Lanthanide Complexes of $[\alpha\text{-}2\text{-}P_2W_{17}O_{61}]^{10-}$: Solid State and Solution Studies

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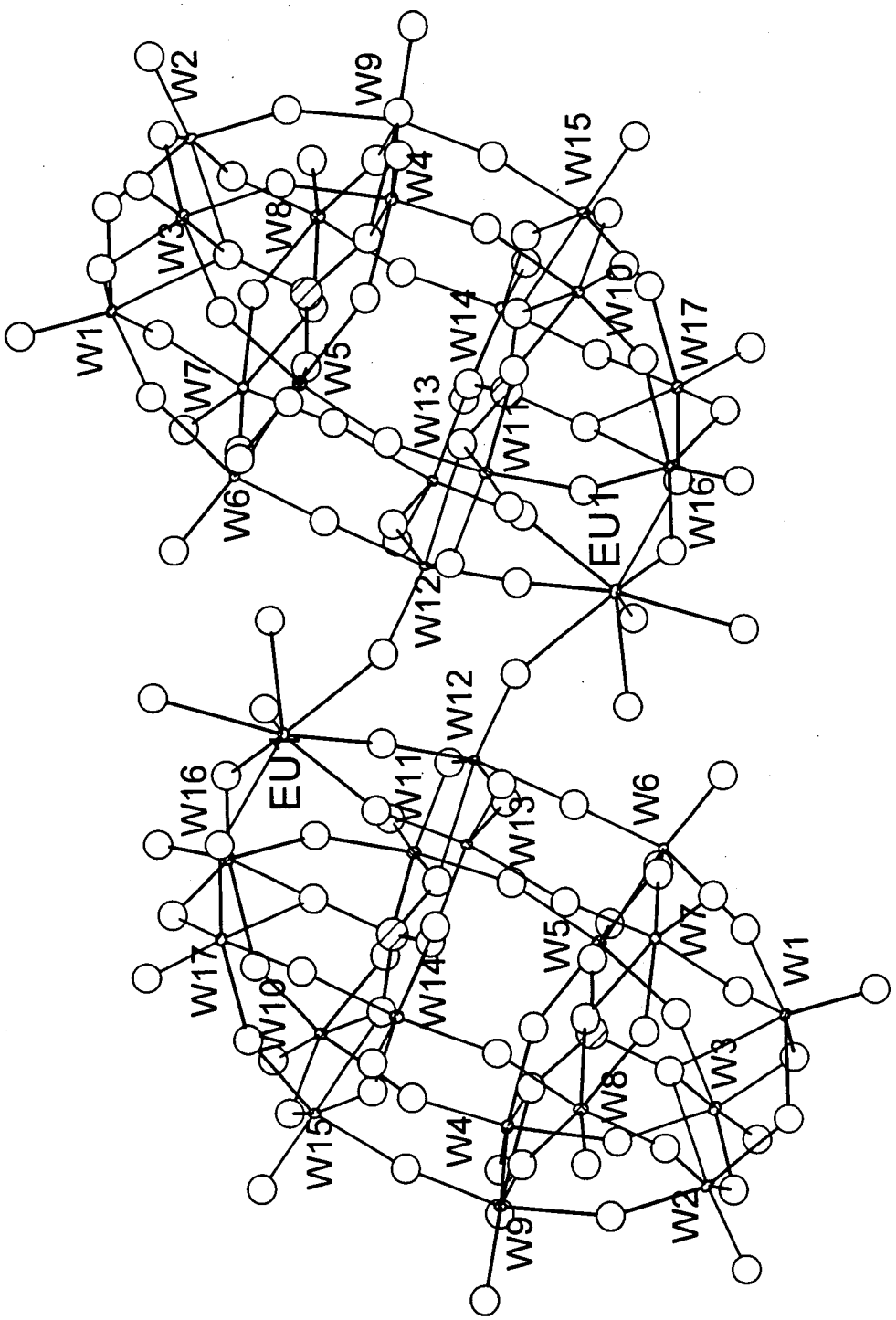
Supplementary Figure Captions.

