Supplementary Information for

Positive thermal expansion facilitates the formation of argentophilic forces following an order-disorder phase transition

Navkiran Juneja,^a Daniel K. Unruh,^a Ryan H. Groeneman,^b and Kristin M. Hutchins^a*

^a Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX, 79409, USA. Email: kristin.hutchins@ttu.edu

^b Department of Biological Sciences, Webster University, St. Louis, MO, 63119, USA.

1.	Materials and synthesis of the crystal	Page S2
2.	X-ray diffraction information and data tables	Page S3-S11
3.	Thermal expansion data and intermolecular interaction distances	Page S12-S13
4.	DSC data	Page S14
5.	Expansivity indicatrix images	Page S15
6.	Variation of the unit cell parameters	Page S16
7.	Colossal TE coefficients for organic and metal-organic systems	Page S17
8.	References	Page S18

1. Materials and synthesis of the crystal

Materials

The compounds 4-stilbazole (**4-SB**), silver(I) trifluoromethanesulfonate (**AgCF₃SO₃**), and the solvents reagent grade ethanol (95%) and acetonitrile were all purchased from Sigma-Aldrich Chemical (St. Louis, MO, USA) and used as received. All crystallization studies were performed in 20 mL scintillation vials.

Synthesis of [Ag₂(CF₃SO₃)₂(4-SB)₄]

The formation of the complex has been previously reported,¹ and a similar approach was utilized in this paper. In particular, crystals were synthesized by dissolving 25.0 mg of **4-SB** in 2.0 mL of ethanol and combining it with a dissolved 17.7 mg solution of **AgCF₃SO₃** in 2.0 mL of acetonitrile (2:1 molar ratio). Within two days crystals suitable for X-ray diffraction were realized via slow solvent evaporation.

2. X-ray diffraction information and data tables

Data were collected on a Rigaku XtaLAB Synergy-*i* Kappa diffractometer equipped with a PhotonJet-*i* X-ray source operated at 50 W (50kV, 1 mA) to generate Cu K α radiation (λ = 1.54178 Å) and a HyPix-6000HE HPC detector. Crystals were transferred from the vial and placed on a glass slide in polyisobutylene. A Zeiss Stemi 305 microscope was used to identify a suitable specimen for X-ray diffraction from a representative sample of the material. The crystal and a small amount of the oil were collected on a MiTeGen 50 micron MicroLoop and transferred to the instrument where it was placed under a cold nitrogen stream (Oxford 700 series). The mounting and data collection were done at different temperatures as outlined below. The transition rate between temperatures was 2 K/minute. The samples were optically centered with the aid of a video camera to insure that no translations were observed as the crystal was rotated through all positions. A unit cell collection was then carried out. Then, a data collection strategy was calculated by *CrysAlisPro.*² The crystal was measured for size, morphology, and color.

Refinement Details

After data collection, the unit cell was re-determined using a subset of the full data collection. Intensity data were corrected for Lorentz, polarization, and background effects using the *CrysAlisPro*.² A numerical absorption correction was applied based on a Gaussian integration over a multifaceted crystal and followed by a semi-empirical correction for adsorption applied using the program *SCALE3 ABSPACK*.³ The *SHELX-2014*,⁴ series of programs was used for the solution and refinement of the crystal structure within the OLEX2 software.⁵ Throughout the temperature range in this study, the ethylene moiety (C6 and C7) was positionally disorder over two sites (A and B). At 270 K and 290 K, the triflate molecule being modeled over two sites (A and B) with SOFs of nearly 0.5:0.5, respectively. To help maintain reasonable ADP values and bond lengths for the disordered sites, SIMU and free variable DFIX restraints were applied. For data collected at 270 K and 290 K, the RIGU restraint was also applied globally due to the significant amount of disorder throughout the structure. Hydrogen atoms bound to carbon atoms were located in the difference Fourier map and were geometrically constrained using the appropriate AFIX commands.

