Table 1S. Crystal data and structure refinement for $[Fe_4(sae)_4(MeOH)_4]$.

Identification code	fe4sae	
Empirical formula	C40 H52 Fe4 N4 O12	
Formula weight	1004.26	
Temperature	-70 °C	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 13.3625(7) Å	α = 66.538(1)°
	b = 13.7572(7) Å	β = 74.973(1)°
	c = 14.2004(7) Å	γ = 71.105(1)°
Volume	2239.9(2) $Å^3$	
Z	2	
Density (calculated)	1.489 Mg/m^3	
Absorption coefficient	1.332 mm^{-1}	
F(000)	1040	
Crystal size	0.2 x 0.2 x 0.3 mm^3	
Theta range for data collection	1.58 to 26.04°.	
Index ranges	-16<=h<=16, -16<=k<=16, -17<=l<=17	
Reflections collected	18347	
Independent reflections	8707 [R(int) = 0.0189]	
Completeness to theta = 26.04∞	98.4 %	
Absorption correction max/minimum	empirical 1.000/0.872	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8707 / 0 / 541	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0338, wR2 = 0.0898	
R indices (all data)	R1 = 0.0477, wR2 = 0.0959	
Largest diff. peak and hole	0.662 and -0.421 $e.Å^{-3}$	

$R1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo|$.

$wR2 = [\Sigma[w(Fo^2 - Fc^2)^2] / \Sigma[w(Fo^2)^2]]^{0.5}$,

calc $w=1/[\sigma^2(Fo^2)+(0.0570P)^2+0.2617P]$, where $P=(Fo^2+2Fc^2)/3$.

Table 2S. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[Fe_4(sae)_4(MeOH)_4]$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	2422(1)	3911(1)	2246(1)	30(1)
Fe(2)	1791(1)	2743(1)	4644(1)	32(1)
Fe(3)	2337(1)	1459(1)	2889(1)	33(1)
Fe(4)	114(1)	3114(1)	3241(1)	34(1)
O(1)	2958(1)	4999(1)	2427(1)	37(1)
O(2)	1554(1)	3032(1)	1998(1)	30(1)
O(3)	757(1)	2560(2)	5946(1)	39(1)
O(4)	2977(1)	2464(1)	3414(1)	31(1)
O(5)	3671(2)	1014(2)	2001(2)	46(1)
O(6)	1163(1)	1755(1)	4098(1)	34(1)
O(7)	-749(2)	2528(2)	2754(2)	46(1)
O(8)	961(1)	4002(1)	3488(1)	31(1)
O(9)	3931(2)	3153(2)	1317(1)	44(1)
O(10)	2446(2)	4138(2)	4531(2)	46(1)
O(11)	1129(2)	1000(2)	2356(2)	67(1)
O(12)	-849(2)	2931(3)	4910(2)	83(1)
N(1)	1839(2)	5072(2)	932(2)	31(1)
N(2)	2961(2)	1571(2)	5480(2)	34(1)
N(3)	2679(2)	-69(2)	4024(2)	43(1)
N(4)	-884(2)	4650(2)	2703(2)	38(1)
C(1)	2974(2)	6015(2)	1800(2)	30(1)
C(2)	3443(2)	6620(2)	2082(2)	36(1)
C(3)	3464(2)	7689(2)	1481(2)	41(1)
C(4)	3037(2)	8194(2)	565(2)	41(1)
C(5)	2594(2)	7615(2)	259(2)	37(1)
C(6)	2539(2)	6532(2)	856(2)	30(1)
C(7)	1997(2)	6036(2)	467(2)	33(1)
C(8)	1198(2)	4684(2)	520(2)	37(1)
C(9)	1488(2)	3440(2)	919(2)	37(1)
C(10)	905(2)	1951(2)	6909(2)	34(1)
C(11)	33(2)	1989(2)	7709(2)	41(1)
C(12)	143(3)	1387(3)	8732(2)	52(1)
C(13)	1114(3)	693(3)	9010(2)	61(1)
C(14)	1977(2)	628(3)	8244(2)	54(1)
C(15)	1906(2)	1246(2)	7192(2)	38(1)
C(16)	2876(2)	1090(2)	6471(2)	39(1)
C(17)	3960(2)	1254(2)	4821(2)	40(1)
C(18)	3991(2)	2105(2)	3731(2)	39(1)
C(19)	4314(2)	28(2)	2111(2)	44(1)

