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Table 1. Crystal data and structure refinement for 2.

Identification code	2
Empirical formula	$Co_1\ Cl_4\ C_{18}\ O_{7.5}\ H_{41}$
Formula weight	606.15
Temperature	293(2) K
Wavelength	0.71070 A
Crystal system	Trigonal
Space group	R $\bar{3}$ c
Unit cell dimensions	*a* = 11.146(2) A α = 90 deg. *b* = 11.146(2) A β = 90 deg. *c* = 76.47(2) A γ = 120 deg.
Volume	8228(2) Å^3
Z	12
Density (calculated)	1.47 Mg/m^3
Absorption coefficient	1.053 mm^{-1}
F(000)	3648
Crystal size	0.30 x 0.35 x 0.40 mm
Theta range for data collection	2 to 46 °.
Index ranges	-12<=h<=8, -11<=k<=12, -84<=l<=77
Reflections collected	9302
Independent reflections	1330 [R(int) = 0.0340]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1330 / 0 / 103
Goodness-of-fit on F^2	1.167
Final R indices [I>2σ(I)]	R1 = 0.0322, wR2 = 0.0914
R indices (all data)	R1 = 0.0349, wR2 = 0.0930
Largest diff. peak and hole	0.386 and -0.181 e.Å^3

After anisotropic refinement of all non-hydrogen atoms, methylene hydrogen atoms were placed in calculated positions (d_{C-H} = 1.0 Å) and refined as riding atoms with fixed thermal parameters based upon the atoms to which they are bonded. Quaternary ammonium hydrogen atoms were located *via* inspection of a difference Fourier map and refined as riding atoms with fixed thermal parameters based upon the atoms to which they are bonded. The three water molecules were observed to lie upon a crystallographic *3 2* site with O3 being disordered around the two-fold axes. Owing to this crystallographic disorder, O3 was refined with a site occupancy of 0.5 and the water hydrogen atoms were not locateable. Structure solution was accomplished with the aid of SHELXS-86 [Sheldrick, G. M. *Acta Crystallogr.* **1990**, *A46*, 467] and refinement was conducted using SHELX93 [Sheldrick, G. M. *SHELX-76*, University of Cambridge (1976)] locally implemented on a pentium-based IBM compatible computer.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 2.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Co(1)	0	0	521(1)	38(1)
Cl(1)	0	0	227(1)	49(1)
Cl(2)	-464(1)	-2133(1)	618(1)	59(1)
O(1)	-2123(2)	-1433(2)	1703(1)	38(1)
O(2)	-1800(2)	-2204(2)	1328(1)	40(1)
O(3)	5482(13)	3843(18)	794(2)	209(6)
N(1)	0	0	1934(1)	31(1)
N(2)	0	0	1100(1)	33(1)
C(1)	-1484(3)	-643(3)	1991(1)	38(1)
C(2)	-2415(3)	-1881(3)	1879(1)	39(1)
C(3)	-3134(3)	-2436(3)	1587(1)	41(1)
C(4)	-2833(3)	-1942(3)	1402(1)	45(1)
C(5)	-1922(3)	-2419(3)	1145(1)	47(1)
C(6)	-1427(3)	-1097(3)	1043(1)	42(1)

Table 3. Bond lengths (Å) and angles (°) for 2.

Distances

Co(1)-Cl(1)		2.2410(13)	
Co(1)-Cl(2)#1		2.2901(8)	
Co(1)-Cl(2)#2		2.2901(8)	
Co(1)-Cl(2)		2.2901(8)	
O(1)-C(2)		1.420(3)	
O(1)-C(3)		1.430(3)	
O(2)-C(5)		1.419(3)	
O(2)-C(4)		1.436(3)	
N(1)-C(1)#1		1.501(3)	
N(1)-C(1)#2		1.501(3)	
N(1)-C(1)		1.501(3)	
N(2)-C(6)		1.507(3)	
N(2)-C(6)#1		1.507(3)	
N(2)-C(6)#2		1.507(3)	
C(1)-C(2)		1.508(4)	
C(3)-C(4)		1.497(4)	
C(5)-C(6)		1.506(4)	
N(1)-HN(1)	0.944	N(2)-HN(2)	0.915
O(1)...HN(1)	2.246	O(2)...HN(2)	2.412
O(1)...N(1)	2.736(2)	O(2)...N(2)	2.858(2)
O(3)...O(3)#1	2.91(3)		
O(3)...O(3)#2	2.91(3)		
N(1)...N(2)	6.37		

