Slow Magnetization Relaxation in A Tetrahedrally Coordinated Mononuclear Co(II) Complex Exclusively Ligated with Phenanthroline Ligands

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Table 1S L-Co-L	plane angle	and D vaule c	omparison	of other	literat
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complex	L-Co-L	D (cm ⁻¹)
$[CoL_2](ClO_4)_2^a$	62.024°	-47.0
$[Co(dmbpy)_2](ClO_4)_2^{17(b)}$	88.7°	-57.0
$[Co{(NtBu)_3SMe}_2]^{23}$	88.700°	-58
$[\text{Co}(\text{pdms})_2](\text{HNEt}_3)_2{}^{27}$	84.825°	-115
$(HNEt_3)_2[Co(L_1)_2] \cdot H_2O (H_2L_1 =$		
N,N'-bis(p-toluene-sulfony1)	87.308°	-144.31
oxamide ³³		
$(Bu_4N)_2[Co(L_2)_2] \cdot H_2O$ $(H_2L_2 =$	05 72(0	120.0
N,N'-diphenyloxamide)33	85.720°	-130.8



Figure 1S Field dependent magnetic relaxation times at 2K, variable-field observe QTM was shut down above 1000G.



Figure 2S CASSCF(7 in 5) No.185 to No.189 Molecular Orbital draw in LUSCUS

Co basic set (ANO-RCC)	MB	VDZ	VDZP	VTZP	VQZP	VQZP
C H N basic set(ANO-RCC)	MB	VDZ	VDZ	VDZ	VDZ	VDZP
D	-39.7180	-45.8895	-45.8232	-44.8076	-44.0497	-43.0816
E	6.8603	7.1480	7.1772	7.1747	7.0206	6.9386
gx	2.0972	2.1045	2.1049	2.1065	2.1063	2.1058
gy	2.2909	2.3005	2.3010	2.3020	2.2997	2.2964
gz	2.6839	2.7393	2.7401	2.7304	2.7272	2.7145

Table 2S, the result of using Molcas8.2 *ab initio* in SEWARD / CASSCF / RASSI / SINGLE_ANISO ,Complete-active-space self-consistent field(CASSCF 7 in 5) consider 10 triplet and 40 doublet states.



Figure 3S. Powder X-ray measurements of Compound 1 (top) and its theoretical simulations (bottom).

Table 3S. Crystal data and structure refinement for ic16900.

Identification code	ic16900	
Empirical formula	C48 H32 Cl2 Co N4 O8	
Formula weight	922.61	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.8409(4) Å	α= 88.1321(11)°.
	b = 12.8630(6) Å	β= 89.0043(11)°.
	c = 20.4373(10) Å	$\gamma = 79.0659(10)^{\circ}$.
Volume	2022.63(17) Å ³	
Z	2	
Density (calculated)	1.515 Mg/m ³	
Absorption coefficient	0.621 mm ⁻¹	
F(000)	946	
Crystal size	$0.35 \ge 0.30 \ge 0.15 \text{ mm}^3$	
Theta range for data collection	1.00 to 27.50°.	
Index ranges	-10<=h<=10, -16<=k<=16, -26	5<=1<=26
Reflections collected	26412	
Independent reflections	9268 [R(int) = 0.0311]	
Completeness to theta = 27.50°	99.8 %	
Absorption correction	Semi-empirical from equivalen	its
Max. and min. transmission	0.9127 and 0.8121	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9268 / 0 / 568	
Goodness-of-fit on F ²	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0480, wR2 = 0.1153	
R indices (all data)	R1 = 0.0595, wR2 = 0.1225	
Largest diff. peak and hole	0.717 and -0.381 e.Å ⁻³	

Table 4S. Atomic coordinates ($x \ 10^4$) and equivalent isotropic displacement parameters (Å²x 10³)

