Supporting information materials (8 pages):

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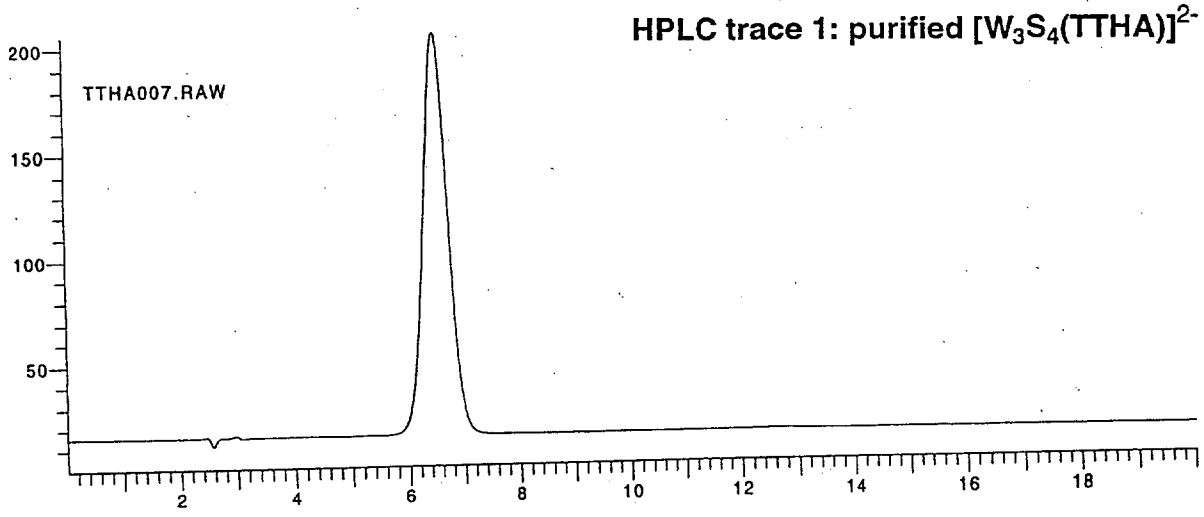
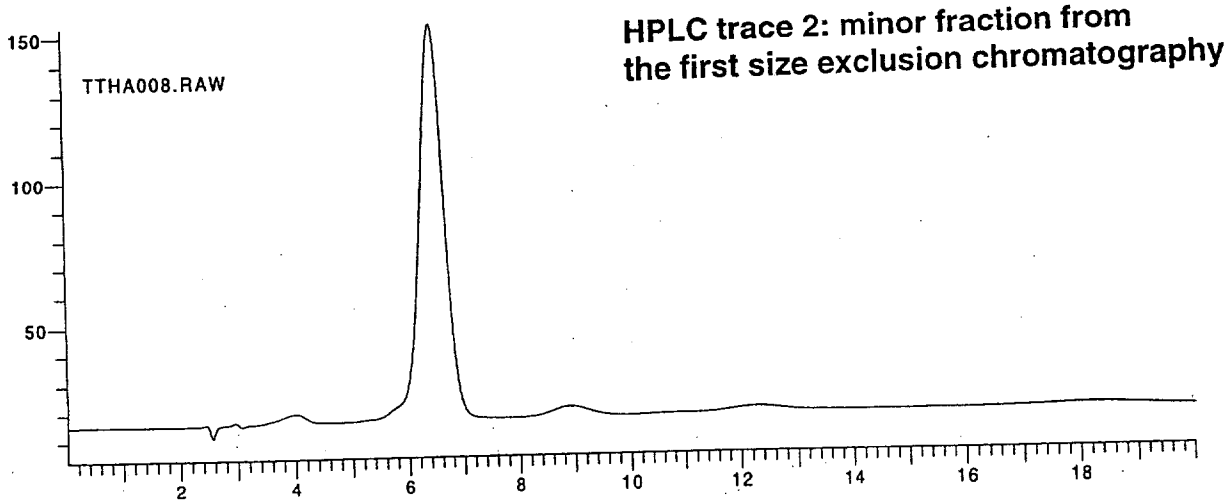
1. Figure S1. HPLC traces from the purification steps of $[W_3S_4(TTHA)]^{2-}$.





