Electronic Supporting Information

Formation of emissive nanoparticles from tetraphenylethylene-containing boronate macrocycles: preparation, characterization and functionalization

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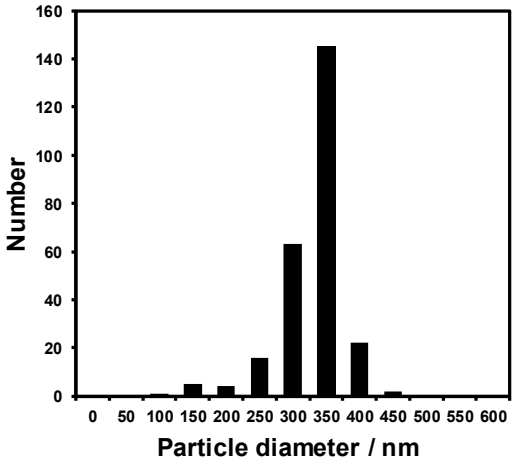


Fig. S1 The size distribution of 258 nanoparticles of **1a** in the FE-SEM image.

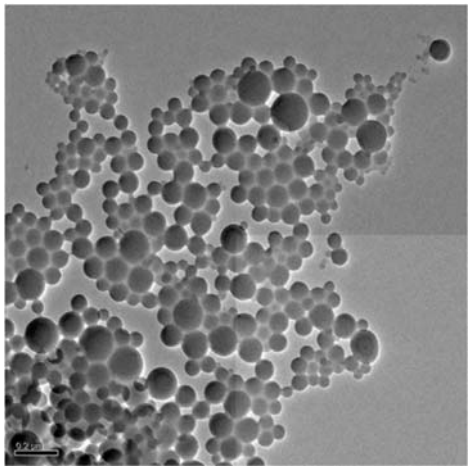


Fig. S2 TEM image of the nanoparticles formation of **1a**, scale bar: 0.2 μm.

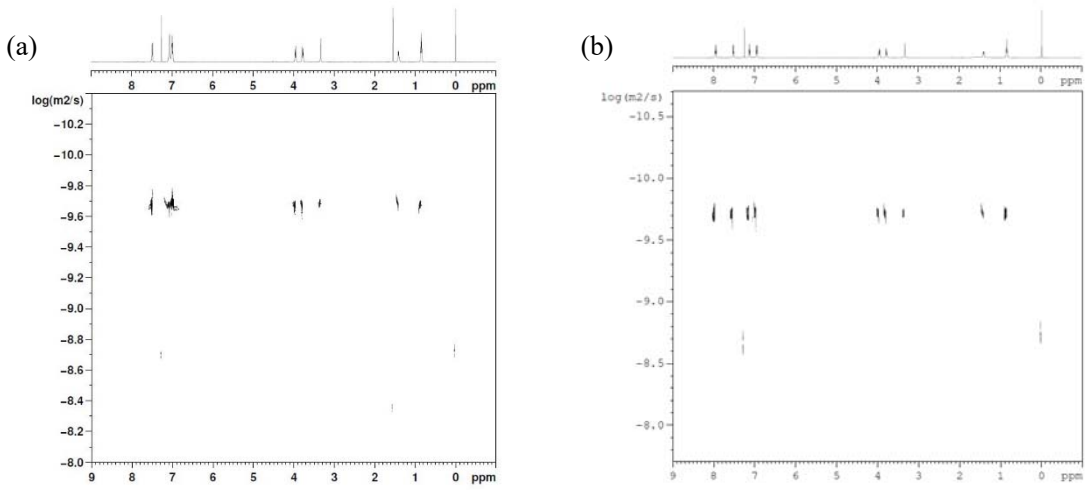


Fig. S3 DOSY NMR spectra ($CDCl_3$) of products isolated from the reactions of **2a** with **3** (a) and **2b** with **3** (b) in MeOH at ambient conditions.

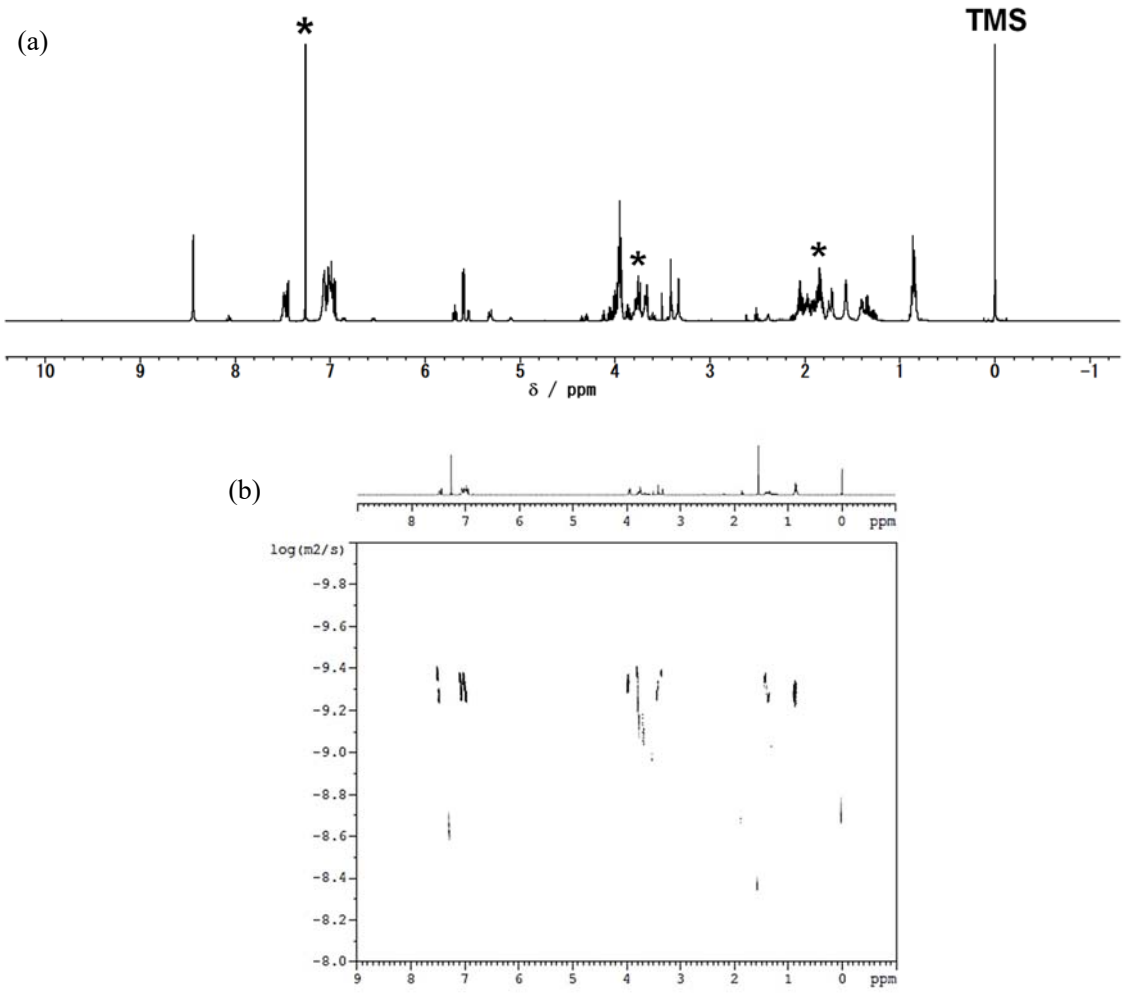


Fig. S4 ^{1}H NMR (a) and DOSY NMR (b) spectra ($CDCl_3$) of product after the reaction of **2a** with **3** in dry THF at ambient conditions. Asterisks show the signals of solvent.

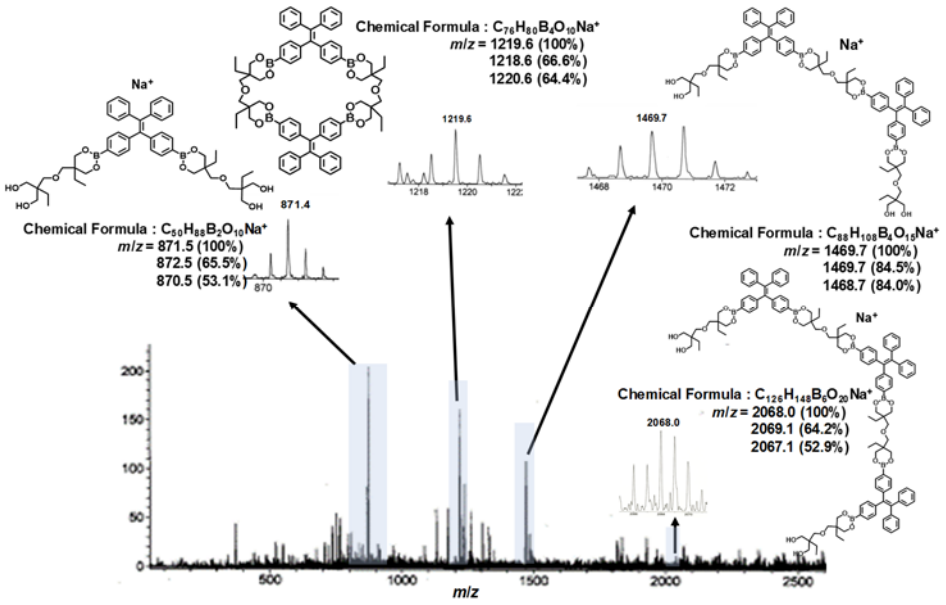


Fig. S5 ESI-MS spectrum of mixing **2a** and **3** in dry THF. [**2a**] = [**3**] = 0.05 mM, positive mode.

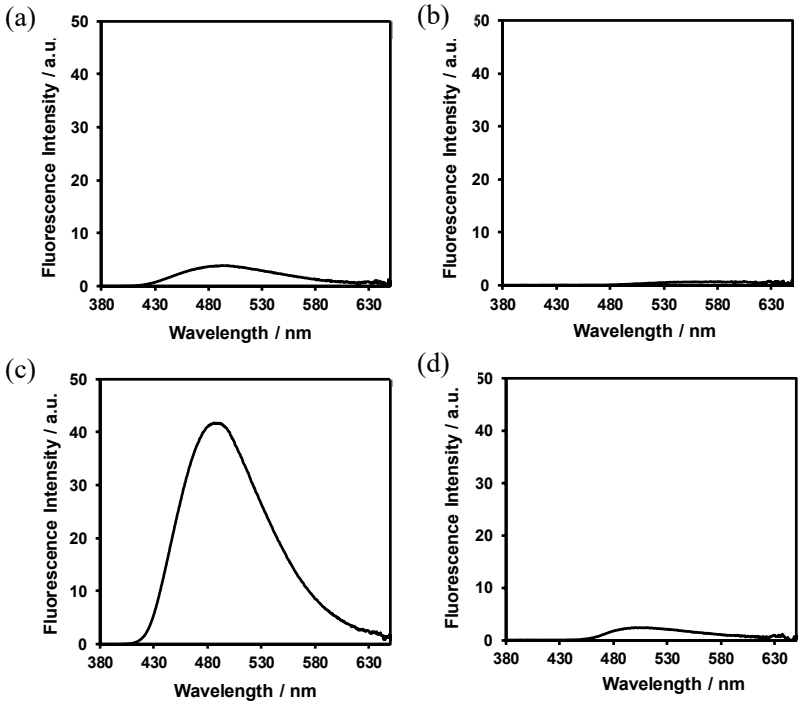


Fig. S6 Fluorescence spectra of as-prepared solid of (a) **1a**, (b) **1b**, (c) **6** and (d) **7**, λ_{ex} = 365 nm, r.t.

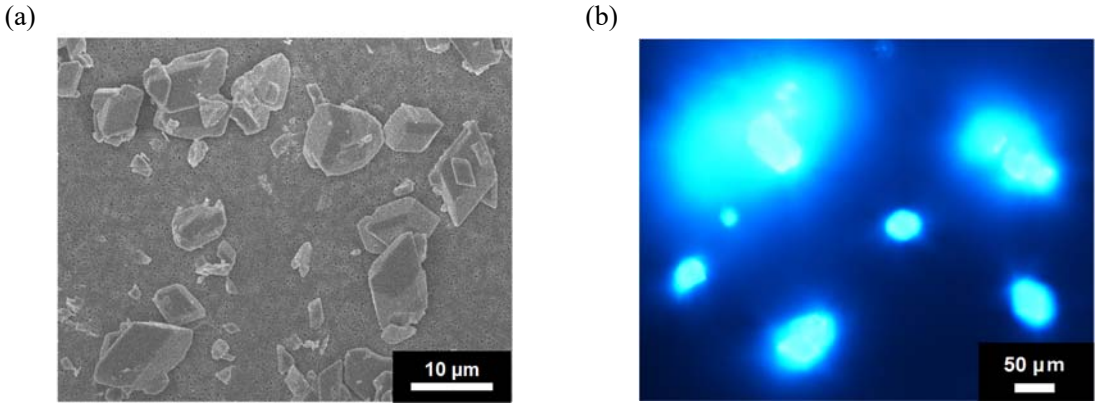


Fig. S7 FE-SEM (a) and fluorescent microscopic images (b) of bis(pinacol)boryl-substituted TPE **6**.

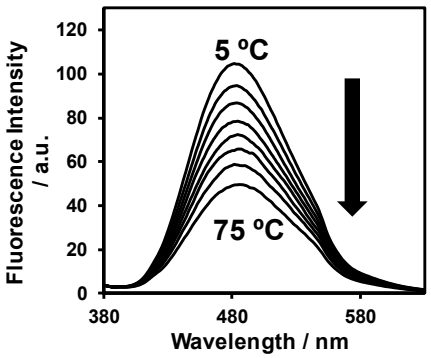


Fig. S8 Fluorescence spectra of **1a**-based nanoparticles dispersed in H_2O at various temperatures. [**1a**] = 0.05 mg mL^{-1}, λ_{ex} = 365 nm.

