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TABLE S1. Crystallographic data

Formula	$C_5H_8CsN_2O_2S$
Formula weight	293.10
System	orthorhombic
Space group	# 61 Pbca
a	8.300(2) Å
b	10.221(1) Å
c	22.673(6) Å
V	1923.3(9) $Å^3$
Z	8
Dcalc	2.024 g/cm^3
Radiation	Mo-Kα (0.71073 Å)
μ	39.9 cm^{-1}
F(000)	1112
Temperature (K)	293 ± 1°
No. of reflections measured	2455 total, 2093 unique
Crystal color	white
Instrument	Enraf-Nonius CAD4 diffractometer
Corrections:	Lorentz-polarization empirical absorption (from 1.00 to 1.13 on I) extinction (coefficient = 0.0000010)
Maximum 2θ	54°
h data range	0 to 10
k data range	0 to 13
l data range	0 to 28
Reflections included	1837 with $Fo^2 > 3.0\sigma(Fo^2)$
Monochromator	graphite crystal, incident beam
Attenuator	Zr foil, factor 17.5
Detector aperture	2.0 to 2.8 mm horizontal 4.0 mm vertical
Scan type	ω-θ
Scan rate	2 -20°/min (in omega)
Scan width, deg	1.0 + 0.350 tanθ
Anomalous dispersion	all non-hydrogen atoms
Parameters refined	101
Unweighted agreement factor	0.025
Weighted agreement factor	0.041
Factor including unobs. data	0.036
Esd of obs. of unit weight	1.77
Convergence, largest shift	0.05σ
Refinement	full-matrix least-squares
Minimization function	$\Sigma w(\|Fo\| - \|Fc\|)^2$
Least-squares weights	$4Fo^2/\sigma^2(Fo^2)$
High peak in final diff. map	0.65(9) e/$Å^3$
Computer hardware:	80486/33
Computer software:	Personal SDP B. A. Frenz & Associates, Inc.

TABLE S2. Fractional atomic coordinates and equivalent displacement parameters with e.s.d's.

Atom	x	y	z	$B_{eq}/B(Å^2)$
Cs	0.27040(3)	0.20524(2)	0.19543(1)	3.156(5)
S6	0.34415(8)	-0.05346(7)	0.08386(3)	2.90(1)
OH	0.4781(3)	0.4991(3)	0.24523(8)	4.21(5)
O7	0.8491(3)	-0.1965(2)	0.18212(9)	3.27(4)
N1	0.6562(3)	-0.0792(2)	0.05735(8)	2.51(4)
N3	0.5942(3)	-0.1405(2)	0.14954(9)	2.43(4)
C2	0.5388(3)	-0.0926(2)	0.09704(9)	2.04(4)
C4	0.7549(3)	-0.1557(3)	0.1436(1)	2.19(4)
C5	0.8124(3)	-0.1110(3)	0.0831(1)	2.15(4)
C8	0.9017(5)	-0.2162(3)	0.0491(1)	3.38(6)
C9	0.9143(4)	0.0120(3)	0.0904(1)	3.29(6)
HN1	0.6250	-0.0566	0.0292	4.00
H8b	0.9285	-0.1841	0.0109	4.40
H8c	0.9975	-0.2388	0.0695	4.40
H8a	0.8350	-0.2912	0.0453	4.40
H9a	0.8550	0.0757	0.1118	4.28
H9c	0.9411	0.0458	0.0526	4.28
H9b	1.0102	-0.0088	0.1112	4.28

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3)[a^2ß(1,1) + b^2ß(2,2) + c^2ß(3,3)]$