Figure S1. ORTEP representation of Packing diagram of $K_{13}(H_3O)[Eu(H_2O)_3(P_2W_{17}O_{61})]_2 \bullet 2KCl \bullet 50\ H_2O$

Figure S2. Packing diagram of of $K_{13}(H_3O)[Eu(H_2O)_3(P_2W_{17}O_{61})]_2 \bullet 2KCl \bullet 50\ H_2O$.

Figure S3. ^{183} W NMR spectrum of $[Lu(H_2O)_3(P_2W_{17}O_{61})]^{7-}$ (0.1M, 16.7 MHz, H_2O, D_2O); Chemical shifts given in Table 3. The ^{183}W NMR spectrum for the 1:2 Lu: $[\alpha\text{-}2\ P_2W_{17}O_{61}]^{10-}$ is presented for comparison. [Bartis, 1997 #20]


W2
W9
W15
W4
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W16
EU1
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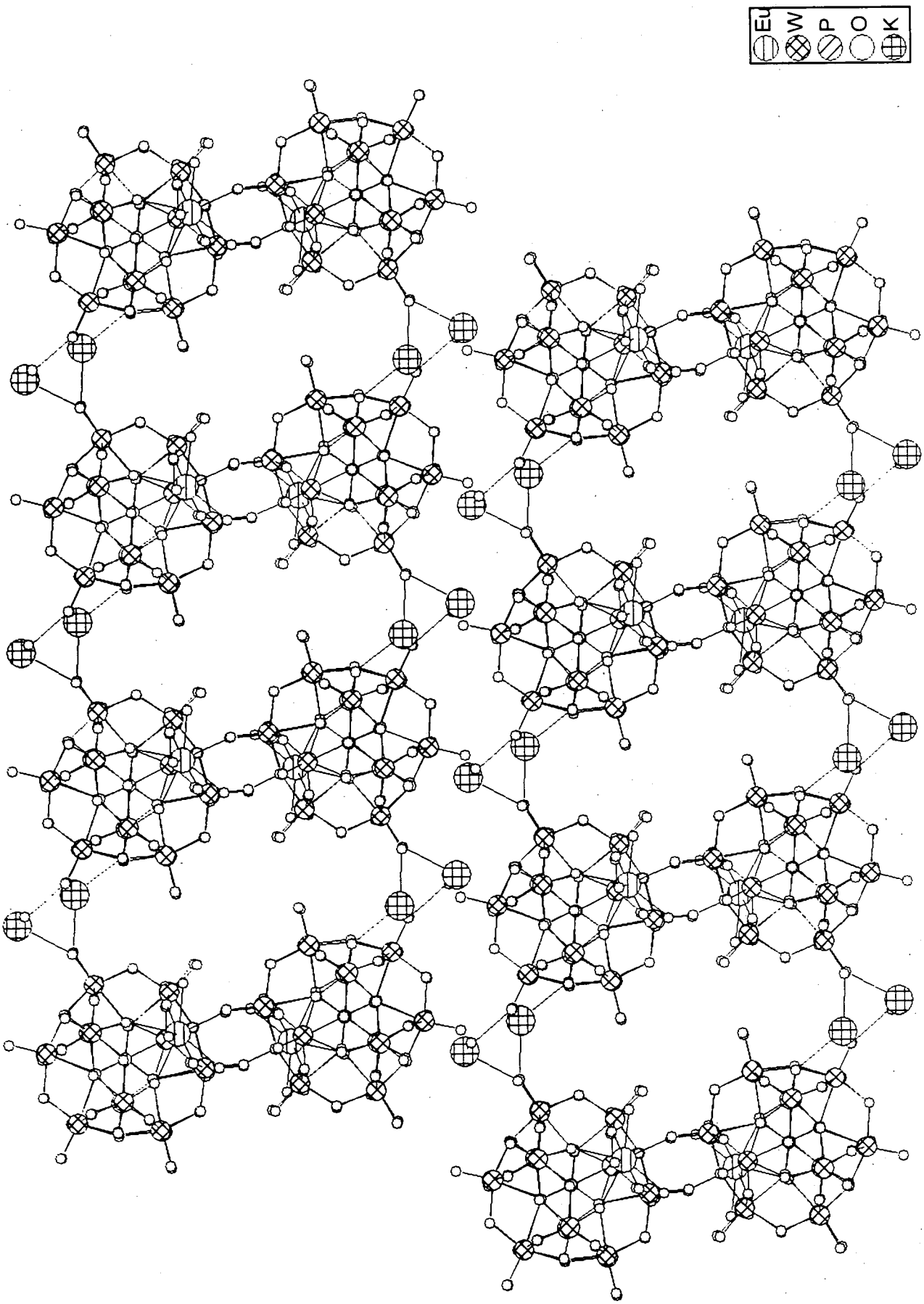

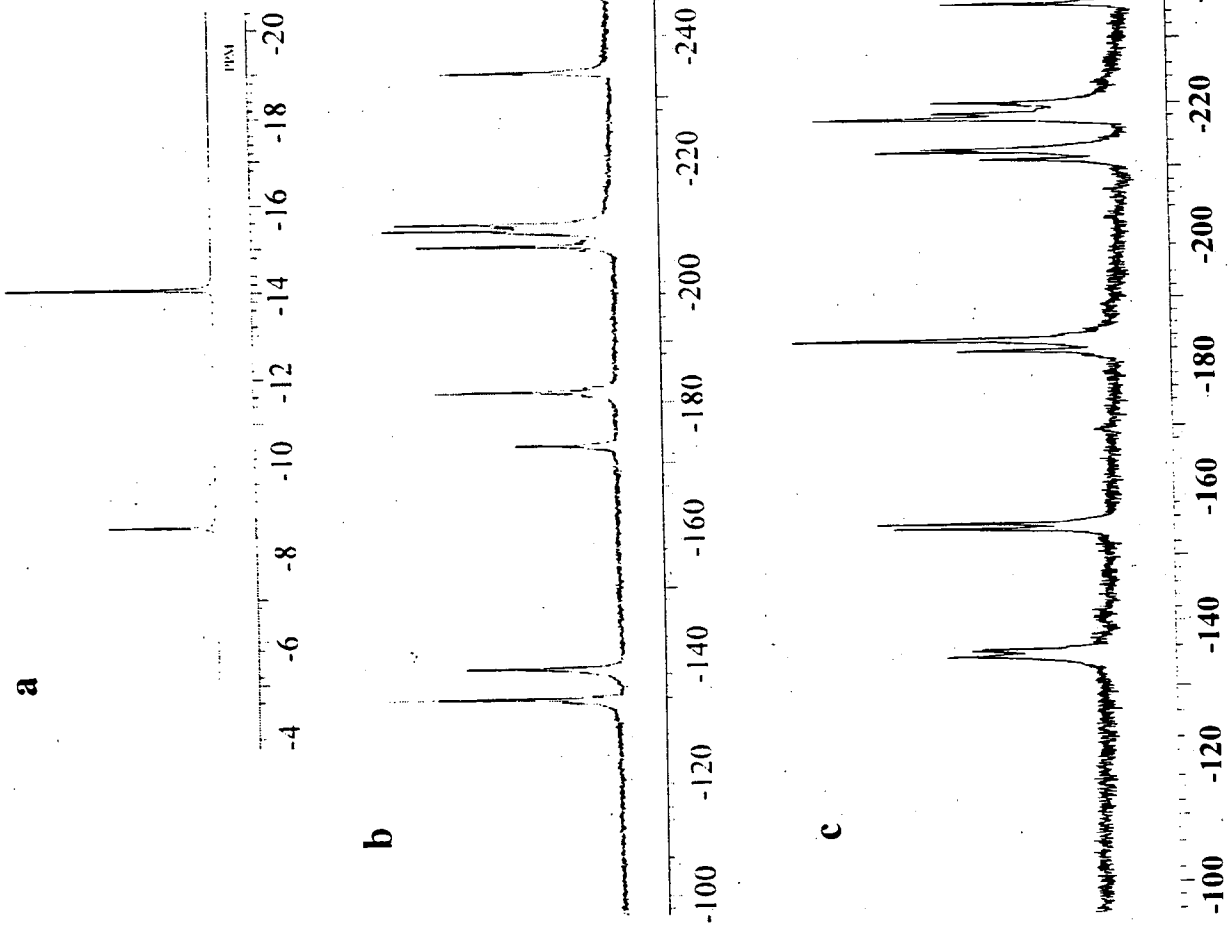
a
PPM
-4
-6
-8
-10
-12
-14
-16
-18
-20
b
PPM
-100
-120
-140
-160
-180
-200
-220
-240
-260
c
-100
-120
-140
-160
-180
-200
-220
-240
-260

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for $(H_3O)K_{13}[Eu(H_2O)_3P_2W_{17}O_{61})]_2 \cdot 2KCl \cdot 56\ H_2O$, **1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Eu(1)	5052(1)	7728(1)	46(1)	5(1)
W(1)	6448(1)	10266(1)	3647(1)	5(1)
W(2)	6778(1)	8006(1)	4719(1)	5(1)
W(3)	8975(1)	8708(1)	3941(1)	5(1)
W(4)	9697(1)	6476(1)	3383(1)	4(1)
W(5)	9332(1)	8970(1)	2271(1)	5(1)
W(6)	6843(1)	10470(1)	1956(1)	4(1)
W(7)	4456(1)	9672(1)	2832(1)	4(1)