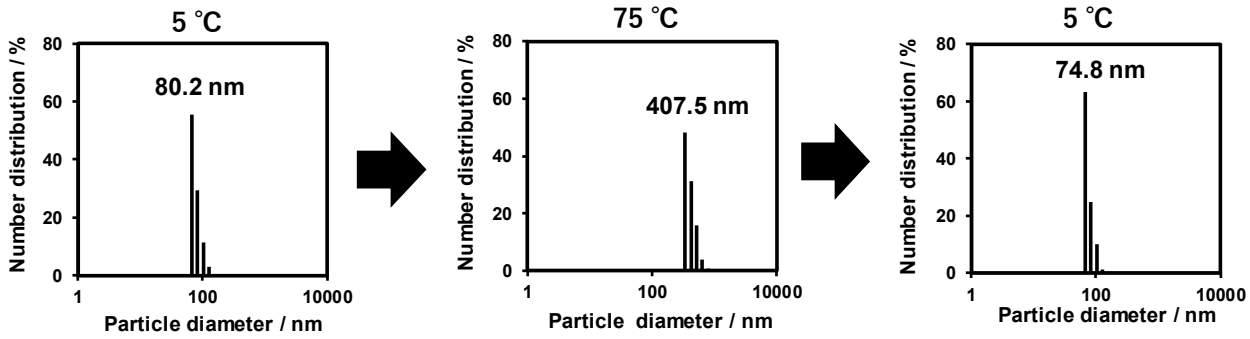


Fig. S9 Temperature-dependent change in particle diameter of nanoparticles **1a** dispersed in H_2O. [**1a**] = 0.05 mg mL^{-1}.

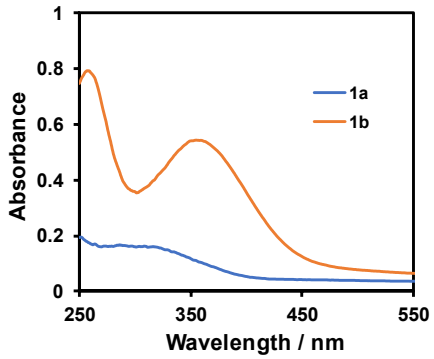


Fig. S10 Absorption spectra of **1a**- and **1b**-based nanoparticles dispersed in H_2O/MeOH (3:2 *v*/*v*). [**1a**] = [**1b**] = 0.041 mM, r.t.

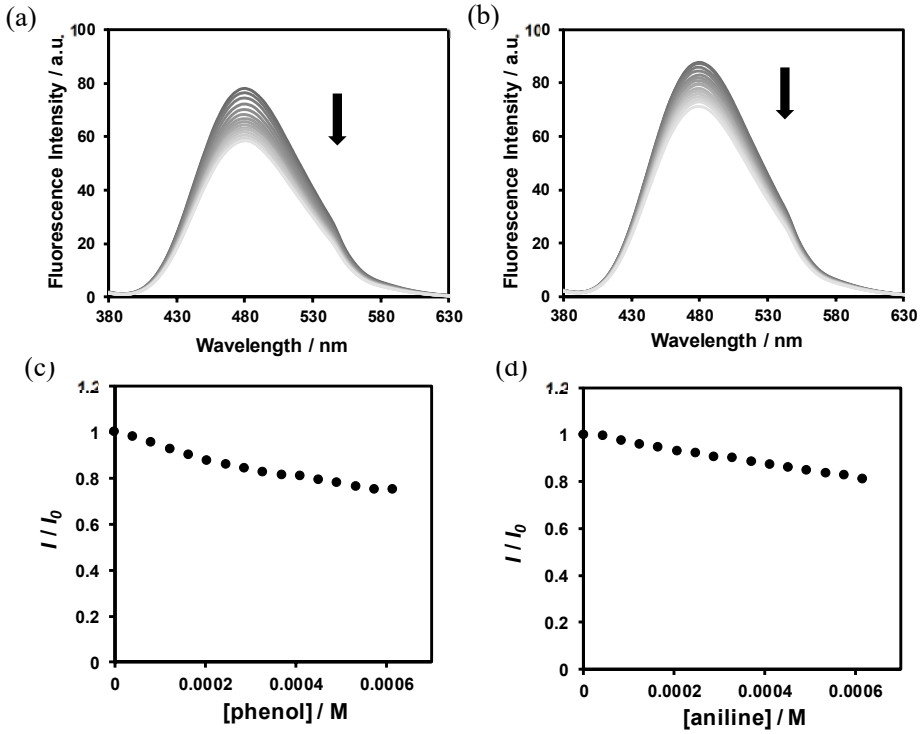


Fig. S11 Fluorescence spectra of **1a**-based nanoparticles dispersed in H_2O/MeOH (3:2 *v*/*v*) upon adding phenol (a) and aniline (b). Change in fluorescence intensity (I/I_0) of **1a**-based nanoparticles at 483 nm upon adding incremental amounts of phenol (c) and aniline (d): [**1a**] = 0.041 mM, [phenol] = [aniline] = 0.041, 0.082, 0.123, 0.164, 0.205, 0.246, 0.287, 0.328, 0.369, 0.41, 0.451, 0.492, 0.533, 0.574, and 0.615 mM, λ_{ex} = 365 nm, r.t.

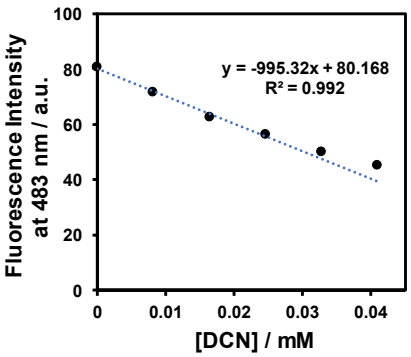


Fig. S12 Determination of detection limit of **1a**-based nanoparticles to DCN: [**1a**] = 0.041 mM, [DCN] = 0.0082, 0.0164, 0.0246, 0.0328 and 0.041 mM, λ_{ex} = 365 nm, r.t.

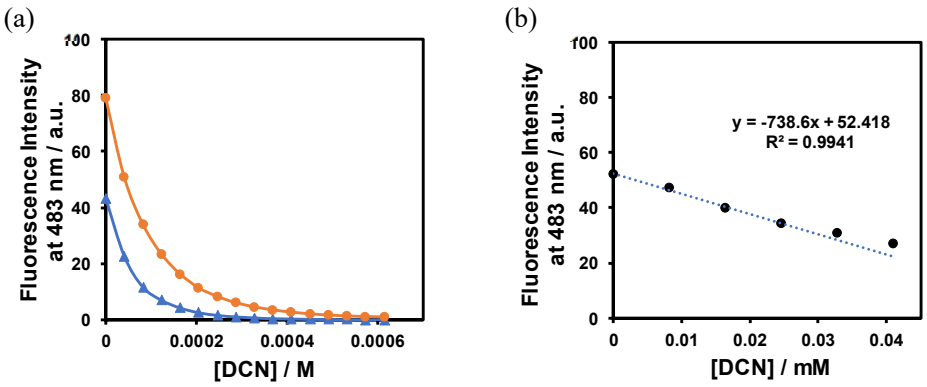


Fig. S13 (a) Plots of fluorescence intensity at 483 nm of **1a**-based nanoparticles (orange line, ●) and **6** (blue line, ▲) dispersed in H_2O/MeOH (3:2 *v*/*v*) upon adding incremental amounts of DCN: [**1a**] = 0.041 mM, [**6**] = 0.082 mM, [DCN] = 0.041, 0.082, 0.123, 0.164, 0.205, 0.246, 0.287, 0.328, 0.369, 0.41, 0.451, 0.492, 0.533, 0.574, and 0.615 mM, λ_{ex} = 365 nm, r.t., (b) Determination of detection limit of **6** to DCN: [**6**] = 0.082 mM, [DCN] = 0.0082, 0.0164, 0.0246, 0.0328 and 0.041 mM, λ_{ex} = 365 nm, r.t.

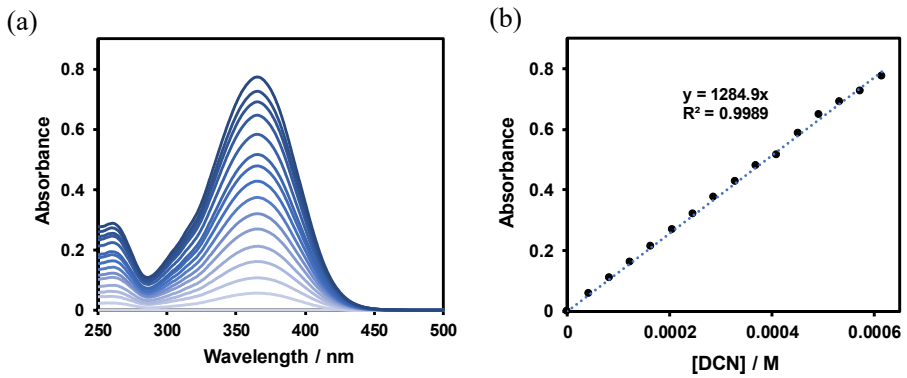


Fig. S14 (a) Absorption spectra of different concentration of DCN in H_2O/MeOH (3:2 *v*/*v*). (b) Lambert–Beer plot of DCN at 365 nm. [DCN] = 0.041, 0.082, 0.123, 0.164, 0.205, 0.246, 0.287, 0.328, 0.369, 0.41, 0.451, 0.492, 0.533, 0.574, and 0.615 mM, Light path: 1 mm, r.t.

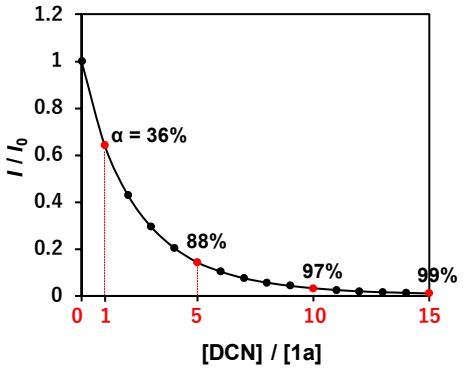


Fig. S15 Fluorescence titration of **1a**-based nanoparticles with DCN in H_2O/MeOH (3:2 *v*/*v*). [**1a**] = 0.041 mM, λ_{ex} = 365 nm, r.t. The apparent complexation ratio (α) of **1a**@DCN was calculated by $(I_0 - I) / I_0$.

Characterization

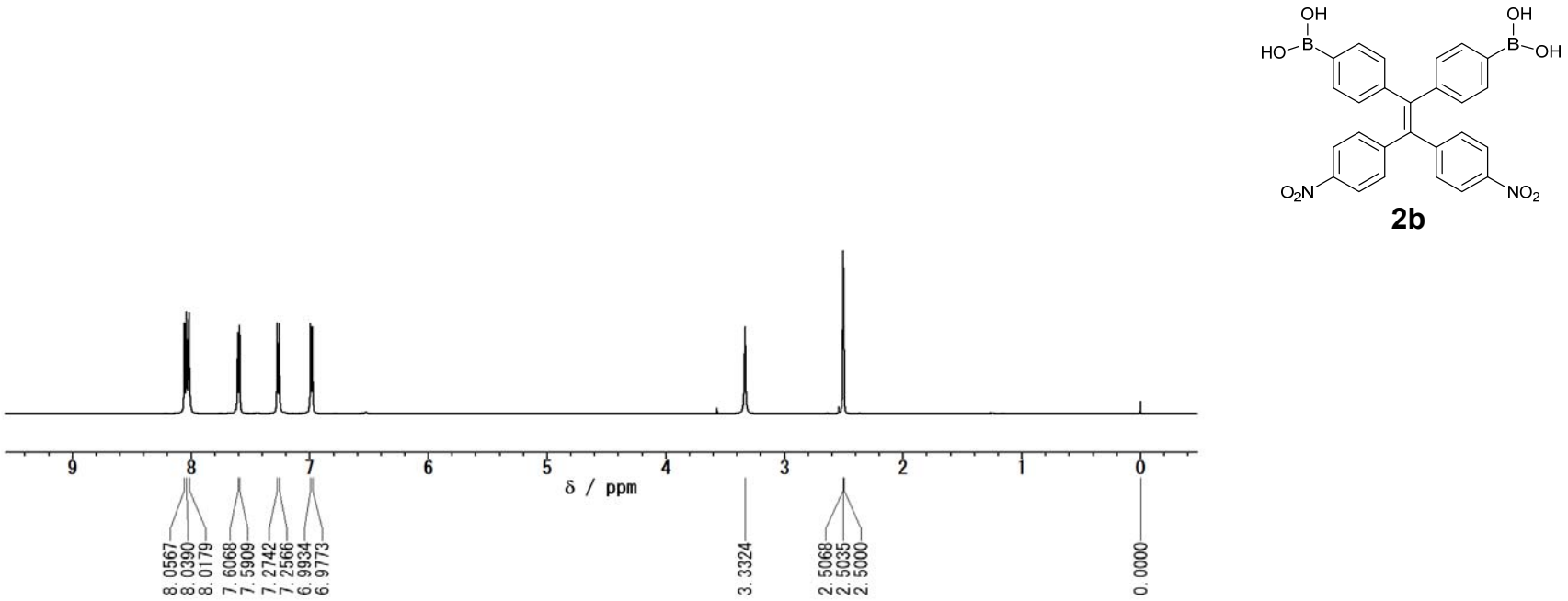
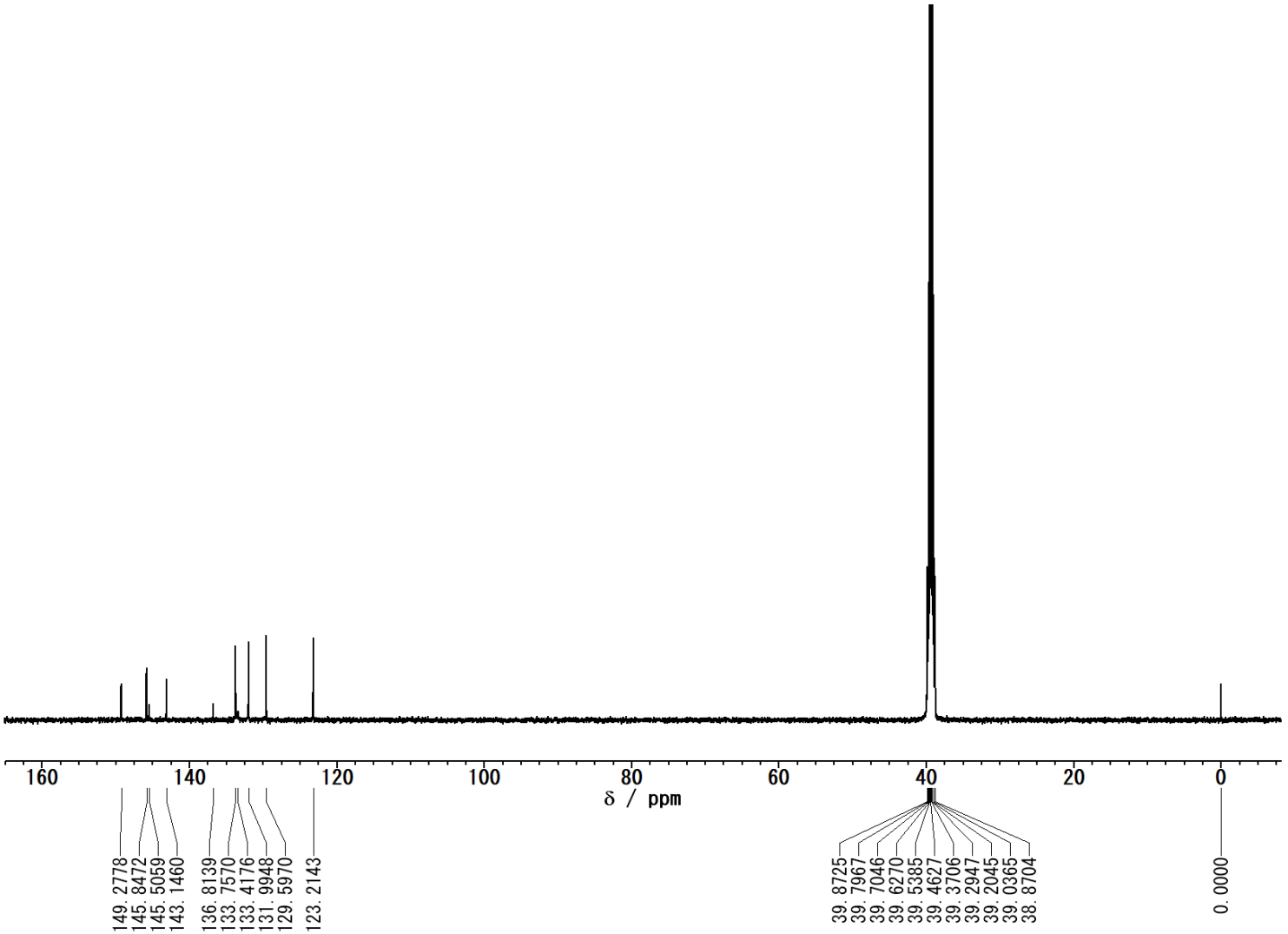
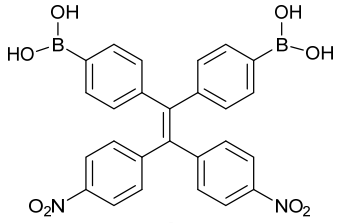