TABLE S3. General Displacement Parameter Expressions - U's

Atom	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Cs	0.0421(1)	0.0395(1)	0.0383(1)	0.00033(7)	0.00416(7)	-0.00060(7)
S6	0.0239(3)	0.0526(4)	0.0338(3)	0.0022(3)	0.0010(3)	0.0016(3)
OH	0.065(1)	0.055(1)	0.040(1)	0.008(1)	0.010(1)	0.0083(9)
O7	0.046(1)	0.050(1)	0.0287(8)	0.005(1)	-0.006(1)	0.0107(8)
N1	0.024(1)	0.051(1)	0.0202(8)	0.0024(9)	-0.0007(8)	0.0074(9)
N3	0.031(1)	0.037(1)	0.0240(9)	-0.0012(9)	0.0046(8)	0.0025(8)
C2	0.026(1)	0.028(1)	0.023(1)	-0.0003(9)	0.0022(9)	-0.0024(9)
C4	0.031(1)	0.027(1)	0.026(1)	-0.001(1)	-0.002(1)	0.002(1)
C5	0.023(1)	0.032(1)	0.027(1)	0.002(1)	0.0010(9)	0.005(1)
C8	0.048(2)	0.042(1)	0.039(1)	0.006(1)	0.012(1)	-0.003(1)
C9	0.035(1)	0.036(1)	0.054(2)	-0.005(1)	0.001(1)	0.006(1)

The form of the anisotropic displacement parameter is:

$\exp\{-2\pi^2[h^2a^{*2}U(1,1)+k^2b^{*2}U(2,2)+l^2c^{*2}U(3,3)+2hka^*b^*U(1,2)+2hla^*c^*U(1,3)+$

$+ 2klb^*c^*U(2,3)]\}$ where a^*, b^*, and c^* are reciprocal lattice constants.

TABLE S4. Interatomic distances (Å) and angles (deg)

Cs	Cs	5.1218 ± 0.0000	(-2 0 0 0)		
Cs	Cs	4.8315 ± 0.0001	(-4 0 0 0)		
Cs	S6	3.7102 ± 0.0006	(1 0 0 0)		
Cs	S6	3.6586 ± 0.0006	(-2 0 0 0)		
Cs	OH	3.6420 ± 0.0021	(1 0 0 0)		
Cs	OH	3.1572 ± 0.0019	(-2 0-1 0)		
Cs	OH	3.2572 ± 0.0021	(3 1-1 0)		
Cs	O7	3.3274 ± 0.0019	(-2 1 0 0)		
Cs	O7	3.1144 ± 0.0016	(3 1 0 0)		
Cs	N3	3.5670 ± 0.0017	(-2 0 0 0)		
S6	Cs	S6	92.98 ± 0.01	(1 0 0 0)	(-2 0 0 0)
S6	Cs	OH	136.13 ± 0.03	(1 0 0 0)	(1 0 0 0)