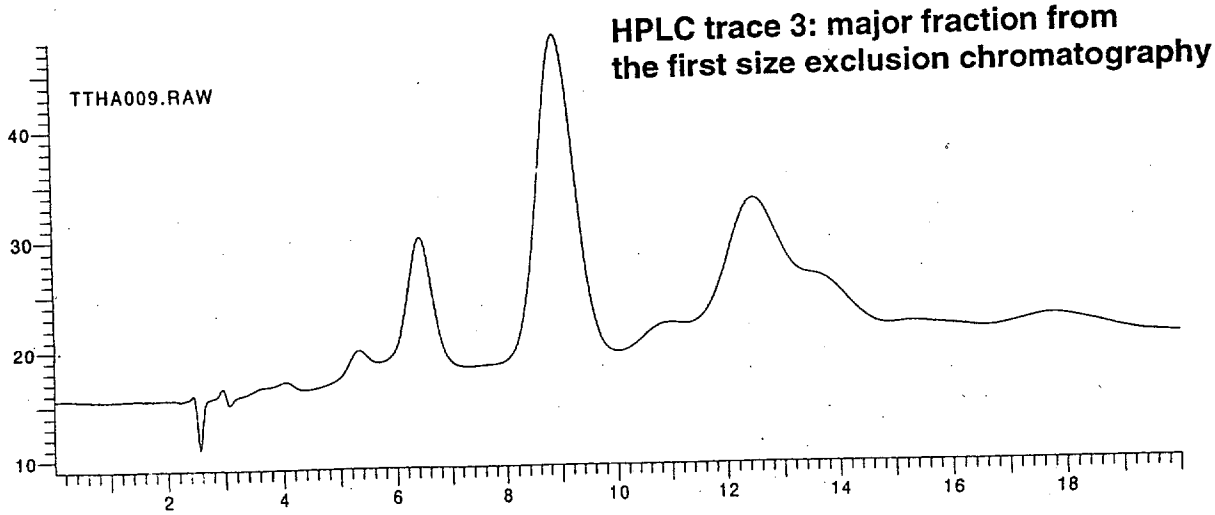


TABLE I -- Crystal and Data Parameters
Compound : SALU2 - amine ligand dimer

Empirical formula: $W_6 S_8 NA_3 O_{40} N_8 C_{36} H_{69}$

A)Crystal Parameters at T = -95°C [a,b]

a = 13.348(6) Å	Space Group: $P2_1/c$
b = 16.737(8) Å	Formula weight = 2682.6 amu
c = 15.810(7) Å	Z = 2
α = 90.0 °	d(calc) = 2.55 g cm^{-3}
β = 98.42(3) °	d(obs) = _____
γ = 90.0 °	μ(calc) = 104.0 cm^{-1}
V = 3494(5) $Å^3$	
Size: 0.05x0.18x0.20 mm	

B) Data Measurement Parameters [8]
Radiation : Mo Kα (λ = 0.71073Å)
Monochromator : Highly-oriented graphite (2θ = 12.2)
Detector : Crystal scintillation counter, with PHA.
Reflections measured : + H, + K, +/-L
2θ range: 3 -> 46 deg Scan Type: theta-2theta
Scan width: $\Delta\theta = 0.95 + 0.35 \tan\theta$
Scan speed: 5.49 (θ, deg/min)
Background: Measured over 0.25*($\Delta\theta$) added to each end of the scan.
Vert. aperture = 6.0 mm Horiz. aperture = 2.2 + 1.0 $\tan\theta$ mm
No. of reflections collected: 5055
No. of unique reflections: 4344

Intensity standards: (-2,9,2),(623),(1,6-7); measured every 0 hours of x-ray exposure time. Over the data collection period no net decrease in intensity was observed.
Orientation: Three reflections were checked after every 250 measurements. Crystal orientation was redetermined if any of the reflections were offset by more than 0.14 degree from their predicted positions. Reorientation was needed numerous times during data collection.

