Supplementary Material (ESI) for Chemical Communications

Electronic Supplementary Information

Host–guest transformational correlations for a gas inclusion co-crystal on changing gas pressure and temperature

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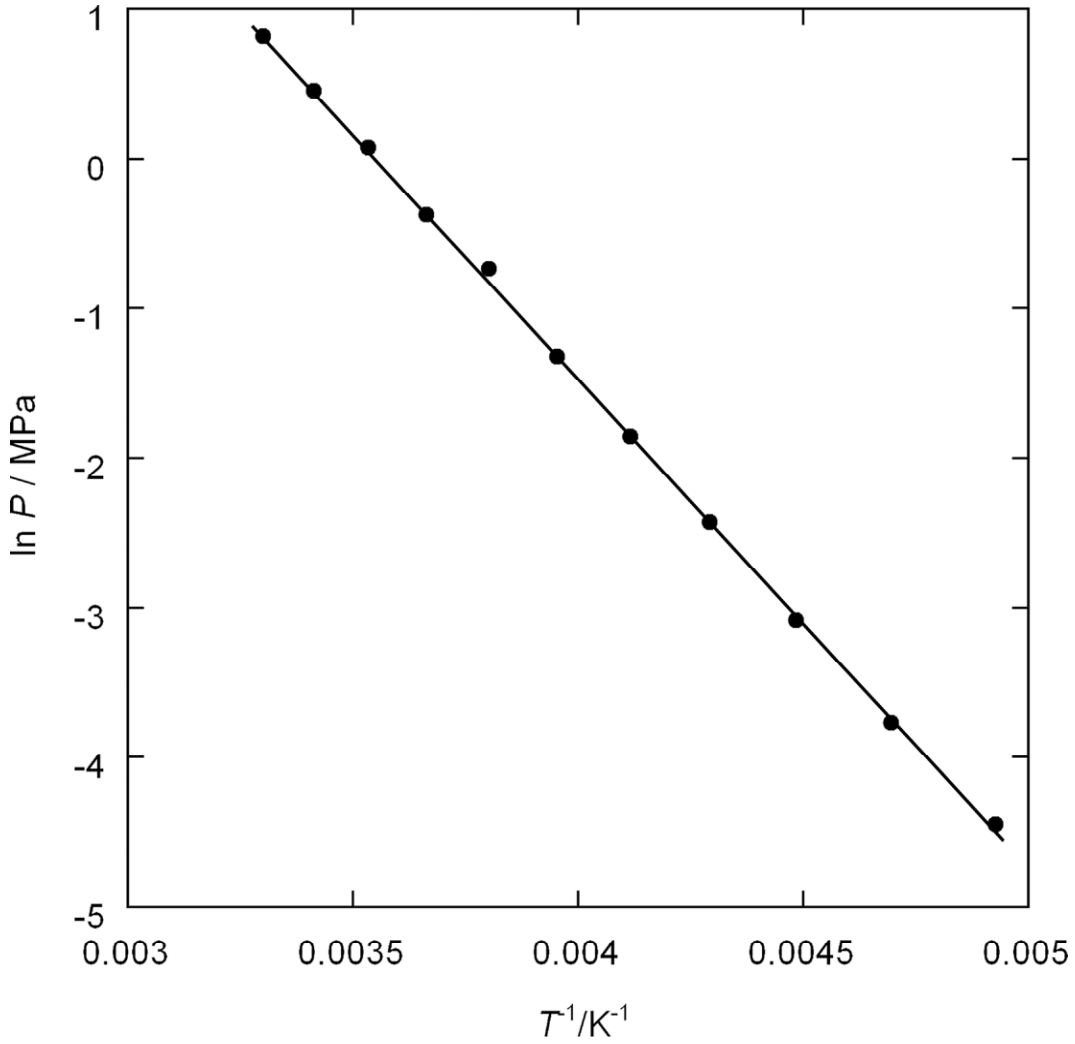

Figure S1. Plot of ln$P$ versus 1/T. Since the gradient was -3.27x10^{-3} MPa K, the isosteric adsorption enthalpy (ΔH_{iso}) was calculated as 27.2 kJ mol^{-1}.