	х	у	Z	U(eq)
Со	5876(1)	7450(1)	2546(1)	27(1)
N(1)	7124(2)	6502(1)	3265(1)	27(1)
N(2)	4097(2)	7933(1)	3255(1)	28(1)
N(3)	6386(2)	8691(2)	2001(1)	31(1)
N(4)	5844(2)	6776(1)	1670(1)	28(1)
C(1)	8559(3)	5750(2)	3242(1)	30(1)
C(2)	9099(3)	5106(2)	3800(1)	37(1)
C(3)	8182(3)	5254(2)	4372(1)	39(1)
C(4)	6675(3)	6038(2)	4408(1)	34(1)
C(5)	5647(4)	6249(2)	4990(1)	42(1)
C(6)	4217(3)	7016(2)	5001(1)	41(1)
C(7)	3674(3)	7633(2)	4422(1)	34(1)
C(8)	2239(3)	8477(2)	4404(1)	38(1)
C(9)	1792(3)	9023(2)	3833(1)	35(1)
C(10)	2706(3)	8721(2)	3250(1)	30(1)
C(11)	6177(3)	6633(2)	3835(1)	29(1)
C(12)	4608(3)	7417(2)	3835(1)	28(1)
C(13)	9513(3)	5586(2)	2616(1)	31(1)
C(14)	10206(3)	4560(2)	2422(1)	39(1)
C(15)	10953(4)	4394(2)	1813(1)	47(1)
C(16)	11056(4)	5239(2)	1388(1)	48(1)
C(17)	10448(3)	6262(2)	1580(1)	40(1)
C(18)	9689(3)	6436(2)	2192(1)	34(1)
C(19)	2144(3)	9255(2)	2620(1)	32(1)
C(20)	2188(3)	8684(2)	2050(1)	38(1)
C(21)	1675(4)	9192(2)	1460(1)	50(1)
C(22)	1108(4)	10274(3)	1434(2)	57(1)
C(23)	1042(4)	10847(2)	1994(2)	54(1)
C(24)	1540(3)	10347(2)	2588(1)	42(1)
C(25)	6514(3)	9660(2)	2188(1)	37(1)
C(26)	6609(4)	10472(2)	1718(2)	52(1)
C(27)	6672(4)	10260(2)	1069(2)	56(1)

for ic16900. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

C(28)	6596(4)	9239(2)	862(1)	45(1)
C(29)	6716(4)	8932(3)	197(1)	56(1)
C(30)	6626(4)	7937(3)	33(1)	54(1)
C(31)	6361(3)	7159(2)	523(1)	41(1)
C(32)	6297(4)	6105(2)	393(1)	47(1)
C(33)	6023(4)	5417(2)	891(1)	41(1)
C(34)	5766(3)	5776(2)	1535(1)	32(1)
C(35)	6386(3)	8488(2)	1352(1)	34(1)
C(36)	6180(3)	7450(2)	1177(1)	32(1)
C(37)	6552(3)	9812(2)	2900(1)	36(1)
C(38)	5523(3)	10689(2)	3188(2)	46(1)
C(39)	5473(4)	10764(2)	3860(2)	53(1)
C(40)	6445(4)	9988(2)	4253(1)	48(1)
C(41)	7489(3)	9127(2)	3975(1)	42(1)
C(42)	7550(3)	9049(2)	3302(1)	36(1)
C(43)	5458(3)	5062(2)	2085(1)	32(1)
C(44)	4283(3)	5416(2)	2585(1)	35(1)
C(45)	4078(4)	4760(2)	3114(1)	42(1)
C(46)	5046(4)	3747(2)	3157(1)	48(1)
C(47)	6200(4)	3381(2)	2663(1)	48(1)
C(48)	6396(3)	4029(2)	2122(1)	39(1)
Cl(1)	655(1)	2302(1)	4220(1)	43(1)
O(1)	1850(3)	2683(2)	3786(1)	79(1)
O(2)	1344(4)	1254(2)	4434(1)	76(1)
O(3)	-923(3)	2342(3)	3885(1)	94(1)
O(4)	297(3)	2956(2)	4773(1)	64(1)
Cl(2)	8358(1)	2697(1)	352(1)	45(1)
O(5)	6737(4)	2730(2)	709(1)	84(1)
O(6)	8052(5)	3522(2)	-103(2)	128(1)
O(7)	9582(5)	2799(3)	804(2)	131(2)
O(8)	8859(4)	1705(2)	44(1)	74(1)

