C\textsubscript{4}H\textsubscript{6}NO) (IWIHEB) | 1.926(1) | 1.913(1) | 1.939(1) | – | [2] |
| | 1.933(1) | 1.923(2) | 1.983(1) | | |

[Image of chemical structure]
| Complex                          | \( \Delta \) | \( \Delta \mu \) | \( \Delta \) | \( \Delta \mu \) | Ref  |
|---------------------------------|----------------|----------------|----------------|----------------|------|
| \([\text{Cu}(L)(\text{H}_2\text{O})]_n\) (REFJIX) | 2.010          | 1.951          |                |                | [3]  |
| ![Cu(L)(H_2O)_n](image)        |                |                |                |                |      |
| \(\text{Cu}(\text{HL})(\text{N}_2)(\text{pTol})_2\) (GEPNEX) | 1.946(4)       | 1.901(3)       |                |                | [4]  |
| ![Cu(HL)(N_2)(pTol)_2](image)  | 1.950(4)       | 1.900(4)       |                |                |      |
| Complex | Cu-Cu [Å] | Cu—O [Å] | Cu—N [Å] | Ref. |
|---------|-----------|-----------|-----------|------|
| [Cu₂L(O₂CC₆H₄-o-NH₂)] (ABIWIS) | 1.941(4)  | 1.933(5)  | 1.844(4)  | 1.896(3)  | 1.914(3)  | –    | [5] |
| [Cu₂L(O₂CC₆H₄-p-NH₂)] (ABIWOY) | 1.943(4)  | 1.926(4)  | 1.891(3)  | 1.913(3)  | 1.927(3)  | –    | [6] |
| Complex                     | d(Cu–Cu) | d(Cu–N) | d(Cu–O) | Solv. | Ref. |
|-----------------------------|----------|---------|---------|-------|------|
| [Cu\textsuperscript{II}2(L\textsuperscript{-1}F)(μ-prz)] (AWAWAW) | 1.942(2) | 1.886(2) | 1.902(1) | –     | [6]  |
| Complex                                           | Bond Length 1 (Å) | Bond Length 2 (Å) | Bond Length 3 (Å) | Bond Length 4 (Å) | Bond Length 5 (Å) | Ref. |
|---------------------------------------------------|-------------------|-------------------|-------------------|-------------------|-------------------|------|
| $[\text{Cu}^{II}_2(\text{L}^1\text{-2OMe})\,(\mu\text{-prz})]\cdot0.5\text{CH}_3\text{CN}$ (AWAWEA) | 1.933(8)          | 1.870(6)          | 1.917(6)          | –                 | –                 | [6]  |
| $[\text{Cu}^{II}_2(\text{L}^\text{F})(\mu\text{-C}_7\text{H}_5\text{N}_2)]$ (AYEYOS)        | 1.956(6)          | 1.907(6)          | 1.959(4)          | –                 | –                 | [7]  |
| Structure                                      | Bond Lengths          | References |
|------------------------------------------------|-----------------------|------------|
| ![CuII_2(L−H)(µ-C_3H_5N_2)_·CH_3OH (AYEYUY)]  | 1.919(9) 1.907(9) 1.957(7) 1.955(6) | [7]        |
| ![CuII_2C_17H_15N_2O_3(CF_3COO)-CH_3OH (BATVEZ)] | 1.929(4) 1.915(4) 1.942(3) 1.902(3) | [8]        |
| Compound                        | Bond Lengths          | | | |
|--------------------------------|-----------------------|---|---|---|
| $[\text{Cu}_2(\text{L}^1)\text{(m-C}_6\text{H}_5\text{CO}_2)]$ (DEXNAV01) | 1.930(3)  | 1.890(3)  | 1.913(3)  | –  | [9] |
| $\text{C}_{20}\text{H}_{18}\text{Cu}_2\text{N}_4\text{O}_3, \text{H}_2\text{O}$ (DICDEY) | 1.93(1)   | 1.92(1)   | 1.89(1)   | –  | [10] |
| Compound                                      | Bond Length 1 (Å) | Bond Length 2 (Å) | Bond Length 3 (Å) | Bond Length 4 (Å) | Bond Length 5 (Å) | Reference |
|-----------------------------------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-----------|
| [{Cu2L(O2CC3H7N)} · C2H5OH]x (DINCUY)        | 1.956(6)          | 1.908(6)          | 1.932(6)          | –                 | –                 | [11]      |
| C17H16CuN2O3 (DUNPIL)                        | 1.937(3)          | 1.899(2)          | –                 | –                 | –                 | [12]      |
| Compound                                | Bond Length 1 | Bond Length 2 | Bond Length 3 | Bond Length 4 | Ref. |
|----------------------------------------|---------------|---------------|---------------|---------------|------|
| C_{27}H_{36}CuN_{2}O_{3} (FANLUB)      | 1.974(6)      | 1.904(5)      | –             | –             | [13] |
| [Cu_2(L^2)(O_2CMe)]·MeOH (FAPGOS)     | 1.93(1)       | 1.85(1)       | 1.878(9)      | –             | [14] |
| Structure                                      | Bond Length 1 (Å) | Bond Length 2 (Å) | Bond Length 3 (Å) | Notes      |
|------------------------------------------------|-------------------|-------------------|-------------------|------------|
| \([\text{Cu}_2(\text{L}^5)(\text{O}_2\text{CPh})]\cdot\text{H}_2\text{O}\) (FAPGUY) | 1.915(7)          | 1.924(7)          | 1.883(6)          |            |
|                                                 | 1.925(6)          | 1.885(6)          | 1.918(6)          |            |
| \(\text{C}_{19}\text{H}_{18}\text{Cu}_2\text{N}_2\text{O}_5\cdot\text{C}_4\text{H}_4\text{O}\) (FAPGOS01) | 1.929(3)          | 1.892(3)          | 1.913(3)          |            |
|                                                 | 1.922(3)          | 1.904(3)          | 1.909(3)          |            |