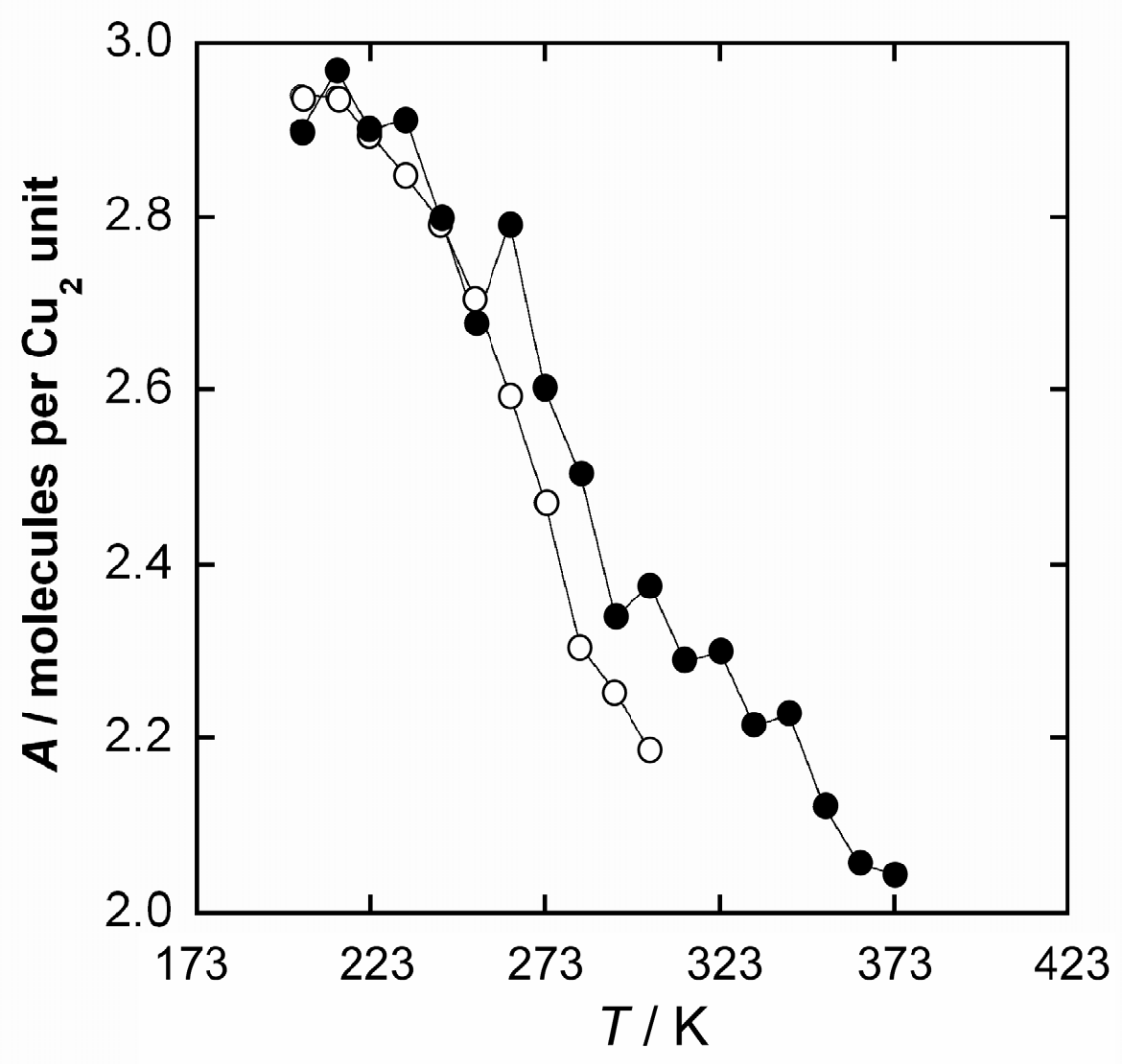

Figure S2. Plot of maximum adsorption amount of CO_2 in **1** in adsorption measurement (open circle: adsorption amount at relative pressure of 0.9, 0.7 for 303 K) and from X-ray crystal structural analyses of CO_2 included crystal (closed circle: included amount of CO_2 in **1**) at various temperatures from 203 to 373 K.

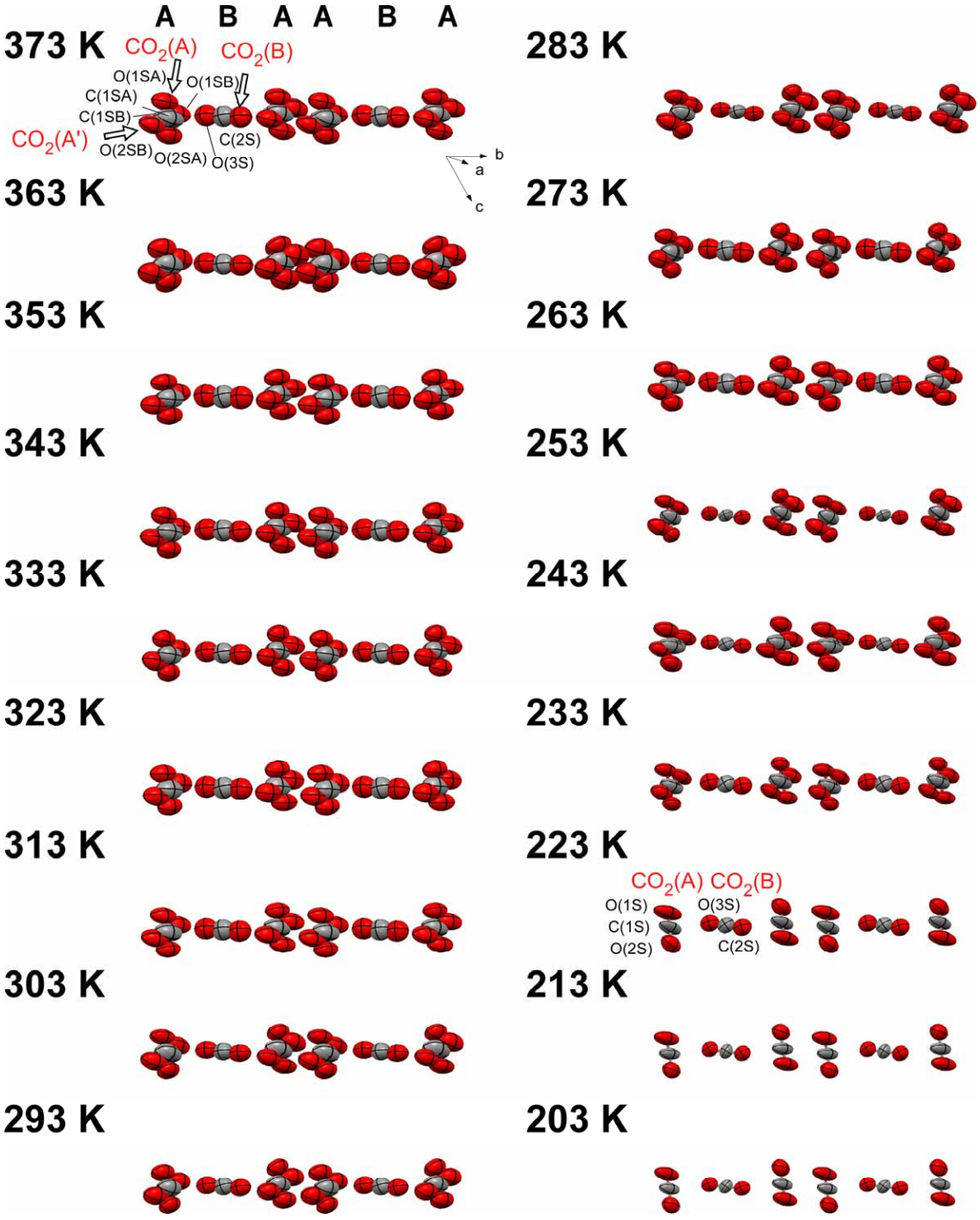

Figure S3. Thermal ellipsoid diagrams of the guest configurations for **1** (50% probability) at various temperatures (from 373 K to 203 K). Bold A and B represent A site and B site of CO_2 molecules in the channel of **1**, respectively. The names of the atoms and CO_2 molecules were the same as that shown in the data of 373 K (from 373 K to 233 K) and that shown in the data of 223 K (from 223 K to 203 K).