S6	Cs	OH	82.87 ± 0.03	(1 0 0 0)	(-2 0-1 0)
S6	Cs	OH	73.43 ± 0.03	(1 0 0 0)	(3 1-1 0)
S6	Cs	O7	89.81 ± 0.03	(1 0 0 0)	(-2 1 0 0)
S6	Cs	O7	152.88 ± 0.03	(1 0 0 0)	(3 1 0 0)
S6	Cs	N3	104.83 ± 0.03	(1 0 0 0)	(-2 0 0 0)
S6	Cs	OH	77.37 ± 0.03	(-2 0 0 0)	(1 0 0 0)
S6	Cs	OH	121.83 ± 0.03	(-2 0 0 0)	(-2 0-1 0)
S6	Cs	OH	152.66 ± 0.03	(-2 0 0 0)	(3 1-1 0)
S6	Cs	O7	88.88 ± 0.03	(-2 0 0 0)	(-2 1 0 0)
S6	Cs	O7	108.44 ± 0.03	(-2 0 0 0)	(3 1 0 0)
S6	Cs	N3	43.94 ± 0.03	(-2 0 0 0)	(-2 0 0 0)
OH	Cs	OH	138.47 ± 0.05	(1 0 0 0)	(-2 0-1 0)
OH	Cs	OH	95.86 ± 0.01	(1 0 0 0)	(3 1-1 0)
OH	Cs	O7	47.94 ± 0.04	(1 0 0 0)	(-2 1 0 0)
OH	Cs	O7	66.95 ± 0.04	(1 0 0 0)	(3 1 0 0)
OH	Cs	N3	97.32 ± 0.04	(1 0 0 0)	(-2 0 0 0)
OH	Cs	OH	80.74 ± 0.04	(-2 0-1 0)	(3 1-1 0)
OH	Cs	O7	148.62 ± 0.05	(-2 0-1 0)	(-2 1 0 0)
OH	Cs	O7	71.85 ± 0.04	(-2 0-1 0)	(3 1 0 0)
OH	Cs	N3	81.09 ± 0.05	(-2 0-1 0)	(-2 0 0 0)
OH	Cs	O7	67.94 ± 0.04	(3 1-1 0)	(-2 1 0 0)
OH	Cs	O7	92.55 ± 0.04	(3 1-1 0)	(3 1 0 0)
OH	Cs	N3	161.82 ± 0.04	(3 1-1 0)	(-2 0 0 0)
O7	Cs	O7	106.61 ± 0.05	(-2 1 0 0)	(3 1 0 0)
O7	Cs	N3	130.19 ± 0.04	(-2 1 0 0)	(-2 0 0 0)
O7	Cs	N3	81.22 ± 0.04	(3 1 0 0)	(-2 0 0 0)
S6	C2	1.6910 ± 0.0020	(1 0 0 0)		
O7	C4	1.2443 ± 0.0026	(1 0 0 0)		
N1	C2	1.3333 ± 0.0023	(1 0 0 0)		
N1	C5	1.4586 ± 0.0025	(1 0 0 0)		
N1	HN1	0.7245 ± 0.0015	(1 0 0 0)		
C2	N1	C5	110.87 ± 0.15	(1 0 0 0)	(1 0 0 0)
C2	N1	HN1	111.34 ± 0.19	(1 0 0 0)	(1 0 0 0)
C5	N1	HN1	137.77 ± 0.19	(1 0 0 0)	(1 0 0 0)
N3	C2	1.3668 ± 0.0023	(1 0 0 0)		
N3	C4	1.3491 ± 0.0027	(1 0 0 0)		
C2	N3	C4	106.66 ± 0.16	(1 0 0 0)	(1 0 0 0)