Temperature Details

The data outlined in Tables S1-S4 below was collected by mounting a crystal of $[Ag_2(CF_3SO_3)_2(4-SB)_4]$ at 100 K (flash cooled) and a full data set was collected. Then the crystal was warmed to 110 K for the next full data set, followed by temperature increases of 20 K/data set up to 290 K (room temperature).

Compound formula	C ₂₇ H ₂₂ AgF ₃ N ₂ O ₃ S	$C_{27}H_{22}AgF_3N_2O_3S$	C ₂₇ H ₂₂ AgF ₃ N ₂ O ₃ S
Formula Mass	619.39	619.39	619.39
Crystal System	Monoclinic	Monoclinic	Monoclinic
Space Group	C2/c	C2/c	C2/c
a/Å	22.6960(7)	22.6717(5)	22.1453(2)
b/Å	12.8357(5)	12.8018(4)	12.74270(10)
c/Å	18.1558(5)	18.1125(4)	18.37430(10)
α/°	90	90	90
β/°	94.635(3)	94.823(2)	97.2980(10)
γ/°	90	90	90
$V/Å^3$	5271.8(3)	5238.3(2)	5143.05(7)
ρ_{calc} / g cm ⁻³	1.561	1.571	1.601
T/K	290	270	250
Z	8	8	8
Radiation Type	CuKa	СиКа	CuKα
Wavelength, Å	1.54184	1.54184	1.54184
Absorption coefficient, μ/mm^{-1}	7.339	7.386	7.529
F(000)	2496	2496	2496
Reflections collected	30335	32359	31828
No. of independent reflections	5144	5179	5214
No. of reflection $(I > 2\sigma(I))$	3021	3432	4549
Data/restraints/parameter	5144 / 449 / 454	5179 / 443 / 454	5214 / 258 / 397
R _{int}	0.0820	0.0757	0.0624
$R1 (I > 2\sigma(I))$	0.0651	0.0582	0.0506
$wR(F2) (I > 2\sigma(I))$	0.2036	0.1702	0.1399
R1 (all data)	0.0913	0.0793	0.0553
wR(F2) (all data)	0.2313	0.1895	0.1441
Goodness-of-fit on F ²	1.057	1.052	1.055
CCDC deposition number	2055941	2055940	2055939

Table S1. X-ray data for [Ag2(CF3SO3)2(4-SB)4] at 290, 270, and 250 K.

Compound formula	C ₂₇ H ₂₂ AgF ₃ N ₂ O ₃ S	$C_{27}H_{22}AgF_3N_2O_3S$	C ₂₇ H ₂₂ AgF ₃ N ₂ O ₃ S
Formula Mass	619.39	619.39	619.39
Crystal System	Monoclinic	Monoclinic	Monoclinic
Space Group	C2/c	C2/c	C2/c
a/Å	22.10270(10)	22.07840(10)	22.05900(10)
b/Å	12.71470(10)	12.69100(10)	12.67000(10)
c/Å	18.36400(10)	18.34850(10)	18.32840(10)
α/°	90	90	90
β/°	97.5790(10)	97.7740(10)	97.9270(10)
γ/°	90	90	90
V/Å ³	5115.73(6)	5093.94(6)	5073.61(6)
ρ_{calc} / g cm ⁻³	1.608	1.615	1.622
T/K	230	210	190
Z	8	8	8
Radiation Type	CuKa	CuKa	CuKa
Wavelength, Å	1.54184	1.54184	1.54184
Absorption coefficient, μ/mm^{-1}	7.563	7.595	7.626
F(000)	2496	2496	2496
Reflections collected	30792	26895	29905
No. of independent reflections	5184	5082	5136
No. of reflection $(I > 2\sigma(I))$	4684	4723	4843
Data/restraints/parameter	5184 / 258 / 397	5082 / 258 / 397	5136 / 258 / 397
R _{int}	0.0601	0.0539	0.0558
R1 (I > $2\sigma(I)$)	0.0448	0.0412	0.0374
wR(F2) (I > $2\sigma(I)$	0.1233	0.1119	0.0984
R1 (all data)	0.0477	0.0432	0.0389
wR(F2) (all data)	0.1258	0.1135	0.0996
Goodness-of-fit on F ²	1.047	1.046	1.031
CCDC deposition number	2055938	2055937	2055936

Table S2. X-ray data for [Ag2(CF3SO3)2(4-SB)4] at 230, 210, and 190 K.