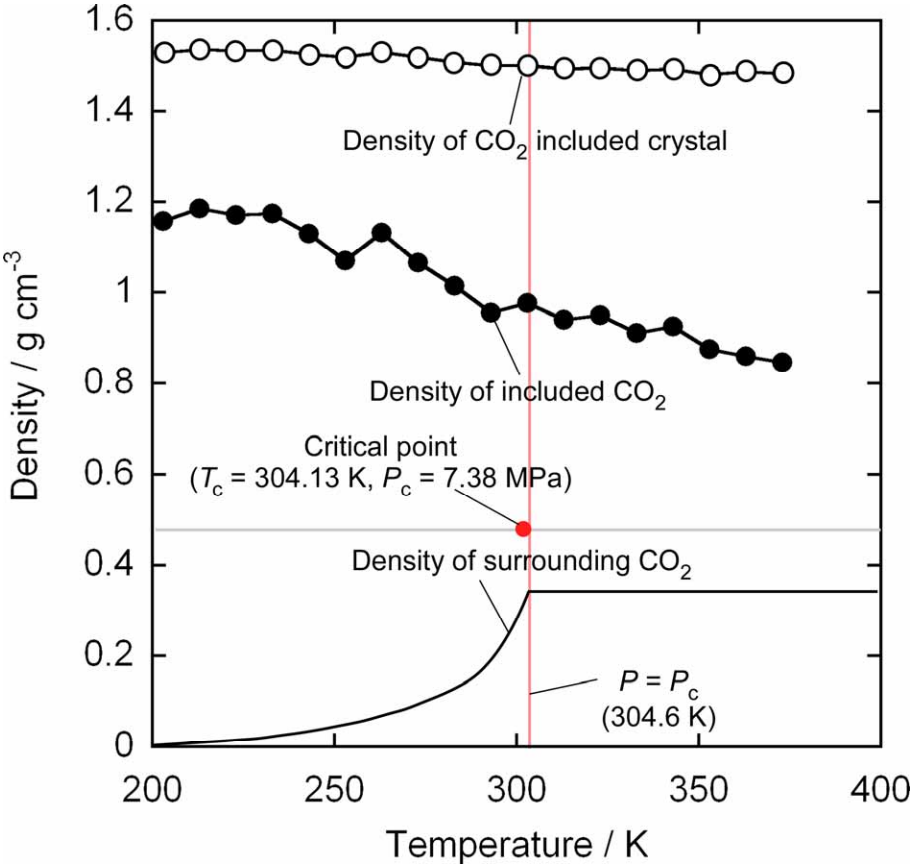

Figure S4. Temperature dependence of the density of CO_2 included crystal (empty circle), included CO_2 in the channel of **1** (solid circle), and surrounding CO_2 (black line). The density of included CO_2 molecules in the channel was calculated as density in void space. The density of supercritical CO_2 fluid at its critical point (red circle) and temperature at which the pressure of surrounding CO_2 reaches over the critical pressure (P_c) are shown as gray line and red line, respectively.

<Crystal structure of CO_2 inclusion of 1>

Table S1. Crystallographic data for single-crystal **1** under the saturated pressure of CO_2 gas at various temperatures (from 203 K to 373 K)

Complex	**1**•2.90 (CO_2)	**1**•2.97 (CO_2)	**1**•2.90 (CO_2)	**1**•2.91 (CO_2)
Empirical formula	$C_{34.89}H_{24}Cu_2N_2O_{13.79}$	$C_{34.97}H_{24}Cu_2N_2O_{13.94}$	$C_{34.90}H_{24}Cu_2N_2O_{13.80}$	$C_{34.91}H_{24}Cu_2N_2O_{13.82}$
Crystal size / mm^3	0.30 × 0.30 × 0.05	0.30 × 0.30 × 0.05	0.30 × 0.30 × 0.05	0.30 × 0.30 × 0.05
M / g mol^{-1}	819.00	822.26	819.26	819.78
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1	*P*-1
T / K	203	213	223	233
a / Å	9.694(2)	9.693(2)	9.687(2)	9.6898(19)
b / Å	10.424(3)	10.424(2)	10.420(2)	10.420(2)
c / Å	10.971(3)	10.967(2)	10.945(2)	10.939(2)
α / °	70.894(5)	70.883(4)	71.008(4)	71.090(4)
β / °	66.197(4)	66.181(4)	66.135(4)	66.112(4)
γ / °	63.016(5)	63.010(4)	63.024(4)	63.052(4)
V / $Å^3$	889.6(4)	889.1(3)	886.5(3)	886.8(3)
Z	1	1	1	1
D_{calcd} / g cm^{-3}	1.529	1.536	1.534	1.535
μ(Mo-Kα) / mm^{-1}	1.266	1.267	1.270	1.270
Reflections collected	6472	6496	5627	5624
Independent reflections (Rint)	4348 (0.0429)	4349 (0.0436)	3612 (0.0383)	3610 (0.0409)
Goodness of fit	0.997	0.976	0.999	1.015
$R1$ (I>2σ (all data))	0.0727 (0.1362)	0.0643 (0.1205)	0.0629 (0.1105)	0.0625 (0.1132)
w$R2$ (I>2σ (all data))	0.1726 (0.2127)	0.1523 (0.1908)	0.1522 (0.1859)	0.1473 (0.1847)
Least diff. peak (hole) /e $Å^{-3}$	0.971 (-1.133)	0.883 (-0.956)	1.035 (-0.761)	0.904 (-0.810)

Complex	**1**•2.80 (CO_2)	**1**•2.68 (CO_2)	**1**•2.79 (CO_2)	**1**•2.61 (CO_2)
Empirical formula	$C_{34.80}H_{24}Cu_2N_2O_{13.59}$	$C_{34.68}H_{24}Cu_2N_2O_{13.36}$	$C_{34.79}H_{24}Cu_2N_2O_{13.58}$	$C_{34.61}H_{24}Cu_2N_2O_{13.22}$
Crystal size / mm^3	0.30 × 0.30 × 0.05	0.35 × 0.30 × 0.04	0.30 × 0.30 × 0.05	0.30 × 0.30 × 0.05
M / g mol^{-1}	814.68	809.58	814.34	806.58
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1	*P*-1
T / K	243	253	263	273
a / Å	9.691(2)	9.6831(14)	9.689(2)	9.6874(19)
b / Å	10.420(2)	10.4150(15)	10.408(2)	10.4009(19)
c / Å	10.932(2)	10.9296(16)	10.911(2)	10.899(2)
α / °	70.150(4)	71.211(3)	71.321(4)	71.390(4)
β / °	66.075(4)	66.074(3)	65.986(4)	65.922(4)
γ / °	63.057(4)	63.040(3)	63.085(4)	63.111(4)
V / $Å^3$	886.3(3)	885.0(2)	883.5(3)	881.9(3)
Z	1	1	1	1
D_{calcd} / g cm^{-3}	1.526	1.519	1.530	1.519
μ(Mo-Kα) / mm^{-1}	1.270	1.271	1.274	1.275
Reflections collected	5625	5944	5406	5634
Independent reflections (Rint)	3606 (0.0441)	3743 (0.0258)	3568 (0.0380)	3585 (0.0385)
Goodness of fit	1.007	1.020	0.978	1.018
$R1$ (I>2σ (all data))	0.0651 (0.1181)	0.0426 (0.0625)	0.0698 (0.1246)	0.0659 (0.1185)
w$R2$ (I>2σ (all data))	0.1591 (0.1908)	0.1096 (0.1241)	0.1699 (0.2076)	0.1558 (0.1922)
Least diff. peak (hole) /e $Å^{-3}$	0.956 (-0.762)	0.651 (-0.820)	0.852 (-0.780)	0.953 (-0.776)