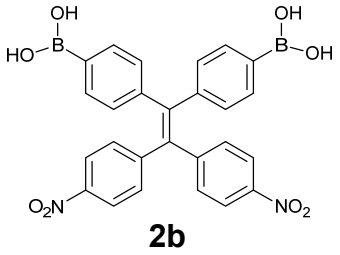
Fig. S16 ^{1}H NMR spectrum of **2b** in DMSO-d_6.





2b

Fig. S17 ^{13}C NMR spectrum of **2b** in DMSO-d_6.



2b

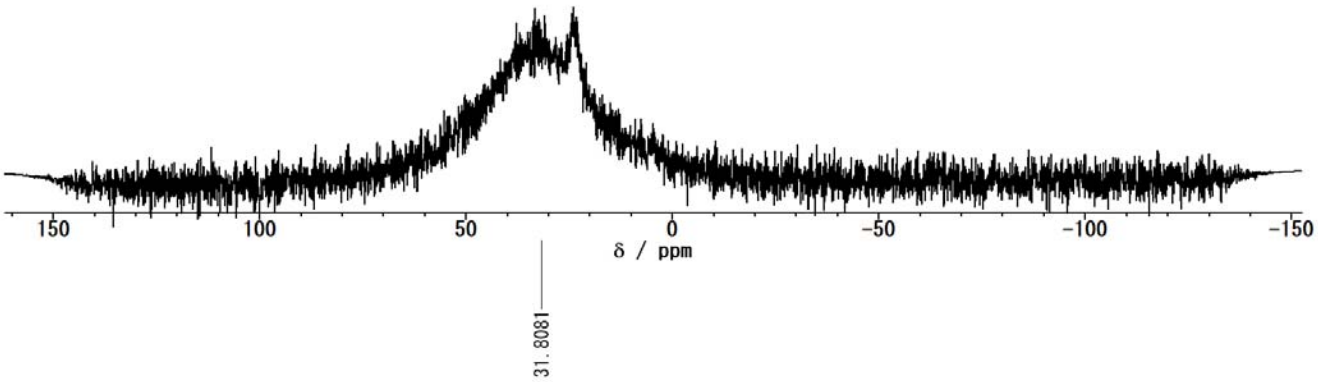


Fig. S18 ^{11}B NMR spectrum of **2b** in DMSO-d_6.

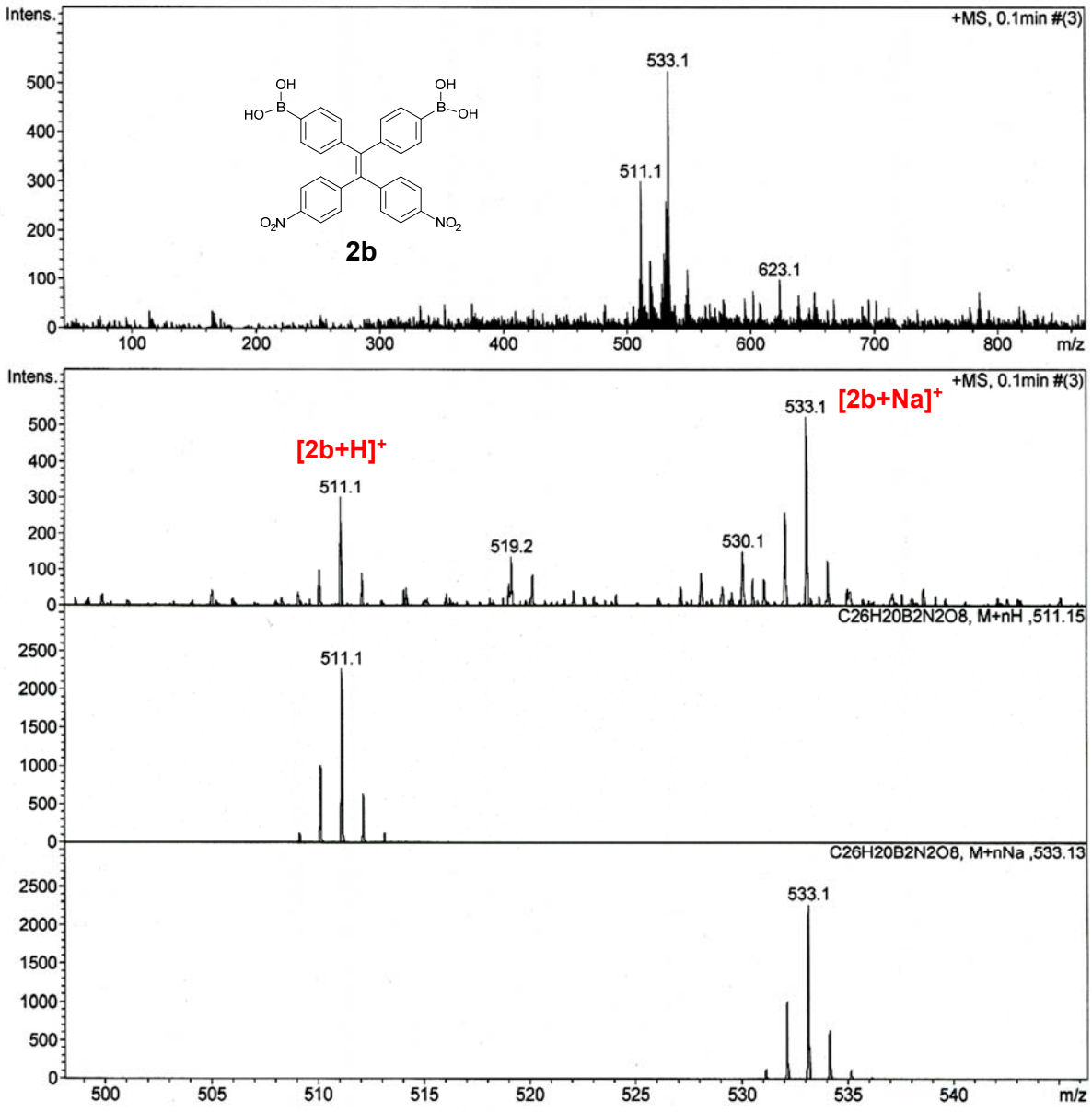
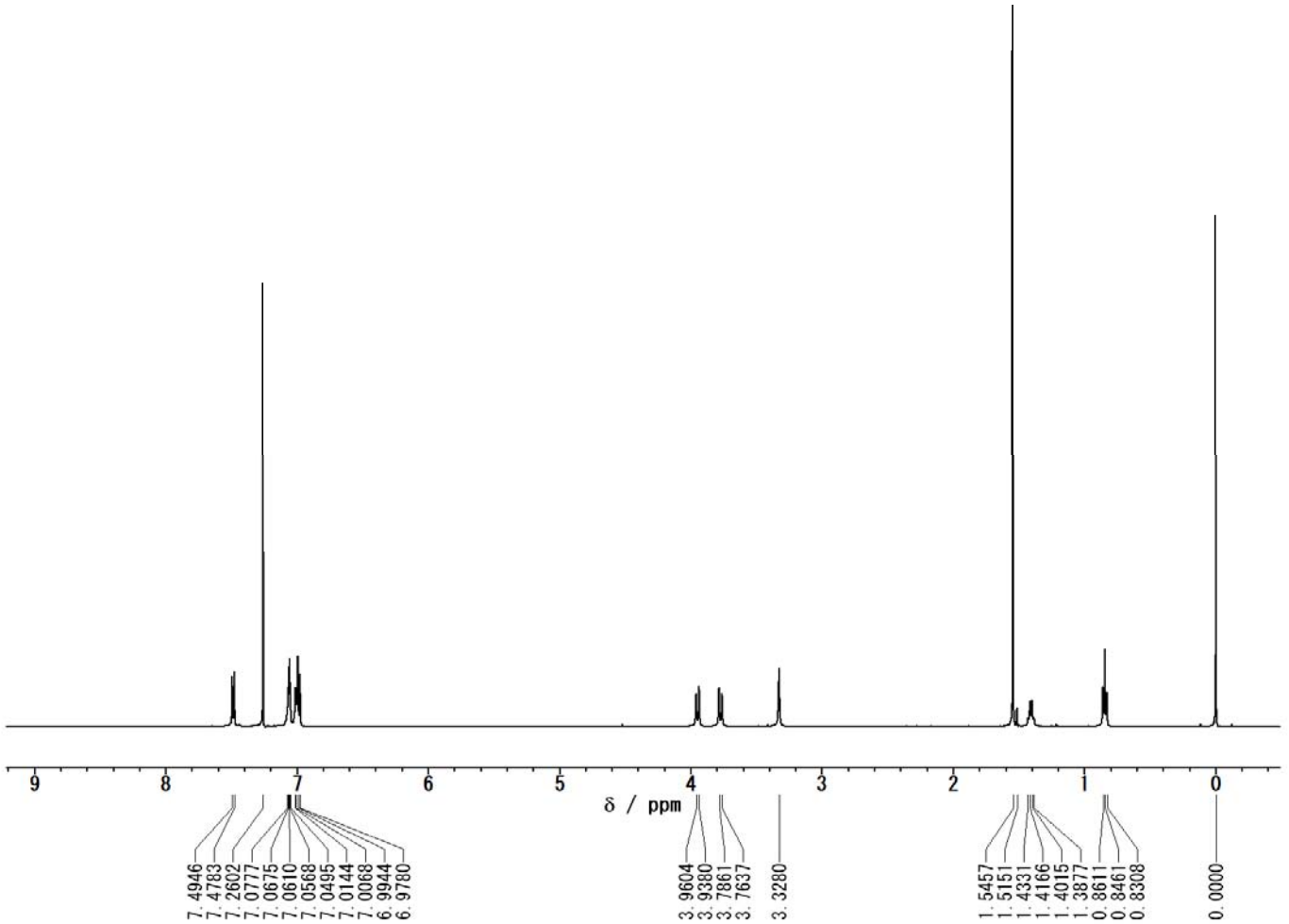


Fig. S19 ESI-MS spectrum (positive mode) of **2b**.



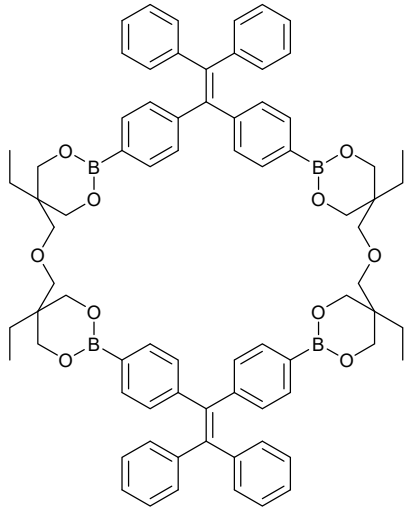


Fig. S20 ^{1}H NMR spectrum of **1a** in $CDCl_3$.