Compound formula	C ₂₇ H ₂₂ AgF ₃ N ₂ O ₃ S	C ₂₇ H ₂₂ AgF ₃ N ₂ O ₃ S	C ₂₇ H ₂₂ AgF ₃ N ₂ O ₃ S
Formula Mass	619.39	619.39	619.39
Crystal System	Monoclinic	Monoclinic	Monoclinic
Space Group	C2/c	C2/c	C2/c
a/Å	22.0404(2)	22.0352(2)	22.0261(2)
b/Å	12.65120(10)	12.63540(10)	12.61900(10)
c/Å	18.30820(10)	18.28730(10)	18.2707(2)
α/°	90	90	90
β/°	98.0560(10)	98.1460(10)	98.2460(10)
γ/°	90	90	90
V/Å ³	5054.63(7)	5040.24(7)	5025.79(8)
ρ_{calc} / g cm ⁻³	1.628	1.633	1.637
T/K	170	150	130
Z	8	8	8
Radiation Type	CuKα	СиКа	CuKα
Wavelength, Å	1.54184	1.54184	1.54184
Absorption coefficient, μ/mm^{-1}	7.655	7.676	7.698
F(000)	2496	2496	2496
Reflections collected	30135	33921	33089
No. of independent reflections	5157	5242	5220
No. of reflection $(I > 2\sigma(I))$	4890	5004	5002
Data/restraints/parameter	5157 / 258 / 397	5242 / 258 / 397	5220 / 258 / 397
R _{int}	0.0556	0.0574	0.0573
R1 (I > $2\sigma(I)$)	0.0365	0.0364	0.0351
wR(F2) (I > $2\sigma(I)$	0.0968	0.0967	0.0931
R1 (all data)	0.0379	0.0376	0.0363
wR(F2) (all data)	0.0979	0.0976	0.0939
Goodness-of-fit on F ²	1.048	1.046	1.060
CCDC deposition number	2055935	2055934	2055933

Table S3. X-ray data for [Ag2(CF3SO3)2(4-SB)4] at 170, 150, and 130 K.

Compound formula	C ₂₇ H ₂₂ AgF ₃ N ₂ O ₃ S	$C_{27}H_{22}AgF_3N_2O_3S$
Formula Mass	619.39	619.39
Crystal System	Monoclinic	Monoclinic
Space Group	C2/c	C2/c
a/Å	22.0143(2)	22.0074(2)
b/Å	12.60480(10)	12.59700(10)
c/Å	18.2550(2)	18.2478(10)
α/°	90	90
β/°	98.3420(10)	98.3810(10)
$\gamma/^{\circ}$	90	90
V/Å ³	5011.91(8)	5004.76(8)
ρ_{calc} / g cm ⁻³	1.642	1.644
T/K	110	100
Z	8	8
Radiation Type	CuKa	CuKa
Wavelength, Å	1.54184	1.54184
Absorption coefficient, μ/mm^{-1}	7.720	7.731
F(000)	2496	2496
Reflections collected	29078	26877
No. of independent reflections	5125	5085
No. of reflection $(I > 2\sigma(I))$	4913	4881
Data/restraints/parameter	5125 / 258 / 397	5085 / 258 / 397
R _{int}	0.0587	0.0568
$R1 (I > 2\sigma(I))$	0.0364	0.0367
$wR(F2) (I > 2\sigma(I))$	0.0962	0.0981
R1 (all data)	0.0374	0.0377
wR(F2) (all data)	0.0971	0.0990
Goodness-of-fit on F ²	1.050	1.053
CCDC deposition number	2055932	2055931

Table S4. X-ray data for [Ag2(CF3SO3)2(4-SB)4] at 110 and 100 K.