[14] [15]
| Compound                        | 1.943(2) | 1.909(1) | –       | –       | [16] |
|--------------------------------|----------|----------|---------|---------|------|
| Cu₂(L)(prz) (FUXVAV)           | 1.932(4) | 1.871(4) | 1.918(4)| –       | [17] |
| Chemical Formula | Data 1  | Data 2  | Data 3  | Data 4  | Ref. |
|------------------|---------|---------|---------|---------|------|
| $\text{C}_{22}\text{H}_{18}\text{Cu}_2\text{N}_4\text{O}_3$ (IYETEL) | 1.962(6) | 1.922(5) | 1.907(6) | –       | [18] |
| $[\text{Cu}_2(\text{L})(\text{OAc})]\cdot3\text{DMF}$ (HOWYEY) | 1.984(2) | 1.916(2) | 1.953(2) | –       | [19] |
| Complex                      | μ (Å)  | μ (Å)  | μ (Å)  | μ (Å)  | Reference |
|------------------------------|--------|--------|--------|--------|-----------|
| [Cu₂(L)(OAc)]₂·3DMF (HOWYIC) | 1.916(5)| 1.920(4)| 1.972(4)| –      | [19]      |
| [Cu₂(L)(Fa)]·2DMF (HOWYOI)  | 1.929(2)| 1.897(2)| 1.941(2)| –      | [19]      |
| Compound | Bond Length (Å) | Reference |
|----------|----------------|------------|
| [Cu₂(L)(Pa)]·DMF (HOWYUO) | 1.923(5) | 1.900(4) | 1.935(4) | – | [19] |
| [Cu₂(L)(μ-6-meo-pur)(dmf)] (IGEJEK) | 1.905(3) | 1.895(2) | 1.961(2) | – | [20] |
| | 1.923(6) | 1.893(4) | 1.906(4) | | |
| | 1.919(3) | 1.906(3) | 1.966(3) | | |
| Formula                  | 1.952 | 1.930 |       |       | [22] |
|-------------------------|-------|-------|-------|-------|------|
| C_{17}H_{14}CuN_{4}O_{7} (LIBNAM01) |       |       |       |       |      |

| Formula                  | 1.932(8) | 1.902(8) | 1.926(6) | – | [21] |
|-------------------------|----------|----------|----------|---|--|
| [Cu\textsubscript{2}L(O_{2}CCHCHC\textsubscript{6}H\textsubscript{4}p-OH)] (IVAXIM) |          |          |          |   |

| Formula                  | 1.936(8) | 1.905(7) | 1.910(7) | – | – | [21] |
|-------------------------|----------|----------|----------|---|--|--|
| [Cu\textsubscript{2}L(O_{2}CCHCHC\textsubscript{6}H\textsubscript{4}p-OH)] (IVAXIM) |          |          |          |   |   |

