

Title

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Abstract

Related literature

Computing details

Data collection: *APEX3* v2019.3-2click4 (Bruker Nano, 2019); cell refinement: *SAINT* V8.38A (Bruker AXS Inc., 2017); data reduction: *SAINT* V8.38A (Bruker AXS Inc., 2017); program(s) used to solve structure: *XT*, VERSION 2014/5; program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2018); molecular graphics: *shelXle* (C.B. Huebschle, rev 924); software used to prepare material for publication: *XP*, VERSION 5.

Acknowledgements

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Funding information

References

Sheldrick, G. M. (2015). Crystal structure refinement with *SHELXL*. *Acta Cryst. C* 71, 3-8.

Figure 1

Fig. 1. *ORTEP* diagram of the molecule with thermal ellipsoids at 50% probability level. Riding hydrogen atoms, disordered parts and solvent molecules are omitted for clarity.

(mo_CHEM0913)

Crystal data

$C_{112}H_{100} \cdot 4(C_2H_4Cl_2)$

$M_r = 1841.72$

Triclinic, $P\bar{1}$

$a = 10.7131$ (7) Å

$b = 16.1974$ (11) Å

$c = 16.5188$ (11) Å

$\alpha = 118.419$ (2)°

$\beta = 93.901$ (2)°

$\gamma = 100.021$ (2)°

$V = 2444.6$ (3) Å³

$Z = 1$

$F(000) = 972$

$D_x = 1.251$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5320 reflections

$\theta = 2.2$ – 22.3 °

$\mu = 0.28$ mm⁻¹

$T = 158$ K

Plate, red

$0.15 \times 0.11 \times 0.07$ mm

Data collection

Bruker D8 VENTURE FIXED-CHI PHOTON 100

CMOS

diffractometer

Radiation source: $I\mu$ S HB micro-focus sealed tube

Detector resolution: 10.4167 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan

SADABS 2016/2: Krause, L., Herbst-Irmer, R.,

Sheldrick G.M. & Stalke D., *J. Appl. Cryst.* 48 (2015)

3-10

$T_{\min} = 0.416$, $T_{\max} = 0.745$

32457 measured reflections

9602 independent reflections

5553 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.083$
 $\theta_{\text{max}} = 26.1^\circ$, $\theta_{\text{min}} = 2.2^\circ$
 $h = -13 \rightarrow 12$

$k = -20 \rightarrow 20$
 $l = -19 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.079$
 $wR(F^2) = 0.236$
 $S = 1.03$
9602 reflections
630 parameters
57 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.1021P)^2 + 2.2067P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.43 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.61 \text{ e } \text{\AA}^{-3}$
Extinction correction: *SHELXL2018/3* (Sheldrick 2018), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0042 (12)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.3775 (3)	0.4358 (2)	0.4914 (2)	0.0280 (7)	
C2	0.2625 (3)	0.3814 (2)	0.4921 (2)	0.0280 (7)	
H2	0.215889	0.329290	0.433862	0.034*	
C3	0.2090 (3)	0.3984 (2)	0.5744 (2)	0.0279 (7)	
C4	0.2741 (3)	0.4806 (2)	0.6565 (2)	0.0268 (7)	
C5	0.3914 (3)	0.5357 (2)	0.6564 (2)	0.0283 (7)	
C6	0.4469 (3)	0.5163 (2)	0.5777 (2)	0.0268 (7)	
C7	0.5651 (3)	0.5818 (2)	0.5915 (2)	0.0281 (7)	
C8	0.6181 (3)	0.6556 (2)	0.6819 (2)	0.0287 (7)	
H8	0.696366	0.699050	0.690451	0.034*	
C9	0.5636 (3)	0.6708 (2)	0.7628 (2)	0.0277 (7)	
C10	0.4445 (3)	0.6114 (2)	0.7467 (2)	0.0270 (7)	
C11	0.1293 (3)	0.5160 (2)	0.7818 (2)	0.0291 (7)	
C12	0.2493 (3)	0.5296 (2)	0.7518 (2)	0.0279 (7)	
C13	0.3517 (3)	0.6077 (2)	0.8059 (2)	0.0280 (7)	
C14	0.3475 (3)	0.6844 (2)	0.8969 (2)	0.0292 (7)	
C15	0.2221 (3)	0.6729 (2)	0.9241 (2)	0.0339 (8)	
H15	0.209594	0.722436	0.982059	0.041*	
C16	0.1228 (3)	0.5963 (2)	0.8721 (2)	0.0335 (8)	
H16	0.044324	0.594581	0.895485	0.040*	
C17	0.0983 (3)	0.3287 (2)	0.5715 (2)	0.0289 (7)	
C18	0.0186 (3)	0.3479 (2)	0.6421 (2)	0.0279 (7)	
C19	-0.0832 (3)	0.2707 (2)	0.6260 (2)	0.0321 (8)	
H19	-0.138845	0.283495	0.670743	0.039*	
C20	-0.1088 (3)	0.1780 (2)	0.5504 (2)	0.0346 (8)	
C21	-0.0271 (3)	0.1607 (2)	0.4850 (2)	0.0353 (8)	
H21	-0.039498	0.097978	0.432434	0.042*	
C22	0.0715 (3)	0.2342 (2)	0.4962 (2)	0.0330 (8)	