Table S5. Site occupancies of disordered **4-SB** ligand and the trifluoromethanesulfonate anion (CF_3SO_3) within $[Ag_2(CF_3SO_3)_2(4-SB)_4]$ as a function of temperature. The data is from the 100-290 K heating experiment in Tables S1-S4 above.

Temperature	4-SB disorder	CF ₃ SO ₃ ⁻ disorder
	(major/minor)	(major/minor)
100 K	0.91 / 0.09	1.00 / 0.00
110 K	0.91 / 0.09	1.00 / 0.00
130 K	0.91 / 0.09	1.00 / 0.00
150 K	0.91 / 0.09	1.00 / 0.00
170 K	0.94 / 0.06	1.00 / 0.00
190 K	0.93 / 0.07	1.00 / 0.00
210 K	0.92 / 0.08	1.00 / 0.00
230 K	0.90 / 0.10	1.00 / 0.00
250 K	0.88 / 0.12	1.00 / 0.00
270 K	0.81 / 0.19	0.51 / 0.49
290 K	0.81 / 0.19	0.51 / 0.49

Temperature details

The data outlined below in Table S6 was collected by mounting a crystal of [Ag₂(CF₃SO₃)₂(4-SB)₄] at 190 K and a full data set was collected. Then the crystal was warmed and full data sets were collected at 210, 230, 250, 270, and 290 K.

Table S6. Unit cell parameters for [Ag₂(CF₃SO₃)₂(4-SB)₄] from 190-290 K. The CCDC number for each structure is included below the temperature value.

Temperature	a/Å	b/Å	c/Å	β/°	$V/Å^3$
190 K	22.0621(2)	12 6447(10)	18 3556(2)	07.857(10)	5072 8(1)
(2057199)	22.0031(2)	12.0447(10)	18.3330(2)	97.857(10)	5072.8(1)
210 K	22.0810(2)	12 6642(10)	18 2777(2)	07.712(10)	5002.83(1)
(2057200)	22.0819(2)	12.0042(10)	10.3777(2)	97.712(10)	5092.85(1)
230 K	22.1074(2)	12 6992(2)	18 2044(2)	07.522(10)	5115 21(1)
(2057201)	22.1074(2)	12.0885(2)	16.3944(2)	97.332(10)	5115.21(1)
250 K	22.1276(2)	12 71 (2(2)	19 4026(2)	07 208(10)	512976(1)
(2057202)	22.1370(3)	12.7102(2)	18.4030(2)	97.298(10)	3138.70(1)
270 K	22 6055(4)	12 7820(2)	19 1157(2)	04 668(2)	5228 6(2)
(2057203)	22.0933(4)	12.7639(3)	10.1137(3)	94.008(2)	3238.0(2)
290 K	22 6805(5)	12 8202(4)	19 1655(2)	04 500(2)	5270 74(2)
(2057204)	22.0893(3)	12.8292(4)	16.1035(3)	94.399(2)	3270.74(2)

Table S7. Site occupancies of disordered **4-SB** ligand and the trifluoromethanesulfonate anion (CF_3SO_3) within $[Ag_2(CF_3SO_3)_2(4-SB)_4]$ as a function of temperature. The data is from the 190-290 K heating experiment in Table S6 above.

Temperature	4-SB disorder	CF ₃ SO ₃ ⁻ disorder
	(major/minor)	(major/minor)
190 K	0.96 / 0.04	1.00 / 0.00
210 K	0.95 / 0.05	1.00 / 0.00
230 K	0.93 / 0.07	1.00 / 0.00
250 K	0.91 / 0.09	1.00 / 0.00
270 K	0.81 / 0.19	0.50 / 0.50
290 K	0.82 / 0.18	0.48 / 0.52

Temperature details

The data outlined below in Table S8 was collected by mounting a crystal of $[Ag_2(CF_3SO_3)_2(4-SB)_4]$ at 290 K and a full data set was collected. Then the crystal was cooled and full data sets were collected every 20 K from 270-100 K. The data collected by this method, however, was very poor quality due to significant disorder in the anion that does not resolve until 190 K. This is a much lower temperature for ordering compared to the two data sets outlined above. The unit cell parameters are usable, but the data could not be fully solved due to poor quality.