Table 5S.	Bond lengths [Å] and angles [°] for		
ic16900.			
Co-N(3)	2.0152(19)	C(21)-C(22)	1.378(4)
Co-N(4)	2.0177(18)	C(22)-C(23)	1.377(4)
Co-N(1)	2.0206(18)	C(23)-C(24)	1.381(4)
Co-N(2)	2.0228(18)	C(25)-C(26)	1.407(4)
N(1)-C(1)	1.339(3)	C(25)-C(37)	1.475(4)
N(1)-C(11)	1.368(3)	C(26)-C(27)	1.361(4)
N(2)-C(10)	1.341(3)	C(27)-C(28)	1.405(4)
N(2)-C(12)	1.367(3)	C(28)-C(35)	1.397(3)
N(3)-C(25)	1.338(3)	C(28)-C(29)	1.425(4)
N(3)-C(35)	1.361(3)	C(29)-C(30)	1.349(4)
N(4)-C(34)	1.337(3)	C(30)-C(31)	1.433(4)
N(4)-C(36)	1.362(3)	C(31)-C(36)	1.398(3)
C(1)-C(2)	1.410(3)	C(31)-C(32)	1.399(4)
C(1)-C(13)	1.473(3)	C(32)-C(33)	1.369(4)
C(2)-C(3)	1.361(3)	C(33)-C(34)	1.406(3)
C(3)-C(4)	1.403(3)	C(34)-C(43)	1.475(3)
C(4)-C(11)	1.397(3)	C(35)-C(36)	1.433(3)
C(4)-C(5)	1.430(3)	C(37)-C(42)	1.389(3)
C(5)-C(6)	1.346(4)	C(37)-C(38)	1.397(4)
C(6)-C(7)	1.429(3)	C(38)-C(39)	1.380(4)
C(7)-C(12)	1.402(3)	C(39)-C(40)	1.379(4)
C(7)-C(8)	1.407(3)	C(40)-C(41)	1.379(4)
C(8)-C(9)	1.360(3)	C(41)-C(42)	1.382(4)
C(9)-C(10)	1.406(3)	C(43)-C(48)	1.392(3)
C(10)-C(19)	1.474(3)	C(43)-C(44)	1.393(3)
C(11)-C(12)	1.435(3)	C(44)-C(45)	1.376(3)
C(13)-C(14)	1.397(3)	C(45)-C(46)	1.379(4)
C(13)-C(18)	1.398(3)	C(46)-C(47)	1.377(4)
C(14)-C(15)	1.372(4)	C(47)-C(48)	1.388(4)
C(15)-C(16)	1.383(4)	Cl(1)-O(2)	1.412(2)
C(16)-C(17)	1.380(4)	Cl(1)-O(3)	1.415(3)
C(17)-C(18)	1.381(3)	Cl(1)-O(1)	1.421(2)
C(19)-C(20)	1.394(3)	Cl(1)-O(4)	1.424(2)
C(19)-C(24)	1.395(3)	Cl(2)-O(7)	1.370(3)
C(20)-C(21)	1.382(4)	Cl(2)-O(6)	1.377(3)