H22	0.124880	0.219834	0.449848	0.040*
C23	−0.2193 (3)	0.0974 (3)	0.5396 (2)	0.0411 (9)
C24	−0.3013 (4)	0.1340 (3)	0.6162 (3)	0.0618 (12)
H24A	−0.336195	0.185577	0.615050	0.093*
H24B	−0.247887	0.159130	0.677228	0.093*
H24C	−0.372281	0.080719	0.605227	0.093*
C25	−0.3078 (4)	0.0541 (3)	0.4456 (3)	0.0625 (12)
H25A	−0.258470	0.027996	0.394956	0.094*
H25B	−0.344104	0.104418	0.442785	0.094*
H25C	−0.377758	0.002207	0.438824	0.094*
C26	−0.1623 (5)	0.0196 (3)	0.5445 (4)	0.0725 (14)
H26A	−0.231596	−0.030750	0.541235	0.109*
H26B	−0.101954	0.048426	0.603436	0.109*
H26C	−0.116681	−0.009017	0.491939	0.109*
C27	0.6368 (3)	0.7383 (2)	0.8573 (2)	0.0295 (7)
C28	0.5840 (3)	0.7798 (2)	0.9412 (2)	0.0289 (7)
C29	0.6725 (3)	0.8419 (2)	1.0250 (2)	0.0310 (7)
H29	0.638677	0.873083	1.080806	0.037*
C30	0.8047 (3)	0.8607 (2)	1.0319 (2)	0.0344 (8)
C31	0.8538 (3)	0.8174 (2)	0.9494 (2)	0.0380 (8)
H31	0.944214	0.828400	0.951065	0.046*
C32	0.7718 (3)	0.7590 (2)	0.8662 (2)	0.0358 (8)
H32	0.808007	0.730829	0.811062	0.043*
C33	0.8978 (3)	0.9250 (3)	1.1254 (2)	0.0420 (9)
C34	0.8260 (4)	0.9656 (3)	1.2076 (3)	0.0628 (12)
H34A	0.768875	1.002163	1.197409	0.094*
H34B	0.888235	1.008363	1.265458	0.094*
H34C	0.774942	0.912333	1.212554	0.094*
C35	0.9851 (4)	0.8669 (3)	1.1406 (3)	0.0613 (12)
H35A	0.932438	0.810331	1.139390	0.092*
H35B	1.042232	0.907318	1.201261	0.092*
H35C	1.036887	0.845699	1.090806	0.092*
C36	0.9804 (4)	1.0104 (3)	1.1219 (3)	0.0509 (10)
H36A	1.031993	0.986285	1.072333	0.076*
H36B	1.037567	1.053546	1.182112	0.076*
H36C	0.924216	1.046009	1.108874	0.076*
C37	0.0255 (3)	0.4381 (2)	0.7308 (2)	0.0301 (7)
C38	−0.0951 (3)	0.4459 (2)	0.7728 (2)	0.0319 (8)
C39	−0.1110 (3)	0.4273 (2)	0.8463 (2)	0.0380 (8)
C40	−0.2176 (4)	0.4479 (3)	0.8897 (3)	0.0498 (10)
H40	−0.228740	0.436117	0.940108	0.060*
C41	−0.3081 (4)	0.4852 (3)	0.8613 (3)	0.0516 (10)
C42	−0.2942 (4)	0.4971 (3)	0.7853 (3)	0.0498 (10)
H42	−0.358035	0.518848	0.762931	0.060*
C43	−0.1894 (3)	0.4783 (2)	0.7403 (3)	0.0386 (8)
C44	−0.0156 (4)	0.3863 (3)	0.8778 (3)	0.0531 (10)
H44A	−0.005696	0.326792	0.824295	0.080*
H44B	−0.046417	0.372093	0.925376	0.080*
H44C	0.067614	0.433392	0.904403	0.080*
C45	−0.4171 (5)	0.5128 (4)	0.9145 (4)	0.0787 (15)
H45A	−0.494186	0.500009	0.870911	0.118*
H45B	−0.392673	0.581621	0.961357	0.118*

