X-ray Structure Report

for

190424R

April 26, 2019

Experimental

Data Collection

A colorless prism crystal of $C_{28}H_{18}$ having approximate dimensions of 0.200 x 0.200 x 0.100 mm was mounted on a glass fiber. All measurements were made on a Rigaku R-AXIS RAPID diffractometer using multi-layer mirror monochromated Cu-Kα radiation.

The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 9.5683(5) Å
b = 35.080(2) Å β = 107.439(8)^o
c = 5.8336(4) Å
V = 1868.1(2) Å^3

For Z = 4 and F.W. = 354.45, the calculated density is 1.260 g/cm^3. The reflection conditions of:

h0l: l = 2n
0k0: k = 2n

uniquely determine the space group to be:

$P2_1/c$ (#14)

The data were collected at a temperature of 23 $\pm$ 1^{o}C to a maximum 2θ value of 136.5^o. A total of 60 oscillation images were collected. A sweep of data was done using ω scans from 80.0 to 260.0^o in 15.00^o step, at χ=54.0^o and ϕ = 0.0^o. The exposure rate was 32.0 [sec./^{o}]. A second sweep was performed using ω scans from 80.0 to 260.0^o in 15.00^o step, at χ=54.0^o and ϕ = 90.0^o. The exposure rate was 32.0 [sec./^{o}]. Another sweep was performed using ω scans from 80.0 to 260.0^o in 15.00^o step, at χ=54.0^o and ϕ = 180.0^o. The exposure rate was 32.0 [sec./^{o}]. Another sweep was performed using ω scans from 80.0 to 260.0^o in 15.00^o step, at χ=54.0^o and ϕ = 270.0^o. The

exposure rate was 32.0 [sec./^{o}]. Another sweep was performed using ω scans from 80.0 to 260.0^{o} in 15.00^{o} step, at χ=0.0^{o} and ϕ = 0.0^{o}. The exposure rate was 32.0 [sec./^{o}]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 20141 reflections were collected, where 3407 were unique (R_{int} = 0.1312); equivalent reflections were merged.

The linear absorption coefficient, μ, for Cu-Kα radiation is 5.418 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.436 to 0.947. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[2] on F^{2} was based on 3407 observed reflections and 253 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0701$$

$$wR2 = [\Sigma \, (w \, (Fo^{2} - Fc^{2})^{2}) / \Sigma \, w(Fo^{2})^{2}]^{1/2} = 0.2163$$

The goodness of fit[3] was 1.05. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.21 and -0.18 e^{-}/Å^{3}, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 [4]. Anomalous dispersion effects were included in Fcalc[5]; the values for Δf' and Δf'' were those of Creagh and McAuley[6]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[7]. All calculations were performed using the CrystalStructure[8] crystallographic software package except for refinement, which was performed using SHELXL Version 2013/4[9].

References

(1) SHELXT Version 2014/4: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(2) Least Squares function minimized: (SHELXL Version 2013/4)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(3) Goodness of fit is defined as:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(4) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(5) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(6) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(7) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(8) CrystalStructure 4.3: Crystal Structure Analysis Package, Rigaku Corporation (2000-2019). Tokyo 196-8666, Japan.

(9) SHELXL Version 2013/4: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{28}H_{18}$
Formula Weight	354.45
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.200 X 0.200 X 0.100 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 9.5683(5) Å b = 35.080(2) Å c = 5.8336(4) Å β = 107.439(8) ^{o} V = 1868.1(2) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.260 g/cm^3
F_{000}	744.00
μ(CuKα)	5.418 cm^{-1}

