**X-ray Crystallography Data for:**

**Stereoisomerization of human constitutive androstane receptor agonist CITCO**

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**Contents:**

[Species *E-CITCO* 1](#__RefHeading___Toc44987_3210615111)

[Species *Z*-CITCO 15](#__RefHeading___Toc44989_3210615111)

# Species *E-CITCO*

**Table X-1**. Crystal data and structure refinement for *E*-CITCO

Identification code *E*-CITCO

Empirical formula C22.50H16Cl3N3OS

Formula weight 482.79

Temperature 150(2) K

Wavelength 1.54178 Å

Crystal system Monoclinic

Space group C2/c

Unit cell dimensions a = 35.774(11) Å = 90°.

b = 6.935(3) Å = 121.277(14)°.

c = 20.419(4) Å  = 90°.

Volume 4330(3) Å3

Z 8

Density (-123ºC) 1.481 Mg/m3

Absorption coefficient 4.905 mm-1

F(000) 1976

Crystal size 0.070 x 0.027 x 0.010 mm3

Theta range for data collection 2.890 to 68.239°.

Index ranges -42<=h<=42, -8<=k<=8, -23<=l<=19

Reflections collected 12918

Independent reflections 3786 [Rint = 0.0720]

Completeness to theta = 67.679° 95.5 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.7538 and 0.4269

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 3786 / 343 / 372

Goodness-of-fit on F2 1.136

Final R indices [I>2sigma(I)] R1 = 0.0727, wR2 = 0.1872

R indices (all data) R1 = 0.0877, wR2 = 0.1938

Largest diff. peak and hole 0.342 and -0.404 e.Å-3

**Table X-2**. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for *E*-CITCO. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

x y z U(eq)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C(4") 2942(4) 6019(15) 2881(9) 47(2)

C(5") 3361(3) 4881(16) 3215(7) 42(2)

C(6") 3365(3) 3093(15) 2901(5) 42(2)

C(7") 3753(3) 2056(11) 3193(4) 42(2)

Cl(7A) 3746(1) -119(3) 2777(1) 58(1)

C(8") 4135(2) 2767(13) 3821(4) 41(1)

Cl(8A) 4622(1) 1478(4) 4203(1) 61(1)

C(9") 4134(2) 4513(12) 4145(4) 48(2)

C(10") 3747(3) 5563(14) 3830(6) 48(2)

C(4B) 2978(19) 5620(100) 2890(50) 47(2)

C(5B) 3364(15) 4420(80) 3170(30) 35(7)

C(6B) 3294(15) 2800(70) 2730(30) 40(8)

C(7B) 3633(10) 1470(60) 2990(20) 44(7)

C(8B) 4049(8) 1900(40) 3600(20) 50(7)

C(9B) 4105(9) 3660(60) 3956(18) 56(10)

C(10B) 3766(13) 4910(60) 3810(30) 42(7)

Cl(8B) 4475(5) 250(20) 3876(10) 83(4)

Cl(9B) 4588(4) 4170(20) 4814(8) 104(5)

S(1) 3752(1) 4365(2) 6869(1) 49(1)

C(2) 3906(2) 4239(8) 6182(3) 46(1)

Cl(2) 650(1) 5864(3) 4409(1) 62(1)

C(3) 3567(2) 4440(8) 5463(3) 41(1)

N(4) 3172(1) 4655(6) 5436(2) 36(1)

C(5) 2730(2) 4851(7) 4895(3) 34(1)

C(6) 2525(2) 4941(7) 5318(3) 35(1)

N(7) 2833(1) 4806(6) 6103(2) 40(1)

C(8) 3213(2) 4638(7) 6139(3) 39(1)

C(1") 2571(2) 4854(7) 4082(3) 39(1)

N(2") 2845(1) 5306(7) 3874(2) 43(1)

O(3") 2642(1) 5158(6) 3072(2) 49(1)

C(11") 2063(2) 5144(7) 5067(3) 35(1)

C(12") 1741(2) 5712(7) 4327(3) 38(1)

C(13") 1309(2) 5908(8) 4118(3) 43(1)

C(14") 1192(2) 5545(8) 4652(3) 42(1)

C(15") 1498(2) 4970(8) 5385(3) 43(1)

C(16") 1928(2) 4749(7) 5587(3) 41(1)

C(1S) 5165(5) 3440(30) 6410(8) 80(4)

C(2S) 4848(4) 4490(16) 8094(6) 70(3)

C(3S) 4918(8) 5996(11) 7721(10) 78(4)

C(4S) 5029(7) 5603(12) 7175(9) 70(4)

C(5S) 5069(4) 3705(14) 7002(5) 52(3)

C(6S) 4999(5) 2199(10) 7375(7) 59(3)

C(7S) 4889(4) 2592(13) 7921(6) 77(4)

**Table X-3**. Bond lengths [Å] and angles [°] for *E*-CITCO

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C(4")-O(3") 1.447(8) C(4")-C(5") 1.508(10)

C(4")-H(4"1) 0.9900 C(4")-H(4"2) 0.9900

C(5")-C(10") 1.380(10) C(5")-C(6") 1.399(11)

C(6")-C(7") 1.392(9) C(6")-H(6") 0.9500

C(7")-C(8") 1.392(10) C(7")-Cl(7A) 1.725(8)

C(8")-C(9") 1.381(12) C(8")-Cl(8A) 1.742(7)

C(9")-C(10") 1.391(10) C(9")-H(9") 0.9500

C(10")-H(10") 0.9500 C(4B)-C(5B) 1.450(10)

C(4B)-O(3") 1.460(10) C(4B)-H(4B1) 0.9900

C(4B)-H(4B2) 0.9900 C(5B)-C(6B) 1.389(10)

C(5B)-C(10B) 1.392(10) C(6B)-C(7B) 1.390(10)

C(6B)-H(6B) 0.9500 C(7B)-C(8B) 1.390(10)

C(7B)-H(7B) 0.9500 C(8B)-C(9B) 1.387(10)

C(8B)-Cl(8B) 1.748(10) C(9B)-C(10B) 1.390(10)

C(9B)-Cl(9B) 1.743(10) C(10B)-H(10B) 0.9500

S(1)-C(8) 1.730(5) S(1)-C(2) 1.754(5)

C(2)-C(3) 1.340(7) C(2)-H(2) 0.9500

Cl(2)-C(14") 1.747(5) C(3)-N(4) 1.393(6)

C(3)-H(3) 0.9500 N(4)-C(8) 1.367(6)

N(4)-C(5) 1.389(6) C(5)-C(6) 1.395(6)

C(5)-C(1") 1.447(6) C(6)-N(7) 1.399(6)

C(6)-C(11") 1.460(7) N(7)-C(8) 1.327(7)

C(1")-N(2") 1.293(6) C(1")-H(1") 0.9500

N(2")-O(3") 1.409(5) C(11")-C(12") 1.400(7)

C(11")-C(16") 1.404(6) C(12")-C(13") 1.380(7)

C(12")-H(12") 0.9500 C(13")-C(14") 1.379(7)

C(13")-H(13") 0.9500 C(14")-C(15") 1.377(8)

C(15")-C(16") 1.379(7) C(15")-H(15") 0.9500

C(16")-H(16") 0.9500 C(1S)-C(5S) 1.427(17)

