Electronic Supplementary Information - Part Three

Chloride, carboxylate and carbonate transport by *ortho*-phenylenediamine-based bisureas

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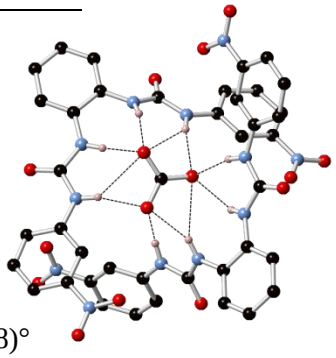
Table S2. Crystal data and structure refinement details.



Identification code	**2011sot0753** (BISMN02 HCO3)	
Empirical formula	$C_{57}H_{72}N_{14}O_{15}$	
	$2(C_{20}H_{16}N_6O_6)$, $2(C_8H_{20}N)$, CO_3	
Formula weight	1193.29	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Triclinic	
Space group	*P*–1	
Unit cell dimensions	a = 14.1445(18) Å	α = 86.271(8)°
	b = 14.338(2) Å	β = 81.687(8)°
	c = 16.719(3) Å	γ = 61.358(5)°
Volume	2944.5(8) Å^3	
Z	2	
Density (calculated)	1.346 Mg / m^3	
Absorption coefficient	0.099 mm^{-1}	
F(000)	1264	
Crystal	Prism; Yellow	
Crystal size	0.12 × 0.10 × 0.08 mm^3	
θ range for data collection	2.91 – 27.48°	
Index ranges	$-16 \le h \le 18$, $-18 \le k \le 18$, $-19 \le l \le 21$	
Reflections collected	33949	
Independent reflections	13317 [R_{int} = 0.0279]	
Completeness to θ = 27.48°	98.5 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9921 and 0.9882	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13317 / 36 / 770	
Goodness-of-fit on F^2	1.078	
Final *R* indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0618, *wR2* = 0.1432	
R indices (all data)	*R1* = 0.0780, *wR2* = 0.1535	
Largest diff. peak and hole	0.630 and –0.513 e Å^{-3}	

Diffractometer: *Rigaku AFC12* goniometer equipped with an enhanced sensitivity (HG) *Saturn724+* detector mounted at the window of an *FR-E+ SuperBright* molybdenum rotating anode generator with HF *Varimax* optics (100µm focus). **Cell determination, Data collection, Data reduction and cell refinement & Absorption correction**: CrystalClear-SM Expert 2.0 r7 (Rigaku, 2011) , **Structure solution**: SHELXS97 (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). S**tructure refinement**: SHELXL97 (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** CrystalMaker: a crystal and molecular structures program for Mac and Windows. CrystalMaker Software Ltd, Oxford, England (www.crystalmaker.com)

Special details: The counter-ions balancing the 2 negative charges of the carbonate ion comprise 1 whole and 2 half TEA molecules. The 2 half molecules lie on inversion centres and were refined using thermal parameter and geometrical restraints.

Table S3. Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [$Å^2$ × 10^3] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
N14	5000	0	0	41(1)	1
C50A	5788(4)	–1031(4)	7(3)	43(1)	0.50
C51A	6690(5)	–1295(5)	556(4)	43(1)	0.50
C52A	4655(4)	–852(4)	343(3)	43(1)	0.50
C53A	4126(5)	–621(4)	1225(3)	43(1)	0.50
C50B	5928(4)	–160(4)	487(3)	43(1)	0.50
C51B	6911(4)	–1187(4)	487(4)	43(1)	0.50
C52B	4390(4)	530(4)	848(3)	43(1)	0.50
C53B	3851(5)	–72(4)	1329(3)	43(1)	0.50
N15	0	0	0	40(1)	1
C54A	1049(4)	–32(4)	166(3)	40(1)	0.50
C55A	1517(5)	–381(5)	891(4)	40(1)	0.50
C56A	–773(4)	282(4)	820(3)	40(1)	0.50
C57A	–1112(4)	1415(4)	1081(3)	40(1)	0.50
C54B	375(4)	–494(4)	681(3)	40(1)	0.50
C55B	1397(5)	–573(5)	945(4)	40(1)	0.50
C56B	–334(4)	1284(4)	–1(3)	40(1)	0.50
C57B	–1094(4)	1836(4)	753(3)	40(1)	0.50
O1	723(2)	2380(2)	712(2)	65(1)	1
O2	1799(2)	2320(1)	1534(1)	55(1)	1
O3	–253(1)	7804(1)	1838(1)	35(1)	1
O4	4069(1)	8005(1)	2750(1)	37(1)	1
O5	7713(1)	2619(1)	2820(1)	48(1)	1
O6	9177(1)	2782(1)	2674(1)	56(1)	1
N1	1026(2)	2812(2)	1152(1)	46(1)	1
N2	762(1)	6030(1)	2122(1)	28(1)	1
N3	972(1)	7267(1)	2755(1)	28(1)	1
N4	2846(1)	7361(1)	2899(1)	24(1)	1
N5	4654(1)	6204(1)	2762(1)	25(1)	1
N6	8184(2)	3163(2)	2747(1)	37(1)	1
C1	851(2)	4469(2)	1621(1)	31(1)	1
C2	432(2)	3979(2)	1209(2)	36(1)	1
C3	–498(2)	4527(2)	841(2)	42(1)	1
C4	–1013(2)	5629(2)	894(2)	42(1)	1
C5	–621(2)	6159(2)	1300(1)	35(1)	1
C6	317(2)	5577(2)	1675(1)	29(1)	1
C7	431(2)	7099(2)	2211(1)	28(1)	1
C8	904(2)	8262(2)	2897(1)	28(1)	1
C9	–93(2)	9189(2)	2966(2)	37(1)	1
C10	–156(2)	10166(2)	3083(2)	43(1)	1
C11	776(2)	10223(2)	3151(2)	39(1)	1