B. Intensity Measurements

Diffractometer	R-AXIS RAPID
Radiation	CuKα (λ = 1.54187 Å) multi-layer mirror monochromated
Voltage, Current	40kV, 30mA
Temperature	23.0^{o}C
Detector Aperture	460.0 x 256.0 mm
Data Images	60 exposures
ω oscillation Range (χ=54.0, ϕ=0.0)	80.0 - 260.0^{o}
Exposure Rate	32.0 sec./^{o}
ω oscillation Range (χ=54.0, ϕ=90.0)	80.0 - 260.0^{o}
Exposure Rate	32.0 sec./^{o}
ω oscillation Range (χ=54.0, ϕ=180.0)	80.0 - 260.0^{o}
Exposure Rate	32.0 sec./^{o}
ω oscillation Range (χ=54.0, ϕ=270.0)	80.0 - 260.0^{o}
Exposure Rate	32.0 sec./^{o}
ω oscillation Range (χ=0.0, ϕ=0.0)	80.0 - 260.0^{o}
Exposure Rate	32.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	136.5^{o}
No. of Reflections Measured	Total: 20141

	Unique: 3407 (R_{int} = 0.1312)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.436 - 0.947)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXT Version 2014/4)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0865 \cdot P)^2 + 0.0000 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	136.5^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	3407
No. Variables	253
Reflection/Parameter Ratio	13.47
Residuals: R1 (I>2.00σ(I))	0.0701
Residuals: R (All reflections)	0.0900
Residuals: wR2 (All reflections)	0.2163
Goodness of Fit Indicator	1.046
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.21 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.18 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
C1	0.5047(3)	0.33668(6)	0.8241(5)	5.34(5)
C2	0.8195(2)	0.39534(7)	0.7247(5)	5.38(5)
C3	0.5858(3)	0.36537(6)	0.7370(4)	5.29(5)
C4	0.5003(2)	0.39493(7)	0.5651(5)	5.44(5)
C5	0.7347(3)	0.36543(6)	0.8095(5)	5.31(5)
C6	0.8165(3)	0.33720(6)	0.9797(5)	5.38(5)
C7	0.7407(3)	0.30891(6)	1.0687(5)	5.60(6)
C8	0.5806(3)	0.30880(7)	0.9896(5)	5.53(5)
C9	0.8230(2)	0.43304(7)	0.8055(5)	5.69(6)
C10	0.4911(3)	0.43240(7)	0.6399(5)	5.65(6)
C11	0.3500(3)	0.33659(7)	0.7543(5)	6.04(6)
C12	0.9053(3)	0.38512(7)	0.5793(5)	6.01(6)
C13	0.9706(3)	0.33735(7)	1.0644(5)	6.08(6)
C14	0.4177(3)	0.38407(7)	0.3337(5)	6.04(6)
C15	0.9977(3)	0.41104(8)	0.5202(5)	6.55(6)
C16	0.7292(3)	0.44696(6)	0.9487(5)	6.36(6)
C17	0.4989(3)	0.28180(7)	1.0731(5)	6.49(6)
C18	0.5829(3)	0.44659(7)	0.8753(5)	6.41(6)
C19	0.8241(3)	0.28211(7)	1.2351(5)	6.52(6)
C20	1.0058(3)	0.44767(8)	0.6056(5)	6.67(7)
C21	0.3255(3)	0.40955(8)	0.1802(5)	6.55(6)
C22	0.3937(3)	0.45730(7)	0.4856(6)	6.73(7)
C23	0.3496(3)	0.28231(8)	1.0015(5)	6.91(7)
C24	0.9194(3)	0.45847(7)	0.7452(5)	6.61(7)
C25	0.2739(3)	0.30991(8)	0.8401(5)	6.69(6)
C26	0.9719(3)	0.28289(8)	1.3120(5)	6.86(7)
C27	1.0465(3)	0.31077(8)	1.2265(5)	6.63(6)
C28	0.3113(3)	0.44605(8)	0.2583(6)	7.09(7)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H11	0.29867	0.35507	0.64767	7.247
H12	0.90030	0.36034	0.52070	7.209
H13	1.02205	0.35589	1.00916	7.294
H14	0.42502	0.35926	0.28222	7.246
H15	1.05426	0.40368	0.42293	7.859
H16	0.77553	0.45667	1.10084	7.635
H17	0.54792	0.26308	1.17994	7.783
H18	0.53505	0.45600	0.98071	7.693
H19	0.77538	0.26329	1.29363	7.826
H20	1.06928	0.46511	0.56931	8.007
H21	0.27322	0.40215	0.02509	7.860
H22	0.38396	0.48200	0.53660	8.078
H23	0.29818	0.26421	1.06061	8.298
H24	0.92522	0.48341	0.80139	7.932
H25	0.17202	0.31021	0.79071	8.030
H26	1.02355	0.26485	1.42170	8.237
H27	1.14828	0.31142	1.27944	7.953
H28	0.24642	0.46305	0.15819	8.503