Cl(2)-O(8)	1.426(2)	N(1)-C(11)-C(4)	122.8(2)
Cl(2)-O(5)	1.448(3)	N(1)-C(11)-C(12)	117.78(19)
N(3)-Co-N(4)	83.60(8)	C(4)-C(11)-C(12)	119.5(2)
N(3)-Co-N(1)	134.94(8)	N(2)-C(12)-C(7)	122.7(2)
N(4)-Co-N(1)	115.52(7)	N(2)-C(12)-C(11)	117.84(19)
N(3)-Co-N(2)	111.07(8)	C(7)-C(12)-C(11)	119.5(2)
N(4)-Co-N(2)	135.41(7)	C(14)-C(13)-C(18)	118.5(2)
N(1)-Co-N(2)	84.29(7)	C(14)-C(13)-C(1)	119.8(2)
C(1)-N(1)-C(11)	119.20(19)	C(18)-C(13)-C(1)	121.6(2)
C(1)-N(1)-Co	130.47(15)	C(15)-C(14)-C(13)	120.2(2)
C(11)-N(1)-Co	110.00(14)	C(14)-C(15)-C(16)	120.6(2)
C(10)-N(2)-C(12)	119.06(19)	C(17)-C(16)-C(15)	120.1(2)
C(10)-N(2)-Co	130.46(15)	C(16)-C(17)-C(18)	119.6(2)
C(12)-N(2)-Co	109.95(14)	C(17)-C(18)-C(13)	120.8(2)
C(25)-N(3)-C(35)	119.5(2)	C(20)-C(19)-C(24)	118.9(2)
C(25)-N(3)-Co	129.22(17)	C(20)-C(19)-C(10)	121.0(2)
C(35)-N(3)-Co	110.78(15)	C(24)-C(19)-C(10)	120.0(2)
C(34)-N(4)-C(36)	119.35(19)	C(21)-C(20)-C(19)	120.7(2)
C(34)-N(4)-Co	129.41(15)	C(22)-C(21)-C(20)	119.8(3)
C(36)-N(4)-Co	110.62(15)	C(23)-C(22)-C(21)	120.1(3)
N(1)-C(1)-C(2)	120.5(2)	C(22)-C(23)-C(24)	120.7(3)
N(1)-C(1)-C(13)	118.41(19)	C(23)-C(24)-C(19)	119.8(3)
C(2)-C(1)-C(13)	121.0(2)	N(3)-C(25)-C(26)	120.4(2)
C(3)-C(2)-C(1)	120.3(2)	N(3)-C(25)-C(37)	116.4(2)
C(2)-C(3)-C(4)	120.2(2)	C(26)-C(25)-C(37)	123.3(2)
C(11)-C(4)-C(3)	117.0(2)	C(27)-C(26)-C(25)	120.1(3)
C(11)-C(4)-C(5)	119.3(2)	C(26)-C(27)-C(28)	120.4(2)
C(3)-C(4)-C(5)	123.7(2)	C(35)-C(28)-C(27)	116.6(2)
C(6)-C(5)-C(4)	121.5(2)	C(35)-C(28)-C(29)	118.9(3)
C(5)-C(6)-C(7)	120.3(2)	C(27)-C(28)-C(29)	124.5(2)
C(12)-C(7)-C(8)	116.9(2)	C(30)-C(29)-C(28)	121.3(2)
C(12)-C(7)-C(6)	119.7(2)	C(29)-C(30)-C(31)	121.0(3)
C(8)-C(7)-C(6)	123.4(2)	C(36)-C(31)-C(32)	116.9(2)
C(9)-C(8)-C(7)	120.0(2)	C(36)-C(31)-C(30)	118.8(3)
C(8)-C(9)-C(10)	120.4(2)	C(32)-C(31)-C(30)	124.3(2)
N(2)-C(10)-C(9)	120.7(2)	C(33)-C(32)-C(31)	120.3(2)
N(2)-C(10)-C(19)	118.6(2)	C(32)-C(33)-C(34)	119.8(2)
C(9)-C(10)-C(19)	120.7(2)	N(4)-C(34)-C(33)	120.7(2)

N(4)-C(34)-C(43)	117.68(19)
C(33)-C(34)-C(43)	121.6(2)
N(3)-C(35)-C(28)	122.8(2)
N(3)-C(35)-C(36)	117.3(2)
C(28)-C(35)-C(36)	119.9(2)
N(4)-C(36)-C(31)	122.8(2)
N(4)-C(36)-C(35)	117.5(2)
C(31)-C(36)-C(35)	119.8(2)
C(42)-C(37)-C(38)	118.6(2)
C(42)-C(37)-C(25)	120.1(2)
C(38)-C(37)-C(25)	121.2(2)
C(39)-C(38)-C(37)	119.9(3)
C(40)-C(39)-C(38)	120.8(3)
C(41)-C(40)-C(39)	120.0(3)
C(40)-C(41)-C(42)	119.5(3)
C(41)-C(42)-C(37)	121.2(2)
C(48)-C(43)-C(44)	119.1(2)
C(48)-C(43)-C(34)	119.9(2)
C(44)-C(43)-C(34)	121.0(2)
C(45)-C(44)-C(43)	120.4(2)
C(44)-C(45)-C(46)	120.3(3)
C(47)-C(46)-C(45)	120.0(2)
C(46)-C(47)-C(48)	120.2(3)
C(47)-C(48)-C(43)	119.9(2)
O(2)-Cl(1)-O(3)	110.48(19)
O(2)-Cl(1)-O(1)	110.04(14)
O(3)-Cl(1)-O(1)	108.50(17)
O(2)-Cl(1)-O(4)	109.25(14)
O(3)-Cl(1)-O(4)	107.94(15)
O(1)-Cl(1)-O(4)	110.62(16)
O(7)-Cl(2)-O(6)	113.6(3)
O(7)-Cl(2)-O(8)	109.09(18)
O(6)-Cl(2)-O(8)	111.24(18)
O(7)-Cl(2)-O(5)	106.7(2)
O(6)-Cl(2)-O(5)	105.9(2)
O(8)-Cl(2)-O(5)	110.20(15)