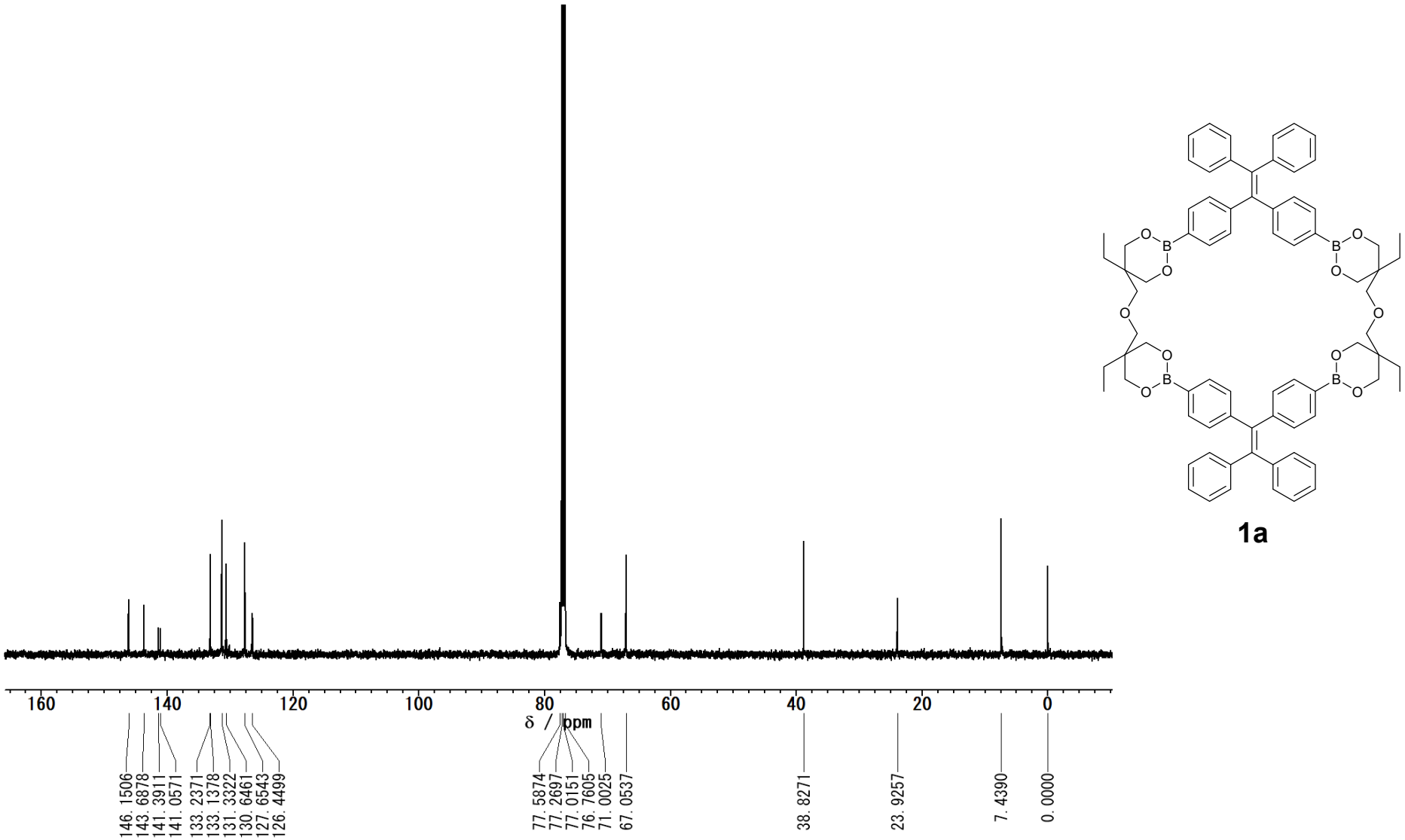
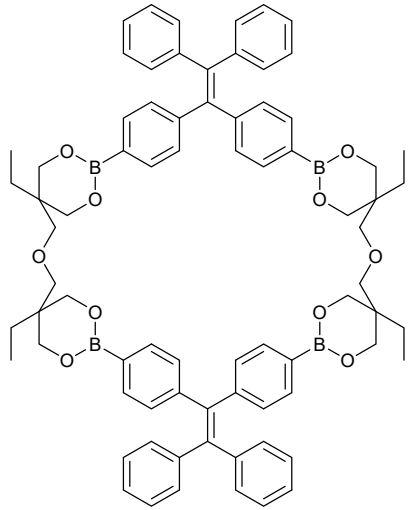


Fig. S21 ^{13}C NMR spectrum of **1a** in $CDCl_3$.



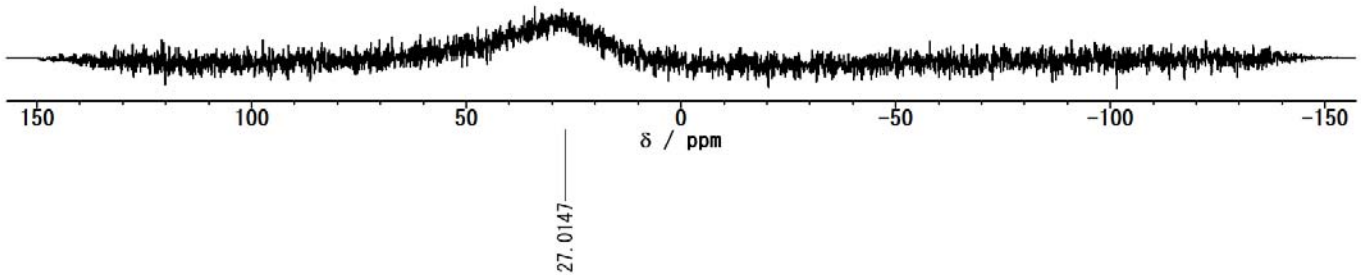


Fig. S22 ^{11}B NMR spectrum of **1a** in $CDCl_3$.

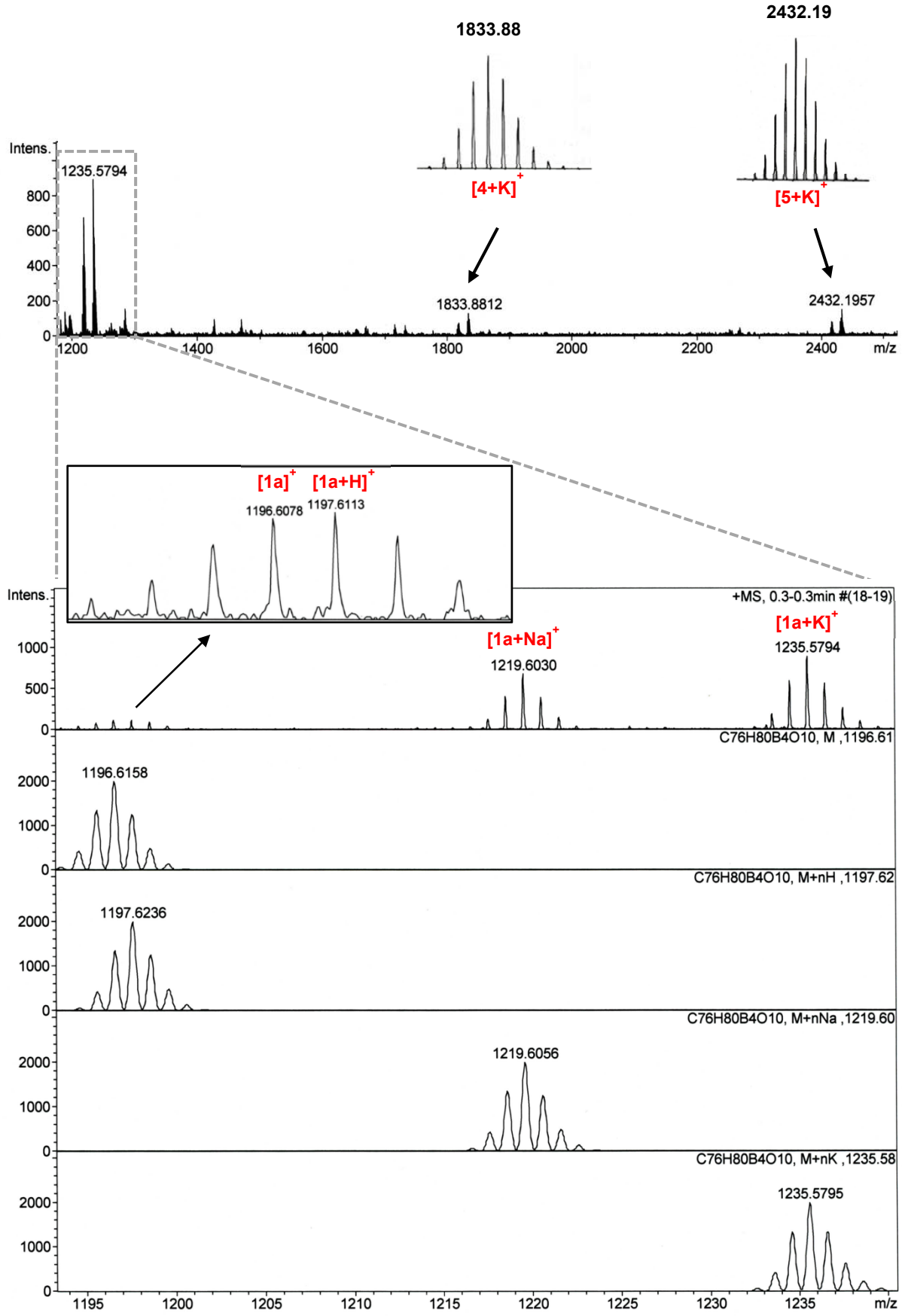
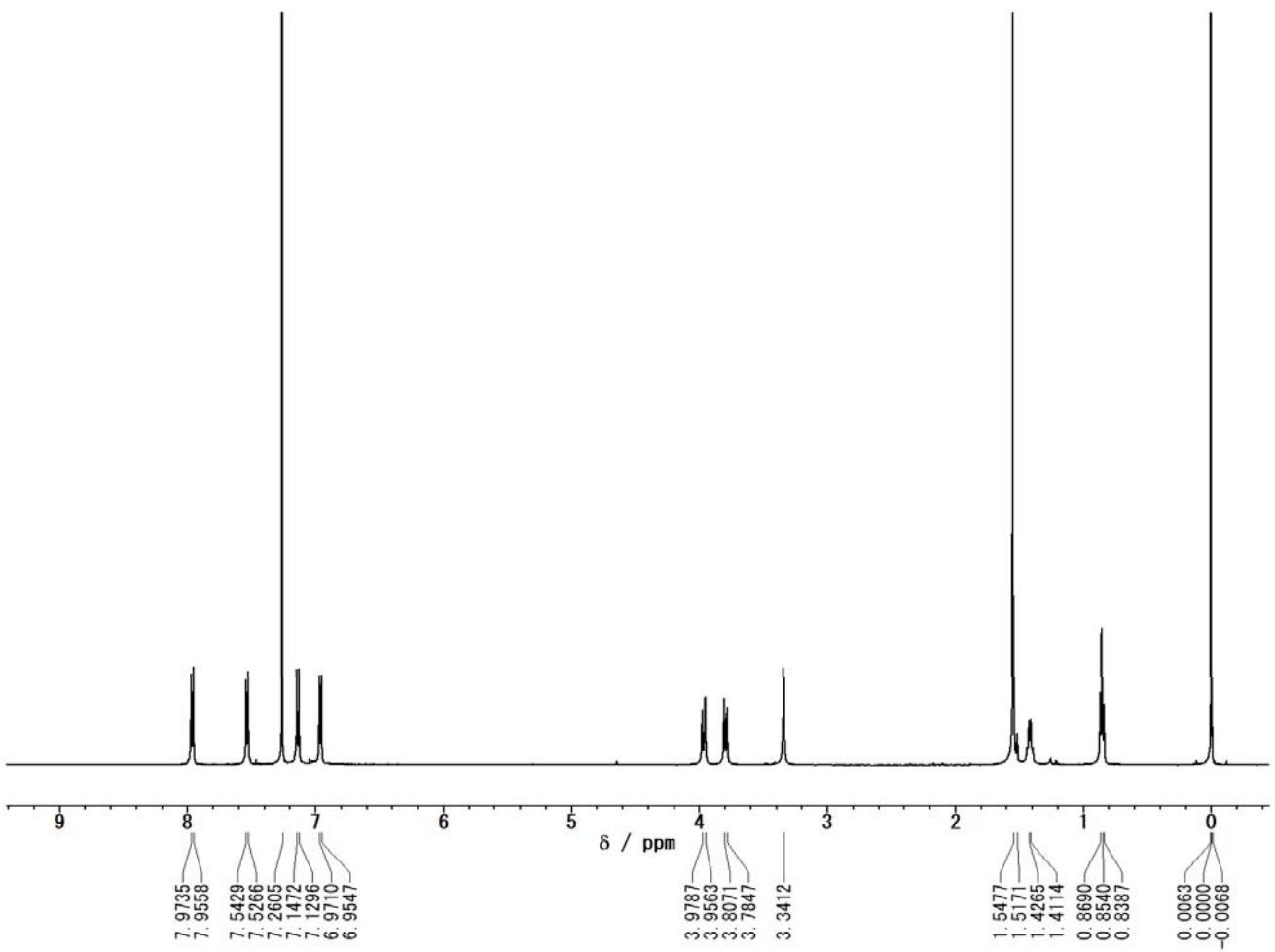
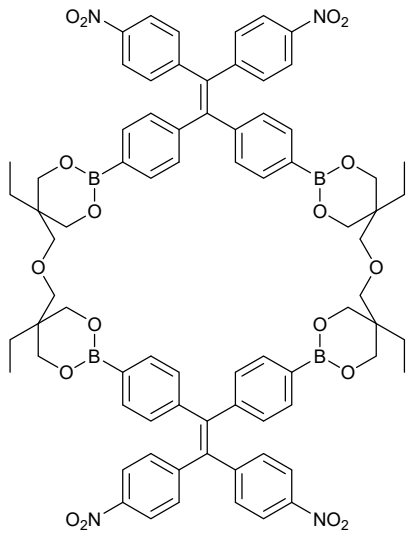


Fig. S23 HR-ESI-MS spectrum (positive mode) of **1a**.





1b

Fig. S24 ^{1}H NMR spectrum of **1b** in $CDCl_3$.

