Electronic Supplementary Information for

Polymorphism and the influence of crystal structure on the luminescence of the opto-electronic material 4,4'-bis(9-carbazolyl)biphenyl

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Full reference for reference 31: Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Packing diagrams for the three **CBP** polymorphs:

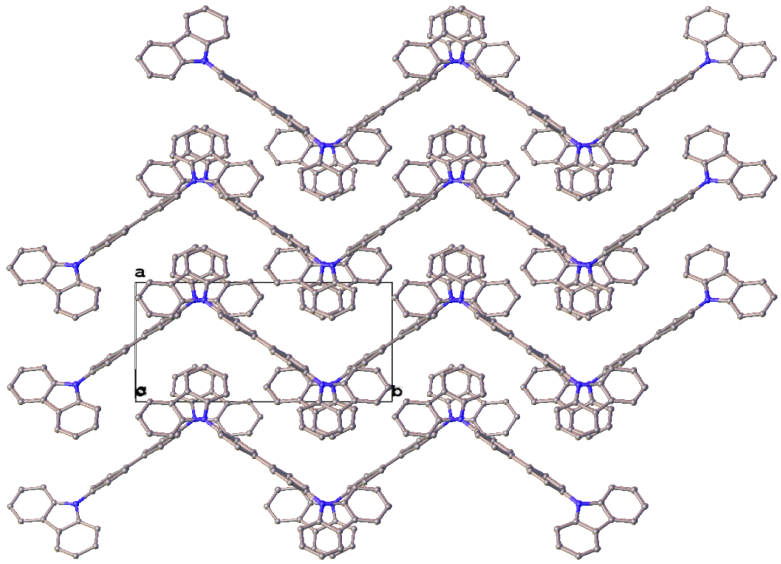

Figure S1. Packing diagram of ***α*-CBP** viewed down the *c*-axis.

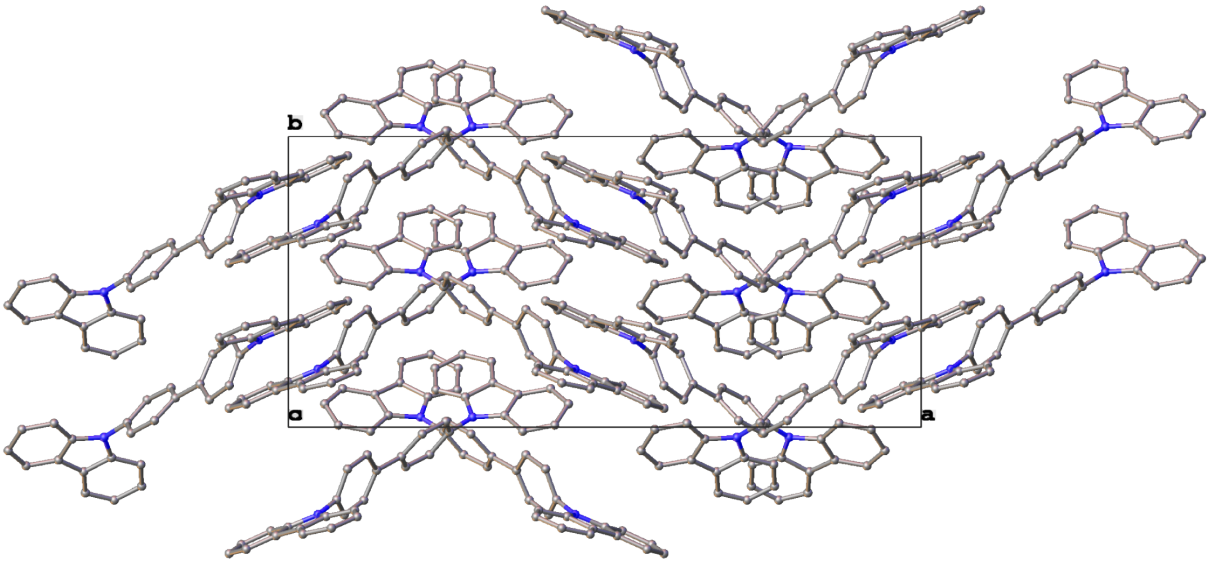

Figure S2. Packing diagram of ***β*-CBP** viewed down the *c*-axis.