Complex	**1**•2.50 (CO_2)	**1**•2.34 (CO_2)	**1**•2.38 (CO_2)	**1**•2.29 (CO_2)
Empirical formula	$C_{34.50}H_{24}Cu_2N_2O_{13.01}$	$C_{34.34}H_{24}Cu_2N_2O_{12.68}$	$C_{34.38}H_{24}Cu_2N_2O_{12.75}$	$C_{34.29}H_{24}Cu_2N_2O_{12.58}$
Crystal size / mm^3	0.35 × 0.30 × 0.04	0.30 × 0.30 × 0.05	0.35 × 0.30 × 0.04	0.30 × 0.30 × 0.05
M / g mol^{-1}	801.84	794.96	796.24	792.94
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1	*P*-1
T / K	283	293	303	313
a / Å	9.6862(17)	9.6878(18)	9.690(3)	9.701(2)
b / Å	10.4076(18)	10.3938(18)	10.403(3)	10.400(2)
c / Å	10.9028(19)	10.884(2)	10.889(3)	10.890(2)
α / °	71.465(4)	71.478(4)	71.578(6)	71.566(4)
β / °	65.916(3)	65.848(4)	65.775(5)	65.771(4)
γ / °	63.096(4)	63.144(4)	63.088(5)	63.127(4)
V / $Å^3$	882.8(3)	880.2(3)	881.1(4)	882.1(3)
Z	1	1	1	1
D_{calcd} / g cm^{-3}	1.508	1.500	1.501	1.493
μ(Mo-Kα) / mm^{-1}	1.273	1.275	1.274	1.272
Reflections collected	5933	5686	5902	5631
Independent reflections (Rint)	3734 (0.0252)	3577 (0.0416)	3728 (0.0253)	3584 (0.0368)
Goodness of fit	0.973	1.001	0.975	0.997
$R1$ (I>2σ (all data))	0.0411 (0.0638)	0.0688 (0.1177)	0.0436 (0.0674)	0.0647 (0.1231)
w$R2$ (I>2σ (all data))	0.0997 (0.1174)	0.1630 (0.1871)	0.1101 (0.1272)	0.1512 (0.1835)
Least diff. peak (hole) /e $Å^{-3}$	0.785 (-0.527)	0.915 (-0.501)	0.751 (-0.528)	0.742 (-0.524)

Complex	**1**•2.30 (CO_2)	**1**•2.22 (CO_2)	**1**•2.23 (CO_2)	**1**•2.12 (CO_2)
Empirical formula	$C_{34.30}H_{24}Cu_2N_2O_{12.61}$	$C_{34.22}H_{24}Cu_2N_2O_{12.43}$	$C_{34.23}H_{24}Cu_2N_2O_{12.45}$	$C_{34.12}H_{24}Cu_2N_2O_{12.24}$
Crystal size / mm^3	0.30 × 0.30 × 0.05	0.30 × 0.30 × 0.05	0.30 × 0.30 × 0.05	0.30 × 0.30 × 0.05
M / g mol^{-1}	793.04	788.98	789.52	784.84
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1	*P*-1
T / K	323	333	343	353
a / Å	9.697(2)	9.6955(18)	9.694(2)	9.703(2)
b / Å	10.392(2)	10.3885(19)	10.383(2)	10.389(2)
c / Å	10.879(2)	10.873(2)	10.866(2)	10.871(3)
α / °	71.587(4)	71.614(4)	71.642(5)	71.664(5)
β / °	65.735(4)	65.704(4)	65.662(4)	65.611(4)
γ / °	63.130(4)	63.135(4)	63.139(4)	63.120(5)
V / $Å^3$	880.1(3)	879.0(3)	877.8(3)	879.1(4)
Z	1	1	1	1
D_{calcd} / g cm^{-3}	1.496	1.490	1.493	1.482
μ(Mo-Kα) / mm^{-1}	1.275	1.275	1.277	1.275
Reflections collected	5814	5825	5799	5782
Independent reflections (Rint)	3729 (0.0402)	3724 (0.0387)	3716 (0.0412)	3720 (0.0397)
Goodness of fit	1.040	0.998	1.005	1.002
$R1$ (I>2σ (all data))	0.0701 (0.1307)	0.0657 (0.1261)	0.0690(0.1312)	0.0683 (0.1365)
w$R2$ (I>2 σ (all data))	0.1635 (0.1990)	0.1562 (0.1923)	0.1573(0.1920)	0.1554 (0.1919)
Least diff. peak (hole) /e $Å^{-3}$	0.783 (-0.552)	0.703 (-0.545)	0.678(-0.454)	0.731 (-0.623)

Complex	**1**•2.06 (CO_2)	**1**•2.04 (CO_2)
Empirical formula	$C_{34.06}H_{24}Cu_2N_2O_{12.11}$	$C_{34.04}H_{24}Cu_2N_2O_{12.09}$
Crystal size / mm^3	0.35 × 0.30 × 0.04	0.30 × 0.30 × 0.05
M / g mol^{-1}	782.16	781.94
Crystal system	Triclinic	Triclinic
Space group	*P*-1	*P*-1
T / K	363	373
a / Å	9.6913(19)	9.691(2)
b / Å	10.366(2)	10.373(2)
c / Å	10.835(2)	10.850(3)
α / °	71.867(4)	71.718(5)
β / °	65.426(4)	65.541(4)
γ / °	63.151(4)	63.159(5)
V / $Å^3$	872.9(3)	875.0(3)
Z	1	1
D_{calcd} / g cm^{-3}	1.488	1.484
μ(Mo-Kα) / mm^{-1}	1.283	1.280
Reflections collected	5858	5788
Independent reflections (Rint)	3685 (0.0277)	3697 (0.0616)
Goodness of fit	0.986	0.885
$R1$ (I>2σ (all data))	0.0464 (0.0797)	0.0732 (0.1660)
w$R2$ (I>2σ (all data))	0.1173 (0.1368)	0.1680 (0.2012)
Least diff. peak (hole) /e $Å^{-3}$	0.552(-0.537)	0.865 (-0.939)