Angles

Cl(1)-Co(1)-Cl(2)#1	108.97(2)
Cl(1)-Co(1)-Cl(2)#2	108.97(2)
Cl(2)#1-Co(1)-Cl(2)#2	109.97(2)
Cl(1)-Co(1)-Cl(2)	108.97(2)
Cl(2)#1-Co(1)-Cl(2)	109.97(2)
Cl(2)#2-Co(1)-Cl(2)	109.97(2)
C(2)-O(1)-C(3)	111.2(2)
C(5)-O(2)-C(4)	113.6(2)
C(1)#1-N(1)-C(1)#2	111.90(14)
C(1)#1-N(1)-C(1)	111.90(14)
C(1)#2-N(1)-C(1)	111.90(14)
C(6)-N(2)-C(6)#1	111.87(14)
C(6)-N(2)-C(6)#2	111.87(14)
C(6)#1-N(2)-C(6)#2	111.87(14)
N(1)-C(1)-C(2)	111.3(2)
O(1)-C(2)-C(1)	106.4(2)
O(1)-C(3)-C(4)	110.8(2)
O(2)-C(4)-C(3)	110.5(2)
O(2)-C(5)-C(6)	112.9(2)
C(5)-C(6)-N(2)	111.4(2)
N(1)-HN(1)-O(1)	111.4
N(2)-HN(2)-O(2)	110.1

Symmetry transformations used to generate equivalent atoms:
#1 -y,x-y,z #2 -x+y,-x,z #3 x-y+1/3,-y+2/3,-z+1/6

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 2.

The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Co(1)	43(1)	43(1)	29(1)	0	0	21(1)
Cl(1)	59(1)	59(1)	29(1)	0	0	29(1)
Cl(2)	82(1)	48(1)	48(1)	3(1)	1(1)	35(1)
O(1)	33(1)	32(1)	38(1)	0(1)	1(1)	9(1)
O(2)	41(1)	44(1)	37(1)	3(1)	3(1)	23(1)
O(3)	211(11)	339(22)	168(12)	92(9)	54(8)	205(14)
N(1)	32(1)	32(1)	28(2)	0	0	16(1)
N(2)	37(1)	37(1)	26(2)	0	0	18(1)
C(1)	34(1)	42(2)	38(1)	2(1)	5(1)	19(1)
C(2)	34(1)	37(1)	41(1)	4(1)	3(1)	13(1)
C(3)	35(1)	36(1)	42(1)	-5(1)	1(1)	10(1)
C(4)	45(2)	52(2)	44(2)	-1(1)	-2(1)	29(1)
C(5)	51(2)	39(2)	41(2)	-3(1)	3(1)	15(1)
C(6)	38(2)	47(2)	34(1)	1(1)	-4(1)	16(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 2.

	x	y	z	U(eq)
HN(1)	0	0	1810	50
HN(2)	0	0	1220	50
H(1B)	-1780(3)	38(3)	1982(1)	45
H(1A)	-1562(3)	-929(3)	2112(1)	45
H(2B)	-2227(3)	-2631(3)	1900(1)	47
H(2A)	-3380(3)	-2206(3)	1906(1)	47
H(3B)	-4047(3)	-2605(3)	1619(1)	49
H(3A)	-3132(3)	-3302(3)	1598(1)	49
H(4B)	-3676(3)	-2416(3)	1333(1)	54
H(4A)	-2508(3)	-956(3)	1398(1)	54
H(5B)	-2885(3)	-3052(3)	1116(1)	57
H(5A)	-1389(3)	-2849(3)	1110(1)	57
H(6B)	-2069(3)	-759(3)	1060(1)	51
H(6A)	-1409(3)	-1282(3)	919(1)	51