C(1S)-H(1S1) 0.9800 C(1S)-H(1S2) 0.9800

C(1S)-H(1S3) 0.9800 C(2S)-C(3S) 1.3900

C(2S)-C(7S) 1.3900 C(2S)-H(2S) 0.9500

C(3S)-C(4S) 1.3900 C(3S)-H(3S) 0.9500

C(4S)-C(5S) 1.3900 C(4S)-H(4S) 0.9500

C(5S)-C(6S) 1.3900 C(6S)-C(7S) 1.3900

C(6S)-H(6S) 0.9500 C(7S)-H(7S) 0.9500

O(3")-C(4")-C(5") 111.4(8) O(3")-C(4")-H(4"1) 109.3

C(5")-C(4")-H(4"1) 109.3 O(3")-C(4")-H(4"2) 109.3

C(5")-C(4")-H(4"2) 109.3 H(4"1)-C(4")-H(4"2) 108.0

C(10")-C(5")-C(6") 118.5(8) C(10")-C(5")-C(4") 121.5(9)

C(6")-C(5")-C(4") 120.0(9) C(7")-C(6")-C(5") 120.4(7)

C(7")-C(6")-H(6") 119.8 C(5")-C(6")-H(6") 119.8

C(8")-C(7")-C(6") 119.7(7) C(8")-C(7")-Cl(7A) 121.2(6)

C(6")-C(7")-Cl(7A) 119.1(6) C(9")-C(8")-C(7") 120.4(6)

C(9")-C(8")-Cl(8A) 119.1(5) C(7")-C(8")-Cl(8A) 120.5(7)

C(8")-C(9")-C(10") 119.2(7) C(8")-C(9")-H(9") 120.4

C(10")-C(9")-H(9") 120.4 C(5")-C(10")-C(9") 121.8(8)

C(5")-C(10")-H(10") 119.1 C(9")-C(10")-H(10") 119.1

C(5B)-C(4B)-O(3") 121(4) C(5B)-C(4B)-H(4B1) 107.1

O(3")-C(4B)-H(4B1) 107.1 C(5B)-C(4B)-H(4B2) 107.1

O(3")-C(4B)-H(4B2) 107.1 H(4B1)-C(4B)-H(4B2) 106.8

C(6B)-C(5B)-C(10B) 124(4) C(6B)-C(5B)-C(4B) 113(5)

C(10B)-C(5B)-C(4B) 123(5) C(5B)-C(6B)-C(7B) 117(4)

C(5B)-C(6B)-H(6B) 121.3 C(7B)-C(6B)-H(6B) 121.3

C(8B)-C(7B)-C(6B) 121(4) C(8B)-C(7B)-H(7B) 119.4

C(6B)-C(7B)-H(7B) 119.4 C(9B)-C(8B)-C(7B) 117(2)

C(9B)-C(8B)-Cl(8B) 123(3) C(7B)-C(8B)-Cl(8B) 120(2

C(8B)-C(9B)-C(10B) 125(3) C(8B)-C(9B)-Cl(9B) 120(3)

C(10B)-C(9B)-Cl(9B) 113(3) C(9B)-C(10B)-C(5B) 114(4)

C(9B)-C(10B)-H(10B) 123.0 C(5B)-C(10B)-H(10B) 123.0

C(8)-S(1)-C(2) 89.5(2) C(3)-C(2)-S(1) 113.0(4)

C(3)-C(2)-H(2) 123.5 S(1)-C(2)-H(2) 123.5

C(2)-C(3)-N(4) 112.1(4) C(2)-C(3)-H(3) 124.0

N(4)-C(3)-H(3) 124.0 C(8)-N(4)-C(5) 107.0(4)

C(8)-N(4)-C(3) 113.9(4) C(5)-N(4)-C(3) 139.0(4)

N(4)-C(5)-C(6) 105.0(4) N(4)-C(5)-C(1") 121.3(4)

C(6)-C(5)-C(1") 133.7(5) C(5)-C(6)-N(7) 110.7(4)

C(5)-C(6)-C(11") 130.4(4) N(7)-C(6)-C(11") 118.8(4)

C(8)-N(7)-C(6) 104.1(4) N(7)-C(8)-N(4) 113.2(4)

N(7)-C(8)-S(1) 135.2(4) N(4)-C(8)-S(1) 111.5(4)

N(2")-C(1")-C(5) 117.7(5) N(2")-C(1")-H(1") 121.2

C(5)-C(1")-H(1") 121.2 C(1")-N(2")-O(3") 110.2(4)

N(2")-O(3")-C(4") 106.0(7) N(2")-O(3")-C(4B) 106(4)

C(12")-C(11")-C(16") 117.2(4) C(12")-C(11")-C(6) 123.6(4)

C(16")-C(11")-C(6) 119.2(4) C(13")-C(12")-C(11") 121.6(4)

C(13")-C(12")-H(12") 119.2 C(11")-C(12")-H(12") 119.2

C(14")-C(13")-C(12") 119.3(5) C(14")-C(13")-H(13") 120.3

C(12")-C(13")-H(13") 120.3 C(15")-C(14")-C(13") 121.0(5)

C(15")-C(14")-Cl(2) 118.9(4) C(13")-C(14")-Cl(2) 120.0(4)

C(14")-C(15")-C(16") 119.4(4) C(14")-C(15")-H(15") 120.3

C(16")-C(15")-H(15") 120.3 C(15")-C(16")-C(11") 121.5(5)

C(15")-C(16")-H(16") 119.3 C(11")-C(16")-H(16") 119.3

C(5S)-C(1S)-H(1S1) 109.5 C(5S)-C(1S)-H(1S2) 109.5

H(1S1)-C(1S)-H(1S2) 109.5 C(5S)-C(1S)-H(1S3) 109.5

H(1S1)-C(1S)-H(1S3) 109.5 H(1S2)-C(1S)-H(1S3) 109.5

C(3S)-C(2S)-C(7S) 120.0 C(3S)-C(2S)-H(2S) 120.0

C(7S)-C(2S)-H(2S) 120.0 C(4S)-C(3S)-C(2S) 120.0

C(4S)-C(3S)-H(3S) 120.0 C(2S)-C(3S)-H(3S) 120.0

C(3S)-C(4S)-C(5S) 120.0 C(3S)-C(4S)-H(4S) 120.0

C(5S)-C(4S)-H(4S) 120.0 C(4S)-C(5S)-C(6S) 120.0

C(4S)-C(5S)-C(1S) 116.2(10) C(6S)-C(5S)-C(1S) 123.8(10)

C(7S)-C(6S)-C(5S) 120.0 C(7S)-C(6S)-H(6S) 120.0

C(5S)-C(6S)-H(6S) 120.0 C(6S)-C(7S)-C(2S) 120.0

C(6S)-C(7S)-H(7S) 120.0 C(2S)-C(7S)-H(7S) 120.0

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**Table X-4**. Anisotropic displacement parameters (Å2x 103)for *E*-CITCO. The anisotropic displacement factor exponent takes the form: -22[h2a\*2U11 + ... + 2 h k a\* b\* U12]

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

U11 U22 U33 U23 U13 U12

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C(4") 48(3) 65(6) 40(3) 10(4) 32(3) 13(3)

C(5") 43(3) 60(6) 37(3) 9(4) 30(3) 5(3)

C(6") 40(4) 61(5) 28(4) 5(3) 20(3) 1(3)

C(7") 45(4) 54(4) 37(3) 5(3) 30(3) 0(3)

Cl(7A) 75(1) 53(1) 54(1) 1(1) 39(1) 9(1)

C(8") 38(3) 56(4) 37(3) 12(3) 24(2) 7(3)

Cl(8A) 47(1) 87(2) 59(1) 19(1) 34(1) 21(1)

C(9") 36(3) 69(4) 44(3) -1(3) 24(3) 1(3)

C(10") 43(3) 62(5) 45(3) -1(4) 27(3) 3(3)