C12	1779(2)	9310(2)	3101(1)	32(1)	1
C13	1856(2)	8318(2)	2966(1)	26(1)	1
C14	3864(2)	7264(2)	2792(1)	25(1)	1
C15	5772(2)	5830(2)	2741(1)	24(1)	1
C16	6266(2)	6482(2)	2701(1)	32(1)	1
C17	7380(2)	6029(2)	2698(2)	37(1)	1
C18	8028(2)	4943(2)	2719(1)	35(1)	1
C19	7523(2)	4321(2)	2742(1)	29(1)	1
C20	6413(2)	4732(2)	2759(1)	25(1)	1
O7	–2273(2)	6287(2)	4688(1)	64(1)	1
O8	–1096(2)	6438(2)	3776(1)	52(1)	1
O9	2893(1)	1112(1)	3682(1)	38(1)	1
O10	6538(1)	1634(1)	813(1)	27(1)	1
O11	5913(2)	6696(1)	794(1)	54(1)	1
O12	6813(2)	6597(1)	–384(1)	43(1)	1
N7	–1384(2)	5912(2)	4262(2)	47(1)	1
N8	2094(1)	2911(2)	3434(1)	29(1)	1
N9	3798(1)	1840(1)	2826(1)	28(1)	1
N10	5454(1)	2196(1)	2032(1)	24(1)	1
N11	5627(1)	3403(1)	1164(1)	26(1)	1
N12	6382(2)	6239(1)	145(1)	31(1)	1
C21	361(2)	4350(2)	3861(1)	33(1)	1
C22	–641(2)	4768(2)	4335(2)	38(1)	1
C23	–960(2)	4155(2)	4868(2)	46(1)	1
C24	–236(2)	3086(2)	4902(2)	45(1)	1
C25	770(2)	2633(2)	4430(1)	38(1)	1
C26	1082(2)	3269(2)	3911(1)	31(1)	1
C27	2919(2)	1885(2)	3344(1)	28(1)	1
C28	4860(2)	979(2)	2734(1)	25(1)	1
C29	5124(2)	–49(2)	3013(1)	31(1)	1
C30	6193(2)	–848(2)	2931(1)	35(1)	1
C31	7025(2)	–655(2)	2563(1)	33(1)	1
C32	6771(2)	354(2)	2267(1)	28(1)	1
C33	5701(2)	1171(2)	2341(1)	24(1)	1
C34	5924(2)	2350(2)	1295(1)	22(1)	1
C35	6065(2)	3811(2)	514(1)	23(1)	1
C36	6496(2)	3317(2)	–243(1)	28(1)	1
C37	6903(2)	3776(2)	–860(1)	31(1)	1
C38	6883(2)	4739(2)	–745(1)	28(1)	1
C39	6440(2)	5212(2)	9(1)	23(1)	1
C40	6033(2)	4777(2)	639(1)	24(1)	1
O13	2902(1)	4141(1)	2567(1)	34(1)	1
O14	2707(1)	5515(1)	3252(1)	33(1)	1
O15	4338(1)	4377(1)	2638(1)	28(1)	1
C49	3316(2)	4671(2)	2818(1)	23(1)	1
N13	5921(2)	2116(1)	4766(1)	30(1)	1
C41	5281(2)	3028(2)	4217(1)	33(1)	1
C42	4451(2)	4050(2)	4652(2)	40(1)	1

C43	5164(2)	1819(2)	5331(1)	34(1)	1
C44	4489(2)	1488(2)	4918(2)	39(1)	1
C45	6722(2)	1190(2)	4223(1)	38(1)	1
C46	7465(2)	201(2)	4653(2)	49(1)	1
C47	6495(2)	2444(2)	5300(1)	37(1)	1
C48	7294(2)	2782(3)	4863(2)	53(1)	1

Table S4. Bond lengths [Å] and angles [°].