H45C	−0.435226	0.474599	0.945659	0.118*	
C46	−0.1773 (4)	0.4957 (3)	0.6592 (3)	0.0569 (11)	
H46A	−0.134293	0.449077	0.614735	0.085*	
H46B	−0.126467	0.561394	0.681947	0.085*	
H46C	−0.263150	0.487892	0.628069	0.085*	
C47	0.4462 (3)	0.7645 (2)	0.9529 (2)	0.0292 (7)	
C48	0.4130 (3)	0.8453 (2)	1.0370 (2)	0.0294 (7)	
C49	0.4218 (3)	0.8496 (2)	1.1240 (2)	0.0350 (8)	
C50	0.3924 (3)	0.9289 (3)	1.1991 (2)	0.0427 (9)	
H50	0.400328	0.933353	1.258795	0.051*	
C51	0.3525 (3)	1.0007 (2)	1.1896 (3)	0.0425 (9)	
C52	0.3389 (3)	0.9922 (2)	1.1023 (3)	0.0413 (9)	
H52	0.308361	1.039877	1.094179	0.050*	
C53	0.3684 (3)	0.9159 (2)	1.0257 (2)	0.0339 (8)	
C54	0.4605 (4)	0.7715 (3)	1.1371 (3)	0.0492 (10)	
H54A	0.395436	0.710770	1.099295	0.074*	
H54B	0.467573	0.789413	1.203182	0.074*	
H54C	0.543837	0.763142	1.117401	0.074*	
C55	0.3235 (4)	1.0859 (3)	1.2741 (3)	0.0661 (13)	
H55A	0.293318	1.128604	1.254706	0.099*	
H55B	0.401811	1.121713	1.321286	0.099*	
H55C	0.256601	1.062003	1.300519	0.099*	
C56	0.3492 (4)	0.9088 (3)	0.9312 (3)	0.0463 (9)	
H56A	0.423618	0.891435	0.901067	0.069*	
H56B	0.340377	0.971154	0.938669	0.069*	
H56C	0.271141	0.859116	0.892252	0.069*	
Cl1_1	0.0393 (4)	0.7496 (3)	0.7113 (3)	0.0675 (8)	0.6816 (19)
Cl2_1	0.3396 (2)	0.7919 (2)	0.67664 (17)	0.1031 (7)	0.6816 (19)
C57_1	0.1244 (9)	0.6614 (5)	0.6479 (7)	0.102 (3)	0.6816 (19)
H57A_1	0.172531	0.647197	0.691233	0.122*	0.6816 (19)
H57B_1	0.062360	0.601050	0.601093	0.122*	0.6816 (19)
C58_1	0.2144 (7)	0.6934 (5)	0.6003 (5)	0.095 (3)	0.6816 (19)
H58A_1	0.166515	0.710978	0.559671	0.113*	0.6816 (19)
H58B_1	0.251426	0.638945	0.559594	0.113*	0.6816 (19)
Cl1_2	0.0323 (10)	0.7315 (9)	0.7232 (9)	0.0675 (8)	0.265 (2)
Cl2_2	0.3504 (5)	0.7146 (5)	0.5763 (5)	0.1031 (7)	0.265 (2)
C57_2	0.1332 (15)	0.6841 (9)	0.6402 (16)	0.102 (3)	0.265 (2)
H57A_2	0.166565	0.634469	0.647699	0.122*	0.265 (2)
H57B_2	0.082180	0.652541	0.576440	0.122*	0.265 (2)
C58_2	0.2411 (13)	0.7592 (8)	0.6506 (12)	0.095 (3)	0.265 (2)
H58A_2	0.287003	0.794530	0.716128	0.113*	0.265 (2)
H58B_2	0.207301	0.805893	0.638059	0.113*	0.265 (2)
Cl1_3	0.0467 (16)	0.5765 (12)	0.5584 (15)	0.0675 (8)	0.0530 (17)
Cl2_3	0.369 (2)	0.710 (2)	0.5401 (16)	0.1031 (7)	0.0530 (17)
C57_3	0.1474 (17)	0.6932 (12)	0.604 (3)	0.102 (3)	0.0530 (17)
H57A_3	0.133319	0.717328	0.560211	0.122*	0.0530 (17)
H57B_3	0.123966	0.737652	0.664157	0.122*	0.0530 (17)
C58_3	0.2832 (16)	0.693 (2)	0.6196 (16)	0.095 (3)	0.0530 (17)
H58A_3	0.289786	0.631016	0.615247	0.113*	0.0530 (17)
H58B_3	0.323393	0.745340	0.683704	0.113*	0.0530 (17)
Cl3_4	0.5626 (3)	0.7639 (2)	0.44948 (18)	0.1163 (9)	0.701 (3)
Cl4_4	0.7304 (3)	0.6922 (2)	0.2050 (3)	0.1089 (9)	0.701 (3)