C(4B) 48(3) 65(6) 40(3) 10(4) 32(3) 13(3)

C(5B) 35(7) 45(12) 39(12) 16(9) 29(7) -1(7)

C(6B) 45(11) 49(11) 49(14) 8(10) 40(9) -7(8)

C(7B) 48(9) 53(12) 58(13) 14(9) 46(8) -4(8)

C(8B) 48(9) 59(12) 60(12) 14(8) 40(8) -5(7)

C(9B) 36(8) 64(13) 66(14) 5(10) 26(8) 0(7)

C(10B) 40(8) 54(14) 43(11) 14(10) 28(7) -5(7)

Cl(8B) 75(7) 90(9) 103(9) 21(7) 59(7) 26(7)

Cl(9B) 56(6) 125(12) 89(8) -14(7) 8(5) -8(6)

S(1) 48(1) 62(1) 35(1) 1(1) 22(1) 4(1)

C(2) 46(3) 54(3) 44(3) -1(2) 28(2) 8(2)

Cl(2) 43(1) 94(1) 57(1) -3(1) 31(1) -7(1)

C(3) 48(3) 44(3) 40(2) -2(2) 29(2) 2(2)

N(4) 43(2) 38(2) 35(2) 0(2) 26(2) 3(2)

C(5) 40(2) 34(2) 31(2) 0(2) 21(2) 1(2)

C(6) 48(2) 36(2) 28(2) 0(2) 26(2) -3(2)

N(7) 46(2) 47(2) 33(2) -2(2) 25(2) -3(2)

C(8) 49(3) 39(3) 36(2) 0(2) 26(2) 0(2)

C(1") 48(3) 45(3) 30(2) 2(2) 26(2) 7(2)

N(2") 46(2) 56(3) 28(2) -2(2) 22(2) 6(2)

O(3") 41(2) 81(3) 31(2) 0(2) 22(2) 4(2)

C(11") 44(2) 35(2) 33(2) -3(2) 26(2) -4(2)

C(12") 48(3) 43(3) 35(2) 2(2) 30(2) 1(2)

C(13") 49(3) 48(3) 37(2) 0(2) 27(2) 0(2)

C(14") 46(3) 48(3) 42(2) -6(2) 29(2) -7(2)

C(15") 52(3) 53(3) 40(2) -2(2) 34(2) -8(2)

C(16") 51(3) 48(3) 32(2) -3(2) 27(2) -6(2)

C(1S) 53(7) 117(11) 65(6) -12(7) 27(6) -22(8)

C(2S) 39(7) 101(9) 58(7) 9(6) 16(6) 19(7)

C(3S) 53(8) 99(9) 53(7) 1(7) 7(6) 0(8)

C(4S) 69(11) 58(6) 62(8) -1(5) 18(8) -14(6)

C(5S) 40(7) 51(6) 48(5) -3(5) 10(5) -25(6)

C(6S) 54(6) 56(5) 66(9) 8(5) 30(6) -7(6)

C(7S) 64(9) 103(9) 65(8) 15(6) 34(7) 13(8)

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**Table X-5**. Hydrogen coordinates ( x 104) and isotropic displacement parameters (Å2x 103) for *E*-CITCO

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

x y z U(eq)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

H(4"1) 3009 7354 3081 56

H(4"2) 2802 6077 2317 56

H(6") 3101 2584 2486 50

H(9") 4394 4991 4577 58

H(10") 3749 6782 4043 58

H(4B1) 2832 5658 2328 56

H(4B2) 3080 6945 3080 56

H(6B) 3024 2609 2258 48

H(7B) 3579 250 2744 53

H(10B) 3806 6005 4124 51

H(2) 4199 4047 6307 55

H(3) 3594 4437 5024 49

H(1") 2276 4536 3716 46

H(12") 1822 5969 3960 46

H(13") 1095 6288 3612 51

H(15") 1413 4728 5748 52

H(16") 2137 4320 6089 49

H(1S1) 5189 4694 6218 120

H(1S2) 4929 2692 5991 120

H(1S3) 5441 2734 6616 120

H(2S) 4772 4758 8467 84

H(3S) 4890 7293 7839 94

H(4S) 5077 6632 6920 85

H(6S) 5027 902 7257 71

H(7S) 4841 1562 8176 93

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

**Table X-6**. Torsion angles [°] for *E*-CITCO

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

O(3")-C(4")-C(5")-C(10") -107.4(14) O(3")-C(4")-C(5")-C(6") 72.7(15)

C(10")-C(5")-C(6")-C(7") -1.6(17) C(4")-C(5")-C(6")-C(7") 178.3(11)

C(5")-C(6")-C(7")-C(8") 2.7(14) C(5")-C(6")-C(7")-Cl(7A) -178.6(8)

C(6")-C(7")-C(8")-C(9") -1.5(11) Cl(7A)-C(7")-C(8")-C(9") 179.8(5)

C(6")-C(7")-C(8")-Cl(8A) 179.2(7) Cl(7A)-C(7")-C(8")-Cl(8A) 0.5(8)

C(7")-C(8")-C(9")-C(10") -0.7(10) Cl(8A)-C(8")-C(9")-C(10") 178.6(7)

C(6")-C(5")-C(10")-C(9") -0.7(17) C(4")-C(5")-C(10")-C(9") 179.4(10)

C(8")-C(9")-C(10")-C(5") 1.8(14) O(3")-C(4B)-C(5B)-C(6B) 82(9)

O(3")-C(4B)-C(5B)-C(10B) -100(9) C(10B)-C(5B)-C(6B)-C(7B) 8(9)

C(4B)-C(5B)-C(6B)-C(7B) -174(5) C(5B)-C(6B)-C(7B)-C(8B) -11(7)

C(6B)-C(7B)-C(8B)-C(9B) 3(6) C(6B)-C(7B)-C(8B)-Cl(8B) -176(4)

C(7B)-C(8B)-C(9B)-C(10B) 9(7) Cl(8B)-C(8B)-C(9B)-C(10B) -172(4)

C(7B)-C(8B)-C(9B)-Cl(9B) 170(3) Cl(8B)-C(8B)-C(9B)-Cl(9B) -11(6)

C(8B)-C(9B)-C(10B)-C(5B) -11(8) Cl(9B)-C(9B)-C(10B)-C(5B) -174(4)

C(6B)-C(5B)-C(10B)-C(9B) 2(9) C(4B)-C(5B)-C(10B)-C(9B) -175(5)

C(8)-S(1)-C(2)-C(3) 1.4(5) S(1)-C(2)-C(3)-N(4) -1.5(6)

C(2)-C(3)-N(4)-C(8) 0.7(6) C(2)-C(3)-N(4)-C(5) -177.5(5)

C(8)-N(4)-C(5)-C(6) 0.0(5) C(3)-N(4)-C(5)-C(6) 178.3(6)

C(8)-N(4)-C(5)-C(1") -177.9(4) C(3)-N(4)-C(5)-C(1") 0.4(9)

N(4)-C(5)-C(6)-N(7) 0.0(5) C(1")-C(5)-C(6)-N(7) 177.5(5)

N(4)-C(5)-C(6)-C(11") -180.0(5) C(1")-C(5)-C(6)-C(11") -2.5(9)

C(5)-C(6)-N(7)-C(8) 0.0(5) C(11")-C(6)-N(7)-C(8) 180.0(4)

C(6)-N(7)-C(8)-N(4) 0.0(6) C(6)-N(7)-C(8)-S(1) -178.8(5)

C(5)-N(4)-C(8)-N(7) 0.0(6) C(3)-N(4)-C(8)-N(7) -178.7(4)