S6	C2	N1	123.69 ± 0.14	(1 0 0 0)	(1 0 0 0)
S6	C2	N3	124.05 ± 0.14	(1 0 0 0)	(1 0 0 0)
N1	C2	N3	112.26 ± 0.17	(1 0 0 0)	(1 0 0 0)
C4	C5	1.5225 ± 0.0027		(1 0 0 0)	
O7	C4	N3	126.15 ± 0.20	(1 0 0 0)	(1 0 0 0)
O7	C4	C5	122.38 ± 0.19	(1 0 0 0)	(1 0 0 0)
N3	C4	C5	111.43 ± 0.17	(1 0 0 0)	(1 0 0 0)
C5	C8	1.5170 ± 0.0028		(1 0 0 0)	
C5	C9	1.5238 ± 0.0029		(1 0 0 0)	
N1	C5	C4	98.56 ± 0.15	(1 0 0 0)	(1 0 0 0)
N1	C5	C8	112.85 ± 0.17	(1 0 0 0)	(1 0 0 0)
N1	C5	C9	110.65 ± 0.17	(1 0 0 0)	(1 0 0 0)
C4	C5	C8	113.53 ± 0.17	(1 0 0 0)	(1 0 0 0)
C4	C5	C9	108.93 ± 0.17	(1 0 0 0)	(1 0 0 0)
C8	C5	C9	111.61 ± 0.18	(1 0 0 0)	(1 0 0 0)
C8	H8b	0.9500 ± 0.0023		(1 0 0 0)	
C8	H8c	0.9500 ± 0.0028		(1 0 0 0)	
C8	H8a	0.9500 ± 0.0026		(1 0 0 0)	
C5	C8	H8b	109.47 ± 0.20	(1 0 0 0)	(1 0 0 0)
C5	C8	H8c	109.47 ± 0.20	(1 0 0 0)	(1 0 0 0)
C5	C8	H8a	109.47 ± 0.23	(1 0 0 0)	(1 0 0 0)
H8b	C8	H8c	109.47 ± 0.27	(1 0 0 0)	(1 0 0 0)
H8b	C8	H8a	109.47 ± 0.23	(1 0 0 0)	(1 0 0 0)
H8c	C8	H8a	109.47 ± 0.23	(1 0 0 0)	(1 0 0 0)
C9	H9a	0.9500 ± 0.0024		(1 0 0 0)	
C9	H9c	0.9500 ± 0.0023		(1 0 0 0)	
C9	H9b	0.9500 ± 0.0024		(1 0 0 0)	
C5	C9	H9a	109.47 ± 0.20	(1 0 0 0)	(1 0 0 0)
C5	C9	H9c	109.47 ± 0.21	(1 0 0 0)	(1 0 0 0)
C5	C9	H9b	109.47 ± 0.20	(1 0 0 0)	(1 0 0 0)
H9a	C9	H9c	109.47 ± 0.22	(1 0 0 0)	(1 0 0 0)
H9a	C9	H9b	109.47 ± 0.24	(1 0 0 0)	(1 0 0 0)
H9c	C9	H9b	109.47 ± 0.23	(1 0 0 0)	(1 0 0 0)
OH	Cs	3.6420 ± 0.0021		(1 0 0 0)	
OH	Cs	3.1572 ± 0.0019		(-2 0 0 0)	
OH	Cs	3.2572 ± 0.0021		(3 1 0 0)	
OH	O7	2.8462 ± 0.0025		(-2 1 0 0)	
OH	O7	3.7527 ± 0.0027		(3 1 0 0)	
OH	O7	3.6797 ± 0.0025		(-4-1 1 0)	
Cs	OH	Cs	97.50 ± 0.05	(1 0 0 0)	(-2 0 0 0)
Cs	OH	Cs	164.76 ± 0.06	(1 0 0 0)	(3 1 0 0)
Cs	OH	O7	60.23 ± 0.05	(1 0 0 0)	(-2 1 0 0)
Cs	OH	O7	49.79 ± 0.04	(1 0 0 0)	(3 1 0 0)
Cs	OH	O7	134.30 ± 0.06	(1 0 0 0)	(-4-1 1 0)
Cs	OH	Cs	97.73 ± 0.06	(-2 0 0 0)	(3 1 0 0)
Cs	OH	O7	128.19 ± 0.06	(-2 0 0 0)	(-2 1 0 0)
Cs	OH	O7	92.29 ± 0.06	(-2 0 0 0)	(3 1 0 0)
Cs	OH	O7	53.54 ± 0.04	(-2 0 0 0)	(-4-1 1 0)
Cs	OH	O7	109.82 ± 0.07	(3 1 0 0)	(-2 1 0 0)
Cs	OH	O7	128.83 ± 0.05	(3 1 0 0)	(3 1 0 0)

Cs	OH	O7	56.94 ± 0.04	(3 1 0 0)	(-4-1 1 0)
O7	OH	O7	102.19 ± 0.07	(-2 1 0 0)	(3 1 0 0)
O7	OH	O7	164.91 ± 0.08	(-2 1 0 0)	(-4-1 1 0)
O7	OH	O7	92.49 ± 0.04	(3 1 0 0)	(-4-1 1 0)

Symmetry codes:

(1 0 0 0) = x, y, z

(-2 0 0 0) = 1/2-x, 1/2+y, z

(-2 1 0 0) = 3/2-x, 1/2+y, z

(-2 0-1 0) = 1/2-x, y-1/2, z

(3 1 0 0) = 1-x, 1/2+y, 1/2-z

(3 1-1 0) = 1-x, y-1/2, 1/2-z

(-4 0 0 0) = 1/2+x, y, 1/2-z

(-4-1 1 0) = x-1/2, 1+y, 1/2-z