[a] Unit cell parameters and their esd's were derived by a least-squares fit to the setting angles of the unresolved Mo Kα components of 24 reflections with 2θ between 22° and 24°.
[b] In this and all subsequent tables the esd's of all parameters are given in parentheses, right-justified to the least significant digit(s) of the reported value.

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Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(Å^2)
W1	0.1544(1)	0.04829(6)	0.27295(8)	1.58(2)
W2	0.2083(1)	0.08021(6)	0.11721(7)	1.56(2)
W3	0.0407(1)	0.15333(6)	0.16857(7)	1.53(2)
S1	0.2134(6)	0.1729(4)	0.2294(4)	1.8(1)*
S2	0.1834(6)	-0.0445(4)	0.1731(4)	1.7(1)*
S3	0.0510(6)	0.0982(4)	0.0370(5)	2.1(1)*
S4	-0.0155(6)	0.0485(4)	0.2419(5)	2.2(1)*
NA1	0.495(1)	0.0858(7)	0.5765(8)	3.8(3)*
NA2	0.388(3)	-0.130(2)	0.649(2)	5.3(7)*
O1	0.305(2)	0.026(1)	0.340(1)	3.1(4)*
O2	0.392(2)	0.020(1)	0.470(1)	3.5(5)*
O3	0.141(2)	-0.050(1)	0.356(1)	2.1(4)*
O4	0.118(2)	-0.091(1)	0.487(1)	2.7(4)*
O5	0.050(1)	0.269(1)	0.120(1)	1.7(4)*
O6	0.118(2)	0.389(1)	0.151(1)	3.2(4)*
O7	-0.329(2)	0.249(1)	0.044(1)	3.8(5)*
O8	-0.256(2)	0.248(2)	-0.076(2)	6.3(7)*
O9	-0.267(2)	-0.172(1)	-0.046(1)	2.3(4)*
O10	-0.329(2)	-0.203(1)	0.073(1)	2.4(4)*
O11	-0.362(2)	-0.065(1)	-0.148(1)	2.2(4)*
O12	-0.512(2)	-0.014(2)	-0.121(2)	5.9(7)*
O13	0.653(2)	0.138(1)	0.654(2)	5.6(6)*
O14	0.473(3)	-0.002(2)	0.691(2)	8.0(8)*
O15	0.510(2)	0.184(1)	0.447(2)	5.1(6)*
O16	0.401(2)	0.192(1)	0.617(2)	5.9(7)*
O17	0.613(3)	0.179(2)	0.808(2)	9(1)*
O18	0.404(3)	0.149(2)	0.782(2)	8.1(8)*
O19	0.225(3)	-0.057(2)	0.650(2)	10(1)*
O20	0.426(3)	-0.161(2)	0.784(2)	12(1)*
N1	0.146(2)	0.107(1)	0.406(1)	1.1(4)*
N2	0.007(2)	0.242(1)	0.271(1)	1.5(4)*
N3	-0.135(2)	0.175(1)	0.126(1)	2.4(5)*
N4	-0.260(2)	-0.013(1)	-0.006(1)	0.8(4)*
C1	0.249(2)	0.108(1)	0.452(2)	1.8(6)*
C2	0.317(2)	0.049(1)	0.425(2)	1.2(5)*
C3	0.081(2)	0.050(2)	0.446(2)	1.9(5)*
C4	0.116(3)	-0.035(2)	0.427(2)	2.6(6)*
C5	0.103(3)	0.190(2)	0.407(2)	2.8(6)*
C6	0.002(3)	0.212(2)	0.364(2)	2.8(6)*
C7	0.058(2)	0.311(2)	0.265(2)	2.2(6)*
C8	0.083(3)	0.331(2)	0.177(2)	2.8(6)*
C9	-0.105(2)	0.269(2)	0.243(2)	2.0(6)*
C10	-0.170(3)	0.204(2)	0.204(2)	2.8(6)*
C11	-0.156(2)	0.225(1)	0.050(2)	1.3(5)*
C12	-0.252(3)	0.242(2)	0.001(2)	4.1(8)*
C13	-0.205(2)	0.102(1)	0.109(2)	1.1(5)*
C14	-0.176(2)	0.050(1)	0.032(2)	1.5(5)*
C15	-0.267(2)	-0.072(1)	0.064(2)	1.7(5)*
C16	-0.294(2)	-0.158(2)	0.028(2)	1.9(5)*
C17	-0.361(3)	0.026(2)	-0.034(2)	2.6(6)*
C18	-0.419(2)	-0.021(2)	-0.110(2)	1.9(6)*