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.0633(16)	0.0610(15)	0.0785(17)	-0.0017(12)	0.0208(13)	-0.0043(13)
C2	0.0550(14)	0.0688(16)	0.0816(17)	-0.0011(12)	0.0219(13)	0.0043(13)
C3	0.0614(15)	0.0612(14)	0.0784(16)	-0.0004(12)	0.0207(13)	-0.0027(13)
C4	0.0560(14)	0.0657(16)	0.0867(19)	-0.0018(12)	0.0238(13)	0.0028(14)
C5	0.0631(15)	0.0598(14)	0.0787(17)	-0.0014(12)	0.0212(13)	-0.0014(12)
C6	0.0612(15)	0.0652(15)	0.0783(17)	0.0033(12)	0.0210(13)	-0.0039(13)
C7	0.0712(17)	0.0627(15)	0.0785(18)	-0.0000(13)	0.0219(14)	-0.0017(13)
C8	0.0685(17)	0.0611(15)	0.0806(17)	-0.0031(13)	0.0227(14)	-0.0026(13)
C9	0.0553(15)	0.0717(16)	0.0872(19)	-0.0030(12)	0.0186(14)	-0.0006(14)
C10	0.0561(14)	0.0683(16)	0.0925(19)	-0.0007(13)	0.0254(14)	-0.0002(14)
C11	0.0649(17)	0.0793(17)	0.0850(19)	-0.0047(13)	0.0220(14)	0.0006(14)
C12	0.0692(17)	0.0750(16)	0.0878(19)	-0.0026(14)	0.0292(15)	-0.0001(14)
C13	0.0651(17)	0.0812(17)	0.0844(19)	0.0037(14)	0.0221(14)	0.0024(14)
C14	0.0670(16)	0.0755(17)	0.0855(19)	0.0037(14)	0.0207(15)	-0.0003(15)
C15	0.0713(17)	0.0869(19)	0.096(2)	0.0004(15)	0.0325(15)	0.0078(17)
C16	0.0731(18)	0.0779(17)	0.0884(19)	-0.0010(14)	0.0206(16)	-0.0067(15)
C17	0.0792(19)	0.0730(18)	0.096(2)	-0.0060(14)	0.0293(16)	0.0034(15)
C18	0.0743(18)	0.0770(17)	0.098(2)	-0.0030(14)	0.0352(17)	-0.0103(15)
C19	0.082(2)	0.0725(17)	0.092(2)	0.0048(14)	0.0245(17)	0.0090(15)
C20	0.0695(18)	0.0817(19)	0.106(2)	-0.0097(14)	0.0325(17)	0.0103(17)
C21	0.0713(17)	0.088(2)	0.0857(19)	0.0005(15)	0.0183(15)	0.0057(16)
C22	0.0702(17)	0.0717(18)	0.115(2)	0.0070(14)	0.0296(18)	0.0025(17)
C23	0.082(2)	0.084(2)	0.101(2)	-0.0148(16)	0.0334(17)	0.0039(17)
C24	0.0681(17)	0.0743(18)	0.105(2)	-0.0084(14)	0.0200(16)	-0.0033(16)
C25	0.0693(17)	0.0909(19)	0.095(2)	-0.0137(15)	0.0256(16)	-0.0084(17)
C26	0.081(2)	0.0836(19)	0.093(2)	0.0134(16)	0.0212(17)	0.0103(16)
C27	0.0696(18)	0.095(2)	0.084(2)	0.0094(15)	0.0183(15)	-0.0017(16)
C28	0.0696(18)	0.084(2)	0.112(3)	0.0100(15)	0.0223(18)	0.0188(18)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
C1	C3	1.453(4)	C1	C8	1.413(3)
C1	C11	1.413(4)	C2	C5	1.498(4)
C2	C9	1.401(4)	C2	C12	1.393(4)
C3	C4	1.503(3)	C3	C5	1.359(3)
C4	C10	1.396(4)	C4	C14	1.397(3)
C5	C6	1.454(3)	C6	C7	1.416(4)
C6	C13	1.407(3)	C7	C8	1.462(4)
C7	C19	1.414(3)	C8	C17	1.405(4)
C9	C16	1.480(4)	C9	C24	1.402(4)
C10	C18	1.477(4)	C10	C22	1.393(3)
C11	C25	1.369(4)	C12	C15	1.382(4)
C13	C27	1.371(4)	C14	C21	1.381(3)
C15	C20	1.372(4)	C16	C18	1.336(4)
C17	C23	1.363(4)	C19	C26	1.350(4)
C20	C24	1.376(5)	C21	C28	1.379(4)
C22	C28	1.382(4)	C23	C25	1.393(4)
C26	C27	1.388(4)			

