Experimental Details (28).

Identification Code	**28**
Empirical Formula	$Zn_2S_4O_4N_6C25H_{52}I_4Cl_6$
Formula Weight	1480.06
Crystal Color, Habit	yellow, plates
Crystal Dimensions	0.43 x 0.18 x 0.02 mm
Crystal System	Colorless, needlelike
Lattice Type	orthorhombic
Lattice Parameters	a = 10.1023(5) Å b = 18.5926(9) Å c = 32.3936(16) Å
Volume	6084.4(5) $Å^3$
Space Group	$P2_12_12_1$ (#19)
Z value	4
D_{calc}	1.616 g/cm^3
F_{000}	2856.00
μ(MoKμ)	98.77 cm^{-1}
Diffractometer	SMART CCD
Radiation	MoKα (λ= 0.71069 Å) Graphite monochromated
Detector Position	60.00 mm
Exposure Time	20.0 seconds per frame
Scan type	ω (0.3 degrees per frame)
$2\theta_{max}$	46.5°
No. of Reflections Measured	Total: 24935
	Unique: 5123 (R_{int} = 0.088)
Corrections	Lorentz-polarization Absorption (T_{max} = 0.87 T_{min} = 0.61)
Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least squares
Function Minimized	$\Sigma w(\|F_o\|-\|F_c\|)^2$
Least Squares Weights	$w = 1/\sigma^2(F_o)=[\sigma^2_c(F_o)+(p^2/4)F_o^2]^{-1}$
p-factor	0.0300
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	4503
No. Variables	296
Reflection/Parameter Ratio	15.21
Residuals: R; Rw; Rall	0.073; 0.090; 0.129
Goodness of Fit Indicator	2.63
Max Shift/Error in Final Cycle	0.03
Maximum peak in Final Diff. Map	0.90 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.69 $e^-/Å^3$

Table S-5.1 Atomic coordinates and B(eq) Values **(28)**.

atom	x	y	z	B(eq)
I(1)	0.2702(3)	0.0126(1)	0.52060(7)	5.22(7)
I(2)	0.6194(2)	0.0218(1)	0.60332(7)	3.95(6)
I(3)	0.8980(2)	0.3832(1)	0.73684(9)	5.20(7)
I(4)	0.7067(2)	0.2401(1)	0.64192(7)	4.30(7)
Zn(1)	0.4168(4)	0.0788(2)	0.5723(1)	2.48(10)
Zn(2)	0.7449(3)	0.2843(2)	0.7149(1)	2.59(10)
S(1)	0.3069(8)	0.2225(4)	0.5401(2)	2.6(2)
S(2)	0.4750(8)	0.3631(4)	0.7436(3)	2.5(2)
S(3)	0.2241(8)	0.0515(4)	0.6453(2)	2.4(2)
S(4)	0.7249(8)	0.1835(4)	0.7905(2)	2.6(2)
O(1)	0.429(2)	0.1792(10)	0.5542(5)	2.6(5)
O(2)	0.559(2)	0.2979(10)	0.7394(5)	2.4(4)
O(3)	0.297(2)	0.1109(9)	0.6210(5)	1.9(4)
O(4)	0.786(2)	0.1937(9)	0.7492(5)	2.5(4)
N(1)	0.267(2)	0.281(1)	0.5754(7)	2.1(5)
N(2)	0.303(2)	0.324(1)	0.6455(7)	1.8(5)
N(3)	0.367(2)	0.365(1)	0.7072(7)	2.4(6)
N(4)	0.281(3)	0.052(1)	0.6934(7)	2.3(5)
N(5)	0.429(2)	0.085(1)	0.7407(7)	2.5(5)
N(6)	0.594(2)	0.130(1)	0.7838(7)	2.2(5)
C(1)	0.324(3)	0.279(1)	0.6121(8)	1.7(6)
C(2)	0.377(3)	0.324(1)	0.6776(8)	0.8(6)
C(3)	0.364(3)	0.289(2)	0.4967(8)	2.2(7)
C(4)	0.427(3)	0.237(2)	0.4670(10)	4.2(8)
C(5)	0.258(3)	0.332(2)	0.4841(9)	3.4(8)
C(6)	0.489(3)	0.332(2)	0.5187(9)	2.9(7)
C(7)	0.182(3)	0.374(2)	0.640(1)	4.5(8)
C(8)	0.367(3)	0.350(2)	0.7877(9)	3.4(8)
C(9)	0.282(4)	0.274(2)	0.7761(10)	4.6(8)
C(10)	0.462(3)	0.342(2)	0.8257(10)	3.9(9)
C(11)	0.273(3)	0.417(2)	0.7927(9)	3.7(8)
C(12)	0.382(3)	0.083(1)	0.7017(8)	1.5(6)
C(13)	0.540(3)	0.123(2)	0.7486(10)	3.2(8)
C(14)	0.059(3)	0.093(1)	0.6516(8)	1.8(7)
C(15)	0.022(4)	0.043(2)	0.674(1)	4.9(9)
C(16)	0.005(3)	0.102(2)	0.6092(10)	3.4(8)
C(17)	0.081(4)	0.165(2)	0.674(1)	4.5(9)
C(18)	0.355(3)	0.055(2)	0.7742(10)	3.8(8)