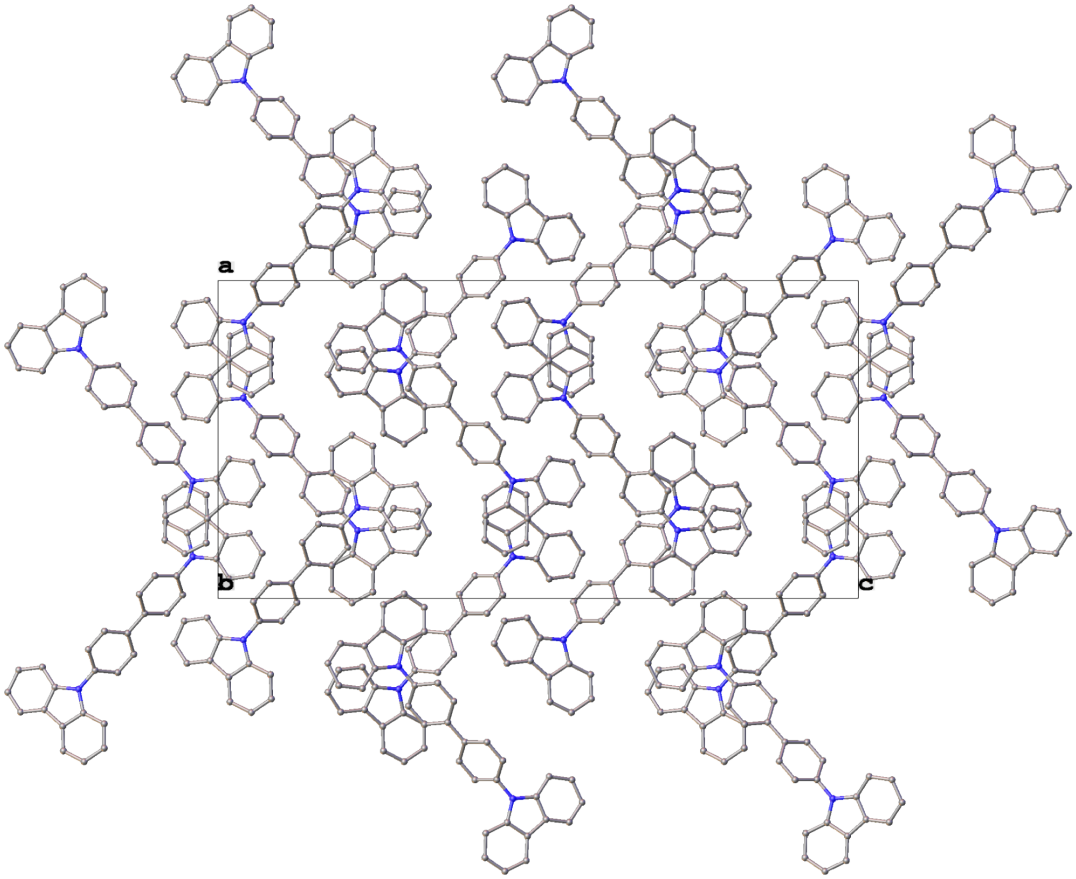

Figure S3. Packing diagram of ***γ*-CBP** viewed down the *b*-axis.

Crystallographic Tables for the three CBP polymorphs:

Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **α-CBP**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N1	1455.3(14)	7308.6(6)	2067.2(11)	13.5(2)
C1	1555.3(17)	8156.0(7)	2412.6(13)	13.9(3)
C2	2826.3(18)	8577.9(8)	3495.8(13)	16.1(3)
C3	2638.8(19)	9436.7(8)	3555.1(14)	19.1(3)
C4	1246.2(19)	9868.5(8)	2562.9(14)	20.7(3)
C5	10.0(19)	9443.9(8)	1483.7(14)	19.4(3)
C6	156.0(18)	8580.5(8)	1397.5(13)	15.3(3)
C7	-832.4(18)	7966.8(8)	392.0(13)	15.7(3)
C8	-2282.5(19)	8017.4(9)	-849.7(14)	21.6(3)
C9	-2879(2)	7303.4(9)	-1619.3(15)	24.3(3)
C10	-2055.5(19)	6533.5(9)	-1155.0(15)	22.0(3)
C11	-618.9(18)	6462.1(8)	72.5(13)	17.7(3)
C12	0.7(17)	7190.8(8)	835.6(13)	14.9(3)
C13	2513.1(17)	6665.7(7)	2911.4(12)	13.2(3)
C14	3279.0(17)	6055.1(7)	2324.3(13)	14.7(3)
C15	2776.6(17)	6632.4(8)	4329.2(13)	15.0(3)
C16	4244.0(17)	5409.8(7)	3140.6(12)	13.1(3)
C17	3755.6(17)	5988.2(8)	5138.9(13)	14.6(3)
C18	4496.6(16)	5352.2(7)	4567.4(12)	11.7(3)

Table S2. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **α-CBP**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	16.4(6)	11.2(5)	11.1(5)	1.0(4)	2.6(4)	1.1(4)
C1	18.7(7)	11.9(6)	13.5(6)	2.2(4)	8.7(5)	2.4(5)
C2	21.4(7)	14.4(6)	13.4(6)	1.9(5)	7.0(5)	1.4(5)
C3	27.6(8)	16.1(6)	16.2(6)	-2.2(5)	10.9(6)	-3.2(5)
C4	31.4(8)	12.0(6)	24.2(7)	1.3(5)	16.9(6)	4.0(5)
C5	23.8(8)	16.1(6)	21.3(7)	5.3(5)	11.8(6)	7.1(5)
C6	16.4(7)	15.8(6)	15.8(6)	2.8(5)	8.3(5)	3.3(5)
C7	14.4(7)	17.8(6)	15.9(6)	2.6(5)	6.5(5)	2.3(5)
C8	17.8(8)	25.4(7)	20.0(7)	5.7(5)	4.3(6)	5.7(5)
C9	16.8(8)	33.2(8)	18.6(7)	1.8(6)	0.4(6)	-0.3(6)
C10	19.3(8)	25.7(7)	19.7(7)	-3.4(6)	5.0(6)	-4.9(6)
C11	18.6(7)	16.8(6)	17.7(6)	0.7(5)	6.1(6)	-1.4(5)