C(5)-N(4)-C(8)-S(1) 179.1(3) C(3)-N(4)-C(8)-S(1) 0.4(5)

C(2)-S(1)-C(8)-N(7) 177.9(6) C(2)-S(1)-C(8)-N(4) -1.0(4)

N(4)-C(5)-C(1")-N(2") -22.3(7) C(6)-C(5)-C(1")-N(2") 160.5(5)

C(5)-C(1")-N(2")-O(3") 177.5(4) C(1")-N(2")-O(3")-C(4") 169.7(5)

C(1")-N(2")-O(3")-C(4B) -178(3) C(5")-C(4")-O(3")-N(2") 64.9(10)

C(5B)-C(4B)-O(3")-N(2") 63(8) C(5)-C(6)-C(11")-C(12") -14.6(8)

N(7)-C(6)-C(11")-C(12") 165.4(5) C(5)-C(6)-C(11")-C(16") 165.1(5)

N(7)-C(6)-C(11")-C(16") -14.8(7) C(16")-C(11")-C(12")-C(13") 1.0(7)

C(6)-C(11")-C(12")-C(13") -179.2(5) C(11")-C(12")-C(13")-C(14") 0.3(8)

C(12")-C(13")-C(14")-C(15") -0.8(8) C(12")-C(13")-C(14")-Cl(2) 177.8(4)

C(13")-C(14")-C(15")-C(16") -0.2(8) Cl(2)-C(14")-C(15")-C(16") -178.8(4)

C(14")-C(15")-C(16")-C(11") 1.6(8) C(12")-C(11")-C(16")-C(15") -2.0(7)

C(6)-C(11")-C(16")-C(15") 178.2(5) C(7S)-C(2S)-C(3S)-C(4S) 0.0

C(2S)-C(3S)-C(4S)-C(5S) 0.0 C(3S)-C(4S)-C(5S)-C(6S) 0.0

C(3S)-C(4S)-C(5S)-C(1S) 177.3(10) C(4S)-C(5S)-C(6S)-C(7S) 0.0

C(1S)-C(5S)-C(6S)-C(7S) -177.1(10) C(5S)-C(6S)-C(7S)-C(2S) 0.0

C(3S)-C(2S)-C(7S)-C(6S) 0.0 \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

# Species *Z*-CITCO

**Table X-7**. Crystal data and structure refinement for *Z*-CITCO

Identification code *Z*-CITCO

Empirical formula C19H12Cl3N3OS

Formula weight 436.73

Temperature 293(2) K

Wavelength 1.54178 Å

Crystal system Monoclinic

Space group P21/c

Unit cell dimensions a = 17.0194(12) Å = 90°.

b = 7.1790(5) Å = 100.064(4)°.

c = 32.056(2) Å  = 90°.

Volume 3856.4(5) Å3

Z 8

Density (20°C) 1.504 Mg/m3

Absorption coefficient 5.441 mm-1

F(000) 1776

Crystal size 0.078 x 0.021 x 0.020 mm3

Theta range for data collection 2.800 to 68.203°.

Index ranges -16<=h<=20, -7<=k<=6, -32<=l<=36

Reflections collected 16585

Independent reflections 5634 [Rint = 0.1280]

Completeness to theta = 67.679° 80.1 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.7531 and 0.5870

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 5634 / 520 / 536

Goodness-of-fit on F2 0.987

Final R indices [I>2sigma(I)] R1 = 0.0934, wR2 = 0.2419

R indices (all data) R1 = 0.3116, wR2 = 0.3291

Largest diff. peak and hole 0.533 and -0.499 e.Å-3

**Table X-8**. Atomic coordinates ( x 104) and equivalent isotropic displacement parameters (Å2x 103) for *Z*-CITCO. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

x y z U(eq)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C(1) 4150(6) 6412(9) 1933(2) 61(2)

C(2) 4038(6) 6452(9) 1497(2) 68(2)

C(3) 4633(6) 7015(10) 1292(3) 67(2)

Cl(4) 4479(2) 7056(3) 743(1) 103(1)

C(5) 5348(6) 7516(10) 1520(3) 68(2)

C(6) 5480(6) 7492(9) 1961(2) 64(2)

C(7) 4879(5) 6957(9) 2170(2) 55(2)

C(8) 5027(5) 6973(9) 2637(2) 56(2)

N(9) 5748(4) 6560(8) 2875(2) 60(2)

C(10) 5619(6) 6693(9) 3267(2) 61(2)

S(11) 6215(2) 6482(3) 3762(1) 77(1)

C(12) 5422(6) 7112(11) 3993(3) 78(2)

C(13) 4762(6) 7451(10) 3720(2) 68(2)

N(14) 4858(4) 7191(7) 3301(2) 59(2)

C(15) 4449(5) 7366(9) 2894(2) 58(2)

C(16) 3627(6) 8054(11) 2771(2) 67(2)

N(17) 3009(5) 7683(9) 2927(2) 77(2)

O(18) 3195(4) 6334(7) 3251(2) 79(2)

C(19) 2450(6) 5768(13) 3383(2) 83(3)

C(20) 2676(6) 4385(13) 3732(3) 79(2)

C(21) 3097(6) 4919(14) 4124(2) 89(3)

C(22) 3370(7) 3660(15) 4428(3) 102(3)

Cl(23) 3896(3) 4423(6) 4896(1) 177(2)

C(24) 3227(7) 1732(16) 4342(3) 105(3)

Cl(25) 3627(2) 87(5) 4710(1) 176(2)

C(26) 2803(7) 1220(16) 3969(3) 120(4)

C(27) 2502(7) 2525(14) 3655(3) 106(3)

C(28) -6(6) 8654(10) 1772(2) 72(2)

C(29) 502(6) 8668(11) 1481(3) 79(2)

C(30) 1299(6) 8262(11) 1613(3) 74(2)

Cl(31) 1928(2) 8243(4) 1241(1) 118(1)

C(32) 1592(6) 7830(10) 2025(3) 70(2)

C(33) 1078(6) 7813(10) 2312(3) 67(2)

C(34) 263(6) 8224(9) 2189(2) 58(2)

C(35) -291(6) 8206(10) 2490(2) 62(2)

N(36) -1092(5) 7831(8) 2332(2) 71(2)

C(37) -1421(6) 7869(10) 2669(3) 69(2)

S(38) -2391(2) 7623(3) 2756(1) 94(1)

C(39) -2060(7) 8067(12) 3277(3) 93(3)

C(40) -1267(7) 8355(12) 3389(3) 84(3)

N(41) -909(5) 8199(8) 3036(2) 67(2)

C(42) -161(6) 8445(9) 2925(2) 59(2)

C(43) 586(6) 8995(10) 3196(2) 71(2)

N(44) 890(5) 8745(10) 3586(2) 95(2)

O(45A) 415(14) 7680(40) 3811(6) 107(3)

C(46A) 915(16) 7350(20) 4220(6) 107(3)

C(47A) 973(11) 9050(17) 4497(4) 111(6)

C(48A) 1590(9) 9088(18) 4845(4) 120(6)

C(49A) 1653(10) 10570(20) 5128(4) 126(7)

C(51A) 1100(12) 12010(20) 5064(5) 135(7)

C(53A) 484(10) 11972(19) 4717(5) 139(8)

C(54A) 420(10) 10490(20) 4434(5) 136(9)

Cl(50) 2416(5) 10555(15) 5541(2) 199(4)

Cl(52) 1218(7) 13793(13) 5427(3) 198(4)

O(45B) 327(17) 7660(60) 3746(9) 107(3)

C(46B) 710(20) 6980(40) 4161(7) 107(3)