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Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(Å^2)
H1A	0.26326(1)	0.13263(1)	0.50690(1)	2.2*
H1B	0.30549(1)	0.11311(1)	0.42292(1)	2.2*
H3A	0.01207(1)	0.05660(1)	0.42248(1)	2.3*
H3B	0.08904(1)	0.05835(1)	0.50611(1)	2.3*
H5A	0.14950(1)	0.22377(1)	0.38387(1)	3.5*
H5B	0.10380(1)	0.20282(1)	0.46585(1)	3.5*
H6A	-0.04120(1)	0.16660(1)	0.36102(1)	3.5*
H6B	-0.02503(1)	0.25329(1)	0.39503(1)	3.5*
H7A	0.11980(1)	0.30807(1)	0.30354(1)	2.7*
H7B	0.01788(1)	0.35346(1)	0.28239(1)	2.7*
H9A	-0.10607(1)	0.31150(1)	0.20271(1)	2.5*
H9B	-0.13121(1)	0.28834(1)	0.29227(1)	2.5*
H10A	-0.16908(1)	0.16151(1)	0.24424(1)	3.5*
H10B	-0.23786(1)	0.22333(1)	0.19051(1)	3.5*
H11A	-0.11737(1)	0.20126(1)	0.01042(1)	1.6*
H11B	-0.12828(1)	0.27535(1)	0.06732(1)	1.6*
H13A	-0.27321(1)	0.12048(1)	0.09465(1)	1.4*
H13B	-0.19978(1)	0.07018(1)	0.15880(1)	1.4*
H14A	-0.16532(1)	0.08522(1)	-0.01308(1)	1.9*
H14B	-0.11544(1)	0.02205(1)	0.05158(1)	1.9*
H15A	-0.31833(1)	-0.05466(1)	0.09601(1)	2.1*
H15B	-0.20386(1)	-0.07357(1)	0.10078(1)	2.1*
H17A	-0.35076(1)	0.07923(1)	-0.04997(1)	3.3*
H17B	-0.39934(1)	0.02506(1)	0.01253(1)	3.3*

Starred atoms were included with isotropic thermal parameters.
The thermal parameter given for anisotropically refined atoms is the isotropic equivalent thermal parameter defined as:
$(4/3)\ [a^2\beta(1,1) + b^2\beta(2,2) + c^2\beta(3,3) + ab(\cos\gamma)\beta(1,2)$
$+ ac(\cos\beta)\beta(1,3) + bc(\cos\alpha)\beta(2,3)]$
where a,b,c are real cell parameters, and $\beta(i,j)$ are anisotropic betas.

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Table of Anisotropic Thermal Parameters - B's

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
W1	1.54(5)	1.53(4)	1.69(4)	0.16(4)	0.24(4)	0.00(4)	1.58(2)
W2	1.41(5)	1.45(4)	1.83(5)	0.17(4)	0.25(4)	-0.03(4)	1.56(2)
W3	1.69(5)	1.31(4)	1.61(4)	0.21(4)	0.26(4)	-0.06(4)	1.53(2)

The form of the anisotropic temperature factor is:
$\exp[-0.25\{h^2a^2B(1,1) + k^2b^2B(2,2) + l^2c^2B(3,3) + 2hkabB(1,2) + 2hlacB(1,3) + 2klbcB(2,3)\}]$ where a,b, and c are reciprocal lattice constants.