C12	14.6(7)	17.0(6)	13.7(6)	2.7(5)	5.6(5)	0.8(5)
C13	13.8(7)	11.2(6)	13.7(6)	1.9(4)	3.5(5)	-0.2(4)
C14	17.1(7)	14.3(6)	12.0(6)	-0.5(4)	4.1(5)	-0.6(5)
C15	19.2(7)	12.6(6)	14.9(6)	0.3(4)	8.2(5)	1.9(5)
C16	15.5(7)	10.4(6)	12.8(6)	-1.7(4)	4.3(5)	1.0(5)
C17	18.9(7)	14.5(6)	11.6(6)	0.5(4)	6.7(5)	1.2(5)
C18	12.8(7)	10.4(5)	12.0(6)	-0.7(4)	4.4(5)	-1.5(4)

Table S3. Bond Lengths for **α-CBP**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1	1.4024(16)	C8	C9	1.380(2)
N1	C12	1.4019(17)	C9	C10	1.405(2)
N1	C13	1.4230(15)	C10	C11	1.384(2)
C1	C2	1.3942(18)	C11	C12	1.3999(18)
C1	C6	1.4119(18)	C13	C14	1.3956(17)
C2	C3	1.3920(18)	C13	C15	1.3924(17)
C3	C4	1.4040(19)	C14	C16	1.3870(16)
C4	C5	1.382(2)	C15	C17	1.3871(17)
C5	C6	1.3978(18)	C16	C18	1.4054(16)
C6	C7	1.4475(19)	C17	C18	1.4043(16)
C7	C8	1.396(2)	C18	C18[1]	1.491(2)
C7	C12	1.4129(18)			

[1]1-X,1-Y,1-Z

Table S4. Bond Angles for **α-CBP**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C13	125.58(10)	C8	C9	C10	120.65(13)
C12	N1	C1	108.39(10)	C11	C10	C9	121.68(13)
C12	N1	C13	125.62(10)	C10	C11	C12	117.40(12)
N1	C1	C6	108.78(11)	N1	C12	C7	108.80(11)
C2	C1	N1	129.45(12)	C11	C12	N1	129.70(12)
C2	C1	C6	121.66(12)	C11	C12	C7	121.49(12)
C3	C2	C1	117.20(12)	C14	C13	N1	120.37(11)
C2	C3	C4	121.93(13)	C15	C13	N1	120.38(11)
C5	C4	C3	120.25(12)	C15	C13	C14	119.24(11)
C4	C5	C6	119.25(13)	C16	C14	C13	120.09(11)
C1	C6	C7	107.06(11)	C17	C15	C13	120.21(11)
C5	C6	C1	119.69(12)	C14	C16	C18	121.75(11)

C5	C6	C7	133.19(13)	C15	C17	C18	121.74(11)
C8	C7	C6	133.29(12)	C16	C18	C18[1]	121.49(13)
C8	C7	C12	119.68(12)	C17	C18	C16	116.92(11)
C12	C7	C6	106.98(11)	C17	C18	C18[1]	121.59(13)
C9	C8	C7	119.08(13)				

[1]1-X,1-Y,1-Z

Table S5. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **α-CBP**.

Atom	*x*	*y*	*z*	U(eq)
H2	3780	8291	4165	19
H3	3478	9740	4288	23
H4	1154	10455	2634	25
H5	-929	9735	808	23
H8	-2851	8536	-1161	26
H9	-3856	7333	-2471	29
H10	-2496	6050	-1698	26
H11	-74	5939	385	21
H14	3139	6081	1364	18
H15	2284	7052	4743	18
H16	4748	4996	2724	16
H17	3929	5977	6106	18

Table S6. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **β-CBP**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N1	4529.6(6)	1992.8(13)	2711.8(11)	17.0(3)
N2	2089.5(6)	5344.9(14)	-1316.9(11)	17.3(4)
C1	4405.3(8)	1926.2(15)	3600.2(13)	18.4(4)
C2	3953.1(8)	2136.0(17)	4000.4(14)	21.9(4)
C3	3915.7(10)	1917.8(18)	4888.4(15)	26.7(5)
C4	4320.7(10)	1528.7(18)	5365.8(14)	26.6(5)
C5	4769.5(9)	1324.2(17)	4965.4(14)	22.9(5)
C6	4811.9(8)	1499.8(16)	4063.2(13)	18.6(4)
C7	5194.2(8)	1264.9(15)	3427.3(14)	17.5(4)
C8	5665.8(8)	803.2(16)	3480.9(15)	20.4(4)
C9	5935.7(8)	651.0(17)	2721.6(15)	22.6(4)
C10	5742.0(8)	960.8(16)	1910.3(14)	21.5(5)

