

Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for co-crystals **I-VI**

**I**

Cl(1)-C(1)	1.753(6)	Cl(3)-C(1)	1.750(5)
Cl(2)-C(1)	1.764(6)	O(1)-C(2)	1.420(5)

Cl(3)-C(1)-Cl(1)	110.5(3)	Cl(1)-C(1)-Cl(2)	109.6(4)
Cl(3)-C(1)-Cl(2)	111.6(3)		

**II**

Cl1-C1S	1.745(2)	C1-C2	1.507(3)
Cl2-C1S	1.752(2)	C2-C3	1.517(4)
Cl3-C1S	1.759(2)	C3-C4	1.518(4)
O1-C1	1.213(2)	C4-C5	1.519(3)
C1-C5	1.494(4)		

Cl1-C1S-Cl2	110.09(12)	C5-C1-C2	108.34(19)
Cl1-C1S-Cl3	109.48(10)	C1-C2-C3	105.0(2)
Cl2-C1S-Cl3	110.98(11)	C2-C3-C4	104.3(2)
O1-C1-C5	126.1(2)	C3-C4-C5	103.7(2)
O1-C1-C2	125.6(2)	C1-C5-C4	105.75(19)

**III**

Cl(1)-C(1S)	1.7508(17)	C(1)-C(6)	1.505(2)
Cl(2)-C(1S)	1.7585(16)	C(2)-C(3)	1.521(2)
Cl(3)-C(1S)	1.7595(16)	C(3)-C(4)	1.525(2)
O(1)-C(1)	1.212(2)	C(4)-C(5)	1.512(3)
C(1)-C(2)	1.499(2)	C(5)-C(6)	1.520(3)

Cl(1)-C(1S)-Cl(2)	110.23(8)	C(1)-C(2)-C(3)	112.54(13)
Cl(1)-C(1S)-Cl(3)	110.45(8)	C(2)-C(3)-C(4)	110.87(14)
Cl(2)-C(1S)-Cl(3)	110.29(9)	C(5)-C(4)-C(3)	110.59(17)
O(1)-C(1)-C(2)	122.44(14)	C(4)-C(5)-C(6)	111.47(14)
O(1)-C(1)-C(6)	122.06(15)	C(1)-C(6)-C(5)	112.70(13)
C(2)-C(1)-C(6)	115.48(16)		

**IV**

Cl1-C5	1.752(3)	N1-C3	1.469(3)
Cl2-C5	1.766(3)	C1-C2	1.518(4)
Cl3-C5	1.757(3)	C3-C4	1.518(3)
N1-C1	1.462(3)		

C1-N1-C3	112.42(16)	Cl1-C5-Cl3	111.05(16)
N1-C1-C2	110.88(19)	Cl1-C5-Cl2	109.20(14)
N1-C3-C4	110.64(18)	Cl3-C5-Cl2	110.10(15)

**V**

Cl(1)-C(1)	1.762(4)	N(1)-C(3)	1.443(6)
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Cl(2)-C(1)	1.770(4)	N(1)-C(4)	1.444(5)
Cl(3)-C(1)	1.753(4)	O(1)-C(2)	1.220(5)
N(1)-C(2)	1.332(4)		

C(2)-N(1)-C(3)	122.2(3)	Cl(3)-C(1)-Cl(2)	110.3(2)
C(2)-N(1)-C(4)	120.1(3)	Cl(1)-C(1)-Cl(2)	109.59(19)
C(3)-N(1)-C(4)	117.7(3)	O(1)-C(2)-N(1)	125.9(3)
Cl(3)-C(1)-Cl(1)	110.9(2)		

## VI

Cl1-Cl	1.7613(7)	C1-Cl1 <sup>1</sup>	1.7613(7)
Cl2-Cl	1.7587(12)		

<sup>1</sup><sub>+X,0.5-Y,+Z</sub>

Cl2-C1-Cl1 <sup>1</sup>	111.16(4)	Cl1 <sup>1</sup> -C1-Cl1	109.65(6)
Cl2-C1-Cl1	111.16(4)		

<sup>1</sup><sub>+X,0.5-Y,+Z</sub>