N14–C50A[i]	1.360(5)	C2–C3	1.381(4)
N14–C50A	1.360(5)	C3–C4	1.389(4)
N14–C50B[i]	1.560(5)	C4–C5	1.388(3)
N14–C50B	1.560(5)	C5–C6	1.401(3)
N14–C52A[i]	1.567(4)	C8–C9	1.395(3)
N14–C52A	1.567(4)	C8–C13	1.409(3)
N14–C52B[i]	1.578(5)	C9–C10	1.385(3)
N14–C52B	1.578(5)	C10–C11	1.380(4)
C50A–C51A	1.563(6)	C11–C12	1.390(3)
C52A–C53A	1.534(6)	C12–C13	1.404(3)
C50B–C51B	1.463(6)	C15–C20	1.391(3)
C50B–C52B	1.926(7)	C15–C16	1.404(3)
C52B–C53B	1.528(6)	C16–C17	1.386(3)
N15–C54B[ii]	1.338(5)	C17–C18	1.379(3)
N15–C54B	1.338(5)	C18–C19	1.381(3)
N15–C54A	1.528(4)	C19–C20	1.385(3)
N15–C54A[ii]	1.528(4)	O7–N7	1.233(3)
N15–C56A[ii]	1.566(4)	O8–N7	1.231(3)
N15–C56A	1.566(4)	O9–C27	1.225(3)
N15–C56B	1.667(5)	O10–C34	1.229(2)
N15–C56B[ii]	1.667(5)	O11–N12	1.230(2)
C54A–C55A	1.413(6)	O12–N12	1.226(2)
C56A–C57A	1.531(5)	N7–C22	1.472(3)
C54B–C55B	1.522(6)	N8–C27	1.371(3)
C56B–C57B	1.514(6)	N8–C26	1.402(3)
O1–N1	1.231(3)	N9–C27	1.386(3)
O2–N1	1.227(3)	N9–C28	1.408(3)
O3–C7	1.225(2)	N10–C34	1.370(2)
O4–C14	1.224(2)	N10–C33	1.417(2)
O5–N6	1.237(3)	N11–C34	1.371(2)
O6–N6	1.229(2)	N11–C35	1.405(2)
N1–C2	1.471(3)	N12–C39	1.467(3)
N2–C7	1.384(3)	C21–C22	1.385(3)
N2–C6	1.402(3)	C21–C26	1.393(3)
N3–C7	1.369(3)	C22–C23	1.390(4)
N3–C8	1.416(3)	C23–C24	1.379(4)
N4–C14	1.365(3)	C24–C25	1.388(3)
N4–C13	1.411(2)	C25–C26	1.397(3)
N5–C14	1.388(2)	C28–C29	1.401(3)
N5–C15	1.401(2)	C28–C33	1.410(3)
N6–C19	1.464(3)	C29–C30	1.385(3)
C1–C2	1.379(3)	C30–C31	1.385(3)
C1–C6	1.396(3)	C31–C32	1.389(3)

C32–C33	1.394(3)	O15–C49	1.290(2)
C35–C40	1.392(3)	N13–C45	1.513(3)
C35–C36	1.399(3)	N13–C43	1.520(3)
C36–C37	1.389(3)	N13–C47	1.520(3)
C37–C38	1.393(3)	N13–C41	1.523(3)
C38–C39	1.384(3)	C41–C42	1.515(3)
C39–C40	1.383(3)	C43–C44	1.511(3)
O13–C49	1.279(2)	C45–C46	1.513(3)
O14–C49	1.291(2)	C47–C48	1.512(3)