C59_4	0.6988 (9)	0.7629 (5)	0.3216 (7)	0.095 (2)	0.701 (3)
H59A_4	0.774264	0.778993	0.368953	0.114*	0.701 (3)
H59B_4	0.678309	0.823604	0.330363	0.114*	0.701 (3)
C60_4	0.5883 (9)	0.7014 (6)	0.3292 (5)	0.101 (2)	0.701 (3)
H60A_4	0.605927	0.637898	0.313414	0.121*	0.701 (3)
H60B_4	0.510967	0.690699	0.285824	0.121*	0.701 (3)
Cl3_5	0.4780 (7)	0.7189 (5)	0.4506 (4)	0.1163 (9)	0.299 (3)
Cl4_5	0.7245 (6)	0.7266 (6)	0.2620 (7)	0.1089 (9)	0.299 (3)
C59_5	0.6496 (15)	0.7692 (8)	0.3646 (10)	0.095 (2)	0.299 (3)
H59A_5	0.710112	0.783221	0.420024	0.114*	0.299 (3)
H59B_5	0.621233	0.828558	0.377182	0.114*	0.299 (3)
C60_5	0.5391 (16)	0.6902 (11)	0.3426 (7)	0.101 (2)	0.299 (3)
H60A_5	0.565800	0.628325	0.318053	0.121*	0.299 (3)
H60B_5	0.471805	0.684416	0.294817	0.121*	0.299 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0277 (17)	0.0273 (16)	0.0280 (17)	0.0049 (13)	0.0087 (14)	0.0131 (14)
C2	0.0274 (17)	0.0254 (16)	0.0258 (17)	0.0002 (13)	0.0036 (14)	0.0106 (14)
C3	0.0256 (16)	0.0280 (16)	0.0302 (17)	0.0045 (13)	0.0077 (14)	0.0148 (14)
C4	0.0237 (16)	0.0261 (16)	0.0285 (17)	0.0038 (13)	0.0065 (13)	0.0123 (14)
C5	0.0241 (16)	0.0303 (17)	0.0289 (17)	0.0038 (13)	0.0083 (14)	0.0138 (14)
C6	0.0246 (16)	0.0271 (16)	0.0266 (17)	0.0051 (13)	0.0070 (13)	0.0117 (14)
C7	0.0277 (16)	0.0240 (16)	0.0313 (18)	0.0045 (13)	0.0100 (14)	0.0127 (14)
C8	0.0234 (16)	0.0268 (16)	0.0304 (18)	−0.0004 (13)	0.0065 (14)	0.0119 (14)
C9	0.0268 (16)	0.0231 (16)	0.0287 (17)	0.0038 (13)	0.0053 (14)	0.0100 (14)
C10	0.0248 (16)	0.0259 (16)	0.0274 (17)	0.0040 (13)	0.0061 (13)	0.0113 (14)
C11	0.0283 (17)	0.0297 (17)	0.0289 (17)	0.0042 (14)	0.0094 (14)	0.0146 (14)
C12	0.0265 (16)	0.0277 (16)	0.0279 (17)	0.0037 (13)	0.0070 (14)	0.0132 (14)
C13	0.0254 (16)	0.0257 (16)	0.0294 (17)	0.0028 (13)	0.0036 (14)	0.0122 (14)
C14	0.0323 (17)	0.0268 (16)	0.0259 (17)	0.0057 (14)	0.0099 (14)	0.0110 (14)
C15	0.0344 (18)	0.0321 (18)	0.0280 (17)	0.0039 (15)	0.0112 (15)	0.0098 (15)
C16	0.0305 (18)	0.0340 (18)	0.0304 (18)	0.0031 (15)	0.0111 (15)	0.0124 (15)
C17	0.0260 (16)	0.0294 (17)	0.0294 (17)	0.0035 (13)	0.0047 (14)	0.0141 (15)
C18	0.0239 (16)	0.0289 (17)	0.0302 (17)	0.0022 (13)	0.0028 (14)	0.0156 (14)
C19	0.0290 (17)	0.0348 (18)	0.0313 (18)	0.0036 (14)	0.0087 (14)	0.0163 (15)
C20	0.0333 (18)	0.0345 (18)	0.0347 (19)	−0.0003 (15)	0.0073 (15)	0.0186 (16)
C21	0.0403 (19)	0.0258 (17)	0.0286 (18)	−0.0009 (15)	0.0079 (15)	0.0075 (14)
C22	0.0339 (18)	0.0313 (18)	0.0278 (17)	0.0016 (15)	0.0072 (15)	0.0117 (15)
C23	0.041 (2)	0.037 (2)	0.038 (2)	−0.0018 (16)	0.0079 (17)	0.0171 (17)
C24	0.053 (3)	0.051 (2)	0.061 (3)	−0.014 (2)	0.023 (2)	0.020 (2)
C25	0.052 (3)	0.057 (3)	0.059 (3)	−0.015 (2)	0.010 (2)	0.022 (2)
C26	0.070 (3)	0.053 (3)	0.099 (4)	−0.003 (2)	0.017 (3)	0.047 (3)
C27	0.0290 (17)	0.0236 (16)	0.0283 (17)	−0.0003 (13)	0.0056 (14)	0.0089 (14)
C28	0.0305 (17)	0.0265 (16)	0.0291 (17)	0.0044 (14)	0.0054 (14)	0.0140 (14)
C29	0.0331 (18)	0.0283 (17)	0.0263 (17)	0.0014 (14)	0.0047 (14)	0.0115 (14)
C30	0.0322 (18)	0.0331 (18)	0.0310 (18)	−0.0007 (15)	0.0010 (15)	0.0139 (15)
C31	0.0295 (18)	0.040 (2)	0.0337 (19)	0.0027 (15)	0.0054 (15)	0.0118 (16)
C32	0.0289 (18)	0.0364 (19)	0.0316 (19)	0.0017 (15)	0.0074 (15)	0.0106 (16)
C33	0.036 (2)	0.047 (2)	0.0310 (19)	−0.0012 (17)	0.0002 (16)	0.0142 (17)
C34	0.051 (2)	0.080 (3)	0.032 (2)	−0.004 (2)	−0.0025 (19)	0.015 (2)