W(8)	4774(1)	7464(1)	3899(1)	5(1)
W(9)	7522(1)	5767(1)	4174(1)	4(1)
W(10)	9273(1)	5432(1)	2120(1)	4(1)
W(11)	8899(1)	7904(1)	1043(1)	4(1)
W(12)	6406(1)	9375(1)	714(1)	3(1)
W(13)	4080(1)	8611(1)	1558(1)	3(1)
W(14)	4402(1)	6425(1)	2651(1)	4(1)
W(15)	7104(1)	4739(1)	2909(1)	4(1)
W(16)	7859(1)	6043(1)	617(1)	4(1)
W(17)	5725(1)	5328(1)	1397(1)	5(1)
P(1)	7115(3)	8181(3)	3133(2)	0(1)
P(2)	6690(3)	7042(3)	1800(2)	0(1)
O(1)	5961(9)	11394(9)	3771(5)	12(2)
O(2)	6485(9)	7697(8)	5503(5)	6(2)
O(3)	10113(10)	8836(9)	4219(5)	12(2)
O(4)	6250(8)	9409(8)	4486(5)	5(2)
O(5)	8221(9)	8200(8)	4706(5)	6(2)
O(6)	7969(9)	9970(8)	3871(5)	7(2)
O(7)	6902(8)	10596(8)	2825(5)	5(2)
O(8)	5214(10)	10028(9)	3432(5)	13(2)
O(9)	5489(9)	7941(8)	4411(5)	8(2)
O(10)	7433(9)	6781(8)	4595(5)	7(2)
O(11)	9461(8)	7444(8)	3862(5)	5(2)
O(12)	9228(9)	9137(8)	3064(5)	7(2)
O(13)	6484(10)	11708(9)	1592(5)	12(2)
O(14)	3340(9)	10639(8)	2776(5)	9(2)
O(15)	3825(10)	7053(9)	4438(5)	14(2)
O(16)	7542(9)	4823(9)	4846(5)	12(2)
O(17)	11039(9)	5998(8)	3581(5)	8(2)
O(18)	10589(9)	9212(8)	2050(5)	11(2)
O(19)	5465(9)	10227(8)	2258(5)	8(2)
O(20)	3969(9)	8782(8)	3558(5)	6(2)
O(21)	6011(9)	6371(8)	4050(5)	7(2)
O(22)	9075(8)	5662(8)	4095(5)	5(2)
O(23)	9771(9)	7588(8)	2686(5)	9(2)
O(24)	8420(9)	10236(8)	1942(5)	9(2)
O(25)	7282(8)	8620(7)	3659(5)	3(2)