Table: Structure and bond lengths for copper complexes.
| Structure | Bond Lengths (Å) | Ref. |
|-----------|-----------------|------|
| C$_{30}$H$_{34}$Cu$_2$N$_4$O$_5$ (LOGPUU) | 1.937(4) 1.903(4) 1.905(4) | [23] |
| | 1.931(4) 1.900(3) 1.903(9) | |
| C$_{19}$H$_{16}$Cl$_2$Cu$_2$N$_2$O$_5$ 0.5(H$_2$O) (MIXXIA) | 1.916(3) 1.891(8) 1.903(9) | [24] |
| | 1.91(1) 1.876(5) 1.903(7) | |
| Chemical Formula | Bond Lengths (Å) | References |
|------------------|------------------|------------|
| \( \text{C}_{20}\text{H}_{21}\text{ClCu}_{2}\text{N}_{2}\text{O}_{6}, \text{CH}_{3}\text{O} \) (NEFFIO) | 1.916(5) 1.938(4) 1.925(4) 1.907(4) – | [25] |
| \([\text{Cu}_2(\text{L})(\mu\text{-pz})]\) (NIWNEP) | 1.962(9) 1.96(1) 1.894(9) 1.88(1) 1.877(9) 1.89(1) – | [26] |
| Chemical Formula          | Bond Length 1 | Bond Length 2 | Bond Length 3 | Reference |
|---------------------------|--------------|--------------|--------------|-----------|
| C_{22}H_{20}Br_2Cu_2N_4O_3 (OCIDOT) | 1.94(2) 1.975(2) 1.916(2) 1.884(1) | - | [27] |
| C_{24}H_{26}Cu_2N_4O_5 (ODAXUM)      | 1.946(3) 1.897(3) 1.890 | - | [28] |
| Structure | Formula | a | b | c | References |
|-----------|---------|---|---|---|------------|
| ![Cu₂L(O₂C-CH₂-C₆H₄-p-OH)]·H₂O (SAQMON) | [Cu₂L(O₂C-CH₂-C₆H₄-p-OH)]·H₂O (SAQMON) | 1.914(7) | 1.911(6) | 1.903(6) | – | [29] |
| ![Cu₂L(O₂C-CH₂-C₆H₄-p-OH)]·H₂O (SAQMON) | [Cu₂L(O₂C-CH₂-C₆H₄-p-OH)]·H₂O (SAQMON) | 1.925(3) | 1.894(2) | 1.894(2) | – | [29] |
Cu₂L(OAc)(CH₃OH)₂CH₃OH (TAWMOV)