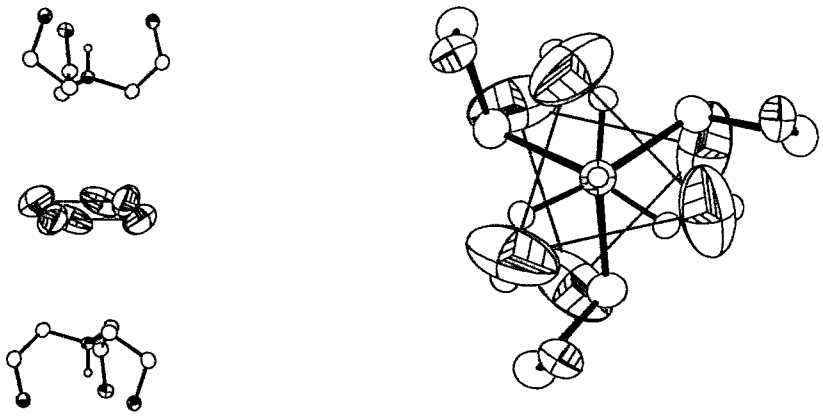

Figure S1. View of the environment above and below the O-O-O plane of $(H_3O)_3$.

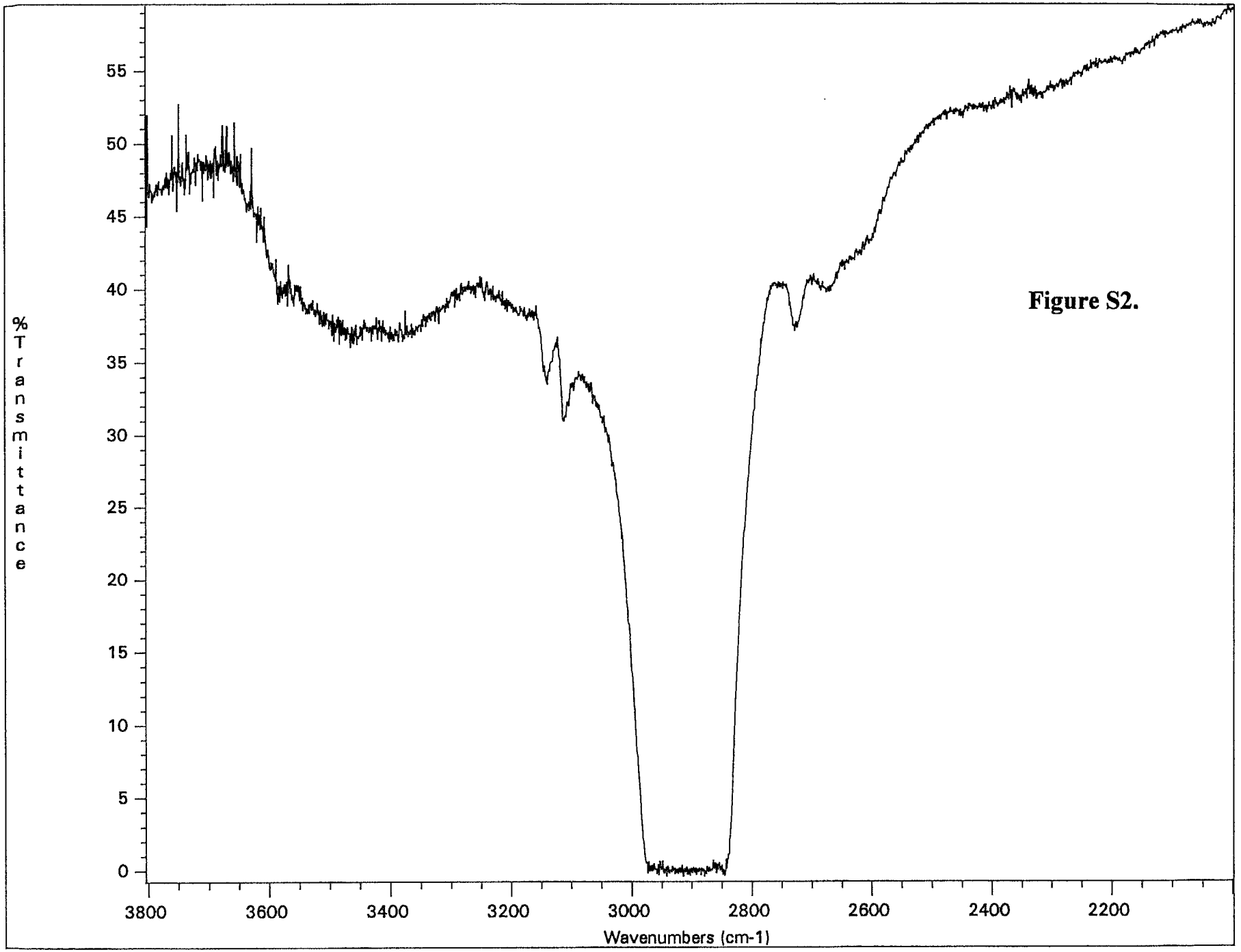

Figure S2.