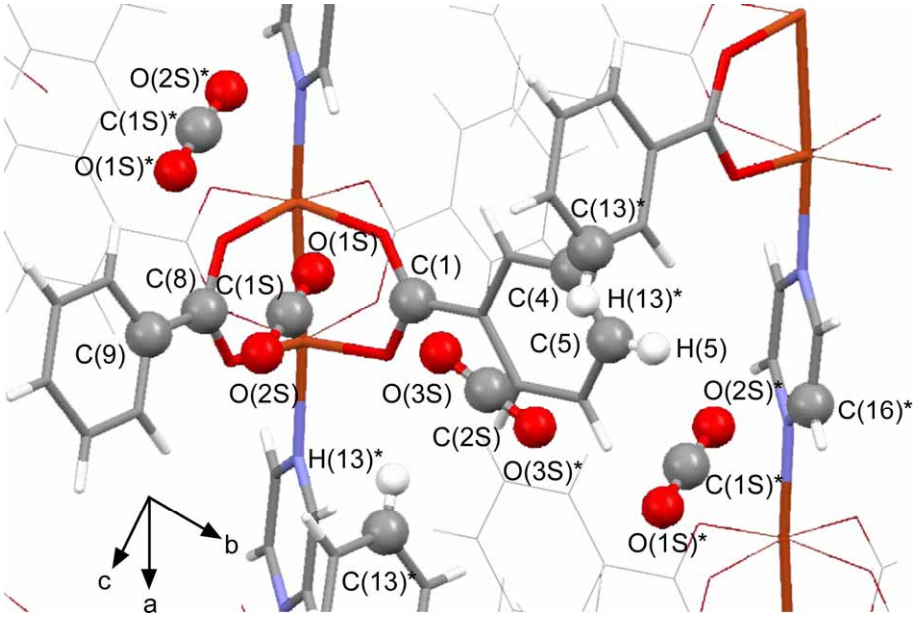

Figure S5. Crystal structure of **1**·n(CO_2) (2.9 < n <3) at 203 - 223 K showing the short contact between guest (CO_2) and host. Atoms that contact the guest or host are represented in a ball and stick model. Distances are listed in Tables S2 and S3.

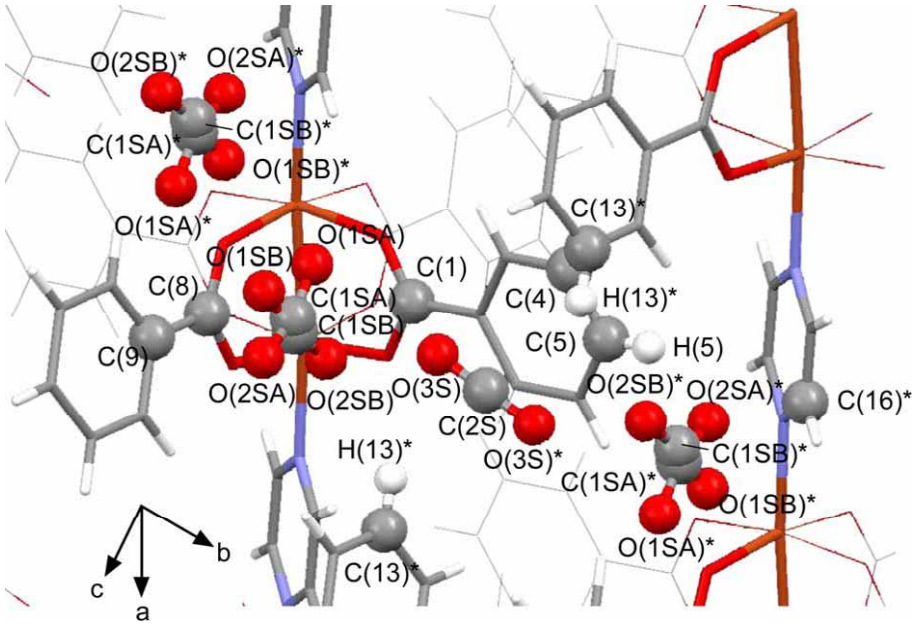

Figure S6. Crystal structure of **1**·n(CO_2) (2 < n < 3) at 233 - 373 K showing the short contact between guest (CO_2) and host. Atoms that contact the guest or host are represented in a ball and stick model. Distances are listed in Tables S2 and S4.