C50A^{i}–N14–C50A	180.0(7)	C54B^{ii}–N15–C54B	180.0(8)
C50A^{i}–N14–C50B^{i}	67.4(3)	C54B^{ii}–N15–C54A	115.2(3)
C50A–N14–C50B^{i}	112.6(3)	C54B–N15–C54A	64.8(3)
C50A^{i}–N14–C50B	112.6(3)	C54B^{ii}–N15–C54A^{ii}	64.8(3)
C50A–N14–C50B	67.4(3)	C54B–N15–C54A^{ii}	115.2(3)
C50B^{i}–N14–C50B	180.0(4)	C54A–N15–C54A^{ii}	180.0(5)
C50A^{i}–N14–C52A^{i}	62.1(3)	C54B^{ii}–N15–C56A^{ii}	59.6(3)
C50A–N14–C52A^{i}	117.9(3)	C54B–N15–C56A^{ii}	120.4(3)
C50B^{i}–N14–C52A^{i}	104.9(3)	C54A–N15–C56A^{ii}	73.1(3)
C50B–N14–C52A^{i}	75.1(3)	C54A^{ii}–N15–C56A^{ii}	106.9(3)
C50A^{i}–N14–C52A	117.9(3)	C54B^{ii}–N15–C56A	120.4(3)
C50A–N14–C52A	62.1(3)	C54B–N15–C56A	59.6(3)
C50B^{i}–N14–C52A	75.1(3)	C54A–N15–C56A	106.9(3)
C50B–N14–C52A	104.9(3)	C54A^{ii}–N15–C56A	73.1(3)
C52A^{i}–N14–C52A	180.0(4)	C56A^{ii}–N15–C56A	180.0(4)
C50A^{i}–N14–C52B^{i}	116.6(3)	C54B^{ii}–N15–C56B	67.0(3)
C50A–N14–C52B^{i}	63.4(3)	C54B–N15–C56B	113.0(3)
C50B^{i}–N14–C52B^{i}	75.7(3)	C54A–N15–C56B	77.6(3)
C50B–N14–C52B^{i}	104.3(3)	C54A^{ii}–N15–C56B	102.4(3)
C52A^{i}–N14–C52B^{i}	81.3(2)	C56A^{ii}–N15–C56B	96.0(2)
C52A–N14–C52B^{i}	98.7(2)	C56A–N15–C56B	84.0(2)
C50A^{i}–N14–C52B	63.4(3)	C54B^{ii}–N15–C56B^{ii}	113.0(3)
C50A–N14–C52B	116.6(3)	C54B–N15–C56B^{ii}	67.0(3)
C50B^{i}–N14–C52B	104.3(3)	C54A–N15–C56B^{ii}	102.4(3)
C50B–N14–C52B	75.7(3)	C54A^{ii}–N15–C56B^{ii}	77.6(3)
C52A^{i}–N14–C52B	98.7(2)	C56A^{ii}–N15–C56B^{ii}	84.0(2)
C52A–N14–C52B	81.3(2)	C56A–N15–C56B^{ii}	96.0(2)
C52B^{i}–N14–C52B	180.00(18)	C56B–N15–C56B^{ii}	180.0(5)
N14–C50A–C51A	116.5(4)	C55A–C54A–N15	125.3(4)
C53A–C52A–N14	111.9(3)	C57A–C56A–N15	110.2(3)
C51B–C50B–N14	120.8(4)	N15–C54B–C55B	121.8(4)
C51B–C50B–C52B	142.1(4)	C57B–C56B–N15	110.9(4)
N14–C50B–C52B	52.6(2)	O2–N1–O1	123.3(2)
C53B–C52B–N14	112.5(4)	O2–N1–C2	119.0(2)
C53B–C52B–C50B	121.2(4)	O1–N1–C2	117.7(2)
N14–C52B–C50B	51.7(2)	C7–N2–C6	127.22(18)