C11	5275.6(8)	1426.2(16)	1831.2(13)	18.1(4)
C12	5003.3(7)	1564.7(15)	2599.1(13)	16.7(4)
C13	4235.9(7)	2512.6(16)	2061.9(13)	16.5(4)
C14	4064.2(8)	3561.4(16)	2213.1(14)	19.0(4)
C15	4115.2(7)	1988.7(16)	1283.7(13)	17.2(4)
C16	3751.8(8)	4049.5(16)	1609.0(14)	18.4(4)
C17	3807.2(7)	2490.2(16)	682.0(13)	16.6(4)
C18	3604.2(7)	3514.8(16)	843.8(13)	15.7(4)
C19	3213.6(8)	3991.7(16)	270.8(13)	16.0(4)
C20	2884.9(8)	4768.6(17)	600.7(14)	20.4(4)
C21	3145.9(7)	3643.2(16)	-592.5(14)	18.2(4)
C22	2511.8(9)	5203.5(16)	86.1(14)	20.8(4)
C23	2768.0(7)	4058.9(17)	-1107.9(13)	19.1(4)
C24	2454.9(7)	4848.8(16)	-770.6(13)	16.9(4)
C25	1581.9(7)	5409.5(16)	-1159.3(13)	15.6(4)
C26	1297.1(8)	4866.9(16)	-535.9(14)	18.4(4)
C27	791.3(8)	5073.2(17)	-531.1(14)	19.9(4)
C28	574.4(8)	5802.9(17)	-1119.9(14)	20.2(4)
C29	858.2(7)	6325.8(16)	-1742.3(14)	17.7(4)
C30	1367.8(7)	6129.6(15)	-1768.6(13)	15.2(4)
C31	1767.1(7)	6531.9(16)	-2312.9(13)	16.7(4)
C32	1792.7(8)	7260.5(16)	-3007.5(13)	19.0(4)
C33	2250.0(9)	7502.9(18)	-3367.8(15)	23.5(5)
C34	2682.2(8)	7026.9(18)	-3037.7(15)	24.0(5)
C35	2667.7(8)	6288.4(17)	-2355.6(15)	21.8(4)
C36	2206.1(8)	6044.0(16)	-2007.6(13)	17.7(4)

Table S7. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **β-CBP**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{23}}$	$\mathbf{U_{13}}$	$\mathbf{U_{12}}$
N1	20.4(9)	14.6(8)	15.9(8)	0.4(7)	-1.1(7)	1.7(6)
N2	16.3(8)	18.2(8)	17.5(8)	1.4(7)	0.3(7)	1.4(7)
C1	27.5(11)	11.4(9)	16.2(10)	-2.2(8)	-2.0(9)	-1.7(8)
C2	27.4(11)	16.1(10)	22.2(11)	-2.6(8)	0.7(9)	1.9(8)
C3	35.9(13)	21.1(11)	23.1(11)	-4.3(9)	7.8(10)	-1.8(10)
C4	45.5(14)	19.0(11)	15.2(10)	-0.4(8)	2.5(10)	-3.5(10)
C5	35.5(13)	14(1)	19.3(10)	0.1(8)	-5.6(9)	-4.2(9)
C6	25.2(10)	11.6(9)	19(1)	-1.3(8)	-3.1(9)	-3.8(8)
C7	22.1(11)	10.1(8)	20.3(10)	1.1(8)	-4.1(8)	-4.5(8)
C8	21.5(11)	14.6(9)	24.9(11)	4.4(8)	-6.9(9)	-3.8(8)