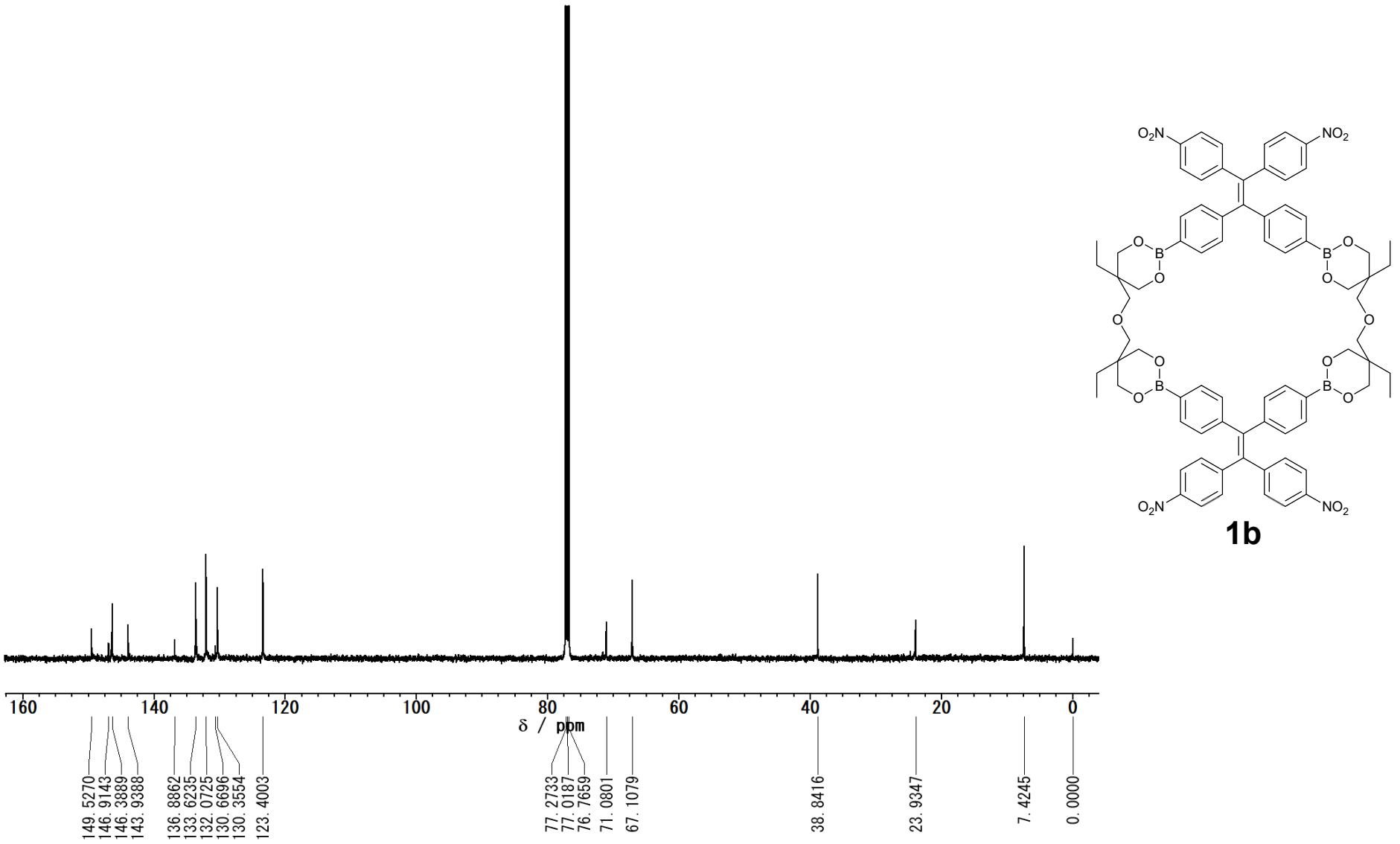
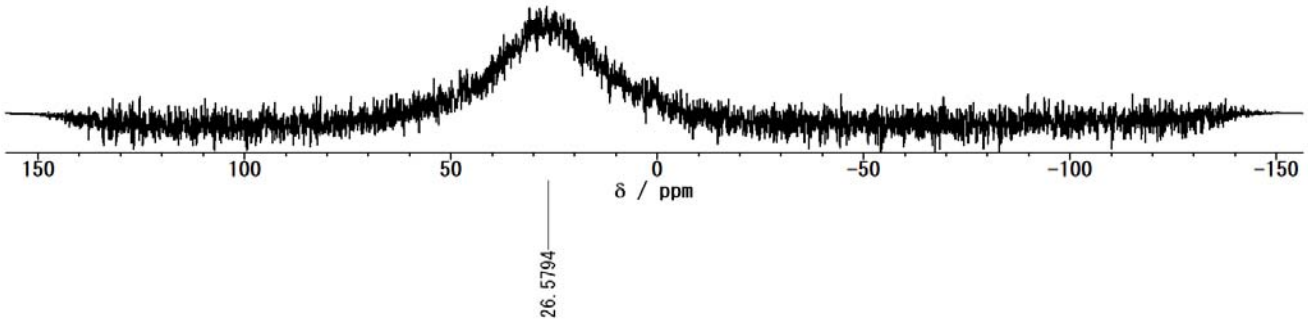
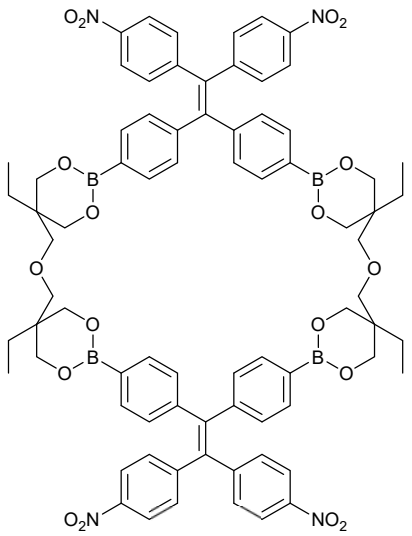


Fig. S25 ^{13}C NMR spectrum of **1b** in $CDCl_3$.





1b

Fig. S26 ^{11}B NMR spectrum of **1b** in $CDCl_3$.

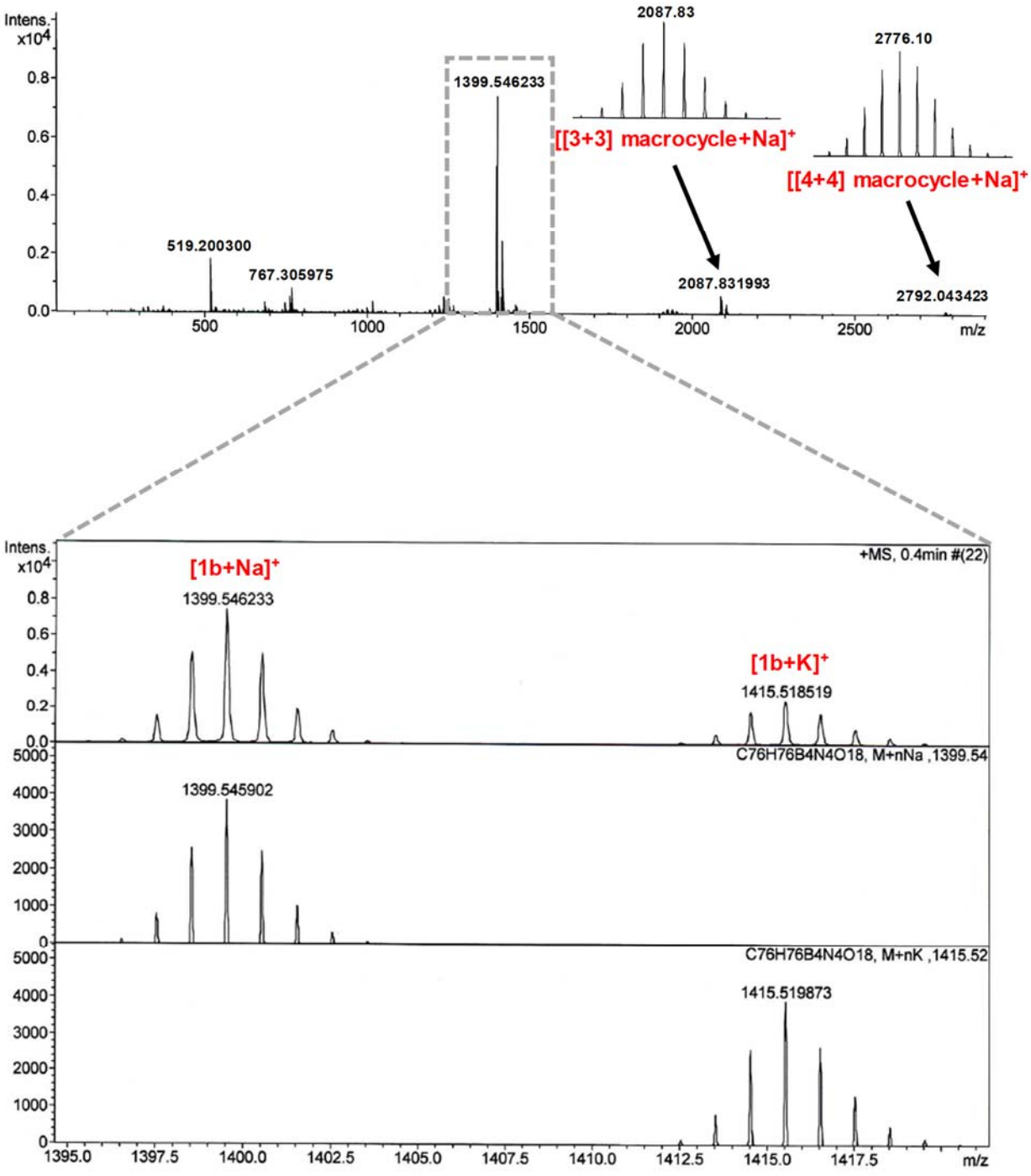


Fig. S27 HR-ESI-MS spectrum (positive mode) of **1b**.

Single crystal X-ray diffraction study

Data Collection

A colorless prism crystal of $C_{78}H_{83}B_4NO_{10}$ having approximate dimensions of 0.290 × 0.245 × 0.132 mm was mounted on a glass fiber. All measurements were made on a diffractometer using graphite monochromated Mo-Kα radiation.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 24952 carefully centered reflections in the range $4.25 < 2\theta < 61.02^o$ corresponded to a primitive monoclinic cell with dimensions:

a = 10.9998(4) Å
b = 32.4732(13) Å β= 104.469(4)°
c = 20.5832(8) Å
V = 7119.1(5) Å3

For Z = 4 and F.W. = 1237.75, the calculated density is 1.155 g/cm^3. The reflection conditions of:

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

uniquely determine the space group to be:

P21/c (#14)

The data were collected at a temperature of 23 + 1°C using the ω-2θ scan technique to a maximum 2θ value of 61.3°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.00° with a take-off angle of 6.0°. Scans of (0.00 + 0.00 tanθ)° were made at a speed of 0.0°/min (in ω).

Data Reduction

Of the 65233 reflections were collected, where 19819 were unique (R_{int} = 0.0464). Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction). [1] No decay correction was applied.

The linear absorption coefficient, μ, for Mo-Kα radiation is 0.741 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.538 to 0.990. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction[2] was applied (coefficient = 0.000760).

Structure Solution and Refinement

The structure was solved by direct methods[3] 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[4] on F^2 was based on 19819 observed reflections and 844 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0926$$

$$wR2 = [\, \Sigma \, (w \, (Fo^2 - Fc^2)^2 \,) / \, \Sigma \, w(Fo^2)^2]^{1/2} = 0.2911$$

The goodness of fit[5] was 1.04. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.91 and -0.39 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 [6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf'' were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All calculations were performed using the CrystalStructure[10] crystallographic software package except for refinement, which was performed using SHELXL Version 2014/7[11].

References

(1) CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.

(2) Larson, A.C. (1970), Crystallographic Computing, 291-294. F.R. Ahmed, ed. Munksgaard, Copenhagen (equation 22, with V replaced by the cell volume).

(3) SHELXT Version 2014/5: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(4) Least Squares function minimized: (SHELXL Version 2014/7)

$\Sigma \, w(Fo^2-Fc^2)^2$ where w = Least Squares weights.

(5) Goodness of fit is defined as:

$[\, \Sigma \, w(Fo^2-Fc^2)^2/(No-Nv)]^{1/2}$

where: No = number of observations

Nv = number of variables

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

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

(8) 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).

(9) 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).

(10) CrystalStructure 4.2.5: Crystal Structure Analysis Package, Rigaku Corporation (2000-2017). Tokyo 196-8666, Japan.

(11) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{78}H_{83}B4NO_{10}$
Formula Weight	1237.75
Crystal Color, Habit	colourless, prism
Crystal Dimensions	0.290×0.245×0.132 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	24952 (4.2 - 61.0°)
Omega Scan Peak Width at Half-height	0.00°
Lattice Parameters	a = 10.9998(4) Å b = 32.4732(13) Å c = 20.5832(8) Å β = 104.469(4) ° V = 7119.1(5) Å^3
Space Group	P21/c (#14)
Z value	4
Dcalc	1.155 g/cm^3
F_{000}	2632.00
μ(MoKα)	0.741 cm^{-1}

B. Intensity Measurements

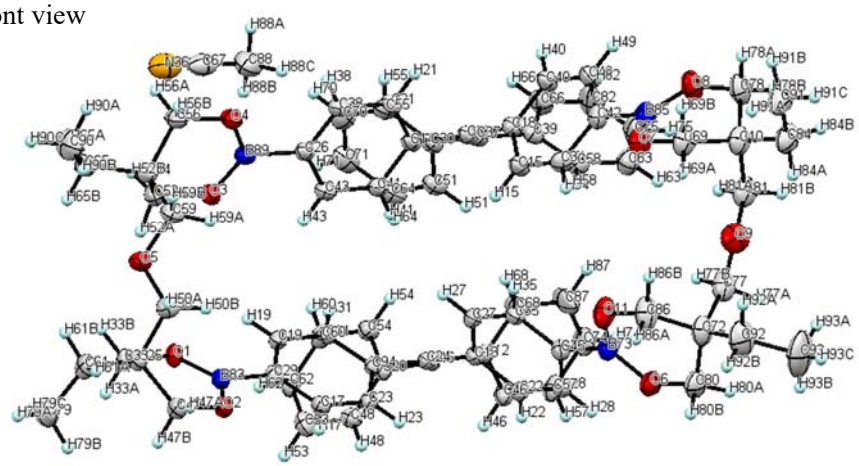
Diffractometer	
Radiation	MoKα (λ= 0.71075 Å) graphite monochromated
Take-off Angle	2.8°
Detector Aperture	2.0 - 2.5 mm horizontal 2.0 mm vertical
Crystal to Detector Distance	21 mm
Temperature	23.0°C
Scan Type	ω-2θ
Scan Rate	0.0°/min (in ω) (up to 0 scans)
Scan Width	(0.00 + 0.00 tanθ)°
$2\theta_{max}$	61.3°
No. of Reflections Measured	Total: 65233 Unique: 19819 (R_{int} = 0.0464)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.538 - 0.990) Secondary Extinction (coefficient: 7.60000e-004)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXT Version 2014/5)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma w (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.1316 . P)^2 + 12.9807 . P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	61.3°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	19819
No. Variables	844
Reflection/Parameter Ratio	23.48
Residuals: R1 (I>2.00σ(I))	0.0926
Residuals: R (All reflections)	0.1215
Residuals: wR2 (All reflections)	0.2911
Goodness of Fit Indicator	1.045
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	1.91 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.39 $e^-/Å^3$

(a) Atom numbering Scheme of **1a**.