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C11	H11	0.930	C12	H12	0.930
C13	H13	0.930	C14	H14	0.930
C15	H15	0.930	C16	H16	0.930
C17	H17	0.930	C18	H18	0.930
C19	H19	0.930	C20	H20	0.930
C21	H21	0.930	C22	H22	0.930
C23	H23	0.930	C24	H24	0.930
C25	H25	0.930	C26	H26	0.930
C27	H27	0.930	C28	H28	0.930

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C3	C1	C8	119.9(2)	C3	C1	C11	121.6(2)
C8	C1	C11	118.4(2)	C5	C2	C9	120.7(2)
C5	C2	C12	119.8(2)	C9	C2	C12	119.3(2)
C1	C3	C4	118.0(2)	C1	C3	C5	120.8(2)
C4	C3	C5	121.1(2)	C3	C4	C10	120.9(2)
C3	C4	C14	119.6(2)	C10	C4	C14	119.2(2)
C2	C5	C3	121.3(2)	C2	C5	C6	117.9(2)
C3	C5	C6	120.7(2)	C5	C6	C7	119.8(2)
C5	C6	C13	122.0(2)	C7	C6	C13	118.1(2)
C6	C7	C8	119.3(2)	C6	C7	C19	118.2(2)
C8	C7	C19	122.5(2)	C1	C8	C7	119.3(2)
C1	C8	C17	118.5(2)	C7	C8	C17	122.1(2)
C2	C9	C16	123.0(2)	C2	C9	C24	117.9(3)
C16	C9	C24	119.2(2)	C4	C10	C18	122.2(2)
C4	C10	C22	118.7(2)	C18	C10	C22	119.1(2)
C1	C11	C25	121.5(2)	C2	C12	C15	121.4(2)
C6	C13	C27	121.5(3)	C4	C14	C21	121.1(2)
C12	C15	C20	119.7(3)	C9	C16	C18	124.8(3)
C8	C17	C23	121.8(2)	C10	C18	C16	125.1(3)
C7	C19	C26	122.3(3)	C15	C20	C24	119.6(3)
C14	C21	C28	119.6(3)	C10	C22	C28	121.3(2)
C17	C23	C25	120.1(3)	C9	C24	C20	122.0(2)
C11	C25	C23	119.8(3)	C19	C26	C27	119.7(2)
C13	C27	C26	120.3(3)	C21	C28	C22	119.9(2)

Table 7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C1	C11	H11	119.3	C25	C11	H11	119.3
C2	C12	H12	119.3	C15	C12	H12	119.3
C6	C13	H13	119.3	C27	C13	H13	119.3
C4	C14	H14	119.4	C21	C14	H14	119.5
C12	C15	H15	120.1	C20	C15	H15	120.1
C9	C16	H16	117.6	C18	C16	H16	117.6
C8	C17	H17	119.1	C23	C17	H17	119.1
C10	C18	H18	117.5	C16	C18	H18	117.5
C7	C19	H19	118.9	C26	C19	H19	118.9
C15	C20	H20	120.2	C24	C20	H20	120.2
C14	C21	H21	120.2	C28	C21	H21	120.2
C10	C22	H22	119.3	C28	C22	H22	119.3
C17	C23	H23	120.0	C25	C23	H23	120.0
C9	C24	H24	119.0	C20	C24	H24	119.0
C11	C25	H25	120.1	C23	C25	H25	120.1
C19	C26	H26	120.2	C27	C26	H26	120.2
C13	C27	H27	119.9	C26	C27	H27	119.9
C21	C28	H28	120.1	C22	C28	H28	120.1