Continued

Table 2S. continued

C(20)	5113(2)	-115(3)	1279(3)	56(1)
C(21)	5812(3)	-1125(4)	1345(4)	73(1)
C(22)	5742(3)	-2023(3)	2246(4)	75(1)
C(23)	4968(3)	-1911(3)	3055(3)	61(1)
C(24)	4235(2)	-910(2)	3027(3)	46(1)
C(25)	3430(2)	-898(2)	3934(2)	47(1)
C(26)	1919(3)	-138(2)	4992(2)	51(1)
C(27)	912(2)	750(2)	4765(2)	45(1)
C(28)	-1738(2)	2952(3)	2568(2)	45(1)
C(29)	-2294(3)	2285(3)	2464(2)	54(1)
C(30)	-3338(3)	2685(4)	2288(2)	66(1)
C(31)	-3887(3)	3752(4)	2201(3)	72(1)
C(32)	-3369(2)	4430(3)	2271(2)	61(1)
C(33)	-2297(2)	4060(3)	2454(2)	46(1)
C(34)	-1825(2)	4852(3)	2506(2)	45(1)
C(35)	-477(2)	5504(2)	2744(2)	44(1)
C(36)	245(2)	4997(2)	3577(2)	41(1)
C(37)	4379(3)	3659(3)	253(2)	62(1)
C(38)	3209(4)	4067(3)	5116(3)	78(1)
C(39)	1120(5)	71(4)	2204(5)	117(2)
C(40)	-1841(3)	2966(4)	5364(3)	90(2)

Table 3S. Bond lengths [Å] and angles [°] for $[Fe_4(sae)_4(MeOH)_4]$.

Fe(1)-O(1)	1.9784(17)	Fe(1)-N(1)	2.053(2)
Fe(1)-O(4)	2.0775(17)	Fe(1)-O(2)	2.0944(16)
Fe(1)-O(8)	2.2736(17)	Fe(1)-O(9)	2.2908(18)
Fe(2)-O(3)	1.9797(17)	Fe(2)-N(2)	2.063(2)
Fe(2)-O(8)	2.0886(17)	Fe(2)-O(4)	2.1012(17)
Fe(2)-O(6)	2.2517(17)	Fe(2)-O(10)	2.2913(19)
Fe(3)-O(5)	1.9714(19)	Fe(3)-N(3)	2.071(2)
Fe(3)-O(6)	2.0775(17)	Fe(3)-O(2)	2.1012(17)