Front view



Side view

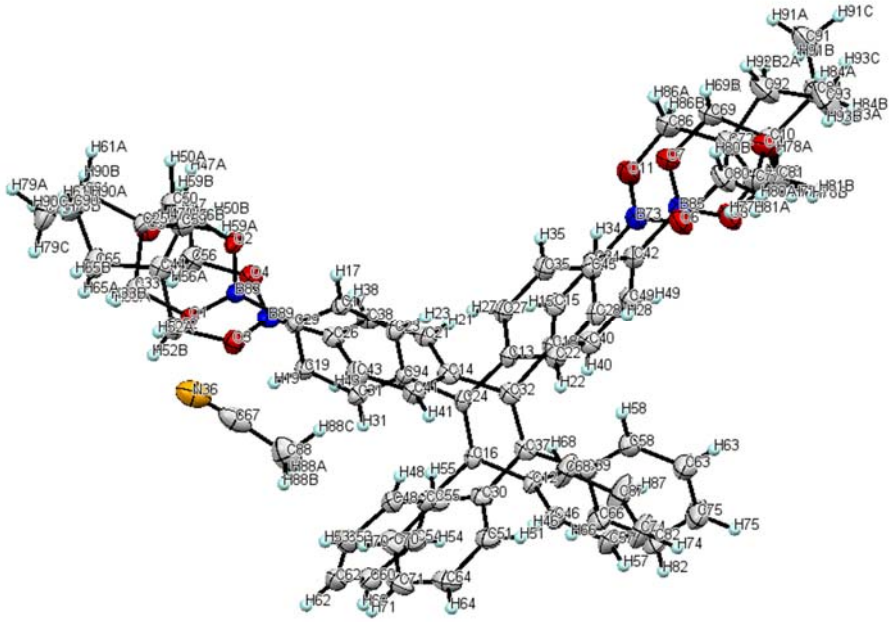


Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
O1	0.41430(19)	0.57996(6)	0.62873(9)	1.92(3)
O2	0.24240(18)	0.54978(6)	0.54646(10)	2.08(3)
O3	0.7712(2)	0.58387(7)	0.59896(10)	2.36(3)
O4	0.8918(2)	0.53370(7)	0.55605(11)	2.40(3)
O5	0.58049(19)	0.49754(7)	0.64170(11)	2.43(4)
O6	0.1379(2)	0.64427(7)	0.05070(11)	2.93(4)

O7	0.6366(2)	0.56400(7)	0.04993(11)	3.02(4)
O8	0.7744(3)	0.60872(8)	0.00931(11)	3.40(5)
O9	0.3836(3)	0.59356(8)	-0.06636(13)	3.65(5)
O11	0.2800(3)	0.58853(7)	0.09048(11)	3.49(5)
N36	1.0962(3)	0.58906(12)	0.67084(19)	4.14(7)
C10	0.5945(4)	0.57628(11)	-0.07053(16)	3.11(6)
C12	0.4084(3)	0.77396(9)	0.32360(14)	1.95(4)
C13	0.3350(3)	0.68601(8)	0.29650(13)	1.80(4)
C14	0.8364(2)	0.65073(9)	0.38004(13)	1.94(4)
C15	0.7074(3)	0.63455(9)	0.23340(14)	2.21(5)
C16	0.3951(2)	0.74437(9)	0.37746(13)	1.79(4)
C17	0.2485(3)	0.61753(8)	0.45521(13)	1.91(4)
C18	0.8200(3)	0.65575(9)	0.25597(13)	1.96(4)
C19	0.4442(3)	0.64105(8)	0.52625(13)	1.85(4)
C20	0.4168(3)	0.76254(8)	0.44631(13)	1.83(4)
C21	0.9063(3)	0.61467(9)	0.39138(14)	1.99(4)
C22	0.2432(3)	0.70321(9)	0.24355(13)	1.97(4)
C23	0.2563(3)	0.64715(9)	0.40778(13)	1.89(4)
C24	0.3661(2)	0.70434(8)	0.36532(12)	1.68(4)
C25	0.3622(3)	0.50726(8)	0.63995(14)	1.94(4)
C26	0.8303(3)	0.59897(9)	0.49010(14)	1.99(4)
C27	0.3928(3)	0.64915(9)	0.28491(14)	2.06(4)
C28	0.2111(3)	0.68397(9)	0.18147(14)	2.11(4)
C29	0.3427(3)	0.61359(8)	0.51527(13)	1.77(4)
C30	0.8988(3)	0.73948(9)	0.39525(14)	2.17(5)
C31	0.4523(2)	0.67064(8)	0.47889(13)	1.82(4)
C32	0.8442(3)	0.67777(9)	0.32186(14)	2.00(4)
C33	0.4049(3)	0.54804(8)	0.67588(13)	1.92(4)
C34	0.6782(3)	0.61501(10)	0.17128(15)	2.37(5)
C35	0.3604(3)	0.63037(9)	0.22244(14)	2.21(5)
C37	0.8698(3)	0.71871(9)	0.32814(14)	2.12(4)

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

atom	x	y	z	B_{eq}
C38	0.9049(3)	0.58915(9)	0.44587(14)	2.03(4)
C39	0.8694(3)	0.74673(9)	0.27040(15)	2.31(5)
C40	0.9056(3)	0.65606(10)	0.21597(15)	2.29(5)
C41	0.7599(3)	0.66041(9)	0.42318(14)	2.21(5)
C42	0.7619(3)	0.61589(9)	0.12977(14)	2.31(5)
C43	0.7580(3)	0.63474(10)	0.47720(14)	2.26(5)

C44	0.7957(3)	0.51357(10)	0.64867(15)	2.35(5)
C45	0.2683(3)	0.64725(9)	0.16935(14)	2.15(4)
C46	0.3343(3)	0.80892(9)	0.31207(15)	2.43(5)
C47	0.2361(3)	0.51533(9)	0.58970(14)	2.11(4)
C48	0.3248(3)	0.76172(9)	0.48183(14)	2.19(4)
C49	0.8762(3)	0.63661(10)	0.15343(15)	2.48(5)
C50	0.4560(3)	0.49354(9)	0.60053(15)	2.27(5)
C51	0.8310(3)	0.77467(10)	0.40373(16)	2.52(5)
C52	0.7810(3)	0.55953(10)	0.65917(14)	2.38(5)
C53	0.3493(3)	0.77714(10)	0.54707(16)	2.71(5)
C54	0.5334(3)	0.77992(9)	0.47670(15)	2.29(5)
C55	0.9916(3)	0.72514(11)	0.44958(16)	2.75(5)
C56	0.9021(3)	0.50751(10)	0.61338(17)	2.76(5)
C57	0.3447(3)	0.83751(10)	0.26328(16)	2.92(6)
C58	0.7750(3)	0.74546(10)	0.21075(16)	2.69(5)
C59	0.6743(3)	0.49578(10)	0.60492(16)	2.56(5)
C60	0.5579(3)	0.79469(10)	0.54202(16)	2.72(5)
C61	0.3483(3)	0.47356(10)	0.69051(16)	2.63(5)
C62	0.4662(3)	0.79344(10)	0.57742(15)	2.78(5)
C63	0.7742(4)	0.77343(11)	0.15940(18)	3.24(6)
C64	0.8520(3)	0.79376(11)	0.46634(18)	3.01(6)
C65	0.8316(3)	0.49281(11)	0.71816(17)	3.02(6)
C66	0.9631(3)	0.77670(11)	0.27722(17)	3.04(6)
C67	1.1019(3)	0.61597(14)	0.6363(2)	3.61(7)
C68	0.4940(4)	0.76794(12)	0.28499(19)	3.53(7)
C69	0.5975(4)	0.54528(10)	-0.01548(16)	3.10(6)
C70	1.0133(3)	0.74455(12)	0.51172(18)	3.42(6)
C71	0.9416(3)	0.77839(12)	0.52043(18)	3.36(6)
C72	0.1912(4)	0.59663(11)	-0.03179(16)	3.29(6)
C74	0.4303(4)	0.83148(13)	0.2260(2)	3.96(8)
C75	0.8663(4)	0.80321(13)	0.1672(2)	3.93(7)

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

atom	x	y	z	B_{eq}
C77	0.3023(4)	0.62121(11)	-0.04367(17)	3.25(6)
C78	0.7271(4)	0.59409(12)	-0.05879(16)	3.48(7)
C79	0.2690(4)	0.48455(13)	0.7396(2)	3.72(7)
C80	0.0963(4)	0.62610(13)	-0.01504(17)	3.54(7)
C81	0.5022(4)	0.61088(11)	-0.06646(18)	3.33(6)
C82	0.9614(4)	0.80462(14)	0.2260(2)	4.15(8)

C84	0.5556(4)	0.55604(12)	-0.14071(17)	3.62(7)
C86	0.2368(4)	0.56728(11)	0.02724(17)	3.80(7)
C87	0.5045(5)	0.79657(15)	0.2365(2)	4.94(10)
C88	1.1082(4)	0.65139(15)	0.5943(2)	4.53(8)
C90	0.8486(5)	0.44597(13)	0.7179(2)	4.64(9)
C91	0.6157(5)	0.51426(14)	-0.14815(19)	4.68(9)
C92	0.1299(5)	0.57127(15)	-0.0945(2)	4.77(9)
C93	0.0818(7)	0.5954(2)	-0.1586(2)	7.11(15)
C94	0.3583(2)	0.67419(8)	0.41887(12)	1.64(4)
B73	0.2273(4)	0.62531(11)	0.09942(17)	2.54(6)
B83	0.3327(3)	0.57911(9)	0.56675(15)	1.83(4)
B85	0.7231(4)	0.59464(12)	0.05888(18)	2.70(6)
B89	0.8318(3)	0.57061(10)	0.55232(16)	2.11(5)

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

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

atom	x	y	z	Biso
H15	0.65079	0.63343	0.26022	2.653
H17	0.17960	0.59994	0.44711	2.287
H19	0.50706	0.63940	0.56590	2.223
H21	0.95501	0.60737	0.36218	2.392
H22	0.20367	0.72762	0.25013	2.366
H23	0.19311	0.64901	0.36829	2.270
H27	0.45349	0.63720	0.31948	2.477
H28	0.15001	0.69579	0.14697	2.531
H31	0.52088	0.68835	0.48700	2.180
H33A	0.34533	0.55634	0.70110	2.298
H33B	0.48594	0.54425	0.70734	2.298
H34	0.60216	0.60116	0.15704	2.846
H35	0.40057	0.60613	0.21562	2.650
H38	0.95386	0.56543	0.45295	2.439
H40	0.98254	0.66927	0.23104	2.745
H41	0.71034	0.68399	0.41571	2.647
H43	0.70703	0.64165	0.50544	2.715
H46	0.27641	0.81344	0.33739	2.914
H47A	0.21102	0.49091	0.56252	2.535
H47B	0.17276	0.52074	0.61399	2.535
H48	0.24616	0.75078	0.46194	2.625

H49	0.93352	0.63742	0.12703	2.977
H50A	0.44004	0.46511	0.58658	2.730
H50B	0.44624	0.51039	0.56064	2.730
H51	0.77147	0.78542	0.36741	3.022
H52A	0.70638	0.56396	0.67530	2.861
H52B	0.85260	0.56912	0.69362	2.861
H53	0.28690	0.77650	0.57032	3.250
H54	0.59502	0.78161	0.45302	2.754
H55	1.03956	0.70239	0.44429	3.295
H56A	0.98177	0.51284	0.64527	3.318
H56B	0.90232	0.47903	0.59921	3.318
H57	0.29350	0.86070	0.25603	3.508
H58	0.71206	0.72571	0.20527	3.232
H59A	0.64784	0.51158	0.56381	3.073
H59B	0.68749	0.46748	0.59322	3.073
H60	0.63653	0.80552	0.56215	3.268

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H61A	0.31166	0.44941	0.66537	3.161
H61B	0.43158	0.46599	0.71645	3.161
H62	0.48281	0.80342	0.62110	3.338
H63	0.71132	0.77205	0.11972	3.887
H64	0.80563	0.81689	0.47167	3.613
H65A	0.90929	0.50498	0.74387	3.628
H65B	0.76707	0.49907	0.74130	3.628
H66	1.02719	0.77791	0.31643	3.653
H68	0.54455	0.74460	0.29164	4.237
H69A	0.51456	0.53344	-0.02111	3.720
H69B	0.65498	0.52320	-0.01887	3.720
H70	1.07600	0.73484	0.54756	4.101
H71	0.95389	0.79064	0.56242	4.032
H74	0.43849	0.85073	0.19391	4.756
H75	0.86473	0.82222	0.13318	4.715
H77A	0.27252	0.64240	-0.07708	3.904
H77B	0.34709	0.63442	-0.00235	3.904
H78A	0.78305	0.57304	-0.06803	4.182
H78B	0.72618	0.61669	-0.08971	4.182
H79A	0.26132	0.46083	0.76609	4.469
H79B	0.18709	0.49327	0.71488	4.469

H79C	0.30895	0.50644	0.76848	4.469
H80A	0.07899	0.64790	-0.04830	4.247
H80B	0.01840	0.61139	-0.01774	4.247
H81A	0.53371	0.62676	-0.02581	3.990
H81B	0.49356	0.62920	-0.10457	3.990
H82	1.02417	0.82440	0.23113	4.977
H84A	0.46518	0.55258	-0.15264	4.347
H84B	0.57604	0.57493	-0.17293	4.347
H86A	0.16880	0.54889	0.03001	4.554
H86B	0.30482	0.55063	0.01920	4.554
H87	0.56201	0.79219	0.21084	5.926
H88A	1.19452	0.65820	0.59769	5.433
H88B	1.06705	0.67439	0.60893	5.433
H88C	1.06732	0.64500	0.54854	5.433
H90A	0.91513	0.43928	0.69714	5.563
H90B	0.77202	0.43336	0.69318	5.563

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H90C	0.86927	0.43592	0.76319	5.563
H91A	0.58595	0.49402	-0.12181	5.610
H91B	0.70532	0.51649	-0.13286	5.610
H91C	0.59336	0.50612	-0.19446	5.610
H92A	0.19074	0.55135	-0.10190	5.718
H92B	0.06023	0.55598	-0.08534	5.718
H93A	0.15054	0.60925	-0.17012	8.527
H93B	0.02133	0.61532	-0.15218	8.527
H93C	0.04283	0.57692	-0.19410	8.527

Table 3. Anisotropic displacement parameters

atom	U11	U22	U33	U12	U13	U23
O1	0.0320(10)	0.0202(9)	0.0203(8)	-0.0046(8)	0.0056(7)	0.0014(7)
O2	0.0244(9)	0.0270(10)	0.0264(9)	-0.0051(8)	0.0039(7)	0.0068(8)
O3	0.0320(10)	0.0321(11)	0.0283(10)		0.0039(9)	0.0122(8)
0.0027(8)						
O4	0.0285(10)	0.0301(11)	0.0353(11)	0.0034(8)	0.0132(8)	
0.0018(8)						
O5	0.0235(10)	0.0364(12)	0.0330(11)	0.0001(8)	0.0084(8)	
0.0011(9)						
O6	0.0387(12)	0.0418(13)	0.0273(10)	0.0038(10)	0.0014(9)	-

0.0043(9)

O7 0.0500(14) 0.0316(12) 0.0315(11) -0.0076(10) 0.0070(10) -0.0049(9)