| Distance (Å) | Cu₁-O₁ | Cu₂-O₂ |
|--------------|--------|--------|
| 1.902(3)     | 1.879(2)| 1.904(2)|
| 1.925(3)     | 1.891(3)| 1.898(3)|
| 1.936(3)     | 1.892(3)| 1.913(3)|
| Compound | Bond Lengths (Å) | References |
|----------|-----------------|------------|
| [Cu$_2$(L$^1$)(μ-HCO$_2$)] (TEFTAA) | | [31] |
| | 1.935(3) 1.925(3) | |
| | 1.886(2) 1.898(2) | |
| | 1.921(2) 1.910(2) | |
| | – | |
| | | |
| [Cu$_2$(L$^2$)(μ-HCO$_2$)] dmf (TEFTII) | | [31] |
| | 1.946(5) 1.957(5) | |
| | 1.906(4) 1.892(5) | |
| | 1.935(3) 1.920(3) | |
| | – | |
| | | |
| Cu$_2$(EGbsdpo)(OAc) (TOMYOK) | | [32] |
| | 1.925(4) 1.921(4) | |
| | 1.893(3) 1.898(3) | |
| | 1.910(3) 1.921(3) | |
| | – | |
| Structure | Formulas | Bond Distances (Å) | References |
|-----------|----------|-------------------|------------|
| ![Structure 1](image1.png) | $\text{C}_{31}\text{H}_{26}\text{Cu}_2\text{N}_2\text{O}_5$, CH$_2$O (VIDBAO) | $1.941(2)$, $1.951(2)$, $1.878(2)$, $1.882(2)$, $1.904(2)$, $1.891(2)$ | [33] |
| ![Structure 2](image2.png) | $\text{[Cu}_2\text{(C}_{17}\text{H}_{15}\text{N}_3\text{O}_3)(\text{HCOO})]}$ (WAZPIW) | $1.937(6)$, $1.921(4)$, $1.960(4)$ | [34] |
| ![Structure 3](image3.png) | $(\text{C}_{19}\text{H}_{22}\text{Cu}_2\text{N}_2\text{O}_6)_n$ (WOBNUY) | $1.983$, $1.938$, $-$ | [35] |
| (C_{19}H_{16}Br_{2}Cu_{2}N_{2}O_{5}), H_{2}O (XAZNOB) | 1.940(3) | 1.890(3) | 1.914(2) | –  | [36] |
| C_{22}H_{36}Cl_{2}Cu_{2}N_{4}O_{3} (XEFSAC) | 1.965(4) | 1.919(4) | 1.900(4) | –  | [37] |
| Chemical Formula | D1 | D2 | D3 | Reference |
|------------------|----|----|----|-----------|
| C37H34Cu2N2O7CH2Cl2 (XEHFIB) | 1.919(2) | 1.898(2) | 1.916(2) | – | [38] |
| C29H36Cu2N2O7 0.5(CH3O) (XEPDOO) | 1.941(2) | 1.895(3) | 1.920(3) | – | [39] |
|                  | 1.928(2) | 1.891(3) | 1.906(3) |         |
|------------------|----------|----------|----------|---------|
| $\text{[Cu}^{II}_6(L_5)(\mu_3\text{-SO}_4)_2(\mu_2$-\text{SO}_4)(\text{MeOH})_2\cdot\text{H}_2\text{O}\cdot15.5(\text{MeOH})\cdot15.5(\text{MeCN})\text{ (BOQMEA)}$ | 1.929(9) | 1.934(7) | 1.929(7) | 2.286(7) | [40] |
|                  | 1.907(9) | 1.883(7) | 1.924(7) |         |
|                  |          |          |          |         |
| Structure                  | Bond Lengths (Å) | Reference |
|---------------------------|------------------|-----------|
| [Cu₂L₂(3-ppz)₂] (CEPKUE)  | 1.942 (5)        | [41]      |
|                           | 1.935 (6)        |           |
|                           | 1.928 (3)        |           |
|                           | 1.890 (4)        |           |
|                           | 1.978 (3)        |           |
|                           | 2.360 (4)        |           |
\[
[Cu_3L^1L^2(1-MeIm)(H_2O)](ClO_4)\] (AWERID)

\[
\begin{array}{cccc}
1.920(3) & 2.061(2) & 1.974(2) & – \\
1.932(2) & 1.897(2) & 1.961(2) & [42]
\end{array}
\]
\[ [\text{Cu}_3(\text{HL})_2\text{L}^+]\text{(ClO}_4^-) \text{(ILAPIU)} \]

- 1.919(7)
- 1.949(7)
- 1.967(7)

- 1.916(5)
- 1.913(6)
- 2.069(5)
- 1.941(5)
- 2.217(5)

- 1.959(5)
- 1.962(4)
- –
- [43]
\[ \text{Cu}_3(\text{HL})_2(\text{ClO}_4) \text{ (ILAPEQ)} \]

| Bond Length (Å) | [Cu$_3$(HL)$_2$(O$_2$CC$_6$H$_4$-p-OH)$_2$] (IVESAD) |
|----------------|-------------------------------------------------|
| 1.958(6)       | 1.982(4)                                        |
| 1.988(6)       | 1.902(4)                                        |
| 1.911(4)       | 1.941(4)                                        |
| 1.906(4)       |                                                 |
| 1.976(5)       |                                                 |
| 1.941(4)       |                                                 |
| 1.896(5)       |                                                 |

\[ \text{Cu}_4\text{L}_2(O_2\text{CC}_6\text{H}_4-p\text{-OH})_2 \text{ (IVESAD)} \]

| Bond Length (Å) | [Cu$_4$L$_2$(O$_2$CC$_6$H$_4$-p-OH)$_2$] (IVESAD) |
|----------------|-------------------------------------------------|
| 1.931(7)       | 1.932(6)                                        |
| 1.930(6)       | 1.926(6)                                        |
| 1.917(5)       | 1.896(5)                                        |
| 2.401(4)       |                                                 |