equivalent atoms:

Symmetry transformations used to generate

	U^{11}	U ²²	U ³³	U ²³	U ¹³	U ¹²
Со	31(1)	27(1)	23(1)	1(1)	1(1)	-4(1)
N(1)	27(1)	29(1)	26(1)	0(1)	-1(1)	-6(1)
N(2)	27(1)	30(1)	25(1)	-1(1)	0(1)	-6(1)
N(3)	30(1)	30(1)	32(1)	3(1)	-2(1)	-6(1)
N(4)	30(1)	31(1)	25(1)	0(1)	0(1)	-6(1)
C(1)	29(1)	30(1)	33(1)	-1(1)	-2(1)	-6(1)
C(2)	34(1)	35(1)	39(1)	5(1)	-4(1)	-2(1)
C(3)	42(1)	42(1)	31(1)	7(1)	-6(1)	-5(1)
C(4)	38(1)	38(1)	27(1)	2(1)	-3(1)	-11(1)
C(5)	49(2)	52(2)	23(1)	5(1)	-1(1)	-10(1)
C(6)	44(1)	55(2)	24(1)	-2(1)	5(1)	-13(1)
C(7)	34(1)	43(1)	27(1)	-4(1)	3(1)	-12(1)
C(8)	35(1)	47(1)	33(1)	-11(1)	9(1)	-10(1)
C(9)	29(1)	37(1)	38(1)	-7(1)	3(1)	-5(1)
C(10)	27(1)	30(1)	34(1)	-5(1)	0(1)	-8(1)
C(11)	29(1)	33(1)	25(1)	-1(1)	-1(1)	-9(1)
C(12)	28(1)	32(1)	27(1)	-3(1)	1(1)	-9(1)
C(13)	26(1)	34(1)	33(1)	-3(1)	-1(1)	-4(1)
C(14)	39(1)	34(1)	44(1)	-4(1)	1(1)	-8(1)
C(15)	50(2)	40(1)	51(2)	-14(1)	7(1)	-7(1)
C(16)	49(2)	59(2)	38(1)	-12(1)	10(1)	-10(1)
C(17)	40(1)	46(2)	36(1)	3(1)	4(1)	-8(1)
C(18)	30(1)	33(1)	36(1)	0(1)	3(1)	-2(1)
C(19)	25(1)	36(1)	36(1)	0(1)	-2(1)	-4(1)
C(20)	36(1)	39(1)	38(1)	-3(1)	-4(1)	-1(1)
C(21)	46(2)	64(2)	38(1)	-1(1)	-6(1)	-2(1)
C(22)	52(2)	66(2)	47(2)	16(2)	-6(1)	-2(2)
C(23)	52(2)	41(2)	65(2)	13(1)	-4(1)	1(1)
C(24)	40(1)	37(1)	48(2)	-1(1)	-1(1)	-1(1)
C(25)	34(1)	30(1)	47(1)	3(1)	-5(1)	-8(1)
C(26)	59(2)	35(1)	63(2)	9(1)	-12(1)	-16(1)
C(27)	70(2)	45(2)	57(2)	24(1)	-13(2)	-25(2)
C(28)	47(2)	49(2)	40(1)	15(1)	-6(1)	-14(1)

Table 6S.Anisotropic displacement parameters $(Å^2x \ 10^3)$ for ic16900. The anisotropicdisplacement factor exponent takes the form: $-2\pi^2 [h^2 \ a^{*2} U^{11} + ... + 2 \ h \ k \ a^* \ b^* \ U^{12}]$