C7–N3–C8	124.56(17)	C27–N9–C28	126.21(17)
C14–N4–C13	126.41(17)	C34–N10–C33	122.69(17)
C14–N5–C15	125.60(17)	C34–N11–C35	125.69(17)
O6–N6–O5	123.45(19)	O12–N12–O11	123.07(18)
O6–N6–C19	118.3(2)	O12–N12–C39	118.79(18)
O5–N6–C19	118.23(17)	O11–N12–C39	118.13(17)
C2–C1–C6	119.1(2)	C22–C21–C26	119.2(2)
C1–C2–C3	123.4(2)	C21–C22–C23	122.7(2)
C1–C2–N1	117.6(2)	C21–C22–N7	117.6(2)
C3–C2–N1	119.0(2)	C23–C22–N7	119.7(2)
C2–C3–C4	116.8(2)	C24–C23–C22	117.1(2)
C5–C4–C3	122.0(2)	C23–C24–C25	122.0(2)
C4–C5–C6	119.7(2)	C24–C25–C26	119.9(2)
C1–C6–C5	119.1(2)	C21–C26–C25	119.1(2)
C1–C6–N2	116.55(19)	C21–C26–N8	115.9(2)
C5–C6–N2	124.4(2)	C25–C26–N8	125.0(2)
O3–C7–N3	124.5(2)	O9–C27–N8	124.94(19)
O3–C7–N2	123.7(2)	O9–C27–N9	124.3(2)
N3–C7–N2	111.78(17)	N8–C27–N9	110.77(18)
C9–C8–C13	119.4(2)	C29–C28–N9	123.76(19)
C9–C8–N3	120.9(2)	C29–C28–C33	118.50(19)
C13–C8–N3	119.66(17)	N9–C28–C33	117.74(17)
C10–C9–C8	120.9(2)	C30–C29–C28	120.6(2)
C11–C10–C9	119.8(2)	C29–C30–C31	121.0(2)
C10–C11–C12	120.7(2)	C30–C31–C32	118.9(2)
C11–C12–C13	120.1(2)	C31–C32–C33	121.1(2)
C12–C13–C8	119.12(18)	C32–C33–C28	119.75(18)
C12–C13–N4	123.29(19)	C32–C33–N10	120.52(18)
C8–C13–N4	117.58(18)	C28–C33–N10	119.72(17)
O4–C14–N4	125.24(19)	O10–C34–N10	124.20(18)
O4–C14–N5	123.59(19)	O10–C34–N11	124.15(18)
N4–C14–N5	111.14(17)	N10–C34–N11	111.65(17)
C20–C15–N5	116.05(18)	C40–C35–C36	119.15(18)
C20–C15–C16	119.37(18)	C40–C35–N11	117.08(17)
N5–C15–C16	124.59(18)	C36–C35–N11	123.75(18)
C17–C16–C15	119.9(2)	C37–C36–C35	120.40(19)
C18–C17–C16	121.6(2)	C36–C37–C38	121.26(19)
C17–C18–C19	117.3(2)	C39–C38–C37	116.79(18)
C18–C19–C20	123.5(2)	C40–C39–C38	123.67(18)
C18–C19–N6	119.11(19)	C40–C39–N12	117.99(18)
C20–C19–N6	117.43(19)	C38–C39–N12	118.33(17)
C19–C20–C15	118.40(19)	C39–C40–C35	118.72(18)
O8–N7–O7	123.6(3)	O13–C49–O15	120.73(18)
O8–N7–C22	118.8(2)	O13–C49–O14	119.93(18)
O7–N7–C22	117.6(2)	O15–C49–O14	119.33(18)
C27–N8–C26	127.30(18)	C45–N13–C43	110.81(17)

C45–N13–C47	111.44(18)	C42–C41–N13	114.99(19)
C43–N13–C47	106.51(16)	C44–C43–N13	115.20(18)
C45–N13–C41	106.94(17)	N13–C45–C46	115.4(2)
C43–N13–C41	110.65(17)	C48–C47–N13	115.9(2)
C47–N13–C41	110.54(17)		

Symmetry transformations used to generate equivalent atoms:
(i) –x+1,–y,–z (ii) –x,–y,–z

Table S5. Anisotropic displacement parameters [Å^2× 10^3]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N14	45(1)	44(1)	39(1)	–1(1)	–7(1)	–25(1)
C50A	54(1)	36(1)	41(1)	3(1)	–5(1)	–24(1)
C51A	54(1)	36(1)	41(1)	3(1)	–5(1)	–24(1)
C52A	54(1)	36(1)	41(1)	3(1)	–5(1)	–24(1)
C53A	54(1)	36(1)	41(1)	3(1)	–5(1)	–24(1)
C50B	54(1)	36(1)	41(1)	3(1)	–5(1)	–24(1)
C51B	54(1)	36(1)	41(1)	3(1)	–5(1)	–24(1)
C52B	54(1)	36(1)	41(1)	3(1)	–5(1)	–24(1)
C53B	54(1)	36(1)	41(1)	3(1)	–5(1)	–24(1)
N15	38(1)	44(1)	43(1)	–12(1)	–2(1)	–22(1)
C54A	36(1)	39(1)	47(1)	–12(1)	2(1)	–20(1)
C55A	36(1)	39(1)	47(1)	–12(1)	2(1)	–20(1)
C56A	36(1)	39(1)	47(1)	–12(1)	2(1)	–20(1)
C57A	36(1)	39(1)	47(1)	–12(1)	2(1)	–20(1)
C54B	36(1)	39(1)	47(1)	–12(1)	2(1)	–20(1)
C55B	36(1)	39(1)	47(1)	–12(1)	2(1)	–20(1)
C56B	36(1)	39(1)	47(1)	–12(1)	2(1)	–20(1)
C57B	36(1)	39(1)	47(1)	–12(1)	2(1)	–20(1)
O1	73(1)	52(1)	80(2)	–16(1)	–11(1)	–35(1)
O2	56(1)	33(1)	71(1)	2(1)	–12(1)	–16(1)
O3	30(1)	26(1)	42(1)	8(1)	–10(1)	–7(1)
O4	32(1)	22(1)	55(1)	1(1)	–1(1)	–13(1)
O5	30(1)	27(1)	77(1)	15(1)	–2(1)	–7(1)
O6	22(1)	39(1)	90(2)	7(1)	–8(1)	–2(1)
N1	50(1)	38(1)	53(1)	–8(1)	3(1)	–25(1)
N2	22(1)	24(1)	35(1)	7(1)	–7(1)	–9(1)
N3	21(1)	23(1)	35(1)	6(1)	–4(1)	–7(1)
N4	23(1)	15(1)	32(1)	–2(1)	–4(1)	–6(1)
N5	20(1)	20(1)	33(1)	0(1)	–3(1)	–9(1)
N6	24(1)	31(1)	45(1)	10(1)	–4(1)	–6(1)
C1	26(1)	31(1)	34(1)	2(1)	0(1)	–13(1)
C2	36(1)	33(1)	38(1)	0(1)	2(1)	–18(1)
C3	43(1)	51(2)	40(1)	–3(1)	–4(1)	–28(1)
C4	34(1)	50(2)	43(1)	4(1)	–10(1)	–20(1)
C5	28(1)	34(1)	40(1)	6(1)	–7(1)	–13(1)
C6	25(1)	31(1)	31(1)	4(1)	–1(1)	–14(1)
C7	20(1)	25(1)	32(1)	6(1)	1(1)	–8(1)
C8	25(1)	21(1)	31(1)	1(1)	0(1)	–6(1)
C9	24(1)	27(1)	49(1)	–2(1)	0(1)	–4(1)
C10	32(1)	24(1)	56(2)	–5(1)	–2(1)	0(1)
C11	39(1)	19(1)	49(1)	–4(1)	–9(1)	–4(1)