C9	18.1(10)	16.5(10)	33.2(12)	2.8(9)	-2.2(9)	-1.1(8)
C10	21.6(11)	16.1(10)	26.6(12)	-0.6(9)	1.5(9)	-3.9(8)
C11	21.7(11)	14.3(9)	18.2(10)	-0.1(8)	-0.9(8)	-3.3(8)
C12	18.7(9)	10.9(8)	20.4(10)	-0.1(8)	-2.6(8)	-2.2(7)
C13	15.9(9)	16(1)	17.8(10)	1.4(8)	-1.2(8)	-0.3(8)
C14	24.4(11)	15.6(10)	16.9(10)	-4.0(8)	-3.3(8)	-0.2(8)
C15	18.8(10)	13.1(9)	19.6(10)	-2.1(8)	0.7(8)	1.6(8)
C16	23.0(11)	12.0(9)	20.1(10)	-2.3(8)	-2.8(8)	1.8(8)
C17	18(1)	16.5(9)	15.3(9)	-2.4(8)	0.8(8)	-0.3(8)
C18	16.0(9)	14.6(9)	16.3(10)	0.5(8)	1.0(8)	-1.2(7)
C19	17.8(10)	12.6(9)	17.6(10)	0.0(8)	0.6(8)	-1.6(8)
C20	25.3(11)	18.7(10)	17.1(10)	-3.2(8)	-1.7(8)	1.0(8)
C21	18.4(10)	17.3(10)	19(1)	-3.5(8)	0.6(8)	3.2(8)
C22	22.4(10)	18.2(10)	21.7(10)	-3.2(9)	1.0(9)	4.0(9)
C23	22.1(11)	20.9(11)	14.2(10)	-3.4(8)	-1.0(8)	0.6(8)
C24	13.9(9)	17.4(10)	19.3(10)	1.8(8)	-1.7(8)	-0.3(8)
C25	17.0(9)	12.8(9)	16.9(10)	-5.2(7)	-0.4(8)	0.1(7)
C26	23.2(10)	15.7(10)	16.5(9)	-1.1(8)	-0.1(8)	-1.9(8)
C27	21.7(10)	17.7(10)	20.3(10)	-4.6(8)	3.1(9)	-4.1(8)
C28	16.2(10)	17.4(10)	27.1(11)	-6.0(9)	1.2(9)	0.0(8)
C29	19.4(10)	13.6(9)	20.2(10)	-3.2(8)	-3.2(8)	2.0(8)
C30	19(1)	10.6(9)	16.1(9)	-4.6(7)	-1.0(8)	-1.0(8)
C31	19.8(10)	14.5(9)	15.7(9)	-4.9(8)	0.3(8)	-0.2(7)
C32	24.9(11)	14.4(9)	17.7(10)	-2.3(8)	-0.7(9)	1.7(8)
C33	33.4(13)	19.6(10)	17.6(10)	0.0(8)	4.9(9)	-3.0(9)
C34	23.7(11)	24.8(11)	23.4(11)	-2.1(9)	7.0(9)	-4.8(9)
C35	18.8(10)	23.6(10)	23.1(10)	-0.9(9)	1.0(9)	-0.1(8)
C36	22.8(11)	14.7(9)	15.6(9)	-2.6(7)	1.0(8)	0.3(8)

Table S8. Bond Lengths for **β-CBP**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1	1.400(3)	C16	C18	1.400(3)
N1	C12	1.392(3)	C17	C18	1.398(3)
N1	C13	1.422(2)	C18	C19	1.490(3)
N2	C24	1.428(3)	C19	C20	1.399(3)
N2	C25	1.391(2)	C19	C21	1.399(3)
N2	C36	1.398(3)	C20	C22	1.384(3)
C1	C2	1.388(3)	C21	C23	1.386(3)
C1	C6	1.406(3)	C22	C24	1.389(3)
C2	C3	1.387(3)	C23	C24	1.388(3)

C3	C4	1.398(3)	C25	C26	1.394(3)
C4	C5	1.379(3)	C25	C30	1.410(3)
C5	C6	1.400(3)	C26	C27	1.387(3)
C6	C7	1.446(3)	C27	C28	1.400(3)
C7	C8	1.395(3)	C28	C29	1.380(3)
C7	C12	1.415(3)	C29	C30	1.395(3)
C8	C9	1.382(3)	C30	C31	1.447(3)
C9	C10	1.398(3)	C31	C32	1.392(3)
C10	C11	1.387(3)	C31	C36	1.407(3)
C11	C12	1.394(3)	C32	C33	1.383(3)
C13	C14	1.393(3)	C33	C34	1.398(3)
C13	C15	1.392(3)	C34	C35	1.384(3)
C14	C16	1.387(3)	C35	C36	1.386(3)
C15	C17	1.384(3)			

Table S9. Bond Angles for **β-CBP**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C13	124.75(17)	C16	C18	C19	120.38(18)
C12	N1	C1	108.48(17)	C17	C18	C16	117.50(18)
C12	N1	C13	126.49(17)	C17	C18	C19	121.93(18)
C25	N2	C24	126.97(17)	C20	C19	C18	120.39(18)
C25	N2	C36	108.43(16)	C20	C19	C21	117.87(19)
C36	N2	C24	123.36(17)	C21	C19	C18	121.66(18)
N1	C1	C6	108.85(18)	C22	C20	C19	121.37(19)
C2	C1	N1	128.76(19)	C23	C21	C19	121.20(19)
C2	C1	C6	122.16(19)	C20	C22	C24	119.58(19)
C3	C2	C1	117.3(2)	C21	C23	C24	119.70(19)
C2	C3	C4	121.4(2)	C22	C24	N2	119.48(18)
C5	C4	C3	121.1(2)	C23	C24	N2	120.18(18)
C4	C5	C6	118.7(2)	C23	C24	C22	120.25(18)
C1	C6	C7	106.99(17)	N2	C25	C26	129.21(19)
C5	C6	C1	119.3(2)	N2	C25	C30	108.92(17)
C5	C6	C7	133.5(2)	C26	C25	C30	121.85(18)
C8	C7	C6	133.76(19)	C27	C26	C25	117.19(19)
C8	C7	C12	119.4(2)	C26	C27	C28	121.7(2)
C12	C7	C6	106.83(17)	C29	C28	C27	120.76(19)
C9	C8	C7	119.05(19)	C28	C29	C30	118.97(19)
C8	C9	C10	120.70(19)	C25	C30	C31	106.90(17)
C11	C10	C9	121.9(2)	C29	C30	C25	119.55(19)
C10	C11	C12	117.02(19)	C29	C30	C31	133.55(19)