Temperature	a/Å	b/Å	c/Å	β/°	$V/Å^3$
290 K	22.72613(6)	12.83102(4)	18.162378(4)	94.5385(2)	5279.5321(2)
270 K	22.62023(13)	12.853073(7)	18.082632(6)	95.0165(4)	5237.1982(5)
250 K	22.51336(2)	12.87484(13)	18.013175(9)	95.4674(6)	5197.4733(8)
230 K	22.46941(3)	12.85892(17)	17.97989(11)	95.8288(8)	5168.114(10)
210 K	22.36904(4)	12.845255(2)	17.93911(16)	96.1158(10)	5125.216(13)
190 K	22.0632(12)	12.717926(9)	18.256624(9)	97.9071(5)	5074.0584(5)
170 K	22.03697(8)	12.707585(6)	18.223340(6)	98.0440(3)	5052.9909(4)
150 K	22.02232(7)	12.696082(5)	18.201706(6)	98.1784(3)	5037.3887(3)
130 K	22.00807(6)	12.680320(4)	18.183391(5)	98.2808(3)	5021.5232(3)
110 K	21.99728(6)	12.666885(4)	18.167226(5)	98.4035(3)	5007.7121(3)
100 K	21.99633(6)	12.661153(4)	18.157837(5)	98.4572(3)	5001.9475(3)

Table S8. Unit cell parameters for [Ag2(CF3SO3)2(4-SB)4] cooling from 290-100 K.

Table S9. Intermolecular interaction distances before and after the phase transition. The distances below are calculated using the data from the 100-290 K experiment. All distances are reported in Å.

Interaction	250 K	270 K	290 K
	(before	(after	(after
	transition)	transition)	transition)
Ag-N bond length	2.162	2.168	2.163
(disordered 4-SB, major site)			
Ag-N bond length	1.046	1.059	1.074
(disordered 4-SB, minor site)	1.940	1.958	1.974
Ag-N bond length	0.127	2 125	2 1 1 7
(ordered 4-SB)	2.157	2.123	2.117
AgAg interactions	3.883	3.527	3.506
Ag-O coordination bonds	2.755	2.788	2.796
$\pi \cdots \pi$ interactions within			
dimer (pyridine-pyridine	3.760	3.644	3.642
centroid)			

3. Thermal expansion data and intermolecular interaction distances

The thermal expansion coefficients were calculated using the PASCal program.⁶ The temperature range used for the calculations is included, and the X-ray data is included in Tables S1-S4 or Table S5.

Temperature	α_{X_1} (MK ⁻¹)	α_{X_2} (MK ⁻¹)	$\alpha_{X_3}(MK^{-1})$	$\alpha_V(\mathrm{MK}^{-1})$
range	[axis]	[axis]	[axis]	
100-250 K	-9(2)	75(3)	111(7)	181(9)
	[1 0 -1]	[0 -1 0]	[2 0 3]	
190-250 K	-21(4)	94(4)	143(4)	217(4)
	[1 0 -1]	[0 -1 0]	[1 0 1]	

Table S10. Thermal expansion coefficients for $[Ag_2(CF_3SO_3)_2(4-SB)_4]$ with errors denoted in the parentheses and approximate crystallographic axes denoted in brackets.

Table S11. Intermolecular interaction distances within $[Ag_2(CF_3SO_3)_2(4-SB)_4]$ that contribute to the thermal expansion. The data below is for the 100-290 K experiment, but only data up to 250 K was used for thermal expansion calculations and interpretations. All distances are reported in Å.