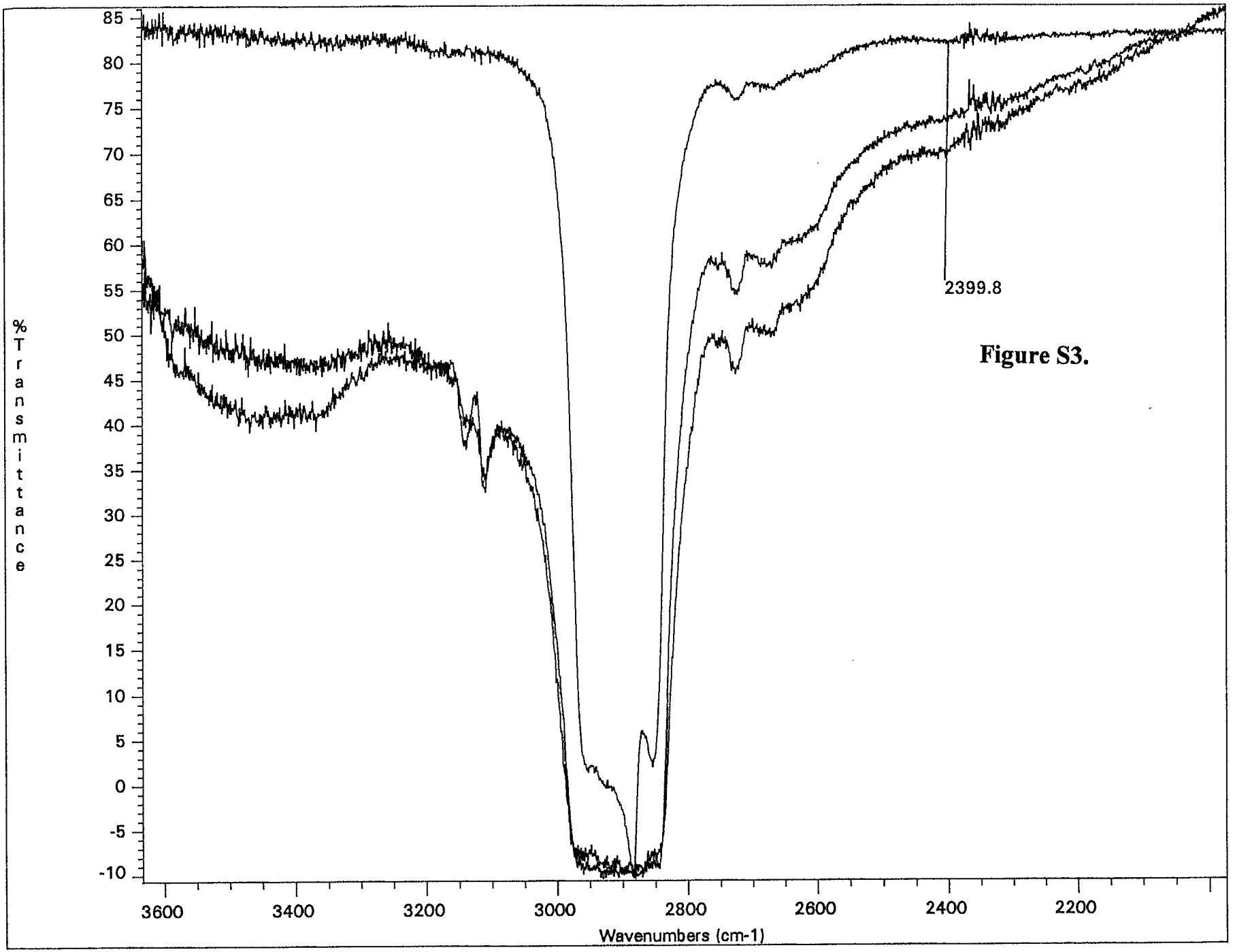

Figure S3.