C(49B) 904(15) 11210(20) 4838(7) 134(7)

C(48B) 690(13) 9960(30) 4507(6) 131(11)

C(47B) 1074(15) 8250(20) 4514(6) 115(7)

C(54B) 1673(13) 7790(20) 4851(6) 130(7)

C(53B) 1887(14) 9040(30) 5182(5) 173(10)

C(51B) 1503(17) 10760(30) 5175(5) 166(12)

Cl(55) 378(8) 13262(13) 4822(3) 194(6)

Cl(56) 1805(12) 12390(20) 5561(4) 245(8)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

**Table X-9**. Bond lengths [Å] and angles [°] for *Z*-CITCO

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C(1)-C(2) 1.379(9) C(1)-C(7) 1.393(11)

C(1)-H(1) 0.9300 C(2)-C(3) 1.360(11)

C(2)-H(2) 0.9300 C(3)-C(5) 1.354(12)

C(3)-Cl(4) 1.734(8) C(5)-C(6) 1.391(10)

C(5)-H(5) 0.9300 C(6)-C(7) 1.373(11)

C(6)-H(6) 0.9300 C(7)-C(8) 1.473(10)

C(8)-N(9) 1.361(10) C(8)-C(15) 1.417(11)

N(9)-C(10) 1.316(9) C(10)-N(14) 1.365(10)

C(10)-S(11) 1.735(8) S(11)-C(12) 1.709(10)

C(12)-C(13) 1.321(12) C(12)-H(12) 0.9300

C(13)-N(14) 1.392(9) C(13)-H(13) 0.9300

N(14)-C(15) 1.374(9) C(15)-C(16) 1.470(11)

C(16)-N(17) 1.271(10) C(16)-H(16) 0.9300

N(17)-O(18) 1.415(8) O(18)-C(19) 1.463(10)

C(19)-C(20) 1.494(11) C(19)-H(19A) 0.9700

C(19)-H(19B) 0.9700 C(20)-C(27) 1.381(12)

C(20)-C(21) 1.386(11) C(21)-C(22) 1.350(12)

C(21)-H(21) 0.9300 C(22)-C(24) 1.424(14)

C(22)-Cl(23) 1.700(11) C(24)-C(26) 1.335(13)

C(24)-Cl(25) 1.723(11) C(26)-C(27) 1.405(13)

C(26)-H(26) 0.9300 C(27)-H(27) 0.9300

C(28)-C(34) 1.368(10) C(28)-C(29) 1.380(11)

C(28)-H(28) 0.9300 C(29)-C(30) 1.381(12)

C(29)-H(29) 0.9300 C(30)-C(32) 1.363(11)

C(30)-Cl(31) 1.737(9) C(32)-C(33) 1.377(11)

C(32)-H(32) 0.9300 C(33)-C(34) 1.406(11)

C(33)-H(33) 0.9300 C(34)-C(35) 1.461(11)

C(35)-C(42) 1.385(10) C(35)-N(36) 1.395(10)

N(36)-C(37) 1.301(9) C(37)-N(41) 1.356(11)

C(37)-S(38) 1.731(9) S(38)-C(39) 1.698(11)

C(39)-C(40) 1.350(13) C(39)-H(39) 0.9300

C(40)-N(41) 1.381(10) C(40)-H(40) 0.9300

N(41)-C(42) 1.391(10) C(42)-C(43) 1.463(11)

C(43)-N(44) 1.279(9) C(43)-H(43) 0.9300

N(44)-O(45B) 1.400(10) N(44)-O(45A) 1.404(9)

O(45A)-C(46A) 1.452(9) C(46A)-C(47A) 1.504(10)

C(46A)-H(46A) 0.9700 C(46A)-H(46B) 0.9700

C(47A)-C(48A) 1.3900 C(47A)-C(54A) 1.3900

C(48A)-C(49A) 1.3900 C(48A)-H(48A) 0.9300

C(49A)-C(51A) 1.3900 C(49A)-Cl(50) 1.684(11)

C(51A)-C(53A) 1.3900 C(51A)-Cl(52) 1.716(10)

C(53A)-C(54A) 1.3900 C(53A)-H(53A) 0.9300

C(54A)-H(54A) 0.9300 O(45B)-C(46B) 1.463(10)

C(46B)-C(47B) 1.497(10) C(46B)-H(46C) 0.9700

C(46B)-H(46D) 0.9700 C(49B)-C(48B) 1.3900

C(49B)-C(51B) 1.3900 C(49B)-Cl(55) 1.718(15)

C(48B)-C(47B) 1.3900 C(48B)-H(48B) 0.9300

C(47B)-C(54B) 1.3900 C(54B)-C(53B) 1.3900

C(54B)-H(54B) 0.9300 C(53B)-C(51B) 1.3900

C(53B)-H(53B) 0.9300 C(51B)-Cl(56) 1.718(13)

C(2)-C(1)-C(7) 119.9(8) C(2)-C(1)-H(1) 120.0

C(7)-C(1)-H(1) 120.0 C(3)-C(2)-C(1) 120.9(9)

C(3)-C(2)-H(2) 119.6 C(1)-C(2)-H(2) 119.6

C(5)-C(3)-C(2) 119.5(8) C(5)-C(3)-Cl(4) 120.4(7)

C(2)-C(3)-Cl(4) 120.1(8) C(3)-C(5)-C(6) 121.1(9)

C(3)-C(5)-H(5) 119.5 C(6)-C(5)-H(5) 119.5

C(7)-C(6)-C(5) 119.8(9) C(7)-C(6)-H(6) 120.1

C(5)-C(6)-H(6) 120.1 C(6)-C(7)-C(1) 118.8(7)

C(6)-C(7)-C(8) 119.0(8) C(1)-C(7)-C(8) 122.3(7)

N(9)-C(8)-C(15) 111.5(7) N(9)-C(8)-C(7) 123.1(7)

C(15)-C(8)-C(7) 125.4(8) C(10)-N(9)-C(8) 103.6(7)

N(9)-C(10)-N(14) 114.5(8) N(9)-C(10)-S(11) 134.2(8)

N(14)-C(10)-S(11) 111.2(6) C(12)-S(11)-C(10) 89.5(4)

C(13)-C(12)-S(11) 114.0(7) C(13)-C(12)-H(12) 123.0

S(11)-C(12)-H(12) 123.0 C(12)-C(13)-N(14) 112.6(9)

C(12)-C(13)-H(13) 123.7 N(14)-C(13)-H(13) 123.7

C(10)-N(14)-C(15) 106.1(6) C(10)-N(14)-C(13) 112.7(7)

C(15)-N(14)-C(13) 141.0(8) N(14)-C(15)-C(8) 104.2(8)

N(14)-C(15)-C(16) 125.8(7) C(8)-C(15)-C(16) 129.5(7)

N(17)-C(16)-C(15) 129.7(8) N(17)-C(16)-H(16) 115.1

C(15)-C(16)-H(16) 115.1 C(16)-N(17)-O(18) 109.7(7)

N(17)-O(18)-C(19) 107.9(6) O(18)-C(19)-C(20) 106.1(7)

O(18)-C(19)-H(19A) 110.5 C(20)-C(19)-H(19A) 110.5

O(18)-C(19)-H(19B) 110.5 C(20)-C(19)-H(19B) 110.5

H(19A)-C(19)-H(19B) 108.7 C(27)-C(20)-C(21) 119.3(9)

C(27)-C(20)-C(19) 119.3(9) C(21)-C(20)-C(19) 121.2(8)

C(22)-C(21)-C(20) 121.8(10) C(22)-C(21)-H(21) 119.1

C(20)-C(21)-H(21) 119.1 C(21)-C(22)-C(24) 119.0(10)