C12	33(1)	23(1)	36(1)	–2(1)	–7(1)	–8(1)
C13	25(1)	19(1)	25(1)	–1(1)	–2(1)	–4(1)
C14	26(1)	22(1)	26(1)	0(1)	–3(1)	–10(1)
C15	21(1)	27(1)	21(1)	–2(1)	–1(1)	–10(1)
C16	27(1)	27(1)	40(1)	–7(1)	0(1)	–12(1)
C17	29(1)	39(1)	47(1)	–13(1)	2(1)	–20(1)
C18	24(1)	44(1)	36(1)	–6(1)	–3(1)	–14(1)
C19	25(1)	27(1)	26(1)	3(1)	–3(1)	–6(1)
C20	23(1)	26(1)	22(1)	4(1)	–3(1)	–10(1)
O7	31(1)	75(2)	74(1)	–35(1)	16(1)	–18(1)
O8	37(1)	47(1)	69(1)	–15(1)	1(1)	–19(1)
O9	37(1)	40(1)	39(1)	8(1)	3(1)	–24(1)
O10	29(1)	22(1)	29(1)	–5(1)	4(1)	–13(1)
O11	95(2)	38(1)	34(1)	–8(1)	10(1)	–40(1)
O12	57(1)	35(1)	41(1)	6(1)	5(1)	–30(1)
N7	29(1)	57(1)	55(1)	–25(1)	2(1)	–20(1)
N8	26(1)	35(1)	28(1)	2(1)	3(1)	–17(1)
N9	23(1)	31(1)	28(1)	9(1)	0(1)	–13(1)
N10	23(1)	19(1)	26(1)	–1(1)	4(1)	–8(1)
N11	28(1)	19(1)	25(1)	–2(1)	7(1)	–8(1)
N12	40(1)	25(1)	30(1)	5(1)	–5(1)	–16(1)
C21	28(1)	46(1)	30(1)	–8(1)	0(1)	–22(1)
C22	28(1)	53(2)	36(1)	–15(1)	2(1)	–21(1)
C23	28(1)	73(2)	40(1)	–12(1)	7(1)	–29(1)
C24	34(1)	72(2)	37(1)	4(1)	3(1)	–33(1)
C25	31(1)	55(2)	33(1)	3(1)	0(1)	–26(1)
C26	25(1)	46(1)	26(1)	–3(1)	–1(1)	–22(1)
C27	28(1)	37(1)	24(1)	4(1)	–3(1)	–20(1)
C28	27(1)	26(1)	22(1)	2(1)	–4(1)	–13(1)
C29	37(1)	31(1)	30(1)	3(1)	–1(1)	–20(1)
C30	43(1)	22(1)	36(1)	2(1)	–4(1)	–14(1)
C31	32(1)	23(1)	38(1)	–1(1)	–4(1)	–8(1)
C32	25(1)	26(1)	33(1)	–1(1)	–3(1)	–11(1)
C33	25(1)	22(1)	24(1)	1(1)	–2(1)	–11(1)
C34	20(1)	22(1)	25(1)	–1(1)	–1(1)	–11(1)
C35	22(1)	22(1)	22(1)	1(1)	0(1)	–8(1)
C36	32(1)	25(1)	26(1)	–5(1)	4(1)	–14(1)
C37	34(1)	33(1)	22(1)	–4(1)	6(1)	–15(1)
C38	27(1)	28(1)	24(1)	3(1)	1(1)	–13(1)
C39	24(1)	21(1)	25(1)	2(1)	–4(1)	–11(1)
C40	26(1)	21(1)	20(1)	1(1)	–2(1)	–9(1)
O13	43(1)	43(1)	29(1)	2(1)	–2(1)	–31(1)
O14	27(1)	18(1)	41(1)	2(1)	6(1)	–3(1)
O15	22(1)	26(1)	32(1)	–7(1)	1(1)	–9(1)
C49	25(1)	18(1)	23(1)	7(1)	–4(1)	–9(1)
N13	34(1)	32(1)	26(1)	4(1)	–4(1)	–17(1)