Table of Root-Mean-Square Amplitudes of Anisotropic Displacement in Angstroms

Atom	Min.	Int'med.	Max.
W1	0.132	0.146	0.146
W2	0.126	0.142	0.153
W3	0.123	0.143	0.150

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Intramolecular Distances

ATOM 1	ATOM 2	DISTANCE
W1	W2	2.718(2)
W1	W3	2.718(2)
W2	W3	2.774(2)
W1	S1	2.367(7)
W2	S1	2.350(7)
W3	S1	2.387(8)
W1	S2	2.287(7)
W1	S4	2.250(9)
W2	S2	2.309(7)
W2	S3	2.309(8)
W3	S3	2.298(8)
W3	S4	2.289(8)
W1	O1	2.15(2)
W1	O3	2.13(2)
W1	N1	2.34(2)
W2	O9	2.13(2)
W2	O11	2.06(2)
W2	N4	2.28(2)
W3	O5	2.09(2)
W3	N2	2.29(2)
W3	N3	2.37(3)

Intramolecular Distances

ATOM 1	ATOM 2	DISTANCE
C2	O1	1.38(3)
C2	O2	1.24(3)
C4	O3	1.25(3)
C4	O4	1.33(3)
C8	O5	1.40(3)
C8	O6	1.17(3)
C12	O7	1.32(5)
C12	O8	1.21(4)
C16	O9	1.30(3)
C16	O10	1.17(3)
C18	O11	1.27(3)
C18	O12	1.24(4)
C1	N1	1.46(3)
C3	N1	1.50(4)
C5	N1	1.50(4)
C6	N2	1.57(4)
C7	N2	1.35(4)
C9	N2	1.57(4)
C10	N3	1.47(4)
C11	N3	1.46(3)
C13	N3	1.54(3)
C14	N4	1.59(3)
C15	N4	1.49(3)
C17	N4	1.51(4)
C1	C2	1.46(4)
C3	C4	1.53(4)
C5	C6	1.47(5)
C7	C8	1.52(4)
C9	C10	1.47(4)
C11	C12	1.44(5)
C13	C14	1.59(4)
C15	C16	1.57(4)
C17	C18	1.55(4)

Intramolecular Angles

ATOM 1	ATOM 2	ATOM 3	ANGLE
W2	W1	W3	61.39(5)
W1	W2	W3	59.30(4)
W1	W3	W2	59.31(5)
S1	W1	S2	107.5(3)
S1	W1	S4	107.6(3)
S1	W1	O1	88.0(6)
S1	W1	O3	157.1(5)
S1	W1	N1	87.2(5)
S2	W1	S4	96.8(3)
S2	W1	O1	89.0(6)
S2	W1	O3	86.6(5)
S2	W1	N1	160.4(5)
S4	W1	O1	160.6(6)
S4	W1	O3	88.0(6)
S4	W1	N1	90.8(6)
O1	W1	O3	73.9(8)
O1	W1	N1	78.4(8)
O3	W1	N1	75.6(7)
S1	W2	S2	107.3(3)
S1	W2	S3	104.6(3)
S1	W2	O9	87.2(5)
S1	W2	O11	89.3(6)
S1	W2	N4	158.4(6)
S2	W2	S3	99.0(3)
S2	W2	O9	160.4(6)
S2	W2	O11	89.5(5)
S2	W2	N4	86.0(5)
S3	W2	O9	89.6(6)
S3	W2	O11	160.5(6)
S3	W2	N4	89.6(6)
O9	W2	O11	77.3(8)
O9	W2	N4	76.5(7)
O11	W2	N4	73.5(8)
S1	W3	S3	103.8(3)
S1	W3	S4	105.7(3)
S1	W3	O5	85.2(6)
S1	W3	N2	84.4(6)
S1	W3	N3	161.8(6)
S3	W3	S4	102.6(3)
S3	W3	O5	91.4(5)
S3	W3	N2	160.7(5)
S3	W3	N3	89.6(6)
S4	W3	O5	159.3(6)
S4	W3	N2	91.6(6)
S4	W3	N3	82.9(6)
O5	W3	N2	71.6(7)
O5	W3	N3	82.1(8)
N2	W3	N3	79.2(8)
W1	N1	C1	106.8(17)
W1	N1	C3	102.5(14)
W1	N1	C5	118.3(17)
C1	N1	C3	110.3(19)
C1	N1	C5	108.5(21)
C3	N1	C5	110.3(23)