Table 8. Torsion Angles(O)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C3	C1	C8	C7	-0.9(4)	C3	C1	C8	C17	179.1(2)
C8	C1	C3	C4	-178.7(2)	C8	C1	C3	C5	1.2(4)
C3	C1	C11	C25	-178.8(2)	C11	C1	C3	C4	-1.1(3)
C11	C1	C3	C5	178.8(2)	C8	C1	C11	C25	-1.1(4)
C11	C1	C8	C7	-178.6(2)	C11	C1	C8	C17	1.3(4)
C5	C2	C9	C16	-8.8(3)	C5	C2	C9	C24	171.67(17)
C9	C2	C5	C3	70.8(3)	C9	C2	C5	C6	-106.9(2)
C5	C2	C12	C15	-172.55(17)	C12	C2	C5	C3	-114.4(2)
C12	C2	C5	C6	68.0(3)	C9	C2	C12	C15	2.4(3)
C12	C2	C9	C16	176.36(18)	C12	C2	C9	C24	-3.2(3)
C1	C3	C4	C10	106.2(2)	C1	C3	C4	C14	-67.8(3)
C1	C3	C5	C2	-178.8(2)	C1	C3	C5	C6	-1.2(4)
C4	C3	C5	C2	1.1(4)	C4	C3	C5	C6	178.7(2)
C5	C3	C4	C10	-73.7(3)	C5	C3	C4	C14	112.3(3)
C3	C4	C10	C18	10.3(4)	C3	C4	C10	C22	-170.6(2)
C3	C4	C14	C21	172.9(2)	C10	C4	C14	C21	-1.3(4)
C14	C4	C10	C18	-175.6(2)	C14	C4	C10	C22	3.4(4)
C2	C5	C6	C7	178.6(2)	C2	C5	C6	C13	-0.1(3)
C3	C5	C6	C7	1.0(4)	C3	C5	C6	C13	-177.7(2)
C5	C6	C7	C8	-0.6(3)	C5	C6	C7	C19	-179.6(2)
C5	C6	C13	C27	179.4(2)	C7	C6	C13	C27	0.7(4)
C13	C6	C7	C8	178.1(2)	C13	C6	C7	C19	-0.8(3)
C6	C7	C8	C1	0.6(4)	C6	C7	C8	C17	-179.3(2)
C6	C7	C19	C26	0.5(4)	C8	C7	C19	C26	-178.4(2)
C19	C7	C8	C1	179.5(2)	C19	C7	C8	C17	-0.4(4)
C1	C8	C17	C23	-1.1(4)	C7	C8	C17	C23	178.8(2)
C2	C9	C16	C18	-60.0(3)	C2	C9	C24	C20	1.9(3)
C16	C9	C24	C20	-177.70(19)	C24	C9	C16	C18	119.5(2)
C4	C10	C18	C16	59.2(4)	C4	C10	C22	C28	-2.7(4)
C18	C10	C22	C28	176.4(3)	C22	C10	C18	C16	-119.8(3)
C1	C11	C25	C23	0.6(4)	C2	C12	C15	C20	-0.0(3)
C6	C13	C27	C26	-0.2(4)	C4	C14	C21	C28	-1.8(4)
C12	C15	C20	C24	-1.4(3)	C9	C16	C18	C10	-0.2(4)
C8	C17	C23	C25	0.5(4)	C7	C19	C26	C27	-0.0(4)
C15	C20	C24	C9	0.4(4)	C14	C21	C28	C22	2.6(4)
C10	C22	C28	C21	-0.4(5)	C17	C23	C25	C11	-0.3(4)
C19	C26	C27	C13	-0.2(4)					