Fe(3)-O(4)	2.2610(17)	Fe(3)-O(11)	2.293(2)
Fe(4)-O(7)	1.9807(18)	Fe(4)-N(4)	2.060(2)
Fe(4)-O(6)	2.0775(18)	Fe(4)-O(8)	2.0830(16)
Fe(4)-O(2)	2.2553(16)	Fe(4)-O(12)	2.343(2)
O(1)-C(1)	1.329(3)	O(2)-C(9)	1.423(3)
O(3)-C(10)	1.316(3)	O(4)-C(18)	1.411(3)
O(5)-C(19)	1.322(3)	O(6)-C(27)	1.419(3)
O(7)-C(28)	1.309(3)	O(8)-C(36)	1.425(3)
O(9)-C(37)	1.445(3)	O(10)-C(38)	1.431(4)
O(11)-C(39)	1.381(4)	O(12)-C(40)	1.310(4)
N(1)-C(7)	1.285(3)	N(1)-C(8)	1.471(3)
N(2)-C(16)	1.287(3)	N(2)-C(17)	1.465(3)
N(3)-C(25)	1.278(4)	N(3)-C(26)	1.470(4)
N(4)-C(34)	1.278(3)	N(4)-C(35)	1.470(3)
C(1)-C(2)	1.406(3)	C(1)-C(6)	1.420(3)
C(2)-C(3)	1.381(4)	C(3)-C(4)	1.382(4)
C(4)-C(5)	1.375(4)	C(5)-C(6)	1.405(3)
C(6)-C(7)	1.458(3)	C(8)-C(9)	1.521(4)
C(10)-C(11)	1.404(4)	C(10)-C(15)	1.422(4)
C(11)-C(12)	1.375(4)	C(12)-C(13)	1.383(5)
C(13)-C(14)	1.372(4)	C(14)-C(15)	1.406(4)
C(15)-C(16)	1.443(4)	C(17)-C(18)	1.524(4)
C(19)-C(20)	1.404(4)	C(19)-C(24)	1.431(4)
C(20)-C(21)	1.383(5)	C(21)-C(22)	1.387(6)
C(22)-C(23)	1.356(5)	C(23)-C(24)	1.399(4)
C(24)-C(25)	1.451(4)	C(26)-C(27)	1.502(4)
C(28)-C(29)	1.421(4)	C(28)-C(33)	1.427(4)
C(29)-C(30)	1.372(5)	C(30)-C(31)	1.383(6)
C(31)-C(32)	1.373(5)	C(32)-C(33)	1.413(4)
C(33)-C(34)	1.457(4)	C(35)-C(36)	1.522(4)