N1	C12	C7	108.77(18)	C32	C31	C30	134.09(19)
N1	C12	C11	129.28(19)	C32	C31	C36	119.14(19)
C11	C12	C7	121.95(18)	C36	C31	C30	106.76(18)
C14	C13	N1	119.18(18)	C33	C32	C31	119.2(2)
C15	C13	N1	121.17(18)	C32	C33	C34	120.6(2)
C15	C13	C14	119.66(18)	C35	C34	C33	121.6(2)
C16	C14	C13	119.62(19)	C34	C35	C36	117.2(2)
C17	C15	C13	120.02(18)	N2	C36	C31	108.95(17)
C14	C16	C18	121.61(19)	C35	C36	N2	128.69(19)
C15	C17	C18	121.37(18)	C35	C36	C31	122.34(19)

Table S10. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **β-CBP**.

Atom	***x***	***y***	***z***	**U(eq)**
H2	3680	2418	3679	26
H3	3608	2035	5178	32
H4	4286	1403	5976	32
H5	5045	1069	5295	28
H8	5799	596	4032	24
H9	6256	333	2751	27
H10	5935	849	1398	26
H11	5147	1641	1278	22
H14	4160	3940	2727	23
H15	4244	1287	1165	21
H16	3635	4764	1717	22
H17	3732	2131	148	20
H20	2918	5003	1190	24
H21	3363	3112	-830	22
H22	2296	5741	318	25
H23	2723	3804	-1689	23
H26	1443	4377	-131	22
H27	587	4710	-118	24
H28	228	5940	-1091	24
H29	709	6812	-2147	21
H32	1500	7587	-3231	23
H33	2271	7997	-3844	28
H34	2993	7215	-3288	29
H35	2962	5963	-2135	26

Table S11. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **γ-CBP**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N1	2860.8(7)	9259.9(17)	2178.8(3)	15.3(3)
N2	-1306.6(7)	7680.4(18)	395.4(3)	17.1(3)
C18	1095.3(8)	8710.3(19)	1412.5(4)	14.2(3)
C12	3608.7(8)	8929.0(19)	2104.7(4)	16.3(3)
C1	2793.0(9)	9768.3(19)	2549.6(4)	17.0(3)
C7	4025.2(9)	9257(2)	2428.0(4)	18.3(3)
C6	3503.5(9)	9754(2)	2713.0(4)	19.5(3)
C13	2265.7(8)	9119.5(19)	1923.5(4)	14.1(3)
C19	476.2(8)	8452.1(19)	1145.6(4)	14.9(3)
C14	2333.5(8)	9810.6(19)	1567.5(4)	14.5(3)
C25	-2059.0(8)	7785(2)	484.0(4)	17.4(3)
C26	-2397.5(9)	8201(2)	819.2(4)	20.4(3)
C24	-706.8(8)	7940(2)	644.9(4)	16.4(3)
C36	-1243.4(9)	7147(2)	27.5(4)	16.9(3)
C31	-1960.4(9)	6984(2)	-123.6(4)	19.4(3)
C23	-712.3(9)	7098(2)	987.0(4)	18.1(3)
C15	1607.1(8)	8282.4(19)	2026.5(4)	15.1(3)
C35	-612.4(9)	6673(2)	-172.5(4)	19.6(3)
C2	2163.4(9)	10297(2)	2745.8(4)	19.9(3)
C17	1032.9(8)	8093.1(19)	1775.2(4)	15.0(3)
C21	-131.7(9)	7354(2)	1231.5(4)	18.0(3)
C20	471.4(9)	9292(2)	799.0(4)	18.2(3)
C34	-713.8(10)	6037(2)	-528.6(4)	24.0(4)
C22	-110.0(9)	9046(2)	553.0(4)	19.3(3)
C16	1759.2(8)	9588.9(19)	1316.6(4)	15.3(3)
C30	-2483.0(9)	7393(2)	167.4(4)	19.3(3)
C10	4714.9(9)	8183(2)	1779.9(5)	23.1(3)
C11	3949.0(9)	8353(2)	1780.2(4)	18.5(3)
C5	3578.3(10)	10183(2)	3085.8(4)	25.1(4)
C3	2255.7(10)	10731(2)	3114.6(4)	25.1(4)
C8	4801.0(9)	9116(2)	2416.3(5)	24.3(4)
C9	5140.8(9)	8591(2)	2092.8(5)	25.8(4)
C4	2954.0(11)	10656(2)	3284.1(4)	27.5(4)
C29	-3256.8(9)	7408(2)	185.8(5)	24.6(4)
C33	-1422.3(10)	5906(2)	-686.1(4)	26.9(4)
C27	-3163.7(9)	8171(2)	831.4(5)	23.9(4)
C32	-2045.2(10)	6383(2)	-485.3(4)	25.7(4)
C28	-3592.4(9)	7787(2)	519.2(5)	25.7(4)