C41	39(1)	34(1)	30(1)	9(1)	–9(1)	–20(1)
C42	41(1)	37(1)	43(1)	3(1)	–11(1)	–17(1)
C43	41(1)	35(1)	28(1)	1(1)	3(1)	–22(1)
C44	46(1)	37(1)	36(1)	–6(1)	2(1)	–24(1)
C45	38(1)	35(1)	32(1)	5(1)	0(1)	–13(1)
C46	51(2)	38(1)	43(1)	9(1)	–2(1)	–10(1)
C47	40(1)	44(1)	33(1)	7(1)	–12(1)	–24(1)
C48	54(2)	73(2)	49(2)	11(1)	–13(1)	–44(2)

Table S6. Hydrogen coordinates [× 10^4] and isotropic displacement parameters [Å^2 × 10^3].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H50A	6144	–1242	–555	51	0.50
H50B	5435	–1476	182	51	0.50
H51A	7212	–2055	513	64	0.50
H51B	6357	–1116	1118	64	0.50
H51C	7067	–880	380	64	0.50
H52A	4137	–862	9	51	0.50
H52B	5304	–1563	306	51	0.50
H53A	3923	–1169	1418	64	0.50
H53B	3475	77	1263	64	0.50
H53C	4642	–623	1560	64	0.50
H50C	6161	373	289	51	0.50
H50D	5603	23	1057	51	0.50
H51D	7534	–1122	204	64	0.50
H51E	6822	–1717	211	64	0.50
H51F	7036	–1410	1046	64	0.50
H52C	4916	556	1166	51	0.50
H52D	3829	1270	765	51	0.50
H53D	3070	408	1457	64	0.50
H53E	4173	–337	1831	64	0.50
H53F	3964	–672	1006	64	0.50
H54A	1617	–472	–271	48	0.50
H54B	941	701	79	48	0.50
H55A	2190	–330	845	59	0.50
H55B	1681	–1121	991	59	0.50
H55C	1007	66	1341	59	0.50
H56A	–1426	221	757	48	0.50
H56B	–395	–225	1241	48	0.50
H57A	–1595	1582	1594	59	0.50
H57B	–1494	1917	666	59	0.50
H57C	–465	1472	1149	59	0.50
H54C	495	–1230	642	48	0.50
H54D	–219	–145	1128	48	0.50
H55D	1533	–957	1458	59	0.50
H55E	1298	142	1016	59	0.50
H55F	2016	–956	532	59	0.50
H56C	332	1356	–28	48	0.50
H56D	–691	1629	–485	48	0.50
H57D	–1279	2589	740	59	0.50
H57E	–736	1503	1232	59	0.50
H57F	–1758	1775	776	59	0.50
H902	1314	5584	2373	33	1
H903	1391	6719	3035	34	1