Table 4S. Bond angles [°] for [Fe4(sae)4(MeOH)4].

O(1)-Fe(1)-N(1)	90.04(7)	O(1)-Fe(1)-O(4)	103.82(7)
N(1)-Fe(1)-O(4)	165.33(7)	O(1)-Fe(1)-O(2)	167.68(7)
N(1)-Fe(1)-O(2)	81.45(7)	O(4)-Fe(1)-O(2)	85.56(6)
O(1)-Fe(1)-O(8)	95.28(7)	N(1)-Fe(1)-O(8)	102.33(7)
O(4)-Fe(1)-O(8)	81.45(6)	O(2)-Fe(1)-O(8)	78.01(6)
O(1)-Fe(1)-O(9)	99.17(7)	N(1)-Fe(1)-O(9)	92.93(7)
O(4)-Fe(1)-O(9)	80.29(7)	O(2)-Fe(1)-O(9)	90.19(7)
O(8)-Fe(1)-O(9)	158.95(6)	O(3)-Fe(2)-N(2)	89.30(8)
O(3)-Fe(2)-O(8)	105.82(7)	N(2)-Fe(2)-O(8)	164.50(7)
O(3)-Fe(2)-O(4)	164.18(7)	N(2)-Fe(2)-O(4)	80.43(7)
O(8)-Fe(2)-O(4)	85.45(6)	O(3)-Fe(2)-O(6)	93.93(7)
N(2)-Fe(2)-O(6)	102.55(8)	O(8)-Fe(2)-O(6)	80.21(6)
O(4)-Fe(2)-O(6)	76.80(6)	O(3)-Fe(2)-O(10)	102.90(8)
N(2)-Fe(2)-O(10)	92.25(8)	O(8)-Fe(2)-O(10)	81.23(7)
O(4)-Fe(2)-O(10)	89.58(7)	O(6)-Fe(2)-O(10)	157.73(7)
O(5)-Fe(3)-N(3)	89.66(9)	O(5)-Fe(3)-O(6)	166.35(8)
N(3)-Fe(3)-O(6)	80.69(8)	O(5)-Fe(3)-O(2)	106.24(7)
N(3)-Fe(3)-O(2)	163.53(8)	O(6)-Fe(3)-O(2)	84.30(7)
O(5)-Fe(3)-O(4)	95.75(7)	N(3)-Fe(3)-O(4)	102.11(8)
O(6)-Fe(3)-O(4)	77.06(6)	O(2)-Fe(3)-O(4)	80.93(6)
O(5)-Fe(3)-O(11)	101.46(9)	N(3)-Fe(3)-O(11)	91.93(9)
O(6)-Fe(3)-O(11)	88.58(8)	O(2)-Fe(3)-O(11)	80.92(8)
O(4)-Fe(3)-O(11)	157.83(7)	O(7)-Fe(4)-N(4)	89.26(8)
O(7)-Fe(4)-O(6)	105.62(8)	N(4)-Fe(4)-O(6)	162.83(8)
O(7)-Fe(4)-O(8)	168.56(8)	N(4)-Fe(4)-O(8)	81.57(8)
O(6)-Fe(4)-O(8)	84.55(6)	O(7)-Fe(4)-O(2)	97.57(7)
N(4)-Fe(4)-O(2)	106.40(8)	O(6)-Fe(4)-O(2)	80.55(6)
O(8)-Fe(4)-O(2)	78.66(6)	O(7)-Fe(4)-O(12)	98.56(9)
N(4)-Fe(4)-O(12)	88.72(10)	O(6)-Fe(4)-O(12)	80.74(8)
O(8)-Fe(4)-O(12)	88.11(8)	O(2)-Fe(4)-O(12)	157.98(7)
C(1)-O(1)-Fe(1)	129.18(15)	C(9)-O(2)-Fe(1)	107.87(13)
C(9)-O(2)-Fe(3)	127.86(15)	Fe(1)-O(2)-Fe(3)	97.60(7)
C(9)-O(2)-Fe(4)	123.55(15)	Fe(1)-O(2)-Fe(4)	101.79(7)
Fe(3)-O(2)-Fe(4)	93.06(6)	C(10)-O(3)-Fe(2)	130.03(16)
C(18)-O(4)-Fe(1)	126.14(14)	C(18)-O(4)-Fe(2)	109.15(15)
Fe(1)-O(4)-Fe(2)	97.86(7)	C(18)-O(4)-Fe(3)	123.20(15)
Fe(1)-O(4)-Fe(3)	93.28(6)	Fe(2)-O(4)-Fe(3)	102.53(6)
C(19)-O(5)-Fe(3)	129.17(18)	C(27)-O(6)-Fe(4)	125.35(16)

Continued

Table 4S. continued.