C35	0.055 (3)	0.068 (3)	0.053 (3)	0.006 (2)	−0.008 (2)	0.029 (2)
C36	0.040 (2)	0.050 (2)	0.043 (2)	−0.0082 (18)	−0.0028 (18)	0.0148 (19)
C37	0.0291 (17)	0.0310 (17)	0.0295 (17)	0.0033 (14)	0.0069 (14)	0.0156 (15)
C38	0.0281 (17)	0.0280 (17)	0.0325 (18)	−0.0011 (14)	0.0087 (14)	0.0115 (15)
C39	0.0355 (19)	0.0364 (19)	0.0329 (19)	−0.0024 (15)	0.0093 (16)	0.0131 (16)
C40	0.054 (2)	0.042 (2)	0.043 (2)	−0.0047 (19)	0.0213 (19)	0.0161 (19)
C41	0.040 (2)	0.042 (2)	0.064 (3)	0.0075 (18)	0.025 (2)	0.018 (2)
C42	0.040 (2)	0.043 (2)	0.067 (3)	0.0127 (18)	0.019 (2)	0.026 (2)
C43	0.0343 (19)	0.0311 (18)	0.046 (2)	0.0040 (15)	0.0125 (17)	0.0163 (17)
C44	0.056 (2)	0.064 (3)	0.046 (2)	0.009 (2)	0.013 (2)	0.034 (2)
C45	0.064 (3)	0.079 (3)	0.097 (4)	0.025 (3)	0.052 (3)	0.039 (3)
C46	0.052 (2)	0.072 (3)	0.067 (3)	0.026 (2)	0.017 (2)	0.045 (2)
C47	0.0321 (17)	0.0298 (17)	0.0268 (17)	0.0049 (14)	0.0102 (14)	0.0151 (14)
C48	0.0271 (16)	0.0239 (16)	0.0292 (17)	−0.0002 (13)	0.0065 (14)	0.0089 (14)
C49	0.0332 (18)	0.0345 (18)	0.0328 (19)	−0.0006 (15)	0.0085 (15)	0.0156 (16)
C50	0.041 (2)	0.042 (2)	0.0289 (19)	−0.0010 (17)	0.0073 (16)	0.0078 (17)
C51	0.035 (2)	0.0299 (19)	0.043 (2)	0.0006 (15)	0.0116 (17)	0.0040 (17)
C52	0.0337 (19)	0.0278 (18)	0.054 (2)	0.0041 (15)	0.0096 (17)	0.0149 (17)
C53	0.0265 (17)	0.0309 (18)	0.0391 (19)	−0.0013 (14)	0.0059 (15)	0.0158 (16)
C54	0.060 (2)	0.050 (2)	0.045 (2)	0.0092 (19)	0.0130 (19)	0.0299 (19)
C55	0.059 (3)	0.045 (2)	0.066 (3)	0.007 (2)	0.020 (2)	0.007 (2)
C56	0.046 (2)	0.047 (2)	0.050 (2)	0.0111 (18)	0.0035 (18)	0.0279 (19)
Cl1_1	0.0625 (9)	0.0707 (19)	0.0666 (15)	0.0049 (11)	0.0151 (8)	0.0351 (9)
Cl2_1	0.0671 (12)	0.144 (2)	0.1042 (16)	0.0167 (12)	0.0211 (11)	0.0678 (15)
C57_1	0.122 (6)	0.076 (5)	0.145 (7)	0.039 (5)	0.052 (5)	0.074 (5)
C58_1	0.075 (5)	0.102 (7)	0.080 (6)	0.045 (5)	0.014 (5)	0.016 (5)
Cl1_2	0.0625 (9)	0.0707 (19)	0.0666 (15)	0.0049 (11)	0.0151 (8)	0.0351 (9)
Cl2_2	0.0671 (12)	0.144 (2)	0.1042 (16)	0.0167 (12)	0.0211 (11)	0.0678 (15)
C57_2	0.122 (6)	0.076 (5)	0.145 (7)	0.039 (5)	0.052 (5)	0.074 (5)
C58_2	0.075 (5)	0.102 (7)	0.080 (6)	0.045 (5)	0.014 (5)	0.016 (5)
Cl1_3	0.0625 (9)	0.0707 (19)	0.0666 (15)	0.0049 (11)	0.0151 (8)	0.0351 (9)
Cl2_3	0.0671 (12)	0.144 (2)	0.1042 (16)	0.0167 (12)	0.0211 (11)	0.0678 (15)
C57_3	0.122 (6)	0.076 (5)	0.145 (7)	0.039 (5)	0.052 (5)	0.074 (5)
C58_3	0.075 (5)	0.102 (7)	0.080 (6)	0.045 (5)	0.014 (5)	0.016 (5)
Cl3_4	0.131 (2)	0.119 (2)	0.1126 (16)	0.0490 (18)	0.0046 (18)	0.0635 (16)
Cl4_4	0.0882 (12)	0.127 (2)	0.136 (3)	0.0560 (14)	0.0340 (18)	0.072 (2)
C59_4	0.086 (4)	0.090 (3)	0.113 (4)	0.046 (3)	0.001 (3)	0.048 (3)
C60_4	0.094 (4)	0.092 (3)	0.120 (4)	0.037 (3)	−0.004 (3)	0.052 (3)
Cl3_5	0.131 (2)	0.119 (2)	0.1126 (16)	0.0490 (18)	0.0046 (18)	0.0635 (16)
Cl4_5	0.0882 (12)	0.127 (2)	0.136 (3)	0.0560 (14)	0.0340 (18)	0.072 (2)
C59_5	0.086 (4)	0.090 (3)	0.113 (4)	0.046 (3)	0.001 (3)	0.048 (3)
C60_5	0.094 (4)	0.092 (3)	0.120 (4)	0.037 (3)	−0.004 (3)	0.052 (3)

Geometric parameters (Å, °)

C1—C2	1.388 (4)	C38—C43	1.401 (5)
C1—C6	1.426 (4)	C39—C40	1.394 (5)
C1—C7 ⁱ	1.462 (4)	C39—C44	1.499 (5)
C2—C3	1.435 (4)	C40—C41	1.391 (6)
C2—H2	0.9500	C40—H40	0.9500
C3—C4	1.388 (4)	C41—C42	1.371 (6)
C3—C17	1.470 (4)	C41—C45	1.511 (5)