O8 0.0494(14) 0.0529(15) 0.0266(11) -0.0144(12) 0.0089(10) -0.0079(10)

O9 0.0539(16) 0.0358(13) 0.0476(14) -0.0032(11) 0.0102(12) -0.0129(11)

O11 0.0663(17) 0.0342(13) 0.0284(11) 0.0093(12) 0.0047(11) -0.0035(9)

N36 0.0428(18) 0.051(2) 0.062(2) -0.0002(15) 0.0101(15) -0.0182(17)

C10 0.051(2) 0.0340(17) 0.0306(15) -0.0015(14) 0.0051(14) -0.0054(13)

C12 0.0232(12) 0.0241(13) 0.0268(13) -0.0004(10) 0.0061(10) 0.0072(10)

C13 0.0228(12) 0.0253(13) 0.0216(12) 0.0007(10) 0.0082(9) 0.0029(10)

C14 0.0191(11) 0.0293(14) 0.0261(12) -0.0047(10) 0.0070(9) -0.0032(10)

C15 0.0246(13) 0.0319(15) 0.0296(13) -0.0042(11) 0.0109(10) -0.0013(11)

C16 0.0194(11) 0.0270(14) 0.0227(12) 0.0006(10) 0.0072(9) 0.0048(10)

C17 0.0241(12) 0.0236(13) 0.0250(12) -0.0037(10) 0.0065(10) 0.0022(10)

C18 0.0247(12) 0.0251(13) 0.0254(12) -0.0015(10) 0.0080(10) -0.0008(10)

C19 0.0246(12) 0.0230(13) 0.0221(12) 0.0007(10) 0.0045(9) 0.0024(10)

C20 0.0242(12) 0.0198(12) 0.0255(12) 0.0009(10) 0.0058(10) 0.0040(10)

C21 0.0226(12) 0.0267(14) 0.0284(13) -0.0033(10) 0.0099(10) -0.0049(10)

C22 0.0240(12) 0.0265(14) 0.0254(12) 0.0033(10) 0.0081(10) 0.0035(10)

C23 0.0229(12) 0.0254(13) 0.0228(12) 0.0003(10) 0.0042(9) 0.0025(10)

C24 0.0196(11) 0.0248(13) 0.0206(11) 0.0023(9) 0.0071(9) 0.0032(9)

C25 0.0256(12) 0.0211(13) 0.0265(12) -0.0020(10) 0.0053(10) 0.0036(10)

C26	0.0207(12)	0.0294(14)	0.0261(12)	-0.0024(10)	0.0065(10)	-0.0025(10)
C27	0.0260(13)	0.0283(14)	0.0245(12)	0.0046(11)	0.0069(10)	0.0058(10)
C28	0.0233(12)	0.0328(15)	0.0242(12)	0.0023(11)	0.0063(10)	0.0044(11)
C29	0.0246(12)	0.0214(13)	0.0227(12)	0.0001(10)	0.0085(9)	0.0018(9)
C30	0.0258(13)	0.0286(14)	0.0298(13)	-0.0077(11)	0.0104(11)	-0.0050(11)
C31	0.0208(12)	0.0212(13)	0.0274(12)	0.0002(9)	0.0068(10)	0.0028(10)
C32	0.0209(12)	0.0306(14)	0.0261(12)	-0.0038(10)	0.0086(10)	-0.0033(10)
C33	0.0293(13)	0.0234(13)	0.0203(11)	-0.0025(10)	0.0065(10)	0.0038(10)
C34	0.0283(14)	0.0310(15)	0.0296(14)	-0.0053(11)	0.0049(11)	-0.0018(11)
C35	0.0282(13)	0.0300(15)	0.0276(13)	0.0044(11)	0.0104(11)	0.0024(11)
C37	0.0226(12)	0.0315(15)	0.0279(13)	-0.0039(11)	0.0090(10)	-0.0042(11)

Table 3. Anisotropic displacement parameters (continued)

atom	U11	U22	U33	U12	U13	U23
C38	0.0218(12)	0.0252(14)	0.0311(13)	-0.0000(10)	0.0083(10)	-0.0033(11)
C39	0.0296(14)	0.0277(14)	0.0337(14)	-0.0041(11)	0.0136(11)	-0.0019(11)
C40	0.0249(13)	0.0336(16)	0.0306(14)	-0.0047(11)	0.0111(11)	-0.0030(11)
C41	0.0235(13)	0.0304(15)	0.0319(14)	0.0030(11)	0.0107(11)	0.0014(11)
C42	0.0349(15)	0.0274(14)	0.0244(13)	-0.0016(12)	0.0058(11)	0.0013(11)
C43	0.0239(13)	0.0350(16)	0.0297(13)	0.0037(11)	0.0115(10)	

0.0004(11)

C44 0.0247(13) 0.0330(16) 0.0332(14) 0.0032(11) 0.0103(11)
0.0037(12)

C45 0.0306(14) 0.0283(14) 0.0232(12) 0.0005(11) 0.0075(10)
0.0013(10)

C46 0.0362(15) 0.0278(15) 0.0274(13) 0.0044(12) 0.0064(11)
0.0041(11)

C47 0.0263(13) 0.0232(13) 0.0300(13) -0.0059(10) 0.0056(10)
0.0062(10)

C48 0.0275(13) 0.0261(14) 0.0311(14) 0.0001(11) 0.0103(11)
0.0003(11)

C49 0.0328(15) 0.0372(17) 0.0276(14) -0.0023(12) 0.0138(11) -
0.0012(12)

C50 0.0273(13) 0.0244(14) 0.0339(14) -0.0024(11) 0.0061(11) -
0.0032(11)

C51 0.0298(14) 0.0302(15) 0.0374(15) -0.0066(12) 0.0119(12) -
0.0042(12)

C52 0.0330(14) 0.0329(16) 0.0257(13) -0.0010(12) 0.0093(11)
0.0009(11)

C53 0.0432(17) 0.0327(16) 0.0308(14) 0.0018(13) 0.0165(13) -
0.0006(12)

C54 0.0269(13) 0.0284(14) 0.0317(14) -0.0029(11) 0.0069(11)
0.0023(11)

C55 0.0282(14) 0.0374(17) 0.0379(16) -0.0046(12) 0.0068(12) -
0.0087(13)

C56 0.0306(15) 0.0345(17) 0.0432(17) 0.0072(12) 0.0152(13)
0.0074(13)

C57 0.0453(18) 0.0282(16) 0.0349(16) 0.0078(13) 0.0050(13)
0.0094(12)

C58 0.0346(16) 0.0316(16) 0.0359(16) -0.0014(12) 0.0083(12)
0.0004(12)

C59 0.0312(14) 0.0329(16) 0.0355(15) 0.0017(12) 0.0126(12) -
0.0029(12)

C60 0.0336(15) 0.0315(16) 0.0343(15) -0.0032(12) 0.0009(12)
0.0023(12)

C61 0.0340(15) 0.0272(15) 0.0370(15) -0.0043(12) 0.0053(12)
0.0111(12)

C62 0.0486(19) 0.0285(15) 0.0271(14) 0.0021(13) 0.0066(13) -
0.0013(11)

C63	0.0436(19)	0.0394(19)	0.0384(17)	-0.0034(14)	0.0071(14)	0.0047(14)
C64	0.0354(16)	0.0356(17)	0.0476(18)	-0.0102(13)	0.0182(14)	-0.0154(14)
C65	0.0331(16)	0.0445(19)	0.0384(17)	0.0028(14)	0.0111(13)	0.0111(14)
C66	0.0360(16)	0.0432(19)	0.0376(16)	-0.0146(14)	0.0115(13)	0.0018(14)
C67	0.0328(17)	0.054(2)	0.049(2)	0.0038(16)	0.0070(14)	-0.0225(19)
C68	0.0447(19)	0.043(2)	0.056(2)	0.0167(15)	0.0311(17)	0.0260(16)
C69	0.050(2)	0.0304(16)	0.0326(15)	-0.0033(14)	0.0021(14)	-0.0065(13)
C70	0.0386(18)	0.051(2)	0.0355(17)	-0.0081(15)	0.0009(13)	-0.0086(15)
C71	0.0409(18)	0.049(2)	0.0385(17)	-0.0167(16)	0.0122(14)	-0.0188(15)
C72	0.056(2)	0.0390(19)	0.0271(15)	-0.0037(16)	0.0047(14)	-0.0061(13)
C74	0.055(2)	0.047(2)	0.052(2)	0.0072(17)	0.0196(18)	0.0292(17)
C75	0.057(2)	0.051(2)	0.0432(19)	-0.0115(18)	0.0152(17)	0.0121(16)

Table 3. Anisotropic displacement parameters (continued)

atom	U11	U22	U33	U12	U13	U23
C77	0.058(2)	0.0310(17)	0.0334(16)	0.0027(15)	0.0085(14)	-0.0019(13)
C78	0.056(2)	0.049(2)	0.0264(15)	-0.0109(17)	0.0099(14)	-0.0074(14)
C79	0.0413(19)	0.053(2)	0.049(2)	0.0016(16)	0.0155(15)	0.0238(17)
C80	0.0455(19)	0.055(2)	0.0282(15)	0.0001(16)	-0.0016(13)	-0.0062(14)
C81	0.054(2)	0.0327(17)	0.0360(17)	-0.0024(15)	0.0042(15)	-0.0056(13)
C82	0.054(2)	0.057(2)	0.048(2)	-0.0259(19)	0.0142(17)	0.0093(18)
C84	0.055(2)	0.045(2)	0.0323(16)	0.0042(17)	0.0013(15)	-0.0079(14)
C86	0.075(3)	0.0341(18)	0.0334(17)	-0.0048(17)	0.0097(17)	-0.0038(14)
C87	0.065(3)	0.066(3)	0.073(3)	0.026(2)	0.048(2)	0.041(2)
C88	0.052(2)	0.074(3)	0.049(2)	0.013(2)	0.0181(18)	-0.007(2)
C90	0.069(3)	0.045(2)	0.067(3)	0.008(2)	0.025(2)	0.022(2)
C91	0.075(3)	0.062(3)	0.0332(18)	0.018(2)	0.0001(18)	-0.0119(17)
C92	0.074(3)	0.066(3)	0.0360(19)	-0.014(2)	0.0041(19)	-0.0161(18)
C93	0.115(5)	0.105(5)	0.033(2)	-0.023(4)	-0.012(3)	-0.010(2)
C94	0.0236(12)	0.0192(12)	0.0204(11)	0.0013(9)	0.0074(9)	0.0028(9)
B73	0.0367(17)	0.0331(18)	0.0257(15)	-0.0002(14)	0.0055(13)	-0.0019(13)
B83	0.0275(14)	0.0206(14)	0.0222(13)	0.0002(11)	0.0080(11)	0.0014(10)

B85	0.0387(18)	0.0338(18)	0.0289(16)	-0.0001(14)	0.0064(13)	-0.0024(13)
B89	0.0223(14)	0.0287(16)	0.0289(15)	-0.0017(12)	0.0061(11)	-0.0027(12)

The general temperature factor expression: exp(-2□2(a*2U11h2 + b*2U22k2 + c*2U33l2 + 2a*b*U12hk + 2a*c*U13hl + 2b*c*U23kl))

Table 4. Fragment Analysis

fragment: 1

O(1)	O(2)	O(3)	O(4)	O(5)
O(6)	O(7)	O(8)	O(9)	O(11)
C(10)	C(12)	C(13)	C(14)	C(15)
C(16)	C(17)	C(18)	C(19)	C(20)
C(21)	C(22)	C(23)	C(24)	C(25)
C(26)	C(27)	C(28)	C(29)	C(30)
C(31)	C(32)	C(33)	C(34)	C(35)
C(37)	C(38)	C(39)	C(40)	C(41)
C(42)	C(43)	C(44)	C(45)	C(46)
C(47)	C(48)	C(49)	C(50)	C(51)
C(52)	C(53)	C(54)	C(55)	C(56)
C(57)	C(58)	C(59)	C(60)	C(61)
C(62)	C(63)	C(64)	C(65)	C(66)
C(68)	C(69)	C(70)	C(71)	C(72)
C(74)	C(75)	C(77)	C(78)	C(79)
C(80)	C(81)	C(82)	C(84)	C(86)
C(87)	C(90)	C(91)	C(92)	C(93)
C(94)	B(73)	B(83)	B(85)	B(89)

Table 4. Fragment Analysis (continued)

fragment: 2

N(36)	C(67)	C(88)

Table 5. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
O1	C33	1.441(3)	O1	B83	1.365(3)

O2	C47	1.442(4)	O2	B83	1.364(3)
O3	C52	1.451(4)	O3	B89	1.368(4)
O4	C56	1.436(4)	O4	B89	1.361(4)
O5	C50	1.425(3)	O5	C59	1.426(4)
O6	C80	1.442(4)	O6	B73	1.363(4)
O7	C69	1.441(4)	O7	B85	1.357(5)
O8	C78	1.448(4)	O8	B85	1.362(5)
O9	C77	1.426(5)	O9	C81	1.421(5)
O11	C86	1.445(4)	O11	B73	1.360(4)
N36	C67	1.138(6)	C10	C69	1.510(5)
C10	C78	1.531(6)	C10	C81	1.530(5)
C10	C84	1.547(5)	C12	C16	1.501(4)
C12	C46	1.383(4)	C12	C68	1.389(5)
C13	C22	1.404(3)	C13	C24	1.495(4)
C13	C27	1.403(4)	C14	C21	1.388(4)
C14	C32	1.504(4)	C14	C41	1.403(4)
C15	C18	1.392(4)	C15	C34	1.391(4)
C16	C20	1.498(4)	C16	C24	1.347(4)
C17	C23	1.388(4)	C17	C29	1.406(3)
C18	C32	1.497(4)	C18	C40	1.397(5)
C19	C29	1.403(4)	C19	C31	1.387(4)
C20	C48	1.389(5)	C20	C54	1.398(4)
C21	C38	1.398(4)	C22	C28	1.386(4)
C23	C94	1.398(4)	C24	C94	1.493(4)
C25	C33	1.532(4)	C25	C47	1.531(4)
C25	C50	1.529(5)	C25	C61	1.544(4)
C26	C38	1.406(4)	C26	C43	1.396(4)
C26	B89	1.574(4)	C27	C35	1.387(4)
C28	C45	1.399(4)	C29	B83	1.564(4)
C30	C37	1.498(4)	C30	C51	1.399(4)
C30	C55	1.393(4)	C31	C94	1.404(3)
C32	C37	1.358(4)	C34	C42	1.404(5)
C35	C45	1.403(4)	C37	C39	1.496(4)
C39	C58	1.396(4)	C39	C66	1.399(5)
C40	C49	1.397(4)	C41	C43	1.394(4)
C42	C49	1.402(4)	C42	B85	1.574(5)