Table 9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
C1	C6	2.847(3)	C1	C10	3.516(3)
C1	C14	3.196(4)	C1	C23	2.799(4)
C2	C4	2.914(3)	C2	C10	3.297(3)
C2	C13	2.905(3)	C2	C18	3.213(4)
C2	C20	2.788(4)	C3	C7	2.854(3)
C3	C9	3.225(3)	C3	C12	3.515(4)
C3	C16	3.253(3)	C3	C18	2.964(3)
C4	C9	3.270(3)	C4	C11	2.903(4)
C4	C16	3.193(3)	C4	C28	2.784(4)
C5	C8	2.855(4)	C5	C10	3.248(3)
C5	C14	3.505(3)	C5	C16	2.978(3)
C5	C18	3.271(4)	C6	C9	3.518(3)
C6	C12	3.193(4)	C6	C26	2.806(3)
C7	C27	2.792(4)	C8	C25	2.800(4)
C9	C10	3.029(3)	C9	C15	2.798(4)
C10	C21	2.793(4)	C11	C14	3.189(4)
C11	C17	2.756(3)	C12	C13	3.186(4)
C12	C24	2.738(4)	C13	C19	2.748(4)
C14	C22	2.749(4)	C16	C22	3.540(4)
C17	C19	2.969(4)	C18	C24	3.547(4)

Table 10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
C1	H14	3.123	C1	H17	3.261
C1	H25	3.265	C2	H13	2.549
C2	H15	3.256	C2	H16	3.189
C2	H24	3.240	C3	H11	2.663
C3	H12	3.599	C3	H14	2.647
C3	H18	3.575	C4	H11	2.543
C4	H18	3.177	C4	H21	3.257
C4	H22	3.238	C5	H12	2.642
C5	H13	2.666	C5	H14	3.581
C5	H16	3.590	C6	H12	3.124
C6	H19	3.266	C6	H27	3.260
C7	H13	3.262	C7	H17	2.669
C7	H26	3.258	C8	H11	3.266
C8	H19	2.681	C8	H23	3.254
C9	H12	3.248	C9	H13	3.318
C9	H18	3.312	C9	H20	3.266
C10	H11	3.287	C10	H14	3.248
C10	H16	3.313	C10	H28	3.255
C11	H14	3.149	C11	H23	3.228
C12	H13	2.628	C12	H20	3.224
C13	H12	3.144	C13	H26	3.231
C14	H11	2.634	C14	H28	3.226
C15	H13	3.396	C15	H24	3.209
C16	H24	2.619	C17	H19	2.653
C17	H25	3.225	C18	H22	2.611
C19	H17	2.650	C19	H27	3.204
C20	H12	3.217	C21	H11	3.402
C21	H22	3.225	C22	H18	2.798
C22	H21	3.230	C23	H11	3.227
C24	H15	3.217	C24	H16	2.813
C25	H17	3.223	C26	H13	3.228
C27	H19	3.204	C28	H14	3.222
H11	H14	2.752	H11	H25	2.291
H12	H13	2.741	H12	H15	2.304
H13	H27	2.288	H14	H21	2.306
H15	H20	2.307	H16	H18	2.195
H16	H24	2.735	H17	H19	2.076

Table 10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H17	H23	2.280	H18	H22	2.718
H19	H26	2.266	H20	H24	2.294
H21	H28	2.313	H22	H28	2.303
H23	H25	2.324	H26	H27	2.319

Table 11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
C22	C22[1]	3.596(4)	C25	C27[2]	3.589(4)
C25	C27[3]	3.572(5)	C27	C25[4]	3.572(5)
C27	C25[5]	3.589(4)			

Symmetry Operators:

(1) -X+1,-Y+1,-Z+1
(2) X-1,Y,Z-1
(3) X-1,Y,Z
(4) X+1,Y,Z
(5) X+1,Y,Z+1

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
C1	H14[1]	3.094	C6	H12[1]	3.122
C7	H12[1]	3.182	C7	H17[2]	3.524
C7	H19[2]	3.069	C8	H14[1]	3.128
C8	H17[2]	3.063	C8	H19[2]	3.529
C10	H22[3]	3.499	C11	H14[1]	3.051
C11	H21[1]	3.003	C11	H27[4]	2.995
C13	H12[1]	3.043	C13	H15[1]	3.070
C13	H25[5]	3.003	C14	H27[4]	3.571
C15	H11[5]	3.379	C15	H16[6]	3.154
C15	H21[7]	3.327	C16	H28[3]	3.240
C17	H14[1]	3.145	C17	H17[2]	2.933
C17	H23[2]	3.433	C18	H22[3]	3.551
C18	H28[3]	3.598	C19	H12[1]	3.180
C19	H19[2]	2.944	C19	H26[2]	3.434
C20	H16[6]	3.120	C20	H20[8]	3.237
C20	H21[7]	3.366	C20	H24[8]	3.586
C20	H28[7]	3.396	C21	H11[6]	3.590
C21	H13[4]	3.351	C21	H15[9]	3.314
C21	H18[6]	3.071	C22	H18[6]	3.591
C22	H20[9]	3.295	C22	H22[3]	3.040
C23	H14[1]	3.127	C23	H17[2]	3.434
C23	H23[2]	2.960	C23	H26[10]	3.437
C23	H27[9]	3.042	C24	H16[6]	3.596
C24	H20[8]	3.269	C24	H22[3]	3.554
C24	H24[11]	3.317	C24	H28[7]	3.332
C24	H28[3]	3.309	C25	H13[9]	3.287
C25	H14[1]	3.083	C25	H21[1]	3.412
C25	H23[2]	3.114	C25	H26[4]	3.269
C25	H27[4]	3.129	C25	H27[9]	3.141
C26	H12[1]	3.136	C26	H19[2]	3.449
C26	H23[12]	3.445	C26	H25[7]	3.030
C26	H26[2]	2.985	C27	H11[7]	3.274
C27	H12[1]	3.060	C27	H15[1]	3.448
C27	H23[5]	3.287	C27	H25[5]	3.121
C27	H25[7]	3.147	C27	H26[2]	3.164
C28	H15[9]	3.255	C28	H18[6]	3.067
C28	H20[9]	3.409	C28	H24[3]	3.301

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H11	C15[9]	3.379	H11	C21[1]	3.590
H11	C27[4]	3.274	H11	H14[1]	3.536
H11	H15[9]	2.874	H11	H21[1]	2.821
H11	H27[4]	2.679	H12	C6[6]	3.122
H12	C7[6]	3.182	H12	C13[6]	3.043
H12	C19[6]	3.180	H12	C26[6]	3.136
H12	C27[6]	3.060	H12	H13[6]	3.517
H12	H25[5]	3.143	H12	H27[6]	3.544
H13	C21[7]	3.351	H13	C25[5]	3.287
H13	H12[1]	3.517	H13	H15[1]	2.879
H13	H21[7]	2.878	H13	H25[5]	2.711
H14	C1[6]	3.094	H14	C8[6]	3.128
H14	C11[6]	3.051	H14	C17[6]	3.145
H14	C23[6]	3.127	H14	C25[6]	3.083
H14	H11[6]	3.536	H14	H25[6]	3.589
H14	H27[4]	3.131	H15	C13[6]	3.070
H15	C21[5]	3.314	H15	C27[6]	3.448
H15	C28[5]	3.255	H15	H11[5]	2.874
H15	H13[6]	2.879	H15	H16[6]	3.331
H15	H21[5]	3.563	H15	H21[7]	3.510
H15	H27[6]	3.526	H15	H28[5]	3.436
H16	C15[1]	3.154	H16	C20[1]	3.120
H16	C24[1]	3.596	H16	H15[1]	3.331
H16	H20[1]	3.294	H16	H20[11]	3.424
H16	H24[11]	3.459	H16	H28[3]	3.173
H17	C7[13]	3.524	H17	C8[13]	3.063
H17	C17[13]	2.933	H17	C23[13]	3.434
H17	H17[2]	3.058	H17	H17[13]	3.058
H18	C21[1]	3.071	H18	C22[1]	3.591
H18	C28[1]	3.067	H18	H18[14]	3.181
H18	H21[1]	3.209	H18	H22[14]	3.457
H18	H28[1]	3.236	H19	C7[13]	3.069
H19	C8[13]	3.529	H19	C19[13]	2.944
H19	C26[13]	3.449	H19	H19[2]	3.062
H19	H19[13]	3.062	H20	C20[8]	3.237
H20	C22[5]	3.295	H20	C24[8]	3.269
H20	C28[5]	3.409	H20	H16[6]	3.294