O(26)	5898(8)	8260(7)	3111(4)	3(2)
O(27)	7783(9)	7088(8)	3318(5)	6(2)
O(28)	7546(9)	8805(8)	2530(5)	6(2)

O(29)	[illegible]	[illegible]	[illegible]	[illegible]
O(30)	4411(9)	7121(8)	3238(5)	9(2)
O(31)	7552(9)	5146(8)	3590(5)	8(2)
O(32)	9546(9)	5785(8)	2874(5)	7(2)
O(33)	9081(8)	8616(8)	1563(5)	5(2)
O(34)	6885(8)	9966(8)	1335(5)	6(2)
O(35)	2895(9)	9510(8)	1292(5)	9(2)
O(36)	3434(9)	5813(9)	3019(5)	12(2)
O(37)	7061(9)	3562(8)	3352(5)	11(2)
O(38)	10576(9)	4709(8)	2075(5)	8(2)
O(39)	10067(9)	7941(8)	596(5)	9(2)
O(40)	5973(9)	10551(8)	197(5)	11(2)
O(41)	3479(9)	7600(8)	2153(5)	9(2)
O(42)	5689(9)	5531(8)	3037(5)	7(2)
O(43)	8632(8)	4466(7)	2703(5)	4(2)
O(44)	9388(9)	6733(8)	1701(5)	9(2)
O(45)	7943(8)	9068(8)	519(5)	5(2)
O(46)	5144(8)	9352(7)	1249(5)	4(2)
O(47)	4349(9)	8006(8)	986(5)	10(2)
O(48)	4759(9)	5869(8)	1975(5)	6(2)
O(49)	6678(9)	4726(8)	2173(5)	8(2)
O(50)	8684(9)	5372(8)	1450(5)	9(2)
O(51)	8434(9)	7093(8)	644(5)	6(2)
O(52)	6141(9)	8604(8)	319(5)	7(2)
O(53)	5297(9)	4279(8)	1510(5)	10(2)
O(54)	8872(9)	5454(8)	201(5)	11(2)
O(55)	5005(9)	6141(8)	727(5)	9(2)
O(56)	7078(9)	5026(8)	952(5)	6(2)
O(57)	6894(8)	6770(7)	37(4)	3(2)
O(58)	3189(10)	7817(9)	-54(6)	17(3)
O(59)	4963(10)	6773(9)	-630(6)	17(3)
O(60)	5798(9)	8579(8)	-955(5)	8(2)
O(61)	5555(8)	7377(7)	2075(5)	4(2)
O(62)	7440(9)	6258(8)	2302(5)	6(2)