[44]
$[\text{Cu}_3\text{L}_2(\mu_1,\mu_3\text{N}_3)_2] \cdot 5\text{H}_2\text{O}$ (GAFQAG)

$$
\begin{array}{cccc}
1.922(2) & 1.904(2) & 1.979(2) & - \\
1.947(3) & 1.874(2) & 1.958(2) & - \\
1.885(2) & 1.971(2) & & \\
1.879(2) & 1.977(2) & & \\
\end{array}
$$
| Chemical Formula                        | Bond Length 1     | Bond Length 2     | Bond Length 3     | Bond Length 4     | Reference |
|----------------------------------------|-------------------|-------------------|-------------------|-------------------|-----------|
| C₃₄H₃₂Cu₃N₆O₁₂, C₂H₆O H₂O (TETCEB)     | 1.947(5)          | 1.940(3)          | –                 | –                 | [46]      |
|                                        | 1.959(4)          | 1.951(4)          | –                 | –                 |           |
| [Cu₄(L-Br)₂(μ-C₄H₆O₄)(dmf)₂] (FIYFAV)  | 1.920(5)          | 1.886(5)          | 1.928(4)          | –                 | [47]      |
|                                        | 1.931(5)          | 1.885(5)          | 1.926(5)          | –                 |           |
\[
[Cu_4(L-Cl)_2(\mu-\text{C}_6\text{H}_4\text{O}_2)(\text{dmf})_2] \text{ (FIYFEZ)}
\]

|   |   |   |   |   |   |
|---|---|---|---|---|---|
|   | 1.942(4) | 1.882(3) | 1.924(3) | – | 48 |
|   | 1.929(4) | 1.883(3) |   |   |   |
| Formula | Bond Lengths (Å) | Temperature (°C) | Disorder | Literature |
|---------|-----------------|------------------|----------|------------|
| \([\text{Cu}_4(L^2)_2(\mu-\text{C}_3\text{H}_6\text{O}_2\cdot 2\text{H}_2\text{O}-2\text{CH}_3\text{CN} \text{ (DOYSOA)})}\) | 1.932(3) | 1.891(2) | 1.904(2) | – | [48] |
| Chemical Formula | Bond Lengths (Å) | Reference |
|------------------|-----------------|-----------|
| C76H78Cu6N8O122+ 2(CH2O) 2(ClO4-) · H2O (MAPDEP) | 1.949(4), 1.932(3), 1.918(3), 1.929(4), 1.930(3), 1.893(3) | [49] |
| C76H78Cu6N8O122+ 2(CH2O) 2(ClO4-) · H2O (MAPDEP) | 1.949(3), 1.932(3), 1.918(3), 1.929(4), 1.930(3), 1.893(3) | [49] |
| [Cu4L2(μ1,1-N3)2] · CH3CN (KUKTAM) | 1.949(3), 1.888(4), 1.938(3), – | [50] |
Figure S1. FTIR spectra of the Schiff base ligand $\text{H}_3\text{L}_1$ and complex 1.

Figure S2. FTIR spectra of the Schiff base ligand $\text{H}_3\text{L}_1$ and complex 2.
Figure S3. FTIR spectra of the complexes 1 and 2.

Figure S4. FTIR spectra of the Schiff base ligand $\text{H}_3\text{L}_2$ and complex 3.
**Figure S5.** FTIR spectra of the Schiff base ligand H$_3$L$_2$ and complex 4.

**Figure S6.** FTIR spectra of the complexes 3 and 4.
### Table S2. Hydrogen bonding and C-H···π interactions geometry [Å, °] for complexes 1-4.

#### Hydrogen bonds

| D-H···A                  | d(D-H) | d(H···A) | d(D···A) | θ DHA |
|-------------------------|--------|----------|----------|-------|
| O(1W)‒H(1W)···O(4)      | 0.83   | 2.28     | 2.884(4) | 130   |
| O(1W)‒H(1W)···O(5)      | 0.83   | 2.11     | 2.897(4) | 157   |
| O(1W)‒H(2W)···O(1)      | 0.83   | 1.97     | 2.803(4) | 174   |
| O(3)‒H(3B)···O(1W)      | 0.84   | 2.02     | 2.734(4) | 142   |
| C(4)‒H(4B)···O(3)       | 0.98   | 2.52     | 3.222(6) | 128   |
| C(11)‒H(11D)···O(3)     | 0.99   | 2.47     | 3.444(5) | 168   |