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H20	H16[11]	3.424	H20	H20[8]	2.786
H20	H21[7]	3.556	H20	H22[5]	3.130
H20	H24[8]	2.830	H20	H28[5]	3.327
H20	H28[7]	3.345	H21	C11[6]	3.003
H21	C15[4]	3.327	H21	C20[4]	3.366
H21	C25[6]	3.412	H21	H11[6]	2.821
H21	H13[4]	2.878	H21	H15[4]	3.510
H21	H15[9]	3.563	H21	H18[6]	3.209
H21	H20[4]	3.556	H21	H25[6]	3.524
H22	C10[3]	3.499	H22	C18[3]	3.551
H22	C22[3]	3.040	H22	C24[3]	3.554
H22	H18[14]	3.457	H22	H20[9]	3.130
H22	H22[3]	2.698	H22	H24[3]	3.258
H23	C17[13]	3.433	H23	C23[13]	2.960
H23	C25[13]	3.114	H23	C26[10]	3.445
H23	C27[9]	3.287	H23	H23[2]	3.082
H23	H23[13]	3.082	H23	H25[13]	3.323
H23	H26[10]	2.706	H23	H27[9]	2.744
H23	H27[10]	3.221	H24	C20[8]	3.586
H24	C24[11]	3.317	H24	C28[3]	3.301
H24	H16[11]	3.459	H24	H20[8]	2.830
H24	H22[3]	3.258	H24	H24[11]	2.605
H24	H28[7]	3.233	H24	H28[3]	2.552
H25	C13[9]	3.003	H25	C26[4]	3.030
H25	C27[4]	3.147	H25	C27[9]	3.121
H25	H12[9]	3.143	H25	H13[9]	2.711
H25	H14[1]	3.589	H25	H21[1]	3.524
H25	H23[2]	3.323	H25	H26[4]	2.711
H25	H26[10]	3.192	H25	H27[4]	2.923
H25	H27[9]	2.927	H26	C19[13]	3.434
H26	C23[12]	3.437	H26	C25[7]	3.269
H26	C26[13]	2.985	H26	C27[13]	3.164
H26	H23[12]	2.706	H26	H25[7]	2.711
H26	H25[12]	3.192	H26	H26[2]	3.097
H26	H26[13]	3.097	H26	H27[13]	3.383
H27	C11[7]	2.995	H27	C14[7]	3.571
H27	C23[5]	3.042	H27	C25[5]	3.141

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H27	C25[7]	3.129	H27	H11[7]	2.679
H27	H12[1]	3.544	H27	H14[7]	3.131
H27	H15[1]	3.526	H27	H23[5]	2.744
H27	H23[12]	3.221	H27	H25[5]	2.927
H27	H25[7]	2.923	H27	H26[2]	3.383
H28	C16[3]	3.240	H28	C18[3]	3.598
H28	C20[4]	3.396	H28	C24[4]	3.332
H28	C24[3]	3.309	H28	H15[9]	3.436
H28	H16[3]	3.173	H28	H18[6]	3.236
H28	H20[4]	3.345	H28	H20[9]	3.327
H28	H24[4]	3.233	H28	H24[3]	2.552

Symmetry Operators:

(1) X,Y,Z+1
(2) X,-Y+1,Z
(3) -X+1,-Y+1,-Z+1
(4) X-1,Y,Z-1
(5) X+1,Y,Z
(6) X,Y,Z-1
(7) X+1,Y,Z+1
(8) -X+2,-Y+1,-Z+1
(9) X-1,Y,Z
(10) X-1,-Y+1,Z
(11) -X+2,-Y+1,-Z+2
(12) X+1,-Y+1,Z+1
(13) X,-Y+1,Z+1
(14) -X+1,-Y+1,-Z+2