O(63)	7193(8)	7926(8)	1483(5)	5(2)
O(64)	6547(8)	6574(8)	1293(5)	5(2)
K(1)	8318(3)	3006(3)	5654(2)	18(1)
K(2)	11836(3)	9803(3)	3920(2)	18(1)
K(3)	2900(4)	4434(3)	4062(2)	20(1)
K(4)	6561(4)	8025(3)	6584(2)	24(1)
K(5)	8013(4)	8413(3)	-631(2)	23(1)
K(6)	7876(4)	5674(4)	-1071(2)	31(1)
K(7)	10000	10000	0	30(1)
K(8)	6002(6)	2625(5)	4454(3)	49(1)
O(65)	8187(12)	1995(11)	2824(7)	28(3)
O(66)	9860(16)	3326(15)	3768(9)	50(5)
O(67)	4891(13)	4639(12)	4421(7)	30(3)
O(68)	8206(14)	2479(12)	4618(8)	34(4)
O(69)	8041(11)	1581(10)	6792(6)	22(3)
O(70)	4660(20)	3638(18)	3385(11)	67(6)
O(71)	1387(10)	6843(9)	8359(6)	17(3)
O(72)	1665(11)	7069(10)	1785(6)	22(3)
O(73)	8169(16)	2744(15)	615(9)	49(5)
O(74)	11728(11)	8766(10)	656(6)	22(3)
O(75)	6646(12)	7480(11)	-1723(7)	25(3)
O(76)	6317(12)	4856(11)	-303(7)	26(3)
O(77)	7183(12)	4934(11)	-1907(7)	29(3)

O(78)	9143(12)	5952(11)	[illegible]	[illegible]
O(79)	9310(17)	6806(16)	-1050(10)	52(5)
Cl(1)	6380(14)	10240(20)	5455(11)	196(12)
O(80)	10018(15)	8975(13)	-831(8)	41(4)
O(81)	2259(15)	3959(14)	3135(8)	42(4)
O(82)	8340(12)	9150(11)	-1944(7)	26(3)
O(83)	11096(11)	9505(10)	5149(6)	23(3)
O(84)	10448(13)	11110(12)	2986(7)	30(3)
O(85)	8421(12)	7412(11)	7447(7)	26(3)
O(86)	11518(11)	11610(10)	4070(6)	22(3)
O(87)	5086(12)	7345(11)	7556(7)	27(3)