| O(1M)‒H(1M)···O(2M)     | 0.84   | 1.86     | 2.700(5) | 174   |
| O(1W)‒H(1W)···O(7)      | 0.87   | 1.97     | 2.834(5) | 176   |
| O(2M)‒H(2M)···O(1W)     | 0.84   | 1.82     | 2.646(5) | 167   |
| O(1W)‒H(2W)···O(5)      | 0.87   | 1.99     | 2.841(3) | 166   |
| O(2W)‒H(3W)···O(1)      | 0.86   | 2.30     | 3.095(4) | 154   |
| O(2W)‒H(3W)···O(6)      | 0.86   | 2.36     | 3.039(4) | 135   |
| O(2W)‒H(4W)···O(2)      | 0.86   | 2.41     | 2.949(5) | 121   |
| O(2W)‒H(4W)···O(2W)     | 0.86   | 2.30     | 2.891(6) | 126   |
| C(8)‒H(8)···O(2M)       | 0.95   | 2.46     | 3.407(5) | 174   |
| C(22)‒H(22A)···Br(2)    | 0.98   | 2.85     | 3.424(5) | 118   |

| O(1M)‒H(1M)···O(3)      | 0.84   | 2.56     | 3.092(3) | 123   |
| O(1M)‒H(1M)···O(5)      | 0.84   | 2.25     | 3.080(3) | 169   |
| O(2M)‒H(2M)···O(1)      | 0.84   | 2.04     | 2.842(3) | 159   |
| C(11)‒H(11B)···O(2M)    | 0.99   | 2.60     | 3.535(3) | 157   |
| C(13)‒H(13C)···O(2M)    | 0.98   | 2.58     | 3.534(4) | 166   |

| O(1W)‒H(1WA)···O(3)     | 0.85   | 2.17     | 2.963(3) | 156   |
| O(1W)‒H(1WA)···O(5)     | 0.85   | 2.40     | 3.049(3) | 134   |
| O(1M)‒H(1M)···O(2W)     | 0.82   | 1.88     | 2.697(4) | 174   |
| O(1W)‒H(1WB)···O(1M)    | 0.85   | 1.97     | 2.820(3) | 176   |
| O(2M)‒H(2M)···O(1W)     | 0.82   | 1.94     | 2.728(4) | 160   |
| O(2W)‒H(2WA)···O(1)     | 0.85   | 2.05     | 2.858(3) | 158   |

#### C-H···π interactions

| C-H···Cg                 | d(D-H) | d(H···Cg) | d(C···Cg) | θ CHCg |
|-------------------------|--------|----------|----------|--------|
| C(9B)‒H(9C)···Cg(5)     | 0.99   | 2.43     | 3.320(10)| 150    |
| C(11)‒H(11C)···Cg(6)    | 0.99   | 2.83     | 3.737(5) | 153    |
| C(10A)‒H(10A)···Cg(6)   | 1.00   | 2.94     | 3.761(11)| 140    |
Symmetry codes for complex 1: (1a) x+1,y,z; (1b) x-1,y,z; (1c) -x,-y+2,-z; (1d) -x,y-2,-z; Cg(5) and Cg(6) are centroids of phenyl C(1)→C(7) and C(13)→C(19) rings
Symmetry codes for complex 2: (2a) x,y,-z+1; (2b) x, y, z-1; (2c) x-1, y-1, z-2; (2d) x-1, y-1, z-1; (2e) x, y+1, -z+1; Cg(8) is centroids of phenyl C(1)→C(7) ring
Symmetry codes for complex 3: (3a) -x+1,-y+1,-z+1; (3b)-x+3/2,y-1/2,-z+1/2; (3c)-x+1,-y+2,-z+1; (3d)-x+3/2,y-1/2,-z+3/2; Cg(7) is centroids of phenyl C(1)→C(6) ring
Symmetry codes for complex 4:(4b)-x,y-1/2,-z+1/2; (4c) -x+1, -y+2, -z+1;(4d) -x+1, y-1/2, -z+1/2; Cg(9) is centroids of phenyl C(1)→C(6) ring.

Figure S7. The packing of structure 1 along the a direction
**Figure S8.** The crystal structure packing of complex 3 showing formed layers via C-H···O interactions.

**Figure S9.** FTIR spectra of gaseous products of complex 2, decomposition in nitrogen.
Figure S10. FTIR spectra of gaseous products of complex 4 decomposition in nitrogen.

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