C(21)-C(22)-Cl(23) 118.9(9) C(24)-C(22)-Cl(23) 122.0(8)

C(26)-C(24)-C(22) 119.3(10) C(26)-C(24)-Cl(25) 120.7(9)

C(22)-C(24)-Cl(25) 120.0(9) C(24)-C(26)-C(27) 122.0(11)

C(24)-C(26)-H(26) 119.0 C(27)-C(26)-H(26) 119.0

C(20)-C(27)-C(26) 118.5(10) C(20)-C(27)-H(27) 120.8

C(26)-C(27)-H(27) 120.8 C(34)-C(28)-C(29) 121.3(9)

C(34)-C(28)-H(28) 119.3 C(29)-C(28)-H(28) 119.3

C(28)-C(29)-C(30) 119.3(8) C(28)-C(29)-H(29) 120.3

C(30)-C(29)-H(29) 120.3 C(32)-C(30)-C(29) 121.2(8)

C(32)-C(30)-Cl(31) 119.9(8) C(29)-C(30)-Cl(31) 118.8(7)

C(30)-C(32)-C(33) 118.8(9) C(30)-C(32)-H(32) 120.6

C(33)-C(32)-H(32) 120.6 C(32)-C(33)-C(34) 121.4(8)

C(32)-C(33)-H(33) 119.3 C(34)-C(33)-H(33) 119.3

C(28)-C(34)-C(33) 117.9(7) C(28)-C(34)-C(35) 120.1(8)

C(33)-C(34)-C(35) 122.1(8) C(42)-C(35)-N(36) 111.2(7)

C(42)-C(35)-C(34) 131.0(9) N(36)-C(35)-C(34) 117.8(7)

C(37)-N(36)-C(35) 103.4(8) N(36)-C(37)-N(41) 114.8(9)

N(36)-C(37)-S(38) 133.7(8) N(41)-C(37)-S(38) 111.5(6)

C(39)-S(38)-C(37) 88.6(5) C(40)-C(39)-S(38) 115.8(8)

C(40)-C(39)-H(39) 122.1 S(38)-C(39)-H(39) 122.1

C(39)-C(40)-N(41) 109.5(10) C(39)-C(40)-H(40) 125.3

N(41)-C(40)-H(40) 125.3 C(37)-N(41)-C(40) 114.5(9)

C(37)-N(41)-C(42) 106.2(7) C(40)-N(41)-C(42) 139.0(9)

C(35)-C(42)-N(41) 104.5(8) C(35)-C(42)-C(43) 126.9(8)

N(41)-C(42)-C(43) 128.4(7) N(44)-C(43)-C(42) 134.6(8)

N(44)-C(43)-H(43) 112.7 C(42)-C(43)-H(43) 112.7

C(43)-N(44)-O(45B) 104.6(13) C(43)-N(44)-O(45A) 114.2(11)

N(44)-O(45A)-C(46A) 104.8(15) O(45A)-C(46A)-C(47A) 111.6(19)

O(45A)-C(46A)-H(46A) 109.3 C(47A)-C(46A)-H(46A) 109.3

O(45A)-C(46A)-H(46B) 109.3 C(47A)-C(46A)-H(46B) 109.3

H(46A)-C(46A)-H(46B) 108.0 C(48A)-C(47A)-C(54A) 120.0

C(48A)-C(47A)-C(46A) 116.8(14) C(54A)-C(47A)-C(46A) 123.1(14)

C(47A)-C(48A)-C(49A) 120.0 C(47A)-C(48A)-H(48A) 120.0

C(49A)-C(48A)-H(48A) 120.0 C(51A)-C(49A)-C(48A) 120.0

C(51A)-C(49A)-Cl(50) 121.9(11) C(48A)-C(49A)-Cl(50) 118.1(11)

C(53A)-C(51A)-C(49A) 120.0 C(53A)-C(51A)-Cl(52) 122.6(11)

C(49A)-C(51A)-Cl(52) 117.4(11) C(54A)-C(53A)-C(51A) 120.0

C(54A)-C(53A)-H(53A) 120.0 C(51A)-C(53A)-H(53A) 120.0

C(53A)-C(54A)-C(47A) 120.0 C(53A)-C(54A)-H(54A) 120.0

C(47A)-C(54A)-H(54A) 120.0 N(44)-O(45B)-C(46B) 107.0(19)

O(45B)-C(46B)-C(47B) 123(2) O(45B)-C(46B)-H(46C) 106.6

C(47B)-C(46B)-H(46C) 106.6 O(45B)-C(46B)-H(46D) 106.6

C(47B)-C(46B)-H(46D) 106.6 H(46C)-C(46B)-H(46D) 106.6

C(48B)-C(49B)-C(51B) 120.0 C(48B)-C(49B)-Cl(55) 117.7(14)

C(51B)-C(49B)-Cl(55) 122.2(14) C(49B)-C(48B)-C(47B) 120.0

C(49B)-C(48B)-H(48B) 120.0 C(47B)-C(48B)-H(48B) 120.0

C(54B)-C(47B)-C(48B) 120.0 C(54B)-C(47B)-C(46B) 126(2)

C(48B)-C(47B)-C(46B) 113(2) C(53B)-C(54B)-C(47B) 120.0

C(53B)-C(54B)-H(54B) 120.0 C(47B)-C(54B)-H(54B) 120.0

C(54B)-C(53B)-C(51B) 120.0 C(54B)-C(53B)-H(53B) 120.0

C(51B)-C(53B)-H(53B) 120.0 C(53B)-C(51B)-C(49B) 120.0

C(53B)-C(51B)-Cl(56) 120.8(17) C(49B)-C(51B)-Cl(56) 119.0(16)

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**Table X-10**. Anisotropic displacement parameters (Å2x 103) for *Z*-CITCO. The anisotropic displacement factor exponent takes the form: -22[h2a\*2U11 + ... + 2 h k a\* b\* U12]

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

U11 U22 U33 U23 U13 U12

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C(1) 79(5) 50(4) 51(4) -3(3) 4(3) 0(4)

C(2) 90(6) 57(4) 50(4) -3(4) -6(4) -2(4)

C(3) 97(6) 45(4) 56(4) 0(3) 7(4) 8(4)

Cl(4) 168(3) 90(2) 48(1) -3(1) 9(2) 4(2)

C(5) 90(6) 67(5) 50(4) 2(3) 17(4) 3(4)

C(6) 76(6) 62(4) 50(4) 1(3) 4(4) -3(4)

C(7) 82(5) 36(4) 46(4) 5(3) 4(3) 6(3)

C(8) 75(5) 36(4) 54(4) 6(3) 8(3) -6(3)

N(9) 74(4) 54(3) 49(3) 9(3) 6(3) 4(3)

C(10) 77(5) 46(4) 57(4) 1(3) 3(3) -8(4)

S(11) 88(2) 76(1) 58(1) 11(1) -9(1) -7(1)

C(12) 109(6) 75(5) 45(4) 6(4) -2(4) -3(5)

C(13) 91(6) 68(5) 47(4) 3(4) 15(4) -3(4)

N(14) 75(4) 56(3) 44(3) 4(3) 4(3) -7(3)

C(15) 72(4) 55(4) 44(4) 5(3) 4(3) -4(3)

C(16) 81(5) 71(5) 47(5) 8(4) 8(4) 4(4)

N(17) 76(5) 94(4) 59(4) 26(3) 7(4) 12(4)

O(18) 89(5) 94(4) 55(3) 24(3) 12(3) 7(3)

C(19) 92(7) 97(5) 60(5) 9(4) 14(4) -5(5)