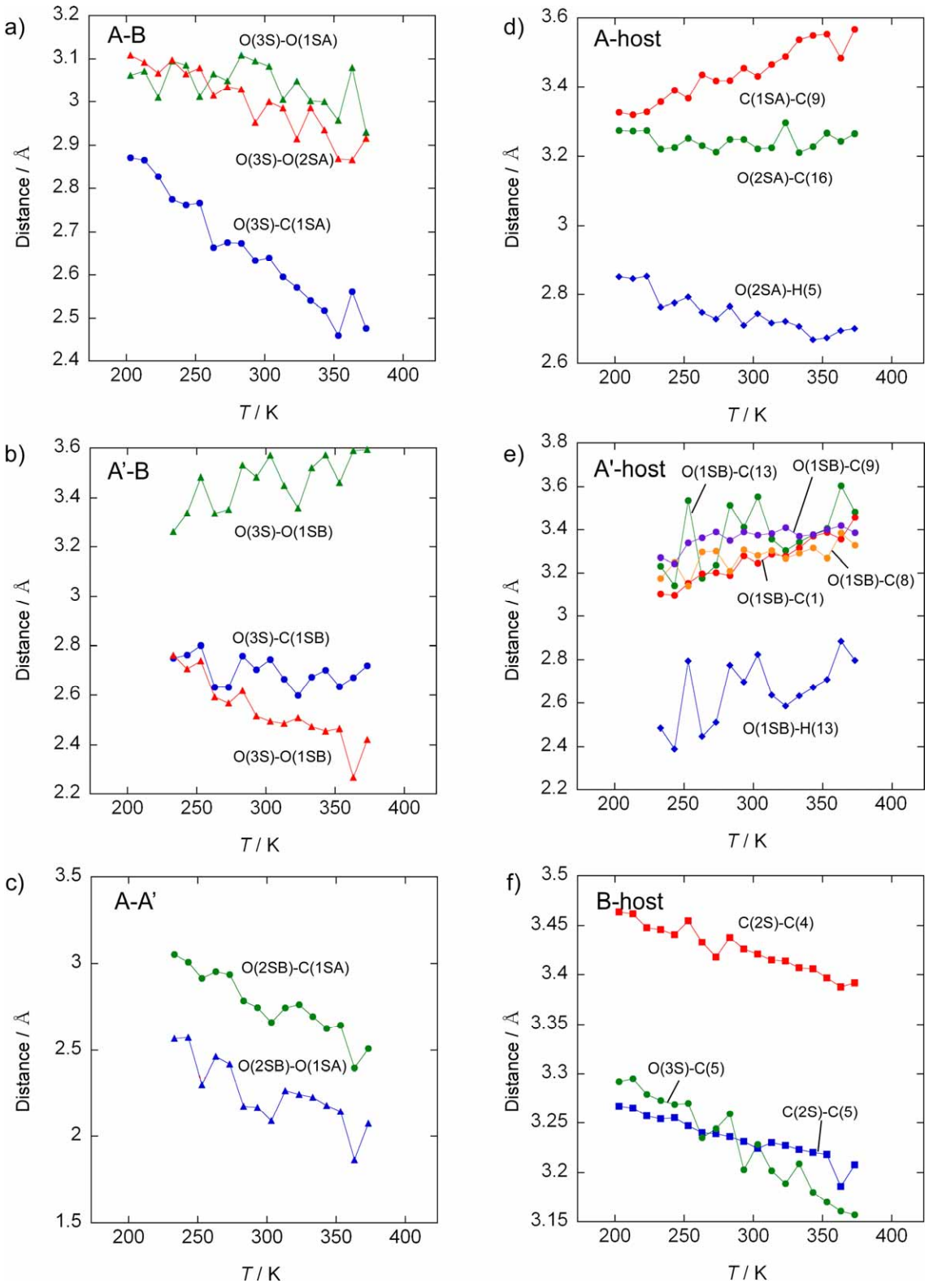

Figure S7. Distances of guest-guest (a-c) and host-guest (d-f) interaction in short distances in CO_2 included crystal of **1**. Data is shown for CO_2(A)-CO_2(B) (a), CO_2(A')-CO_2(B) (b), CO_2(A)-CO_2(A') (c), CO_2(A)-host (d), CO_2(A')-host (e), and CO_2(B)-host (f).

Table S2. Guest-guest interaction in short distances in CO_2 included crystal of **1**

	203 K		213 K		223 K	
CO_2 (A)-CO_2 (B)	C (1S) … O (3S) O (1S) … O (3S) O (2S) … O (3S)	2.87 (2) 3.06 (2) 3.11 (1)	C (1S) … O (3S) O (1S) … O (3S) O (2S) … O (3S)	2.87 (2) 3.07 (2) 3.09 (1)	C (1S) … O (3S) O (1S) … O (3S) O (1S) … O (3S)	2.83 (2) 3.01 (2) 3.07 (2)
	233 K		243 K		253 K	
CO_2 (A)-CO_2 (B)	C(1SA) … O(3S)	2.78(6)	C(1SA) … O(3S)	2.75(6)	C(1SA) … O(3S)	2.76(4)
	O(1SA) … O(3S)	3.10(2)	O(1SA) …O(3S)	3.08(3)	O(1SA) … O(3S)	3.11(2)
	O(2SA) … O(3S)	3.07(2)	O(2SA) … O(3S)	3.06(2)	O(2SA) … O(3S)	3.08(1)
CO_2(A)-CO_2 (A')	C(1SA) … O(2SB)$^{\#1}$	3.05(10)	C(1SA) … O(2SB)$^{\#1}$	3.01(11)	C(1SA)…O(2SB)$^{\#1}$	2.93(6)
	O(1SA) … O(2SB)$^{\#1}$	2.57(7)	O(1SA) … O(2SB)$^{\#1}$	2.57(8)	O(1SA)…O(2SB)$^{\#1}$	2.30(4)
CO_2(A')-CO_2 (B)	C(1SB) … O(3S)	2.75(16)	C(1SB) … O(3S)	2.76(14)	C(1SB) … O(3S)	2.80(8)
	O(1SB) … O(3S)	2.76(4)	O(1SB) … O(3S)	2.71(4)	O(1SB) … O(3S)	2.73(2)
	263 K		273 K		283 K	
CO_2(A)-CO_2 (B)	C(1SA) … O(3S)	2.66(5)	C(1SA) … O(3S)	2.68(5)	C(1SA) … O(3S)	2.67(4)
	O(1SA) … O(3S)	3.06(4)	O(1SA) … O(3S)	3.05(3)	O(1SA) … O(3S)	3.10(4)
	O(2SA) … O(3S)	3.01(3)	O(2SA) … O(3S)	3.03(2)	O(2SA) … O(3S)	3.03(9)
CO_2(A)-CO_2 (A')	C(1SA) … O(2SB)$^{\#1}$	2.95(11)	C(1SA) … O(2SB)$^{\#1}$	2.94(11)	C(1SA)…O(2SB)$^{\#1}$	2.79(7)
	O(1SA) … O(2SB)$^{\#1}$	2.46(9)	O(1SA) … O(2SB)$^{\#1}$	2.42(8)	O(1SA)…O(2SB)$^{\#1}$	2.17(5)
CO_2(A')-CO_2 (B)	C(1SB) … O(3S)	2.63(9)	C(1SB) … O(3S)	2.63(10)	C(1SB) … O(3S)	2.76(7)
	O(1SB) … O(3S)	2.59(4)	O(1SB) … O(3S)	2.57(4)	O(1SB) … O(3S)	2.62(3)
	293 K		303 K		313 K	
CO_2(A)-CO_2 (B)	C(1SA) … O(3S)	2.63(5)	C(1SA) … O(3S)	2.64(4)	C(1SA) … O(3S)	2.60(5)
	O(1SA) … O(3S)	3.10(3)	O(1SA) … O(3S)	3.08(3)	O(1SA) … O(3S)	3.01(4)
	O(2SA) … O(3S)	2.95(3)	O(2SA) … O(3S)	3.00(2)	O(2SA) … O(3S)	2.98(3)
CO_2(A)-CO_2 (A')	C(1SA) … O(2SB)$^{\#1}$	2.75(11)	C(1SA) … O(2SB)$^{\#1}$	2.66(8)	C(1SA)…O(2SB)$^{\#1}$	2.75(11)
	O(1SA) … O(2SB)$^{\#1}$	2.17(8)	O(1SA) … O(2SB)$^{\#1}$	2.09(5)	O(1SA)…O(2SB)$^{\#1}$	2.27(8)
CO_2(A')-CO_2 (B)	C(1SB) … O(3S)	2.70(8)	C(1SB) … O(3S)	2.75(7)	C(1SB) … O(3S)	2.67(9)
	O(1SB) … O(3S)	2.52(5)	O(1SB) … O(3S)	2.49 (3)	O(1SB) … O(3S)	2.49(5)
	323 K		333 K		343 K	
CO_2(A)-CO_2 (B)	C(1SA) … O(3S)	2.57(6)	C(1SA) … O(3S)	2.54(5)	C(1SA) … O(3S)	2.52(5)
	O(1SA) … O(3S)	3.05(4)	O(1SA) … O(3S)	3.00(4)	O(1SA) … O(3S)	3.00(4)
	O(2SA) … O(3S)	2.91(3)	O(2SA) … O(3S)	2.99(3)	O(2SA) … O(3S)	2.94(3)
CO_2(A)-CO_2 (A')	C(1SA) … O(2SB)$^{\#1}$	2.77(13)	C(1SA) … O(2SB)$^{\#1}$	2.70(11)	C(1SA)…O(2SB)$^{\#1}$	2.63(11)
	O(1SA) … O(2SB)$^{\#1}$	2.24(9)	O(1SA) … O(2SB)$^{\#1}$	2.23(7)	O(1SA)…O(2SB)$^{\#1}$	2.18(7)
CO_2(A')-CO_2 (B)	C(1SB) … O(3S)	2.60(8)	C(1SB) … O(3S)	2.67(8)	C(1SB) … O(3S)	2.70(7)
	O(1SB) … O(3S)	2.51(5)	O(1SB) … O(3S)	2.47(5)	O(2SB) … O(3S)	2.46(5)
	353 K		363 K		373 K	
CO_2(A)-CO_2 (B)	C(1SA) … O(3S)	2.46(5)	C(1SA) … O(3S)	2.56(8)	C(1SA) … O(3S)	2.48(6)
	O(1SA) … O(3S)	2.96(5)	O(1SA) … O(3S)	3.08(5)	O(1SA) … O(3S)	2.93(5)
	O(2SA) … O(3S)	2.87(4)	O(2SA) … O(3S)	2.87(4)	O(2SA) … O(3S)	2.92(5)
CO_2(A)-CO_2 (A')	C(1SA) … O(2SB)$^{\#1}$	2.64(12)	C(1SA) … O(2SB)$^{\#1}$	2.40(12)	C(1SA)…O(2SB)$^{\#1}$	2.51(12)
	O(1SA) … O(2SB)$^{\#1}$	2.14(9)	O(1SA) … O(2SB)$^{\#1}$	1.87(7)	O(1SA)…O(2SB)$^{\#1}$	2.07(8)
			O(2SA) …O(2SB)	3.00(8)		
CO_2(A')-CO_2 (B)	C(1SB) … O(3S)	2.63(8)	C(1SB) … O(3S)	2.67(8)	C(1SB) … O(3S)	2.72(8)
	O(1SB) … O(3S)	2.46(5)	O(1SB) … O(3S)	2.27(5)	O(1SB) … O(3S)	2.42(6)