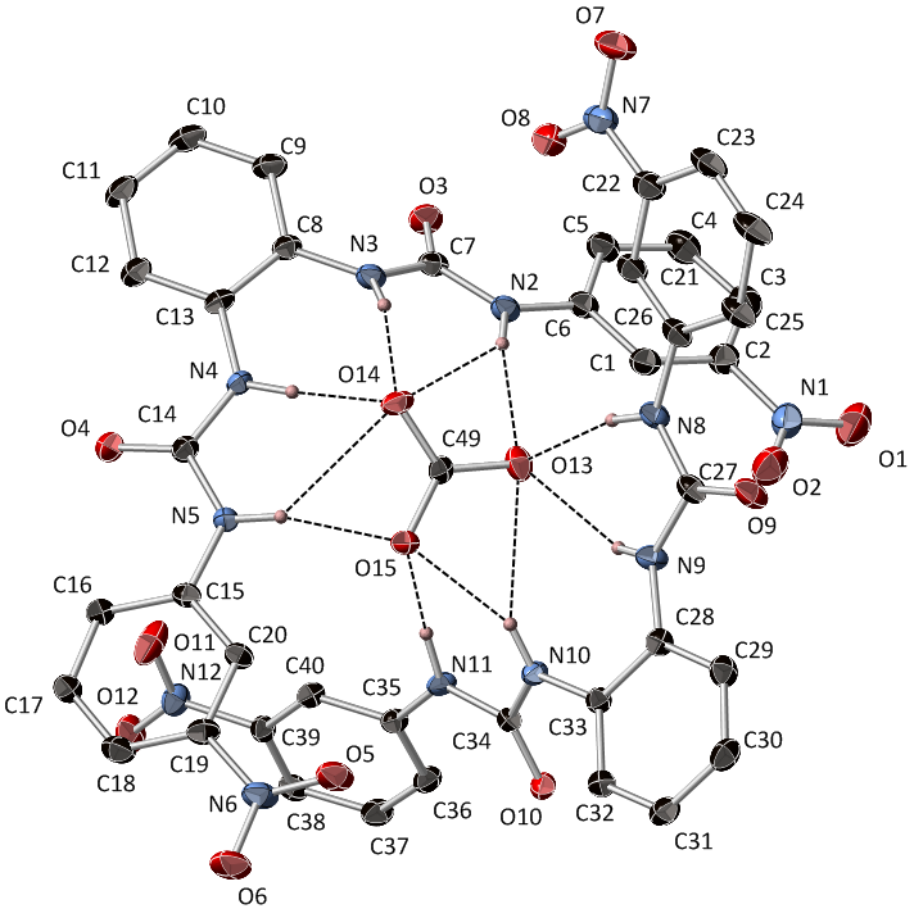
H904	2803	6767	2929	29	1
H905	4434	5726	2755	30	1
H1	1494	4059	1865	37	1
H3	–773	4169	566	50	1
H4	–1653	6032	645	50	1
H5	–987	6914	1323	42	1
H9	–738	9151	2932	45	1
H10	–837	10794	3116	52	1
H11	732	10893	3232	47	1
H12	2413	9357	3159	39	1
H16	5837	7232	2677	38	1
H17	7704	6479	2682	44	1
H18	8792	4636	2716	42	1
H20	6096	4276	2783	30	1
H908	2212	3399	3161	35	1
H909	3682	2403	2525	34	1
H910	4978	2755	2325	29	1
H911	5119	3864	1517	31	1
H21	554	4795	3507	39	1
H23	–1646	4459	5195	55	1
H24	–433	2646	5258	55	1
H25	1247	1892	4461	45	1
H29	4564	–199	3260	38	1
H30	6359	–1538	3129	41	1
H31	7758	–1205	2514	40	1
H32	7337	491	2009	34	1
H36	6512	2663	–337	34	1
H37	7201	3426	–1369	37	1
H38	7160	5057	–1165	33	1
H40	5739	5130	1146	28	1
H41A	5799	3177	3840	40	1
H41B	4900	2796	3889	40	1
H42A	3910	3923	5008	61	1
H42B	4089	4594	4254	61	1
H42C	4817	4294	4974	61	1
H43A	5606	1229	5679	41	1
H43B	4668	2435	5686	41	1
H44A	4035	2070	4579	58	1
H44B	4024	1319	5327	58	1
H44C	4970	859	4580	58	1
H45A	7177	1424	3848	45	1
H45B	6311	1003	3892	45	1
H46A	7940	353	4933	74	1
H46B	7908	–371	4258	74	1
H46C	7027	–19	5048	74	1
H47A	5938	3039	5651	44	1
H47B	6887	1841	5657	44	1
H48A	7882	2185	4542	80	1

H48B	7598	3002	5258	80	1
H48C	6921	3378	4505	80	1

Table S7. Hydrogen bonds [Å and °].

D–H···*A*	*d*(*D*–H)	*d*(H···*A*)	*d*(*D*···*A*)	∠(*D*H*A*)
N2–H902···O13	0.88	2.26	3.095(2)	158.7
N2–H902···O14	0.88	2.59	3.326(2)	142.2
N3–H903···O14	0.88	1.90	2.726(2)	155.7
N4–H904···O14	0.88	1.90	2.765(2)	166.9
N5–H905···O15	0.88	2.03	2.885(2)	165.1
N5–H905···O14	0.88	2.61	3.329(2)	139.0
N8–H908···O13	0.88	1.91	2.765(2)	163.1
N9–H909···O13	0.88	2.19	2.939(2)	142.8
N10–H910···O15	0.88	2.12	2.918(2)	150.2
N10–H910···O13	0.88	2.63	3.368(2)	142.5
N11–H911···O15	0.88	2.02	2.838(2)	154.5

Symmetry transformations used to generate equivalent atoms:
(i) –x+1,–y,–z (ii) –x,–y,–z



Thermal ellipsoids drawn at the 35% probability level, counter ions and selected hydrogens omitted for clarity.