C4—C5	1.410 (4)	C42—C43	1.387 (5)
C4—C12	1.457 (4)	C42—H42	0.9500
C5—C6	1.387 (4)	C43—C46	1.504 (5)
C5—C10	1.398 (4)	C44—H44A	0.9800
C6—C7	1.428 (4)	C44—H44B	0.9800
C7—C8	1.391 (4)	C44—H44C	0.9800
C8—C9	1.424 (4)	C45—H45A	0.9800
C8—H8	0.9500	C45—H45B	0.9800
C9—C10	1.381 (4)	C45—H45C	0.9800
C9—C27	1.469 (4)	C46—H46A	0.9800
C10—C13	1.453 (4)	C46—H46B	0.9800
C11—C37	1.383 (4)	C46—H46C	0.9800
C11—C12	1.428 (4)	C47—C48	1.506 (4)
C11—C16	1.456 (4)	C48—C53	1.399 (5)
C12—C13	1.382 (4)	C48—C49	1.401 (4)
C13—C14	1.434 (4)	C49—C50	1.402 (5)
C14—C47	1.380 (4)	C49—C54	1.500 (5)
C14—C15	1.454 (4)	C50—C51	1.378 (5)
C15—C16	1.346 (4)	C50—H50	0.9500
C15—H15	0.9500	C51—C52	1.376 (5)
C16—H16	0.9500	C51—C55	1.524 (5)
C17—C22	1.400 (4)	C52—C53	1.389 (5)
C17—C18	1.438 (4)	C52—H52	0.9500
C18—C19	1.411 (4)	C53—C56	1.506 (5)
C18—C37	1.482 (4)	C54—H54A	0.9800
C19—C20	1.383 (4)	C54—H54B	0.9800
C19—H19	0.9500	C54—H54C	0.9800
C20—C21	1.392 (5)	C55—H55A	0.9800
C20—C23	1.532 (4)	C55—H55B	0.9800
C21—C22	1.376 (4)	C55—H55C	0.9800
C21—H21	0.9500	C56—H56A	0.9800
C22—H22	0.9500	C56—H56B	0.9800
C23—C26	1.526 (6)	C56—H56C	0.9800
C23—C25	1.527 (5)	Cl1_1—C57_1	1.768 (6)
C23—C24	1.530 (5)	Cl2_1—C58_1	1.745 (7)
C24—H24A	0.9800	C57_1—C58_1	1.460 (10)
C24—H24B	0.9800	C57_1—H57A_1	0.9900
C24—H24C	0.9800	C57_1—H57B_1	0.9900
C25—H25A	0.9800	C58_1—H58A_1	0.9900
C25—H25B	0.9800	C58_1—H58B_1	0.9900
C25—H25C	0.9800	Cl1_2—C57_2	1.768 (7)
C26—H26A	0.9800	Cl2_2—C58_2	1.745 (7)
C26—H26B	0.9800	C57_2—C58_2	1.460 (10)
C26—H26C	0.9800	C57_2—H57A_2	0.9900
C27—C32	1.408 (4)	C57_2—H57B_2	0.9900
C27—C28	1.430 (4)	C58_2—H58A_2	0.9900
C28—C29	1.411 (4)	C58_2—H58B_2	0.9900
C28—C47	1.494 (4)	Cl1_3—C57_3	1.768 (7)
C29—C30	1.381 (4)	Cl1_3—Cl1_3 ⁱⁱ	2.28 (3)
C29—H29	0.9500	Cl2_3—C58_3	1.745 (7)
C30—C31	1.393 (5)	C57_3—C58_3	1.460 (10)
C30—C33	1.537 (5)	C57_3—H57A_3	0.9900

C31—C32	1.365 (5)	C57_3—H57B_3	0.9900
C31—H31	0.9500	C58_3—H58A_3	0.9900
C32—H32	0.9500	C58_3—H58B_3	0.9900
C33—C35	1.524 (6)	Cl3_4—C60_4	1.818 (8)
C33—C34	1.528 (5)	Cl4_4—C59_4	1.805 (10)
C33—C36	1.535 (5)	C59_4—C60_4	1.463 (11)
C34—H34A	0.9800	C59_4—H59A_4	0.9900
C34—H34B	0.9800	C59_4—H59B_4	0.9900
C34—H34C	0.9800	C60_4—H60A_4	0.9900
C35—H35A	0.9800	C60_4—H60B_4	0.9900
C35—H35B	0.9800	Cl3_5—C60_5	1.818 (8)
C35—H35C	0.9800	Cl4_5—C59_5	1.805 (10)
C36—H36A	0.9800	C59_5—C60_5	1.463 (11)
C36—H36B	0.9800	C59_5—H59A_5	0.9900
C36—H36C	0.9800	C59_5—H59B_5	0.9900
C37—C38	1.503 (4)	C60_5—H60A_5	0.9900
C38—C39	1.398 (5)	C60_5—H60B_5	0.9900
C2—C1—C6	118.6 (3)	C39—C38—C37	121.6 (3)
C2—C1—C7 ⁱ	125.4 (3)	C43—C38—C37	118.3 (3)
C6—C1—C7 ⁱ	116.0 (3)	C40—C39—C38	118.4 (3)
C1—C2—C3	124.7 (3)	C40—C39—C44	120.9 (3)
C1—C2—H2	117.7	C38—C39—C44	120.7 (3)
C3—C2—H2	117.7	C41—C40—C39	122.0 (4)
C4—C3—C2	115.6 (3)	C41—C40—H40	119.0
C4—C3—C17	123.1 (3)	C39—C40—H40	119.0
C2—C3—C17	121.2 (3)	C42—C41—C40	118.2 (3)
C3—C4—C5	119.8 (3)	C42—C41—C45	121.6 (4)
C3—C4—C12	134.3 (3)	C40—C41—C45	120.2 (4)
C5—C4—C12	105.9 (3)	C41—C42—C43	121.8 (4)
C6—C5—C10	125.0 (3)	C41—C42—H42	119.1
C6—C5—C4	124.6 (3)	C43—C42—H42	119.1
C10—C5—C4	110.5 (3)	C42—C43—C38	119.4 (3)
C5—C6—C1	116.6 (3)	C42—C43—C46	119.3 (3)
C5—C6—C7	116.2 (3)	C38—C43—C46	121.2 (3)
C1—C6—C7	127.1 (3)	C39—C44—H44A	109.5
C8—C7—C6	118.2 (3)	C39—C44—H44B	109.5
C8—C7—C1 ⁱ	124.9 (3)	H44A—C44—H44B	109.5
C6—C7—C1 ⁱ	116.9 (3)	C39—C44—H44C	109.5
C7—C8—C9	124.7 (3)	H44A—C44—H44C	109.5
C7—C8—H8	117.6	H44B—C44—H44C	109.5
C9—C8—H8	117.6	C41—C45—H45A	109.5
C10—C9—C8	115.9 (3)	C41—C45—H45B	109.5
C10—C9—C27	122.5 (3)	H45A—C45—H45B	109.5
C8—C9—C27	121.3 (3)	C41—C45—H45C	109.5
C9—C10—C5	119.7 (3)	H45A—C45—H45C	109.5
C9—C10—C13	133.9 (3)	H45B—C45—H45C	109.5
C5—C10—C13	106.4 (3)	C43—C46—H46A	109.5
C37—C11—C12	125.2 (3)	C43—C46—H46B	109.5
C37—C11—C16	121.7 (3)	H46A—C46—H46B	109.5
C12—C11—C16	113.0 (3)	C43—C46—H46C	109.5
C13—C12—C11	123.4 (3)	H46A—C46—H46C	109.5