Table S12. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **γ-CBP**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	14.7(7)	17.3(6)	13.8(6)	-0.2(5)	-1.7(5)	-0.8(5)
N2	16.0(7)	20.5(6)	14.7(6)	-0.4(5)	-3.5(5)	-1.2(5)
C18	14.8(7)	13.2(7)	14.7(6)	-1.9(5)	-0.6(5)	1.5(6)
C12	15.2(8)	12.2(7)	21.4(7)	2.7(5)	-3.8(6)	-1.2(6)
C1	25.1(9)	12.6(7)	13.4(7)	1.8(5)	-2.8(6)	-3.9(6)
C7	20.7(8)	13.0(7)	21.3(7)	3.8(6)	-7.3(6)	-2.4(6)
C6	26.0(9)	13.7(7)	18.8(7)	4.6(6)	-5.3(6)	-3.5(6)
C13	15.2(8)	13.1(7)	14.1(6)	-1.8(5)	-2.0(5)	1.3(6)
C19	16.5(8)	14.2(7)	14.1(6)	-1.9(5)	-1.8(5)	0.4(6)
C14	13.4(7)	14.7(7)	15.3(7)	-1.0(5)	1.3(5)	-0.2(6)
C25	18.1(8)	13.5(7)	20.7(7)	2.2(6)	-3.6(6)	-0.5(6)
C26	23.1(9)	17.2(7)	20.7(7)	-0.1(6)	-2.0(6)	1.1(6)
C24	17.0(8)	16.3(7)	15.9(7)	-1.9(5)	-3.6(6)	0.1(6)
C36	21.0(8)	14.7(7)	15.1(7)	2.3(5)	-3.4(6)	-2.9(6)
C31	20.4(8)	19.3(7)	18.6(7)	2.3(6)	-5.1(6)	-3.0(6)
C23	17.7(8)	18.6(7)	17.9(7)	0.8(6)	-2.0(6)	-4.6(6)
C15	16.5(8)	14.8(7)	13.9(6)	1.5(5)	0.1(5)	1.7(6)
C35	20.0(8)	20.5(8)	18.4(7)	1.9(6)	-2.3(6)	-2.4(6)
C2	25.4(9)	16.0(7)	18.3(7)	2.2(6)	1.2(6)	-3.3(6)
C17	13.7(8)	14.9(7)	16.5(7)	-0.5(5)	0.3(5)	-0.3(6)
C21	20.6(8)	19.0(7)	14.4(6)	2.3(6)	-2.1(6)	-1.5(6)
C20	17.6(8)	20.1(7)	17.1(7)	2.0(6)	-1.4(6)	-3.9(6)
C34	26.8(9)	26.0(8)	19.1(7)	-0.2(6)	2.3(6)	-2.3(7)
C22	20.9(8)	23.0(8)	13.9(7)	2.4(6)	-2.4(6)	-2.4(6)
C16	19.0(8)	14.8(7)	12.2(6)	-0.5(5)	1.0(5)	1.5(6)
C30	19.1(8)	17.5(7)	21.2(7)	2.1(6)	-4.4(6)	-1.3(6)
C10	17.8(9)	17.4(7)	34.0(9)	-2.3(6)	1.3(7)	0.6(6)
C11	17.1(8)	14.7(7)	23.6(7)	-1.4(6)	-2.0(6)	-1.1(6)
C5	37.3(10)	18.8(8)	19.3(7)	4.5(6)	-10.9(7)	-9.2(7)
C3	41.2(11)	17.0(8)	17.3(7)	0.6(6)	5.6(7)	-4.4(7)
C8	23.1(9)	17.1(8)	32.6(9)	3.0(6)	-12.7(7)	-0.2(6)
C9	14.8(8)	19.8(8)	42.6(10)	-0.1(7)	-5.5(7)	1.3(6)
C4	49.0(12)	19.7(8)	13.9(7)	2.1(6)	-4.2(7)	-7.3(8)
C29	19.9(9)	25.8(8)	28.1(8)	2.5(7)	-6.7(7)	-0.6(7)
C33	33(1)	31.7(9)	16.0(7)	-2.7(6)	-3.3(7)	-5.1(8)
C27	25.1(9)	20.6(8)	26.1(8)	2.3(6)	3.8(7)	5.5(7)
C32	26.2(9)	31.0(9)	19.9(8)	0.7(7)	-7.8(6)	-5.3(7)

C28	18.5(9)	23.7(8)	34.9(9)	3.9(7)	-1.1(7)	2.2(7)