C(27)-O(6)-Fe(3)	108.27(16)	Fe(4)-O(6)-Fe(3)	99.17(7)
C(27)-O(6)-Fe(2)	122.65(16)	Fe(4)-O(6)-Fe(2)	93.84(7)
Fe(3)-O(6)-Fe(2)	103.61(7)	C(28)-O(7)-Fe(4)	128.18(19)
C(36)-O(8)-Fe(4)	108.84(14)	C(36)-O(8)-Fe(2)	126.25(15)
Fe(4)-O(8)-Fe(2)	98.67(7)	C(36)-O(8)-Fe(1)	124.27(16)
Fe(4)-O(8)-Fe(1)	101.54(7)	Fe(2)-O(8)-Fe(1)	92.37(6)
C(37)-O(9)-Fe(1)	127.05(18)	C(38)-O(10)-Fe(2)	126.78(19)
C(39)-O(11)-Fe(3)	133.8(3)	C(40)-O(12)-Fe(4)	137.5(2)
C(7)-N(1)-C(8)	120.5(2)	C(7)-N(1)-Fe(1)	127.00(16)
C(8)-N(1)-Fe(1)	112.50(15)	C(16)-N(2)-C(17)	119.6(2)
C(16)-N(2)-Fe(2)	127.14(18)	C(17)-N(2)-Fe(2)	113.16(16)
C(25)-N(3)-C(26)	121.1(2)	C(25)-N(3)-Fe(3)	126.6(2)
C(26)-N(3)-Fe(3)	112.28(18)	C(34)-N(4)-C(35)	121.6(2)
C(34)-N(4)-Fe(4)	125.4(2)	C(35)-N(4)-Fe(4)	112.14(16)
O(1)-C(1)-C(2)	118.6(2)	O(1)-C(1)-C(6)	123.7(2)
C(2)-C(1)-C(6)	117.7(2)	C(3)-C(2)-C(1)	121.8(2)
C(2)-C(3)-C(4)	120.4(2)	C(5)-C(4)-C(3)	119.0(2)
C(4)-C(5)-C(6)	122.3(2)	C(5)-C(6)-C(1)	118.7(2)
C(5)-C(6)-C(7)	116.5(2)	C(1)-C(6)-C(7)	124.8(2)
N(1)-C(7)-C(6)	124.8(2)	N(1)-C(8)-C(9)	109.6(2)
O(2)-C(9)-C(8)	110.0(2)	O(3)-C(10)-C(11)	119.0(2)
O(3)-C(10)-C(15)	123.6(2)	C(11)-C(10)-C(15)	117.5(2)
C(12)-C(11)-C(10)	121.6(3)	C(11)-C(12)-C(13)	121.1(3)
C(14)-C(13)-C(12)	118.7(3)	C(13)-C(14)-C(15)	122.1(3)
C(14)-C(15)-C(10)	119.0(2)	C(14)-C(15)-C(16)	116.1(2)
C(10)-C(15)-C(16)	124.9(2)	N(2)-C(16)-C(15)	124.9(2)
N(2)-C(17)-C(18)	110.4(2)	O(4)-C(18)-C(17)	110.0(2)
O(5)-C(19)-C(20)	118.3(3)	O(5)-C(19)-C(24)	123.8(3)
C(20)-C(19)-C(24)	117.8(3)	C(21)-C(20)-C(19)	121.2(4)
C(20)-C(21)-C(22)	120.4(4)	C(23)-C(22)-C(21)	119.5(3)
C(22)-C(23)-C(24)	122.4(4)	C(23)-C(24)-C(19)	118.6(3)
C(23)-C(24)-C(25)	117.2(3)	C(19)-C(24)-C(25)	124.1(3)
N(3)-C(25)-C(24)	125.5(3)	N(3)-C(26)-C(27)	109.4(2)
O(6)-C(27)-C(26)	110.2(2)	O(7)-C(28)-C(29)	118.9(3)
O(7)-C(28)-C(33)	123.6(2)	C(29)-C(28)-C(33)	117.4(3)
C(30)-C(29)-C(28)	121.2(4)	C(29)-C(30)-C(31)	121.3(3)
C(32)-C(31)-C(30)	119.2(3)	C(31)-C(32)-C(33)	121.7(4)
C(32)-C(33)-C(28)	119.0(3)	C(32)-C(33)-C(34)	117.1(3)
C(28)-C(33)-C(34)	123.9(2)	N(4)-C(34)-C(33)	125.5(3)
N(4)-C(35)-C(36)	109.2(2)	O(8)-C(36)-C(35)	109.8(2)