Symmetry code: #1 (1-x, 1-y, 2-z)
The distance between CO_2 (A') and CO_2 (A')#1 was omitted from this table since such a combination cannot exist.

Table S3. Host-guest interaction in short distances in the CO_2 included crystals of **1** in the temperature region of 203 to 223 K.

	203 K		213 K		223K	
CO_2(A)-host	C(1S)…C(9)#1	3.33(2)	C(1S)…C(9)#1	3.32(1)	C(1S)…C(9)#1	3.33(2)
CO_2(B)-host	C(2S)…C(5)	3.27(1)	C(2S)…C(5)	3.26(1)	C(2S)…C(4)	3.26(1)

Symmetry code: #1 (2-x, 1-y, 1-z)

Table S4. Guest-guest interaction in short distances in the CO_2 included crystals of **1** in the temperature region of 233 to 373 K.

	233 K		243 K		253 K	
CO_2(A)-host	C(1SA)…C(9)#1	3.36(4)	C(1SA)…C(9)#1	3.39(4)	C(1SA)…C(9)#1	3.37(3)
CO_2(A')-host	C(1SB)…C(9)#1 O(1SB)…O(1) O(1SB)…C(8) #1 O(1SB)…H(13) #2	3.27(13) 3.10(4) 3.18(4) 2.48(6)	C(1SB)…C(9)#1 O(1SB)…C(1) O(1SB)…C(13) #2 O(1SB)…H(13) #2	3.24(11) 3.10(4) 3.14(7) 2.39(7)	C(1SB)…C(9)#1 O(1SB)…C(1) O(1SB)…C(8) #1	3.34(6) 3.14(2) 3.15(3)
CO_2(B)-host	C(2S) …C(5)	3.25(1)	C(2S) …C(5)	3.25(4)	C(2S) …C(5)	3.25(1)
	263 K		273 K		283 K	
CO_2(A)-host			O(2SA) …C(16)#5	3.21(2)		
CO_2(A')-host	C(1SB)…C(9)#1 O(1SB)…C(1) O(1SB)…C(13) #2 O(1SB)…H(13) #2	3.36(7) 3.20(4) 3.18(8) 2.45(7)	C(1SB)…C(9)#1 O(1SB)…C(1) O(1SB)…C(13) #2	3.36(7) 3.20(4) 3.24(8)	C(1SB)…C(9)#1 O(1SB)…C(1) O(1SB)…C(8) #1	3.35(5) 3.19(3) 3.21(3)
CO_2(B)-host	C(2S) …C(5)	3.24(1)	C(2S) …C(5)	3.24(1)	C(2S) …C(5)	3.24(1)

Symmetry codes: #1 (2-x, 1-y, 1-z), #2 (x, y, 1+z)

Table S4. (continued) Guest-guest interaction in short distances in the CO_2 included crystals of **1** in the temperature region of 233 to 373 K.

	293 K		303 K		313 K	
CO_2(A)-host	O(2SA) …H(5)#3	2.71(3)			O(2SA) …H(5)#3	2.72(3)
CO_2(A')-host	C(1SB)…C(9)#1 O(1SB)…H(13) #2	3.39(6) 2.70(7)	C(1SB)…C(9)#1	3.38(5)	C(1SB)…C(9)#1 O(1SB)…H(13) #2	3.38(7) 2.64(7)
CO_2(B)-host	C(2S) …C(5) O(3S) …C(5)#3	3.23(1) 3.20(2)	C(2S) …C(5)	3.22(1)	C(2S) …C(5) O(3S) …C(5)#3	3.23(1) 3.20(3)
	323 K		333 K		343 K	
CO_2(A)-host			O(2SA) …C(16)#4 O(2SA) …H(5)#3	3.21(2) 2.71(3)	O(2SA) …H(5)#3	2.71(3)
CO_2(A')-host	O(1SB)…H(13) #2	2.59(7)	C(1SB)…C(9)#1 O(1SB)…H(13) #2	3.37(6) 2.63(7)	C(1SB)…C(9)#1 O(1SB)…H(13) #2	3.38(5) 2.67(7)
CO_2(B)-host	C(2S) …C(5) O(3S) …C(5)#3	3.23(1) 3.19(2)	C(2S) …C(5) O(3S) …C(5)#3	3.22(1) 3.21(2)	C(2S) …C(5) O(3S) …C(5)#3	3.22(1) 3.18(2)
	353 K		363 K		373 K	
CO_2(A)-host	O(2SA) …H(5)#3	2.68(4)	O(2SA) …H(5)#3	2.70(4)	O(2SA) …H(5)#3	2.70(4)
CO_2(A')-host	C(1SB)…C(9)#1 O(1SB)…H(13) #2	3.40(6) 2.71(7)			C(1SB)…C(9)#1	3.39(5)
CO_2(B)-host	C(2S) …C(4) C(2S) …C(5) O(3S) …C(5)#3	3.39(1) 3.22(1) 3.18(2)	C(2S) …C(4) C(2S) …C(5) O(3S) …C(5)#5	3.39(1) 3.19(1) 3.16(2)	C(2S) …C(4) C(2S) …C(5) O(3S) …C(5)#3	3.39(1) 3.21(1) 3.16(2)