Table S-5.2 Anisotropic displacement parameters for **(28)**.

atom	U11	U22	U33	U12	U13	U23
I(1)	0.070(2)	0.066(2)	0.062(2)	0.002(2)	-0.022(2)	-0.016(1)
I(2)	0.031(1)	0.053(2)	0.066(2)	0.016(1)	-0.005(2)	0.017(1)
I(3)	0.032(2)	0.043(2)	0.123(2)	-0.010(1)	-0.005(2)	-0.010(2)
I(4)	0.033(2)	0.082(2)	0.048(2)	0.024(2)	-0.004(1)	-0.015(1)
Zn(1)	0.024(2)	0.044(3)	0.027(2)	0.003(2)	0.004(2)	0.005(2)
Zn(2)	0.018(2)	0.031(2)	0.050(2)	0.004(2)	0.002(2)	0.007(2)
Cl(1)	0.18(3)	0.08(2)	0.33(4)	-0.02(2)	0.01(3)	-0.11(2)
Cl(3)	0.07(2)	0.19(3)	0.11(2)	0.10(2)	0.06(2)	0.12(2)
Cl(5)	0.091(9)	0.070(8)	0.114(10)	0.029(7)	-0.039(8)	-0.022(7)
Cl(6)	0.11(2)	0.01(1)	0.42(5)	-0.02(1)	-0.07(3)	0.04(2)
Cl(9)	0.24(4)	0.04(1)	0.08(2)	0.02(2)	-0.01(2)	-0.03(1)
S(1)	0.018(5)	0.042(6)	0.039(5)	-0.001(5)	-0.002(5)	0.018(5)
S(2)	0.024(5)	0.028(6)	0.045(6)	-0.002(4)	0.005(5)	-0.003(4)
S(3)	0.016(5)	0.041(6)	0.033(5)	0.000(4)	0.000(5)	0.000(4)
S(4)	0.022(5)	0.046(6)	0.032(5)	0.013(5)	-0.005(5)	0.007(4)

Table S-5.3. Relevant bond angles **(28)**.

atom	atom	atom	angle	atom	atom	atom	angle
I1	Zn1	I2	122.1(2)	O3	S3	C14	101(1)
I1	Zn1	O1	107.5(6)	N4	S3	C14	102(1)
I1	Zn1	O3	107.3(5)	O4	S4	N6	107(1)
I2	Zn1	O1	118.0(6)	O4	S4	C19	102(1)
I2	Zn1	O3	107.0(5)	N6	S4	C19	99(1)
O1	Zn1	O3	89.5(7)	Zn1	O1	S1	122(1)
I3	Zn2	I4	126.6(2)	Zn2	O2	S2	131(1)
I3	Zn2	O2	111.3(5)	Zn1	O3	S3	117(1)
I3	Zn2	O4	108.9(5)	Zn2	O4	S4	121(1)
I4	Zn2	O2	105.2(5)	S1	N1	C1	120(2)
I4	Zn2	O4	105.6(5)	C1	N2	C2	123(2)
O2	Zn2	O4	94.3(7)	C1	N2	C7	113(2)
O1	S1	N1	110(1)	C2	N2	C7	125(2)
O1	S1	C3	108(1)	S2	N3	C2	120(2)
N1	S1	C3	99(1)	S3	N4	C12	121(2)
O2	S2	N3	110(1)	C12	N5	C13	119(3)
O2	S2	C8	108(1)	C12	N5	C18	121(3)
N3	S2	C8	100(1)	C13	N5	C18	120(3)
O3	S3	N4	108(1)	S4	N6	C13	121(2)
C5	C3	C6	115(2)	N1	C1	N2	128(3)
S2	C8	C9	104(2)	N2	C2	N3	126(3)
S2	C8	C10	105(2)	S1	C3	C4	101(2)
S2	C8	C11	110(2)	S1	C3	C5	110(2)
C9	C8	C10	114(3)	S1	C3	C6	103(2)
C9	C8	C11	112(3)	C4	C3	C5	120(3)
C10	C8	C11	111(2)	C4	C3	C6	105(2)
N4	C12	N5	122(3)	C15	C14	C16	109(3)
N5	C13	N6	126(3)	C15	C14	C17	114(3)
S3	C14	C15	108(2)	C16	C14	C17	113(3)
S3	C14	C16	106(2)	S4	C19	C20	110(2)
S3	C14	C17	107(2)	S4	C19	C21	104(2)
S4	C19	C22	105(2)	C20	C19	C22	107(3)
C20	C19	C21	115(3)	C21	C19	C22	114(3)