C13—C12—C4	108.5 (3)	H46B—C46—H46C	109.5
C11—C12—C4	126.6 (3)	C14—C47—C28	127.5 (3)
C12—C13—C14	123.5 (3)	C14—C47—C48	116.7 (3)
C12—C13—C10	108.5 (3)	C28—C47—C48	115.8 (3)
C14—C13—C10	126.0 (3)	C53—C48—C49	119.9 (3)
C47—C14—C13	125.7 (3)	C53—C48—C47	117.9 (3)
C47—C14—C15	121.7 (3)	C49—C48—C47	122.2 (3)
C13—C14—C15	112.6 (3)	C48—C49—C50	118.2 (3)
C16—C15—C14	124.0 (3)	C48—C49—C54	121.4 (3)
C16—C15—H15	118.0	C50—C49—C54	120.5 (3)
C14—C15—H15	118.0	C51—C50—C49	122.4 (3)
C15—C16—C11	123.4 (3)	C51—C50—H50	118.8
C15—C16—H16	118.3	C49—C50—H50	118.8
C11—C16—H16	118.3	C52—C51—C50	118.1 (3)
C22—C17—C18	116.9 (3)	C52—C51—C55	121.9 (4)
C22—C17—C3	117.5 (3)	C50—C51—C55	120.0 (4)
C18—C17—C3	125.5 (3)	C51—C52—C53	122.0 (3)
C19—C18—C17	116.6 (3)	C51—C52—H52	119.0
C19—C18—C37	113.6 (3)	C53—C52—H52	119.0
C17—C18—C37	129.8 (3)	C52—C53—C48	119.3 (3)
C20—C19—C18	125.5 (3)	C52—C53—C56	120.0 (3)
C20—C19—H19	117.3	C48—C53—C56	120.8 (3)
C18—C19—H19	117.3	C49—C54—H54A	109.5
C19—C20—C21	116.5 (3)	C49—C54—H54B	109.5
C19—C20—C23	122.2 (3)	H54A—C54—H54B	109.5
C21—C20—C23	121.3 (3)	C49—C54—H54C	109.5
C22—C21—C20	120.3 (3)	H54A—C54—H54C	109.5
C22—C21—H21	119.8	H54B—C54—H54C	109.5
C20—C21—H21	119.8	C51—C55—H55A	109.5
C21—C22—C17	124.1 (3)	C51—C55—H55B	109.5
C21—C22—H22	117.9	H55A—C55—H55B	109.5
C17—C22—H22	117.9	C51—C55—H55C	109.5
C26—C23—C25	109.8 (3)	H55A—C55—H55C	109.5
C26—C23—C24	108.7 (3)	H55B—C55—H55C	109.5
C25—C23—C24	107.6 (3)	C53—C56—H56A	109.5
C26—C23—C20	108.5 (3)	C53—C56—H56B	109.5
C25—C23—C20	109.9 (3)	H56A—C56—H56B	109.5
C24—C23—C20	112.3 (3)	C53—C56—H56C	109.5
C23—C24—H24A	109.5	H56A—C56—H56C	109.5
C23—C24—H24B	109.5	H56B—C56—H56C	109.5
H24A—C24—H24B	109.5	C58_1—C57_1—C11_1	111.9 (5)
C23—C24—H24C	109.5	C58_1—C57_1—H57A_1	109.2
H24A—C24—H24C	109.5	C11_1—C57_1—H57A_1	109.2
H24B—C24—H24C	109.5	C58_1—C57_1—H57B_1	109.2
C23—C25—H25A	109.5	C11_1—C57_1—H57B_1	109.2
C23—C25—H25B	109.5	H57A_1—C57_1—H57B_1	107.9
H25A—C25—H25B	109.5	C57_1—C58_1—C12_1	113.4 (5)
C23—C25—H25C	109.5	C57_1—C58_1—H58A_1	108.9
H25A—C25—H25C	109.5	C12_1—C58_1—H58A_1	108.9
H25B—C25—H25C	109.5	C57_1—C58_1—H58B_1	108.9
C23—C26—H26A	109.5	C12_1—C58_1—H58B_1	108.9
C23—C26—H26B	109.5	H58A_1—C58_1—H58B_1	107.7