Intramolecular Angles

ATOM 1	ATOM 2	ATOM 3	ANGLE
W3	N2	C6	119.6(16)
W3	N2	C7	111.1(19)
W3	N2	C9	105.7(15)
C6	N2	C7	115.4(22)
C6	N2	C9	100.4(23)
C7	N2	C9	101.7(21)
W3	N3	C10	104.0(18)
W3	N3	C11	112.6(19)
W3	N3	C13	119.0(16)
C10	N3	C11	117.3(23)
C10	N3	C13	98.4(24)
C11	N3	C13	105.3(20)
W2	N4	C14	109.9(16)
W2	N4	C15	108.2(15)
W2	N4	C17	110.2(16)
C14	N4	C15	106.3(18)
C14	N4	C17	111.7(19)
C15	N4	C17	110.5(22)
W1	O1	C2	113.5(18)
W1	O3	C4	117.5(18)
W3	O5	C8	118.7(16)
W2	O9	C16	121.4(17)
W2	O11	C18	127.4(19)
N1	C1	C2	115.2(22)
O1	C2	O2	115.1(25)
O1	C2	C1	119.1(23)
O2	C2	C1	125.5(24)
N1	C3	C4	107.6(25)
O3	C4	O4	121.7(27)
O3	C4	C3	119.4(26)
O4	C4	C3	118.9(27)
N1	C5	C6	123.2(26)
N2	C6	C5	110.7(28)
N2	C7	C8	115.1(25)
O5	C8	O6	119.8(29)
O5	C8	C7	109.7(25)
O6	C8	C7	130.3(29)
N2	C9	C10	112.6(23)
N3	C10	C9	110.5(29)
N3	C11	C12	128.0(29)
O7	C12	O8	126.0(39)
O7	C12	C11	116.2(32)
O8	C12	C11	117.8(40)
N3	C13	C14	111.0(23)
N4	C14	C13	114.5(23)
N4	C15	C16	111.8(21)
O9	C16	O10	127.8(27)
O9	C16	C15	114.5(25)
O10	C16	C15	117.5(26)
N4	C17	C18	109.7(24)
O11	C18	O12	130.6(30)
O11	C18	C17	113.3(28)
O12	C18	C17	115.8(30)

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Intramolecular Distances

ATOM 1	ATOM 2	DISTANCE
NA1	O2	2.30(3)
NA1	O2	2.50(3)
NA1	O13	2.45(3)
NA1	O14	2.38(3)
NA1	O15	2.65(3)
NA1	O16	2.32(3)
NA2	O8	2.82(4)
NA2	O14	2.48(5)
NA2	O15	2.36(5)
NA2	O19	2.50(6)
NA2	O20	2.19(5)

Intermolecular Distances
Possible Hydrogen bonds

ATOM 1	ATOM 2	DISTANCE
O1	O13	2.82(3)
O4	O19	2.81(4)
O6	O19	3.15(5)
O7	O13	2.60(3)
O7	O15	2.69(4)
O8	O17	2.61(5)
O10	O15	3.06(3)
O10	O18	2.79(4)
O12	O14	2.96(4)
O12	O20	2.94(5)
O13	O17	2.65(5)
O16	O18	2.70(4)
O17	O18	2.80(5)
O17	O20	3.06(5)

Intramolecular Distances
Non-bonding contacts across center

ATOM 1	ATOM 2	DISTANCE
S3	S3'	3.681(14)
S3	S2'	4.311(11)
S3	S4'	5.008(11)
S3	C14	3.13(3)
S3	C14'	3.27(3)

Primed atoms are related to the input
by the inversion center at the origin.