C(29)	66(2)	67(2)	37(2)	21(1)	-2(1)	-22(2)
C(30)	62(2)	71(2)	29(1)	9(1)	2(1)	-16(2)
C(31)	44(1)	51(2)	26(1)	3(1)	1(1)	-6(1)
C(32)	56(2)	57(2)	26(1)	-9(1)	1(1)	-7(1)
C(33)	49(2)	42(1)	33(1)	-9(1)	-2(1)	-7(1)
C(34)	32(1)	34(1)	30(1)	-3(1)	-2(1)	-6(1)
C(35)	34(1)	36(1)	31(1)	7(1)	-1(1)	-8(1)
C(36)	32(1)	39(1)	26(1)	4(1)	-1(1)	-4(1)
C(37)	32(1)	30(1)	49(1)	-4(1)	-3(1)	-11(1)
C(38)	36(1)	30(1)	72(2)	-7(1)	-3(1)	-7(1)
C(39)	40(2)	46(2)	74(2)	-23(2)	11(1)	-8(1)
C(40)	45(2)	56(2)	48(2)	-16(1)	10(1)	-18(1)
C(41)	37(1)	46(2)	46(2)	-5(1)	0(1)	-15(1)
C(42)	32(1)	34(1)	44(1)	-8(1)	-2(1)	-7(1)
C(43)	35(1)	32(1)	30(1)	-2(1)	-4(1)	-12(1)
C(44)	34(1)	37(1)	36(1)	-1(1)	-3(1)	-11(1)
C(45)	44(1)	51(2)	36(1)	-1(1)	4(1)	-20(1)
C(46)	62(2)	46(2)	39(1)	9(1)	-6(1)	-24(1)
C(47)	64(2)	30(1)	51(2)	4(1)	-11(1)	-14(1)
C(48)	46(1)	32(1)	40(1)	-6(1)	-3(1)	-10(1)
Cl(1)	41(1)	40(1)	46(1)	1(1)	8(1)	-3(1)
O(1)	60(1)	73(2)	93(2)	37(1)	31(1)	4(1)
O(2)	114(2)	36(1)	69(2)	5(1)	31(1)	4(1)
O(3)	56(2)	161(3)	69(2)	-28(2)	-6(1)	-24(2)
O(4)	81(2)	42(1)	65(1)	-11(1)	-1(1)	0(1)
Cl(2)	66(1)	33(1)	35(1)	0(1)	0(1)	-6(1)
O(5)	109(2)	63(2)	87(2)	-22(1)	44(2)	-32(2)
O(6)	190(4)	81(2)	89(2)	46(2)	50(2)	19(2)
O(7)	118(3)	125(3)	143(3)	-76(2)	-62(2)	14(2)
O(8)	102(2)	58(1)	61(1)	-28(1)	3(1)	-6(1)

	X	у	Z	U(eq)
H(2)	10107	4565	3777	44
H(3)	8564	4825	4748	47
H(5)	5982	5840	5378	50
H(6)	3565	7146	5396	49
H(8)	1583	8664	4792	45
H(9)	856	9613	3827	42
H(14)	10160	3974	2713	46
H(15)	11404	3692	1683	56
H(16)	11546	5114	963	58
H(17)	10552	6844	1294	49
H(18)	9281	7140	2326	41
H(20)	2576	7937	2067	46
H(21)	1712	8797	1073	60
H(22)	761	10626	1028	68
H(23)	650	11592	1973	65
H(24)	1470	10747	2974	51
H(26)	6630	11168	1854	62
H(27)	6769	10806	754	67
H(29)	6862	9439	-138	67
H(30)	6740	7749	-413	64
H(32)	6445	5867	-43	56
H(33)	6007	4698	803	50
H(38)	4859	11232	2922	55
H(39)	4762	11358	4055	64
H(40)	6394	10046	4716	58
H(41)	8162	8592	4244	50
H(42)	8288	8463	3110	44
H(44)	3619	6115	2561	42
H(45)	3265	5005	3451	51
H(46)	4917	3302	3527	57
H(47)	6865	2682	2694	57
H(48)	7170	3767	1776	47

Table 7S. Hydrogen coordinates ($x \ 10^4$) and isotropic displacement parameters (Å²x 10³) for ic16900.