Table S13. Bond Lengths for **γ-CBP**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C12	1.395(2)	C26	C27	1.381(2)
N1	C1	1.4042(18)	C24	C23	1.390(2)
N1	C13	1.4211(18)	C24	C22	1.391(2)
N2	C25	1.395(2)	C36	C31	1.408(2)
N2	C24	1.4231(18)	C36	C35	1.393(2)
N2	C36	1.3987(18)	C31	C30	1.447(2)
C18	C19	1.490(2)	C31	C32	1.396(2)
C18	C17	1.3992(19)	C23	C21	1.385(2)
C18	C16	1.405(2)	C15	C17	1.387(2)
C12	C7	1.415(2)	C35	C34	1.389(2)
C12	C11	1.395(2)	C2	C3	1.388(2)
C1	C6	1.411(2)	C20	C22	1.389(2)
C1	C2	1.395(2)	C34	C33	1.402(2)
C7	C6	1.446(2)	C30	C29	1.395(2)
C7	C8	1.401(2)	C10	C11	1.385(2)
C6	C5	1.398(2)	C10	C9	1.404(2)
C13	C14	1.3959(19)	C5	C4	1.380(3)
C13	C15	1.389(2)	C3	C4	1.401(3)
C19	C21	1.398(2)	C8	C9	1.381(2)
C19	C20	1.4044(19)	C29	C28	1.383(2)
C14	C16	1.388(2)	C33	C32	1.384(2)
C25	C26	1.397(2)	C27	C28	1.401(2)
C25	C30	1.411(2)			

Table S14. Bond Angles for **γ-CBP**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C12	N1	C1	108.42(12)	C23	C24	C22	118.91(13)
C12	N1	C13	126.10(12)	C22	C24	N2	120.83(13)
C1	N1	C13	125.48(12)	N2	C36	C31	108.79(13)
C25	N2	C24	125.65(12)	C35	C36	N2	129.48(14)
C25	N2	C36	108.38(12)	C35	C36	C31	121.53(14)
C36	N2	C24	125.81(13)	C36	C31	C30	107.07(13)
C17	C18	C19	120.74(13)	C32	C31	C36	119.64(15)
C17	C18	C16	116.94(13)	C32	C31	C30	133.10(15)

C16	C18	C19	122.32(13)	C21	C23	C24	120.46(14)
N1	C12	C7	108.76(13)	C17	C15	C13	120.27(13)
N1	C12	C11	129.82(14)	C34	C35	C36	117.62(15)
C11	C12	C7	121.41(14)	C3	C2	C1	117.45(15)
N1	C1	C6	108.84(13)	C15	C17	C18	121.83(14)
C2	C1	N1	129.50(14)	C23	C21	C19	121.83(13)
C2	C1	C6	121.60(14)	C22	C20	C19	121.62(14)
C12	C7	C6	107.09(14)	C35	C34	C33	121.57(16)
C8	C7	C12	119.37(15)	C20	C22	C24	120.31(14)
C8	C7	C6	133.51(14)	C14	C16	C18	121.70(13)
C1	C6	C7	106.85(13)	C25	C30	C31	106.67(14)
C5	C6	C1	119.58(15)	C29	C30	C25	119.99(14)
C5	C6	C7	133.57(15)	C29	C30	C31	133.32(14)
C14	C13	N1	120.81(13)	C11	C10	C9	121.59(16)
C15	C13	N1	120.02(13)	C10	C11	C12	117.75(14)
C15	C13	C14	119.17(13)	C4	C5	C6	119.01(16)
C21	C19	C18	121.00(13)	C2	C3	C4	121.51(16)
C21	C19	C20	116.87(13)	C9	C8	C7	119.25(15)
C20	C19	C18	122.13(13)	C8	C9	C10	120.50(15)
C16	C14	C13	120.02(13)	C5	C4	C3	120.76(15)
N2	C25	C26	129.60(14)	C28	C29	C30	118.70(15)
N2	C25	C30	109.04(13)	C32	C33	C34	120.32(15)
C26	C25	C30	121.36(15)	C26	C27	C28	121.87(15)
C27	C26	C25	117.42(15)	C33	C32	C31	119.27(15)
C23	C24	N2	120.26(13)	C29	C28	C27	120.64(16)

Table S15. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **γ-CBP**.

Atom	*x*	*y*	*z*	U(eq)
H14	2773	10433	1497	17
H26	-2112	8493	1031	24
H23	-1117	6341	1054	22
H15	1550	7838	2270	18
H35	-130	6782	-69	24
H2	1690	10358	2631	24
H17	585	7529	1851	18
H21	-147	6767	1464	22
H20	876	10047	731	22
H34	-293	5683	-669	29
H22	-100	9637	321	23
H16	1817	10043	1074	18

H10	4958	7782	1563	28
H11	3665	8086	1567	22
H5	4052	10149	3201	30
H3	1836	11087	3255	30
H8	5090	9378	2628	29
H9	5667	8505	2082	31
H4	2998	10934	3538	33
H29	-3547	7164	-27	30
H33	-1475	5487	-932	32
H27	-3407	8418	1058	29
H32	-2525	6302	-592	31
H28	-4119	7787	537	31