C(20) 82(7) 101(5) 55(4) 11(4) 16(4) -9(4)

C(21) 116(8) 103(6) 48(4) 8(4) 13(4) -14(5)

C(22) 114(8) 125(6) 64(5) 31(4) 5(5) -15(5)

Cl(23) 248(5) 192(4) 67(2) 16(2) -39(2) -33(3)

C(24) 105(8) 125(6) 83(5) 36(5) 14(5) -22(5)

Cl(25) 183(4) 175(3) 158(3) 106(3) -9(3) -21(3)

C(26) 139(10) 113(6) 98(6) 33(5) -8(6) -28(6)

C(27) 121(10) 105(5) 84(6) 14(4) -3(6) -23(5)

C(28) 84(6) 81(5) 50(4) 7(4) 7(4) 14(4)

C(29) 96(6) 89(6) 51(4) 10(4) 9(4) 19(5)

C(30) 92(6) 71(5) 62(4) 6(4) 20(4) 9(5)

Cl(31) 142(3) 122(2) 106(2) 26(2) 66(2) 33(2)

C(32) 77(6) 69(5) 61(4) -5(4) 6(4) 3(4)

C(33) 80(5) 70(5) 48(4) 0(4) 3(4) 1(4)

C(34) 78(5) 41(4) 52(4) 3(3) 4(3) 3(4)

C(35) 83(5) 47(4) 54(4) 5(3) 7(3) 10(4)

N(36) 80(5) 72(4) 61(4) -2(3) 12(3) 1(4)

C(37) 80(5) 59(4) 69(4) 3(4) 16(3) 6(4)

S(38) 83(2) 93(2) 112(2) -3(1) 33(2) -1(1)

C(39) 104(6) 71(5) 113(6) 7(5) 44(5) 10(5)

C(40) 102(6) 78(5) 80(5) 6(4) 38(4) 7(5)

N(41) 82(4) 60(4) 63(4) 5(3) 22(3) -1(3)

C(42) 77(5) 46(4) 54(4) 8(3) 13(3) 1(4)

C(43) 100(6) 65(5) 48(4) -2(4) 12(4) -8(4)

N(44) 126(6) 91(5) 65(4) 6(4) 12(4) -11(4)

O(45A) 144(7) 110(4) 63(4) 3(4) 6(4) -33(4)

C(46A) 144(7) 110(4) 63(4) 3(4) 6(4) -33(4)

C(47A) 170(14) 99(9) 59(8) 15(7) 10(8) -40(8)

C(48A) 169(13) 140(11) 51(7) 8(7) 16(7) -33(9)

C(49A) 162(13) 148(11) 66(9) -10(8) 17(9) -41(9)

C(51A) 170(14) 150(11) 80(10) -22(9) 10(9) -33(9)

C(53A) 188(15) 122(12) 96(11) -17(9) -1(10) -28(10)

C(54A) 193(17) 119(11) 85(12) -6(9) -10(11) -18(11)

Cl(50) 188(8) 287(11) 101(5) -6(5) -29(4) -25(7)

Cl(52) 261(12) 194(8) 141(7) -86(6) 40(6) -45(7)

O(45B) 144(7) 110(4) 63(4) 3(4) 6(4) -33(4)

C(46B) 144(7) 110(4) 63(4) 3(4) 6(4) -33(4)

C(49B) 226(18) 125(10) 60(10) -6(8) 51(10) -87(10)

C(48B) 200(20) 124(11) 66(12) -3(8) 23(13) -52(12)

C(47B) 171(16) 122(11) 54(8) 6(8) 26(8) -71(9)

C(54B) 177(16) 165(14) 48(9) 16(9) 23(9) -65(11)

C(53B) 240(20) 196(14) 75(12) -14(10) 13(12) -72(13)

C(51B) 250(20) 181(14) 73(13) -2(11) 31(14) -77(13)

Cl(55) 355(16) 133(7) 102(7) -17(5) 61(8) -22(7)

Cl(56) 320(20) 271(16) 135(9) -81(10) 8(11) -100(14)

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**Table X-11**. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 103) for *Z*-CITCO

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

x y z U(eq)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

H(1) 3739 6021 2069 73

H(2) 3550 6089 1340 81

H(5) 5757 7883 1380 82

H(6) 5975 7837 2113 76

H(12) 5452 7207 4284 94

H(13) 4285 7823 3798 82

H(16) 3549 8886 2545 80

H(19A) 2091 5208 3149 99

H(19B) 2187 6835 3484 99

H(21) 3194 6177 4178 107

H(26) 2705 -40 3915 144

H(27) 2191 2145 3401 127

H(28) -542 8943 1684 86

H(29) 309 8947 1198 95

H(32) 2130 7551 2110 84

H(33) 1274 7523 2594 80

H(39) -2403 8110 3473 112

H(40) -1003 8617 3662 101

H(43) 916 9685 3051 85

H(46A) 1446 6989 4179 129

H(46B) 696 6325 4361 129

H(48A) 1960 8123 4887 145

H(53A) 114 12937 4675 166

H(54A) 7 10467 4202 164

H(46C) 1134 6138 4111 129

H(46D) 322 6222 4270 129

H(48B) 289 10266 4281 157

H(54B) 1930 6646 4856 156

H(53B) 2288 8738 5408 207

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**Table X-12**. Torsion angles [°] for *Z*-CITCO

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C(7)-C(1)-C(2)-C(3) 0.2(11) C(1)-C(2)-C(3)-C(5) 1.0(11)

C(1)-C(2)-C(3)-Cl(4) -179.9(5) C(2)-C(3)-C(5)-C(6) -1.0(12)

Cl(4)-C(3)-C(5)-C(6) 180.0(5) C(3)-C(5)-C(6)-C(7) -0.2(11)

C(5)-C(6)-C(7)-C(1) 1.3(10) C(5)-C(6)-C(7)-C(8) -178.9(6)

C(2)-C(1)-C(7)-C(6) -1.3(10) C(2)-C(1)-C(7)-C(8) 178.9(6)

C(6)-C(7)-C(8)-N(9) -34.3(10) C(1)-C(7)-C(8)-N(9) 145.5(7)

C(6)-C(7)-C(8)-C(15) 147.3(7) C(1)-C(7)-C(8)-C(15) -33.0(10)

C(15)-C(8)-N(9)-C(10) 0.1(7) C(7)-C(8)-N(9)-C(10) -178.6(6)

C(8)-N(9)-C(10)-N(14) -0.8(8) C(8)-N(9)-C(10)-S(11) -177.1(6)

N(9)-C(10)-S(11)-C(12) 175.5(7) N(14)-C(10)-S(11)-C(12) -1.0(5)

C(10)-S(11)-C(12)-C(13) 0.1(7) S(11)-C(12)-C(13)-N(14) 0.9(9)

N(9)-C(10)-N(14)-C(15) 1.2(8) S(11)-C(10)-N(14)-C(15) 178.4(4)

N(9)-C(10)-N(14)-C(13) -175.5(6) S(11)-C(10)-N(14)-C(13) 1.7(7)

C(12)-C(13)-N(14)-C(10) -1.7(9) C(12)-C(13)-N(14)-C(15) -176.6(8)

C(10)-N(14)-C(15)-C(8) -1.0(7) C(13)-N(14)-C(15)-C(8) 174.2(8)

C(10)-N(14)-C(15)-C(16) -173.8(7) C(13)-N(14)-C(15)-C(16) 1.3(13)

N(9)-C(8)-C(15)-N(14) 0.6(7) C(7)-C(8)-C(15)-N(14) 179.3(6)