Table 5S. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Fe_4(sae)_4(MeOH)_4]$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	32(1)	29(1)	30(1)	-5(1)	-7(1)	-13(1)
Fe(2)	31(1)	34(1)	28(1)	-8(1)	-5(1)	-9(1)
Fe(3)	34(1)	28(1)	35(1)	-9(1)	-1(1)	-10(1)
Fe(4)	28(1)	41(1)	38(1)	-17(1)	-5(1)	-12(1)
O(1)	46(1)	34(1)	35(1)	-2(1)	-14(1)	-20(1)
O(2)	33(1)	30(1)	29(1)	-9(1)	-4(1)	-12(1)
O(3)	35(1)	44(1)	31(1)	-10(1)	-6(1)	-4(1)
O(4)	27(1)	32(1)	31(1)	-6(1)	-4(1)	-10(1)
O(5)	46(1)	35(1)	49(1)	-16(1)	4(1)	-7(1)
O(6)	34(1)	34(1)	35(1)	-9(1)	1(1)	-18(1)
O(7)	43(1)	52(1)	52(1)	-18(1)	-12(1)	-21(1)
O(8)	30(1)	32(1)	33(1)	-12(1)	-8(1)	-7(1)
O(9)	41(1)	47(1)	36(1)	-9(1)	6(1)	-15(1)
O(10)	57(1)	47(1)	45(1)	-15(1)	-20(1)	-16(1)
O(11)	71(2)	58(1)	96(2)	-42(1)	-20(1)	-23(1)
O(12)	38(1)	166(3)	43(1)	-36(2)	5(1)	-34(2)
N(1)	31(1)	36(1)	29(1)	-10(1)	-7(1)	-13(1)
N(2)	29(1)	36(1)	36(1)	-10(1)	-5(1)	-8(1)
N(3)	53(1)	30(1)	44(1)	-6(1)	-10(1)	-16(1)
N(4)	33(1)	45(1)	41(1)	-19(1)	-8(1)	-7(1)
C(1)	27(1)	33(1)	32(1)	-11(1)	-2(1)	-12(1)
C(2)	36(1)	40(2)	35(1)	-11(1)	-7(1)	-14(1)
C(3)	43(2)	39(2)	50(2)	-19(1)	-5(1)	-19(1)
C(4)	45(2)	31(1)	47(2)	-8(1)	-5(1)	-17(1)
C(5)	36(1)	35(1)	35(1)	-5(1)	-6(1)	-11(1)
C(6)	27(1)	31(1)	31(1)	-10(1)	-1(1)	-10(1)
C(7)	33(1)	36(1)	27(1)	-6(1)	-8(1)	-10(1)
C(8)	43(2)	45(2)	30(1)	-9(1)	-9(1)	-19(1)
C(9)	40(1)	45(2)	31(1)	-14(1)	-4(1)	-18(1)
C(10)	38(1)	35(1)	31(1)	-10(1)	-5(1)	-15(1)
C(11)	38(2)	42(2)	41(2)	-12(1)	0(1)	-11(1)
C(12)	52(2)	57(2)	38(2)	-10(1)	6(1)	-20(2)
C(13)	57(2)	76(2)	31(2)	-1(2)	-4(1)	-20(2)
C(14)	46(2)	61(2)	39(2)	-1(1)	-11(1)	-11(2)
C(15)	39(2)	41(2)	33(1)	-6(1)	-6(1)	-15(1)
C(16)	35(1)	38(2)	38(2)	-5(1)	-11(1)	-9(1)
C(17)	31(1)	43(2)	41(2)	-12(1)	-8(1)	-4(1)
C(18)	27(1)	44(2)	41(2)	-10(1)	-4(1)	-11(1)
C(19)	35(2)	43(2)	61(2)	-27(2)	-9(1)	-8(1)

Continued

Table 5S. continued.

