

Supplementary Information

Metal-organic frameworks with oxazoline-containing tripodal ligand: structure changes *via* reaction medium and metal-to-ligand ratio

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Table S1 Distances [Å] and angles [°] of hydrogen bonding for complexes **1-6**^a

| D-H...A ^b | Distance (D...A ^b) | D-H-A ^b | Angle (D-H-A ^b) |
|------------------------------------|-----------------------------------|----------------------------------|--------------------------------|
| 1 | | | |
| C(8)-H(8A)...O(1W) | 3.345(12) | C(8)-H(8A)-O(1W) | 135 |
| C(9)-H(9B)...O(15) ^{#1} | 3.428(11) | C(9)-H(9B)-O(15) ^{#1} | 156 |
| C(15)-H(15B)...O(25) ^{#2} | 3.378(15) | C(15)-H(15B)-O(25) ^{#2} | 142 |
| C(23)-H(23B)...O(14) ^{#1} | 3.367(11) | C(23)-H(23B)-O(14) ^{#1} | 156 |
| C(27)-H(27B)...O(17) ^{#3} | 3.029(15) | C(27)-H(27B)-O(17) ^{#3} | 117 |

| | | | |
|-------------------------------------|-----------|-----------------------------------|--------|
| C(41)-H(41B)···O(2W) ^{#4} | 3.119(15) | C(41)-H(41B)-O(2W) ^{#4} | 122 |
| C(44)-H(44A)···O(13) ^{#5} | 3.296(10) | C(44)-H(44A)-O(13) ^{#5} | 143 |
| C(51)-H(51A)···O(21) ^{#6} | 3.338(19) | C(51)-H(51A)-O(21) ^{#6} | 142 |
| C(53)-H(53A)···O(26) ^{#6} | 3.40(3) | C(53)-H(53A)-O(26) ^{#6} | 142 |
| C(54)-H(54A)···O(17) ^{#6} | 3.256(18) | C(54)-H(54A)-O(17) ^{#6} | 133 |
| C(57)-H(57B)···O(18) ^{#5} | 3.34(2) | C(57)-H(57B)-O(18) ^{#5} | 155 |
| C(59)-H(59A)···O(25) ^{#7} | 3.361(17) | C(59)-H(59A)-O(25) ^{#7} | 165 |
| C(59)-H(59B)···O(5) ^{#3} | 3.247(8) | C(59)-H(59B)-O(5) ^{#3} | 147 |
| 2 | | | |
| C(5)-H(5B)···O(6) | 3.406(11) | C(5)-H(5B)-O(6) | 165 |
| C(12)-H(12A)···O(6) ^{#8} | 3.406(15) | C(12)-H(12A)-O(6) ^{#8} | 147 |
| C(12)-H(12C)···O(4) ^{#9} | 3.383(16) | C(12)-H(12C)-O(4) ^{#9} | 156 |
| 3 | | | |
| C(6)-H(3)···O(33) | 3.39(3) | C(6)-H(3)-O(33) | 155 |
| C(32)-H(9)···O(22) ^{#10} | 3.53(2) | C(32)-H(9)-O(22) ^{#10} | 173 |
| C(33)-H(10)···O(31) ^{#10} | 3.16(4) | C(33)-H(10)-O(31) ^{#10} | 158 |
| C(233)-H(31)···O(15) ^{#11} | 3.50(4) | C(233)-H(31)-O(15) ^{#11} | 165 |
| 4 | | | |
| O1W-H1WA···N3 ^{#12} | 2.871(5) | O1W-H1WA-N3 ^{#12} | 160(4) |
| O1W-H1WB···O4 | 2.935(6) | O1W-H1WB-O4 | 164(3) |
| C4-H4A···O1W ^{#12} | 3.315(6) | C4-H4A-O1W ^{#12} | 162 |
| C12-H12A···O6 ^{#13} | 3.369(7) | C12-H12A-O6 ^{#13} | 143 |
| C14-H14A···O6 ^{#14} | 3.338(7) | C14-H14A-O6 ^{#14} | 137 |
| C14-H14B···O5 ^{#15} | 3.433(8) | C14-H14B-O5 ^{#15} | 164 |
| C17-H17A···O1W ^{#16} | 3.251(7) | C17-H17A-O1W ^{#16} | 163(3) |
| 5 | | | |
| C(6)-H(6A)···Br(2) | 3.712(7) | C(6)-H(6A)-Br(2) | 157 |
| 6 | | | |
| C(6)-H(6A)···Br(4) | 3.740(11) | C(6)-H(6A)-Br(4) | 165 |
| C(12)-H(12B)···Br(4) ^{#17} | 3.617(14) | C(12)-H(12B)-Br(4) ^{#17} | 132 |
| C(14)-H(14B)···Br(4) ^{#18} | 3.842(11) | C(14)-H(14B)-Br(4) ^{#18} | 165 |

^a Symmetry transformations are used to generate equivalent atoms: #1 2-x, 1-y, 1-z; #2 1-x, 2-y, 1-z; #3 1-x, 1-y, 1-z; #4 1-x, -1-y, 1-z; #5 1-x, -y, 1-z; #6 -x, 1-y, 1-z; #7 x, -1+y, z; #8

-1/3+x, -2/3+x-y, -1/6+z; #9 1/3-y, -1/3+x-y, -1/3+z; #10 -x, -1/2+y, 1-z; #11 1/2-x, 1/2-y, z;
#12 1-x, 1-y, -z; #13 -1+x, y, -1+z; #14 -1+x, 1+y, z; #15 x, 1+y, z; #16 2-x, 1-y, 1-z; #17
3/2-x, -y, z; #18 x, 1/2-y, 1/2-z.

^bD: donor; A: acceptor.