Interaction	250 K	100 K	Δ
Ag-N coordination bonds	2.162	2.151	0.011
	2.137	2.135	0.002
C-H····O interactions	3.505	3.440	0.065
	3.553	3.522	0.031
	3.373	3.363	0.01
F···F contacts	2.814	2.834	-0.02
C-H···F interactions	3.218	3.190	0.028
	3.261	3.282	-0.021
Ag-O coordination bonds	2.755	2.729	0.026
Ag-Ag interactions	3.883	3.909	-0.026
Ag…C interactions	3.180	3.123	0.057
$\pi \cdots \pi$ interactions within dimer	3.760 (major)	3.750 (major)	0.010
(pyridine-pyridine centroid)	3.724 (minor)	3.721 (minor)	0.003
$\pi \cdots \pi$ interactions between dimers	4.054	4.032	0.022
(pyridine-benzene centroid)			

Table S12. Ag-N bond lengths and Ag-Ag interactions within [Ag₂(CF₃SO₃)₂(4-SB)₄] as a function of temperature during the 100-290 K experiment. All distances are reported in Å.

Temperature	Ag-N bond length	Ag-N bond length	Ag-N bond	Ag-Ag
(K)	(disordered 4-SB,	(disordered 4-SB,	length	interaction
	major site)	minor site)	(ordered 4-SB)	
100	2.151	2.011	2.135	3.909
110	2.154	2.002	2.132	3.910
130	2.155	1.976	2.136	3.909
150	2.154	1.959	2.134	3.908
170	2.150	1.912	2.132	3.897
190	2.152	1.919	2.132	3.899
210	2.156	1.925	2.133	3.900
230	2.158	1.931	2.135	3.897
250	2.162	1.946	2.137	3.883

Table S13. Intermolecular interaction distances within $[Ag_2(CF_3SO_3)_2(4-SB)_4]$ that contribute to the thermal expansion. The data below is for the 190-290 experiment, but only data up to 250 K was used for thermal expansion calculations and interpretations. All distances are reported in Å.

Interaction	250 K	190 K	Δ
Ag-N coordination bonds	2.141	2.140	0.001
	2.133	2.131	0.002
C-H····O interactions	3.503	3.476	0.027
	3.556	3.541	0.015
	3.371	3.359	0.012
F···F contacts	2.830	2.838	-0.008
C-H···F interactions	3.422	3.389	0.033
	3.575	3.556	0.019
Ag-O coordination bonds	2.755	2.759	-0.004
Ag-Ag interactions	3.882	3.888	-0.006
Ag…C interactions	3.181	3.161	0.02
$\pi \cdots \pi$ interactions within dimer	3.767	3.768	-0.001
(pyridine-pyridine centroid)			
$\pi \cdots \pi$ interactions between dimers	4.041	4.027	0.014
(pyridine-benzene centroid)			

4. DSC data

DSC data were collected on a Mettler Toledo DSC 823 with intra cooler (freon cooler). The sample was cooled from 25 to -65 °C at 20 K/min and warmed back to 25 °C at 10 K/min.

The top curve is the cooling curve from 25 to -65 °C, and the bottom curve is the heating curve from -65 to 25 °C. A discernible transition was observed at -16 °C (257.15 K) during cooling and -10 °C (263.15 K) during heating.



Figure S1. DSC curve for [Ag2(CF3SO3)2(4-SB)4].

5. Expansivity indicatrix images



Figure S2. Expansivity indicatrix for [Ag2(CF3SO3)2(4-SB)4] for the 100-250 K warming data set.



Figure S3. Expansivity indicatrix for [Ag2(CF3SO3)2(4-SB)4] for the 190-250 K warming data set.

6. Variation of the unit cell parameters



Figure S4. Absolute values of the percent change in length as a function of temperature for $[Ag_2(CF_3SO_3)_2(4-SB)_4]$ using the 100-290 K data set. The values at 100 K are used as the zero point.