Table S-5.4. Relevant bond lengths **(28)**.

atom	atom	distance	atom	atom	distance
I1	Zn1	2.552(4)	N2	C1	1.39(3)
I2	Zn1	2.516(4)	N2	C2	1.28(3)
I3	Zn2	2.506(4)	N2	C7	1.54(4)
I4	Zn2	2.533(4)	N3	C2	1.24(3)
Zn1	O1	1.96(2)	N4	C12	1.20(3)
Zn1	O3	2.08(2)	N5	C12	1.35(3)
Zn2	O2	2.05(2)	N5	C13	1.34(3)
Zn2	O4	2.06(2)	N5	C18	1.43(3)
S1	O1	1.54(2)	N6	C13	1.27(3)
S1	N1	1.63(2)	C3	C4	1.50(4)
S1	C3	1.96(3)	C3	C5	1.40(4)
S2	O2	1.49(2)	C3	C6	1.65(4)
S2	N3	1.60(2)	C8	C9	1.69(4)
S2	C8	1.81(3)	C8	C10	1.57(4)
S3	O3	1.54(2)	C8	C11	1.57(4)
S3	N4	1.66(2)	C14	C15	1.44(4)
S3	C14	1.84(3)	C14	C16	1.49(4)
S4	O4	1.48(2)	C14	C17	1.55(4)
S4	N6	1.67(2)	C19	C20	1.61(4)
S4	C19	1.78(4)	C19	C21	1.61(4)
N1	C1	1.32(3)	C19	C22	1.59(5)

Table S-5.5. Relevant torsion angles **(28)**.

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
I1	Zn1	O1	S1	45(1)	S1	O1	Zn1	O3	-63(1)
I1	Zn1	O3	S3	60(1)	S1	N1	C1	N2	180(2)
I2	Zn1	O1	S1	-171.7(9)	S2	O2	Zn2	O4	155(1)
I2	Zn1	O3	S3	-73(1)	S2	N3	C2	N2	-175(2)
I3	Zn2	O2	S2	43(2)	S3	O3	Zn1	O1	168(1)
I3	Zn2	O4	S4	85(1)	S3	N4	C12	N5	179(2)
I4	Zn2	O2	S2	-97(1)	S4	O4	Zn2	O2	-29(1)
I4	Zn2	O4	S4	-136(1)	S4	N6	C13	N5	-175(2)
Zn1	O1	S1	N1	107(1)	O1	S1	N1	C1	-10(2)
Zn1	O1	S1	C3	-146(1)	O1	S1	C3	C4	55(2)
Zn1	O3	S3	N4	116(1)	O1	S1	C3	C5	-177(2)
Zn1	O3	S3	C14	-138(1)	O1	S1	C3	C6	-54(2)
Zn2	O2	S2	N3	99(2)	O2	S2	N3	C2	-11(3)
Zn2	O2	S2	C8	-153(2)	O2	S2	C8	C9	-59(2)
Zn2	O4	S4	N6	98(1)	O2	S2	C8	C10	62(2)
Zn2	O4	S4	C19	-159(2)	O2	S2	C8	C11	-179(2)
N1	S1	C3	C6	60(2)	O3	S3	N4	C12	-15(3)
N1	C1	N2	C2	-170(3)	O3	S3	C14	C15	180(2)
N1	C1	N2	C7	10(4)	O3	S3	C14	C16	63(2)
N3	S2	C8	C9	56(2)	O3	S3	C14	C17	-58(2)
N3	S2	C8	C10	177(2)	O4	S4	N6	C13	-21(3)
N3	S2	C8	C11	-64(2)	O4	S4	C19	C20	-59(3)
N3	C2	N2	C1	176(3)	O4	S4	C19	C21	177(2)
N3	C2	N2	C7	-5(5)	O4	S4	C19	C22	57(3)
N4	S3	C14	C15	-69(2)	N1	S1	C3	C4	169(2)
N4	S3	C14	C16	174(2)	N1	S1	C3	C5	-63(2)
N4	S3	C14	C17	53(2)	C1	N1	S1	C3	-122(2)
N4	C12	N5	C13	-177(3)	C2	N3	S2	C8	-125(2)
N4	C12	N5	C18	-5(4)	C12	N4	S3	C14	-121(3)
N6	S4	C19	C20	50(3)	C13	N6	S4	C19	-127(3)
N6	S4	C19	C21	-74(2)	N6	C13	N5	C12	180(3)
N6	S4	C19	C22	166(2)	N6	C13	N5	C18	8(5)

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