O(88)	10150(30)	3810(30)	4822(16)	97(9)
O(89)	10730(40)	4090(30)	4530(20)	128(13)

$(H_2O)K_{13}[Eu(H_2O)_3(P_2W_{17}O_{61})]_2 \cdot 2KCl \cdot 56\ H_2O$, **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \ldots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Eu(1)	7(1)	5(1)	5(1)	-2(1)	0(1)	-2(1)
W(1)	6(1)	4(1)	4(1)	-2(1)	-1(1)	0(1)
W(2)	7(1)	6(1)	3(1)	-2(1)	0(1)	0(1)
W(3)	5(1)	7(1)	6(1)	-3(1)	-1(1)	-1(1)
W(4)	3(1)	6(1)	5(1)	-2(1)	-1(1)	0(1)
W(5)	5(1)	6(1)	5(1)	-2(1)	1(1)	-3(1)
W(6)	6(1)	4(1)	3(1)	-1(1)	-1(1)	-1(1)
W(7)	4(1)	5(1)	4(1)	-2(1)	-1(1)	0(1)
W(8)	4(1)	6(1)	4(1)	-1(1)	1(1)	-1(1)
W(9)	5(1)	4(1)	3(1)	0(1)	0(1)	0(1)
W(10)	3(1)	4(1)	4(1)	-1(1)	0(1)	0(1)
W(11)	3(1)	5(1)	4(1)	-1(1)	1(1)	-2(1)
W(12)	3(1)	3(1)	2(1)	0(1)	-1(1)	0(1)
W(13)	3(1)	4(1)	3(1)	-1(1)	0(1)	0(1)
W(14)	3(1)	5(1)	4(1)	-1(1)	1(1)	-2(1)
W(15)	4(1)	4(1)	4(1)	-1(1)	0(1)	-1(1)
W(16)	4(1)	5(1)	4(1)	-2(1)	1(1)	-1(1)
W(17)	6(1)	5(1)	4(1)	-1(1)	0(1)	-3(1)
K(1)	16(2)	12(2)	24(2)	-2(1)	-9(2)	-3(1)
K(2)	15(2)	21(2)	22(2)	-10(2)	2(1)	-7(2)
K(3)	29(2)	13(2)	14(2)	-1(1)	2(2)	-3(2)
K(4)	35(2)	28(2)	16(2)	-14(2)	-1(2)	-9(2)
K(5)	25(2)	20(2)	20(2)	1(2)	-6(2)	-8(2)
K(6)	32(2)	26(2)	30(2)	-3(2)	6(2)	-9(2)
K(7)	36(4)	16(3)	34(3)	3(2)	-20(3)	-8(3)
K(8)	60(4)	54(4)	38(3)	-18(3)	7(3)	-20(3)
Cl(1)	93(11)	350(30)	210(20)	-200(20)	-1(12)	-26(15)