H26A—C26—H26B	109.5	C58_2—C57_2—Cl1_2	111.8 (5)
C23—C26—H26C	109.5	C58_2—C57_2—H57A_2	109.3
H26A—C26—H26C	109.5	Cl1_2—C57_2—H57A_2	109.3
H26B—C26—H26C	109.5	C58_2—C57_2—H57B_2	109.3
C32—C27—C28	117.4 (3)	Cl1_2—C57_2—H57B_2	109.3
C32—C27—C9	116.5 (3)	H57A_2—C57_2—H57B_2	107.9
C28—C27—C9	126.0 (3)	C57_2—C58_2—Cl2_2	113.4 (5)
C29—C28—C27	116.6 (3)	C57_2—C58_2—H58A_2	108.9
C29—C28—C47	114.9 (3)	Cl2_2—C58_2—H58A_2	108.9
C27—C28—C47	128.6 (3)	C57_2—C58_2—H58B_2	108.9
C30—C29—C28	124.9 (3)	Cl2_2—C58_2—H58B_2	108.9
C30—C29—H29	117.6	H58A_2—C58_2—H58B_2	107.7
C28—C29—H29	117.6	C57_3—Cl1_3—Cl1_3 ⁱⁱ	154 (2)
C29—C30—C31	117.3 (3)	C58_3—C57_3—Cl1_3	111.8 (5)
C29—C30—C33	123.1 (3)	C58_3—C57_3—H57A_3	109.2
C31—C30—C33	119.5 (3)	Cl1_3—C57_3—H57A_3	109.2
C32—C31—C30	119.9 (3)	C58_3—C57_3—H57B_3	109.2
C32—C31—H31	120.0	Cl1_3—C57_3—H57B_3	109.3
C30—C31—H31	120.0	H57A_3—C57_3—H57B_3	107.9
C31—C32—C27	123.8 (3)	C57_3—C58_3—Cl2_3	113.4 (5)
C31—C32—H32	118.1	C57_3—C58_3—H58A_3	108.9
C27—C32—H32	118.1	Cl2_3—C58_3—H58A_3	108.9
C35—C33—C34	109.4 (3)	C57_3—C58_3—H58B_3	108.9
C35—C33—C36	109.3 (3)	Cl2_3—C58_3—H58B_3	108.9
C34—C33—C36	108.0 (3)	H58A_3—C58_3—H58B_3	107.7
C35—C33—C30	109.6 (3)	C60_4—C59_4—Cl4_4	105.0 (5)
C34—C33—C30	111.8 (3)	C60_4—C59_4—H59A_4	110.7
C36—C33—C30	108.7 (3)	Cl4_4—C59_4—H59A_4	110.7
C33—C34—H34A	109.5	C60_4—C59_4—H59B_4	110.7
C33—C34—H34B	109.5	Cl4_4—C59_4—H59B_4	110.7
H34A—C34—H34B	109.5	H59A_4—C59_4—H59B_4	108.8
C33—C34—H34C	109.5	C59_4—C60_4—Cl3_4	106.9 (6)
H34A—C34—H34C	109.5	C59_4—C60_4—H60A_4	110.3
H34B—C34—H34C	109.5	Cl3_4—C60_4—H60A_4	110.3
C33—C35—H35A	109.5	C59_4—C60_4—H60B_4	110.3
C33—C35—H35B	109.5	Cl3_4—C60_4—H60B_4	110.3
H35A—C35—H35B	109.5	H60A_4—C60_4—H60B_4	108.6
C33—C35—H35C	109.5	C60_5—C59_5—Cl4_5	105.0 (5)
H35A—C35—H35C	109.5	C60_5—C59_5—H59A_5	110.8
H35B—C35—H35C	109.5	Cl4_5—C59_5—H59A_5	110.8
C33—C36—H36A	109.5	C60_5—C59_5—H59B_5	110.8
C33—C36—H36B	109.5	Cl4_5—C59_5—H59B_5	110.8
H36A—C36—H36B	109.5	H59A_5—C59_5—H59B_5	108.8
C33—C36—H36C	109.5	C59_5—C60_5—Cl3_5	107.0 (6)
H36A—C36—H36C	109.5	C59_5—C60_5—H60A_5	110.3
H36B—C36—H36C	109.5	Cl3_5—C60_5—H60A_5	110.3
C11—C37—C18	128.7 (3)	C59_5—C60_5—H60B_5	110.3
C11—C37—C38	115.0 (3)	Cl3_5—C60_5—H60B_5	110.3
C18—C37—C38	116.3 (3)	H60A_5—C60_5—H60B_5	108.6
C39—C38—C43	119.9 (3)		

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+1, -z+1$.