C(20)	43(2)	60(2)	74(2)	-39(2)	-1(2)	-11(2)
C(21)	39(2)	87(3)	112(3)	-68(3)	-6(2)	0(2)
C(22)	54(2)	59(2)	127(4)	-55(3)	-40(2)	17(2)
C(23)	55(2)	49(2)	89(3)	-30(2)	-39(2)	5(2)
C(24)	44(2)	37(2)	67(2)	-23(2)	-28(2)	-2(1)
C(25)	58(2)	34(2)	52(2)	-6(1)	-23(2)	-16(1)
C(26)	72(2)	39(2)	42(2)	-4(1)	-2(2)	-30(2)
C(27)	51(2)	44(2)	41(2)	-9(1)	4(1)	-29(1)
C(28)	43(2)	68(2)	29(1)	-7(1)	-6(1)	-32(2)
C(29)	61(2)	73(2)	36(2)	-5(2)	-9(1)	-43(2)
C(30)	60(2)	103(3)	46(2)	-8(2)	-9(2)	-57(2)
C(31)	41(2)	116(4)	60(2)	-14(2)	-14(2)	-37(2)
C(32)	38(2)	86(3)	50(2)	-8(2)	-12(1)	-20(2)
C(33)	37(2)	69(2)	32(1)	-10(1)	-7(1)	-23(2)
C(34)	35(2)	55(2)	39(2)	-14(1)	-10(1)	-5(1)
C(35)	43(2)	39(2)	54(2)	-23(1)	-13(1)	-3(1)
C(36)	40(2)	42(2)	46(2)	-24(1)	-11(1)	-3(1)
C(37)	49(2)	70(2)	43(2)	-4(2)	12(1)	-19(2)
C(38)	111(3)	74(3)	69(2)	-9(2)	-54(2)	-39(2)
C(39)	132(4)	102(4)	172(5)	-95(4)	-47(4)	-18(3)
C(40)	41(2)	159(5)	61(2)	-32(3)	6(2)	-30(2)

Table 6S. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Fe_4(sae)_4(MeOH)_4]$.

	x	y	z	U(eq)
H(2)	3746	6291	2689	43
H(3)	3769	8072	1695	49
H(4)	3050	8914	161	49
H(5)	2320	7951	-365	44
H(7)	1746	6448	-165	39
H(8A)	1336	4957	-233	45
H(8B)	443	4959	737	45
H(9A)	949	3184	804	44
H(9B)	2169	3169	543	44
H(11)	-634	2433	7544	50
H(12)	-445	1448	9246	63
H(13)	1180	278	9702	73
H(14)	2630	159	8428	64
H(16)	3486	604	6743	46
H(17A)	4016	549	4785	48
H(17B)	4564	1186	5122	48
H(18A)	4196	2723	3725	46
H(18B)	4520	1790	3251	46
H(20)	5174	481	672	68
H(21)	6332	-1203	783	88
H(22)	6223	-2698	2293	90
H(23)	4922	-2520	3652	73
H(25)	3464	-1548	4498	56
H(26A)	2235	-56	5490	62
H(26B)	1756	-847	5289	62
H(27A)	490	552	4438	54
H(27B)	489	832	5409	54
H(29)	-1944	1565	2516	65
H(30)	-3683	2229	2227	79
H(31)	-4598	4008	2096	86
H(32)	-3735	5152	2196	73
H(34)	-2245	5564	2387	54
H(35A)	-1071	6074	2902	53
H(35B)	-78	5830	2075	53
H(36A)	649	5503	3500	49
H(36B)	-187	4852	4259	49

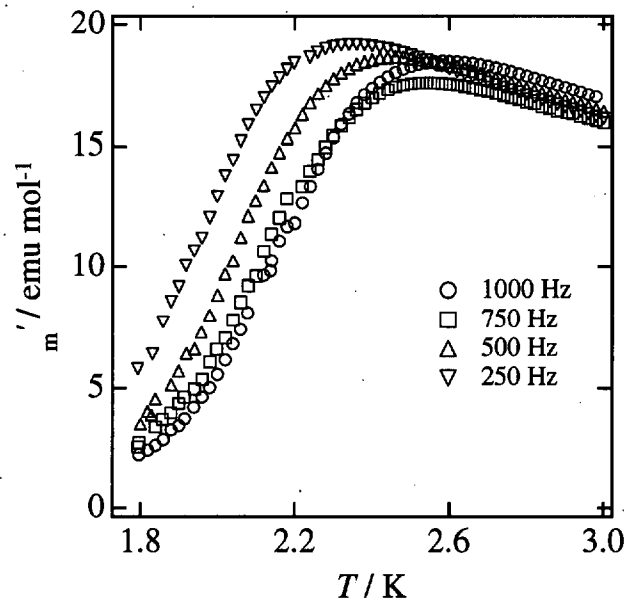

Figure 1S