Symmetry codes: #1 (2-x, 1-y, 1-z), #2 (x, y, 1+z), #3 (1-x, 2-y, 2-z), #4 (1-x, 1-y, 2-z)

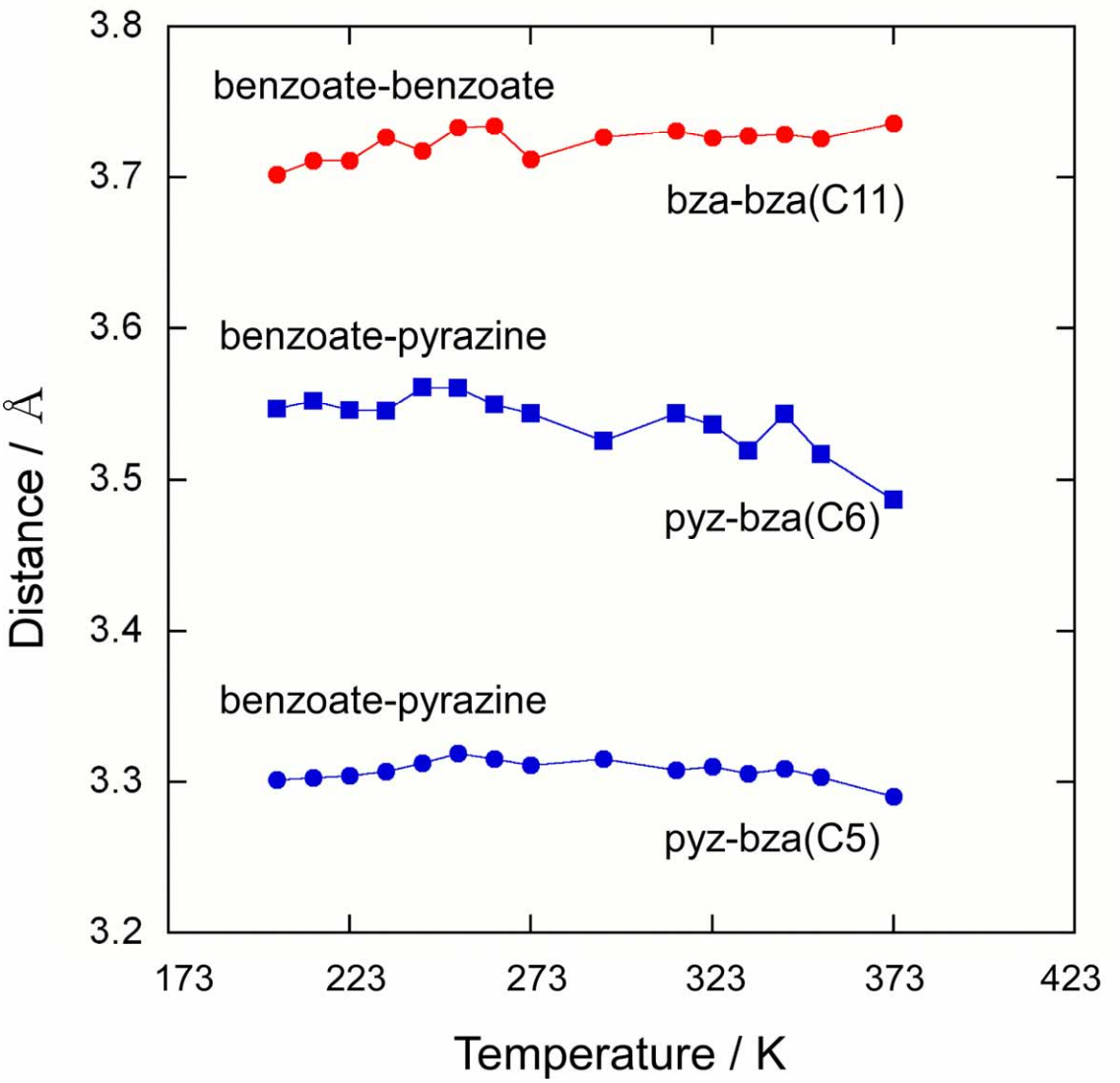

Figure S8. Distances of π-π interaction between aromatic rings in CO_2 included crystal of **1** at various temperatures. Distances were calculated as distance between aromatic plane and signed atom (C5, C6, or C11) in the other aromatic ring. For atom number, please refer to Figure 3c, d in the manuscript.

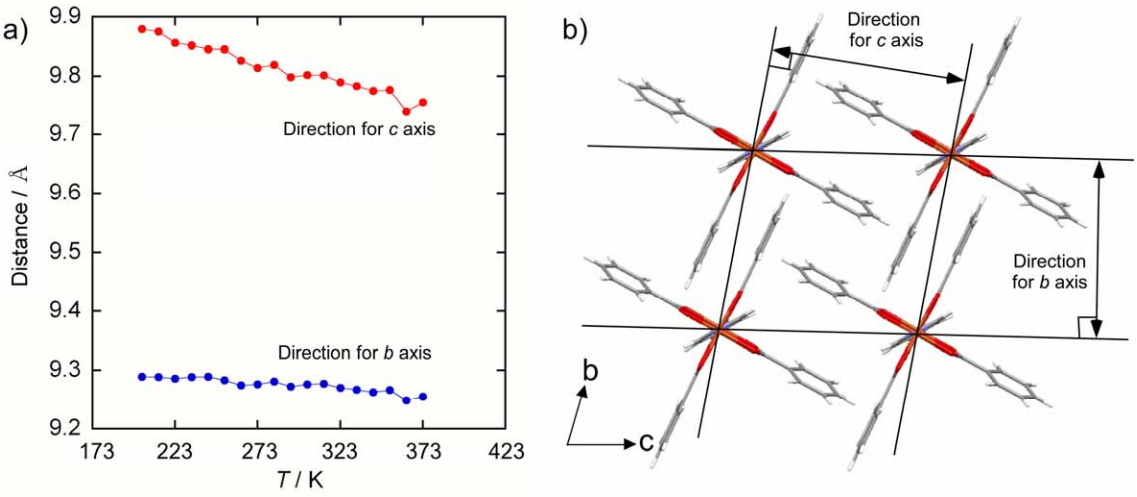

Figure S9. Temperature dependence of the distance between 1D complex layers for the *b* axis direction and *c* axis direction (a) and crystal structure showing the definition of distance between 1D complex layers for each axis direction.