N(9)-C(8)-C(15)-C(16) 173.1(7) C(7)-C(8)-C(15)-C(16) -8.3(12)

N(14)-C(15)-C(16)-N(17) -43.8(13) C(8)-C(15)-C(16)-N(17) 145.2(9)

C(15)-C(16)-N(17)-O(18) -3.1(12) C(16)-N(17)-O(18)-C(19) -172.7(7)

N(17)-O(18)-C(19)-C(20) -178.6(6) O(18)-C(19)-C(20)-C(27) -107.4(10)

O(18)-C(19)-C(20)-C(21) 68.9(10) C(27)-C(20)-C(21)-C(22) 2.6(14)

C(19)-C(20)-C(21)-C(22) -173.7(9) C(20)-C(21)-C(22)-C(24) 0.5(15)

C(20)-C(21)-C(22)-Cl(23) 178.9(7) C(21)-C(22)-C(24)-C(26) -2.2(16)

Cl(23)-C(22)-C(24)-C(26) 179.4(10) C(21)-C(22)-C(24)-Cl(25) 175.5(8)

Cl(23)-C(22)-C(24)-Cl(25) -2.8(14) C(22)-C(24)-C(26)-C(27) 0.8(18)

Cl(25)-C(24)-C(26)-C(27) -177.0(9) C(21)-C(20)-C(27)-C(26) -4.0(15)

C(19)-C(20)-C(27)-C(26) 172.3(9) C(24)-C(26)-C(27)-C(20) 2.4(18)

C(34)-C(28)-C(29)-C(30) -0.8(12) C(28)-C(29)-C(30)-C(32) 0.7(13)

C(28)-C(29)-C(30)-Cl(31) 178.8(6) C(29)-C(30)-C(32)-C(33) -0.4(12)

Cl(31)-C(30)-C(32)-C(33) -178.5(6) C(30)-C(32)-C(33)-C(34) 0.3(11)

C(29)-C(28)-C(34)-C(33) 0.7(11) C(29)-C(28)-C(34)-C(35) -179.5(7)

C(32)-C(33)-C(34)-C(28) -0.4(11) C(32)-C(33)-C(34)-C(35) 179.8(7)

C(28)-C(34)-C(35)-C(42) -155.3(8) C(33)-C(34)-C(35)-C(42) 24.5(11)

C(28)-C(34)-C(35)-N(36) 27.2(9) C(33)-C(34)-C(35)-N(36) -153.0(7)

C(42)-C(35)-N(36)-C(37) 0.6(8) C(34)-C(35)-N(36)-C(37) 178.6(6)

C(35)-N(36)-C(37)-N(41) -1.2(9) C(35)-N(36)-C(37)-S(38) 177.5(6)

N(36)-C(37)-S(38)-C(39) -176.6(9) N(41)-C(37)-S(38)-C(39) 2.2(6)

C(37)-S(38)-C(39)-C(40) -1.1(7) S(38)-C(39)-C(40)-N(41) -0.3(10)

N(36)-C(37)-N(41)-C(40) 176.1(6) S(38)-C(37)-N(41)-C(40) -2.9(8)

N(36)-C(37)-N(41)-C(42) 1.4(9) S(38)-C(37)-N(41)-C(42) -177.6(4)

C(39)-C(40)-N(41)-C(37) 2.1(10) C(39)-C(40)-N(41)-C(42) 174.4(8)

N(36)-C(35)-C(42)-N(41) 0.2(8) C(34)-C(35)-C(42)-N(41) -177.5(7)

N(36)-C(35)-C(42)-C(43) -175.0(7) C(34)-C(35)-C(42)-C(43) 7.4(12)

C(37)-N(41)-C(42)-C(35) -0.9(7) C(40)-N(41)-C(42)-C(35) -173.6(8)

C(37)-N(41)-C(42)-C(43) 174.2(7) C(40)-N(41)-C(42)-C(43) 1.5(13)

C(35)-C(42)-C(43)-N(44) -154.0(9) N(41)-C(42)-C(43)-N(44) 32.0(14)

C(42)-C(43)-N(44)-O(45B) 1(3) C(42)-C(43)-N(44)-O(45A) 1(2)

C(43)-N(44)-O(45A)-C(46A) 172.1(15) N(44)-O(45A)-C(46A)-C(47A) 76(3

O(45A)-C(46A)-C(47A)-C(48A) -163.3(15) O(45A)-C(46A)-C(47A)-C(54A) 20(2)

C(54A)-C(47A)-C(48A)-C(49A) 0.0 C(46A)-C(47A)-C(48A)-C(49A) -176.4(18)

C(47A)-C(48A)-C(49A)-C(51A) 0.0 C(47A)-C(48A)-C(49A)-Cl(50) -179.5(15)

C(48A)-C(49A)-C(51A)-C(53A) 0.0 Cl(50)-C(49A)-C(51A)-C(53A) 179.5(16)

C(48A)-C(49A)-C(51A)-Cl(52) -179.9(15) Cl(50)-C(49A)-C(51A)-Cl(52) -0.4(13)

C(49A)-C(51A)-C(53A)-C(54A) 0.0 Cl(52)-C(51A)-C(53A)-C(54A) 179.9(16)

C(51A)-C(53A)-C(54A)-C(47A) 0.0 C(48A)-C(47A)-C(54A)-C(53A) 0.0

C(46A)-C(47A)-C(54A)-C(53A) 176.1(18) C(43)-N(44)-O(45B)-C(46B) 167(2)

N(44)-O(45B)-C(46B)-C(47B) 57(4) C(51B)-C(49B)-C(48B)-C(47B) 0.0

Cl(55)-C(49B)-C(48B)-C(47B) -177.3(16) C(49B)-C(48B)-C(47B)-C(54B) 0.0

C(49B)-C(48B)-C(47B)-C(46B) 173(2) O(45B)-C(46B)-C(47B)-C(54B) -156(2)

O(45B)-C(46B)-C(47B)-C(48B) 31(4) C(48B)-C(47B)-C(54B)-C(53B) 0.0

C(46B)-C(47B)-C(54B)-C(53B) -173(3) C(47B)-C(54B)-C(53B)-C(51B) 0.0

C(54B)-C(53B)-C(51B)-C(49B) 0.0 C(54B)-C(53B)-C(51B)-Cl(56) -175(2)

C(48B)-C(49B)-C(51B)-C(53B) 0.0 Cl(55)-C(49B)-C(51B)-C(53B) 177.2(17)

C(48B)-C(49B)-C(51B)-Cl(56) 175(2) Cl(55)-C(49B)-C(51B)-Cl(56) -7(2)

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**Table X-13**. Hydrogen bonds for *Z*-CITCO [Å and °]

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

D-H...A d(D-H) d(H...A) d(D...A) <(DHA)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C(12)-H(12)...Cl(23)#1 0.93 2.91 3.714(9) 145.4

C(19)-H(19A)...N(36)#2 0.97 2.69 3.633(12) 162.8

C(19)-H(19B)...N(44) 0.97 2.67 3.554(12) 152.5

C(39)-H(39)...S(11)#3 0.93 2.92 3.732(11) 146.9

C(40)-H(40)...O(45A) 0.93 2.47 2.99(3) 114.9

C(40)-H(40)...O(45B) 0.93 2.34 2.80(4) 110.4

C(43)-H(43)...N(36)#4 0.93 2.61 3.420(10) 145.4

C(46B)-H(46D)...Cl(55)#5 0.97 2.76 3.51(3) 135.5

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Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x,y-1/2,-z+1/2 #3 x-1,y,z

#4 -x,y+1/2,-z+1/2 #5 x,y-1,z