7. Colossal TE coefficients for metal-organic and organic solids

Table S14. TE coefficients for some reported organic and metal-organic solids that exhibit colossal TE behavior. This list represents some examples and is not intended to encompass all systems that exhibit colossal TE. The TE coefficients for the silver complex in this work are listed in Table S10.

Compound	TE Coefficients ^a	Reference
2(res)·2(4,4'-azopyridine)	$\alpha_{X1} = -12 \text{ MK}^{-1}$	7
	$\alpha_{X2} = 87 \ MK^{-1}$	
	$\alpha_{X3} = 151 \ MK^{-1}$	
$2(res) \cdot 2(4,4'-bispyridylethylene)$	$\alpha_{X1} = -36 \text{ MK}^{-1}$	7
	$\alpha_{\rm X2} = 52~\rm MK^{-1}$	
	$\alpha_{X3} = 113 \text{ MK}^{-1}$	
(phenylazophenyl)palladium	$\alpha_a = 124.0(2) \ge 10^{-6} \text{ K}^{-1}$	8
hexafluoroacetylacetonate (β form)	$\alpha_{\rm b} = 105.4(3) \ge 10^{-6} \ {\rm K}^{-1}$	
	$\alpha_{\rm c} = 114.9(3) \ge 10^{-6} {\rm K}^{-1}$	
$Ag_3[Co(CN)_6]$	$\alpha_a = 150 \times 10^{-6} \text{ K}^{-1}$	9
	$\alpha_{\rm c} = -130 \text{ x } 10^{-6} \text{ K}^{-1}$	
(<i>S</i> , <i>S</i>)-octa-3,5-diyn-2,7-diol	$\alpha_a = 515 - 156 \ge 10^{-6} \text{ K}^{-1}$	10
	$\alpha_{\rm b} = -85$ to $-63 \ge 10^{-6}$ K ⁻¹	
	$\alpha_{\rm c} = -204 \text{ to } -45 \text{ x } 10^{-6} \text{ K}^{-1}$	
imidazolium 4-hydroxybenzene carboxylate	$\alpha_{a} = 210 \text{ MK}^{-1}$	11
	$\alpha_b = -115 \text{ MK}^{-1}$	
[Ni(pba)2]·2DMA	$\alpha_a = 153 \times 10^{-6} \text{ K}^{-1}$	12
	$\alpha_{\rm b} = 41 \text{ x } 10^{-6} \text{ K}^{-1}$	
	$\alpha_{\rm c} = -35 \text{ x} \ 10^{-6} \text{ K}^{-1}$	
[Co(pba)2]·2DMA	$\alpha_a = 193 \times 10^{-6} \text{ K}^{-1}$	12
	$\alpha_b = 64 \times 10^{-6} \text{ K}^{-1}$	
	$\alpha_c = -76 \times 10^{-6} \text{ K}^{-1}$	10
[Zn(pba)2]·2DMA	$\alpha_a = 18 / x 10^{-6} K^{-1}$	12
	$\alpha_b = 89 \times 10^{-6} \text{ K}^{-1}$	
$L_{i}(A, arrow)$ (IL O) $1.0.5$ MaO(II)	$\alpha_c = -84 \times 10^{\circ} \text{ K}^{-1}$	12
$L1(4-pyc)-(H_2O)_{0.5}-O.5MeOH_n$	$\alpha_{X1} = -42$ IVIK	15
	$\alpha_{X2} = 5 \text{ MK}^{-1}$	
	$\alpha_{X3} = 200 \text{ MK}^{-1}$	

^aThe program PASCal⁶ is used for TE calculations when the crystal lies in a low-symmetry system and is considered a straightforward method for calculating the expansion coefficients describing these systems completely. The units from PASCal are in inverse megakelvin (MK⁻¹). The writers of the program use 1 MK⁻¹ instead of 1×10^{-6} K⁻¹ for convenience, but the terms are comparable. In this way, literature values can be compared whether the program was used or if the values were calculated by hand.

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