Table 5. Bond lengths (Å) (continued)

atom	atom	distance	atom	atom	distance
C44	C52	1.522(5)	C44	C56	1.537(5)
C44	C59	1.525(4)	C44	C65	1.541(5)
C45	B73	1.568(4)	C46	C57	1.393(5)
C48	C53	1.395(4)	C51	C64	1.396(5)
C53	C62	1.386(5)	C54	C60	1.389(4)
C55	C70	1.392(5)	C57	C74	1.369(6)
C58	C63	1.392(5)	C60	C62	1.385(5)
C61	C79	1.532(6)	C63	C75	1.381(6)
C64	C71	1.383(5)	C65	C90	1.533(6)
C66	C82	1.386(6)	C67	C88	1.451(7)
C68	C87	1.390(6)	C70	C71	1.390(6)
C72	C77	1.529(6)	C72	C80	1.519(6)
C72	C86	1.527(5)	C72	C92	1.538(5)
C74	C87	1.382(6)	C75	C82	1.389(5)
C84	C91	1.533(6)	C92	C93	1.511(6)

Table 6. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C15	H15	0.930	C17	H17	0.930
C19	H19	0.930	C21	H21	0.930
C22	H22	0.930	C23	H23	0.930
C27	H27	0.930	C28	H28	0.930
C31	H31	0.930	C33	H33A	0.970
C33	H33B	0.970	C34	H34	0.930
C35	H35	0.930	C38	H38	0.930
C40	H40	0.930	C41	H41	0.930
C43	H43	0.930	C46	H46	0.930
C47	H47A	0.970	C47	H47B	0.970
C48	H48	0.930	C49	H49	0.930
C50	H50A	0.970	C50	H50B	0.970
C51	H51	0.930	C52	H52A	0.970
C52	H52B	0.970	C53	H53	0.930
C54	H54	0.930	C55	H55	0.930
C56	H56A	0.970	C56	H56B	0.970
C57	H57	0.930	C58	H58	0.930
C59	H59A	0.970	C59	H59B	0.970
C60	H60	0.930	C61	H61A	0.970

C61	H61B	0.970	C62	H62	0.930
C63	H63	0.930	C64	H64	0.930
C65	H65A	0.970	C65	H65B	0.970
C66	H66	0.930	C68	H68	0.930
C69	H69A	0.970	C69	H69B	0.970
C70	H70	0.930	C71	H71	0.930
C74	H74	0.930	C75	H75	0.930
C77	H77A	0.970	C77	H77B	0.970
C78	H78A	0.970	C78	H78B	0.970
C79	H79A	0.960	C79	H79B	0.960
C79	H79C	0.960	C80	H80A	0.970
C80	H80B	0.970	C81	H81A	0.970
C81	H81B	0.970	C82	H82	0.930
C84	H84A	0.970	C84	H84B	0.970
C86	H86A	0.970	C86	H86B	0.970
C87	H87	0.930	C88	H88A	0.960
C88	H88B	0.960	C88	H88C	0.960
C90	H90A	0.960	C90	H90B	0.960

Table 6. Bond lengths involving hydrogens (Å) (continued)

atom	atom	distance	atom	atom	distance
C90	H90C	0.960	C91	H91A	0.960
C91	H91B	0.960	C91	H91C	0.960
C92	H92A	0.970	C92	H92B	0.970
C93	H93A	0.960	C93	H93B	0.960
C93	H93C	0.960			

Table 7. Bond angles (o)

atom	atom	atom	angle	atom	atom	atom	angle
C33	O1	B83	118.3(2)	C47	O2	B83	119.8(2)
C52	O3	B89	118.9(2)	C56	O4	B89	120.4(3)
C50	O5	C59	113.4(2)	C80	O6	B73	120.5(3)
C69	O7	B85	118.1(3)	C78	O8	B85	119.9(3)
C77	O9	C81	113.8(3)	C86	O11	B73	119.1(3)
C69	C10	C78	107.0(3)	C69	C10	C81	109.8(3)

C69	C10	C84	111.5(3)	C78	C10	C81	109.4(3)
C78	C10	C84	109.8(3)	C81	C10	C84	109.3(3)
C16	C12	C46	119.4(3)	C16	C12	C68	122.5(3)
C46	C12	C68	118.1(3)	C22	C13	C24	121.8(2)
C22	C13	C27	118.4(2)	C24	C13	C27	119.6(2)
C21	C14	C32	119.1(3)	C21	C14	C41	118.5(3)
C32	C14	C41	122.4(3)	C18	C15	C34	120.9(3)
C12	C16	C20	115.1(2)	C12	C16	C24	122.9(2)
C20	C16	C24	122.0(3)	C23	C17	C29	121.3(2)
C15	C18	C32	118.7(3)	C15	C18	C40	118.8(3)
C32	C18	C40	122.5(2)	C29	C19	C31	121.0(2)
C16	C20	C48	121.7(2)	C16	C20	C54	119.6(3)
C48	C20	C54	118.7(3)	C14	C21	C38	121.2(3)
C13	C22	C28	120.3(3)	C17	C23	C94	120.6(2)
C13	C24	C16	123.2(2)	C13	C24	C94	113.4(2)
C16	C24	C94	123.4(2)	C33	C25	C47	107.1(2)
C33	C25	C50	110.0(2)	C33	C25	C61	110.9(2)
C47	C25	C50	108.0(2)	C47	C25	C61	110.5(2)
C50	C25	C61	110.2(2)	C38	C26	C43	117.6(3)
C38	C26	B89	120.3(3)	C43	C26	B89	122.1(3)
C13	C27	C35	120.7(2)	C22	C28	C45	121.7(2)
C17	C29	C19	117.8(2)	C17	C29	B83	120.0(2)
C19	C29	B83	122.3(2)	C37	C30	C51	119.1(2)
C37	C30	C55	122.3(3)	C51	C30	C55	118.7(3)
C19	C31	C94	120.8(2)	C14	C32	C18	114.2(2)
C14	C32	C37	123.2(3)	C18	C32	C37	122.6(3)
O1	C33	C25	111.2(2)	C15	C34	C42	120.9(3)
C27	C35	C45	121.2(3)	C30	C37	C32	121.3(3)
C30	C37	C39	114.6(2)	C32	C37	C39	124.1(3)
C21	C38	C26	120.7(3)	C37	C39	C58	122.3(3)
C37	C39	C66	119.2(2)	C58	C39	C66	118.4(3)

Table 7. Bond angles (o) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C18	C40	C49	120.3(3)	C14	C41	C43	120.1(3)
C34	C42	C49	117.8(3)	C34	C42	B85	119.2(3)
C49	C42	B85	123.0(3)	C26	C43	C41	121.9(3)

C52	C44	C56	108.2(3)	C52	C44	C59	110.3(2)
C52	C44	C65	108.0(3)	C56	C44	C59	109.3(3)
C56	C44	C65	109.5(3)	C59	C44	C65	111.5(3)
C28	C45	C35	117.6(3)	C28	C45	B73	120.8(2)
C35	C45	B73	121.6(3)	C12	C46	C57	121.3(3)
O2	C47	C25	112.0(2)	C20	C48	C53	120.6(3)
C40	C49	C42	121.2(3)	O5	C50	C25	109.5(2)
C30	C51	C64	120.5(3)	O3	C52	C44	113.6(2)
C48	C53	C62	120.4(3)	C20	C54	C60	120.5(3)
C30	C55	C70	120.6(3)	O4	C56	C44	113.5(3)
C46	C57	C74	120.0(3)	C39	C58	C63	120.7(3)
O5	C59	C44	108.3(3)	C54	C60	C62	120.6(3)
C25	C61	C79	116.6(3)	C53	C62	C60	119.3(3)
C58	C63	C75	120.2(3)	C51	C64	C71	120.2(3)
C44	C65	C90	115.7(3)	C39	C66	C82	120.6(3)
N36	C67	C88	177.8(5)	C12	C68	C87	120.5(4)
O7	C69	C10	111.4(3)	C55	C70	C71	120.3(3)
C64	C71	C70	119.6(3)	C77	C72	C80	109.2(3)
C77	C72	C86	109.7(3)	C77	C72	C92	110.2(3)
C80	C72	C86	108.7(3)	C80	C72	C92	110.2(3)
C86	C72	C92	108.8(3)	C57	C74	C87	119.5(4)
C63	C75	C82	119.7(4)	O9	C77	C72	108.4(3)
O8	C78	C10	112.0(3)	O6	C80	C72	113.3(3)
O9	C81	C10	109.3(3)	C66	C82	C75	120.4(4)
C10	C84	C91	116.3(3)	O11	C86	C72	112.8(3)
C68	C87	C74	120.5(5)	C72	C92	C93	116.1(4)
C23	C94	C24	118.9(2)	C23	C94	C31	118.5(2)
C24	C94	C31	122.5(2)	O6	B73	O11	123.4(3)
O6	B73	C45	117.3(3)	O11	B73	C45	119.3(3)
O1	B83	O2	124.0(3)	O1	B83	C29	118.5(2)
O2	B83	C29	117.5(2)	O7	B85	O8	123.5(3)
O7	B85	C42	117.8(3)	O8	B85	C42	118.7(3)
O3	B89	O4	123.5(3)	O3	B89	C26	118.6(3)
O4	B89	C26	117.9(3)				

Table 8. Bond angles involving hydrogens (o)

atom	atom	atom	angle	atom	atom	atom	angle

C18	C15	H15	119.5	C34	C15	H15	119.5
C23	C17	H17	119.4	C29	C17	H17	119.3
C29	C19	H19	119.5	C31	C19	H19	119.5
C14	C21	H21	119.4	C38	C21	H21	119.4
C13	C22	H22	119.9	C28	C22	H22	119.9
C17	C23	H23	119.7	C94	C23	H23	119.7
C13	C27	H27	119.7	C35	C27	H27	119.7
C22	C28	H28	119.1	C45	C28	H28	119.1
C19	C31	H31	119.6	C94	C31	H31	119.6
O1	C33	H33A	109.4	O1	C33	H33B	109.4
C25	C33	H33A	109.4	C25	C33	H33B	109.4
H33A	C33	H33B	108.0	C15	C34	H34	119.5
C42	C34	H34	119.5	C27	C35	H35	119.4
C45	C35	H35	119.4	C21	C38	H38	119.7
C26	C38	H38	119.7	C18	C40	H40	119.8
C49	C40	H40	119.8	C14	C41	H41	119.9
C43	C41	H41	120.0	C26	C43	H43	119.1
C41	C43	H43	119.1	C12	C46	H46	119.3
C57	C46	H46	119.3	O2	C47	H47A	109.2
O2	C47	H47B	109.2	C25	C47	H47A	109.2
C25	C47	H47B	109.2	H47A	C47	H47B	107.9
C20	C48	H48	119.7	C53	C48	H48	119.7
C40	C49	H49	119.4	C42	C49	H49	119.4
O5	C50	H50A	109.8	O5	C50	H50B	109.8
C25	C50	H50A	109.8	C25	C50	H50B	109.8
H50A	C50	H50B	108.2	C30	C51	H51	119.8
C64	C51	H51	119.8	O3	C52	H52A	108.8
O3	C52	H52B	108.8	C44	C52	H52A	108.8
C44	C52	H52B	108.8	H52A	C52	H52B	107.7
C48	C53	H53	119.8	C62	C53	H53	119.8
C20	C54	H54	119.8	C60	C54	H54	119.8
C30	C55	H55	119.7	C70	C55	H55	119.7
O4	C56	H56A	108.9	O4	C56	H56B	108.9
C44	C56	H56A	108.9	C44	C56	H56B	108.9
H56A	C56	H56B	107.7	C46	C57	H57	120.0
C74	C57	H57	120.0	C39	C58	H58	119.6
C63	C58	H58	119.6	O5	C59	H59A	110.0

Table 8. Bond angles involving hydrogens (o) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O5	C59	H59B	110.0	C44	C59	H59A	110.0
C44	C59	H59B	110.0	H59A	C59	H59B	108.4
C54	C60	H60	119.7	C62	C60	H60	119.7
C25	C61	H61A	108.1	C25	C61	H61B	108.1
C79	C61	H61A	108.1	C79	C61	H61B	108.1
H61A	C61	H61B	107.3	C53	C62	H62	120.4
C60	C62	H62	120.3	C58	C63	H63	119.9
C75	C63	H63	119.9	C51	C64	H64	119.9
C71	C64	H64	119.9	C44	C65	H65A	108.4
C44	C65	H65B	108.3	C90	C65	H65A	108.3
C90	C65	H65B	108.3	H65A	C65	H65B	107.4
C39	C66	H66	119.7	C82	C66	H66	119.7
C12	C68	H68	119.8	C87	C68	H68	119.8
O7	C69	H69A	109.3	O7	C69	H69B	109.3
C10	C69	H69A	109.3	C10	C69	H69B	109.3
H69A	C69	H69B	108.0	C55	C70	H70	119.9
C71	C70	H70	119.9	C64	C71	H71	120.2
C70	C71	H71	120.2	C57	C74	H74	120.3
C87	C74	H74	120.3	C63	C75	H75	120.2
C82	C75	H75	120.2	O9	C77	H77A	110.0
O9	C77	H77B	110.0	C72	C77	H77A	110.0
C72	C77	H77B	110.0	H77A	C77	H77B	108.4
O8	C78	H78A	109.2	O8	C78	H78B	109.2
C10	C78	H78A	109.2	C10	C78	H78B	109.2
H78A	C78	H78B	107.9	C61	C79	H79A	109.5
C61	C79	H79B	109.5	C61	C79	H79C	109.5
H79A	C79	H79B	109.5	H79A	C79	H79C	109.5
H79B	C79	H79C	109.5	O6	C80	H80A	108.9
O6	C80	H80B	108.9	C72	C80	H80A	108.9
C72	C80	H80B	108.9	H80A	C80	H80B	107.7
O9	C81	H81A	109.8	O9	C81	H81B	109.8
C10	C81	H81A	109.8	C10	C81	H81B	109.8
H81A	C81	H81B	108.3	C66	C82	H82	119.8
C75	C82	H82	119.8	C10	C84	H84A	108.2
C10	C84	H84B	108.2	C91	C84	H84A	108.2
C91	C84	H84B	108.2	H84A	C84	H84B	107.3

O11	C86	H86A	109.0	O11	C86	H86B	109.0

Table 8. Bond angles involving hydrogens (o) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C72	C86	H86A	109.0	C72	C86	H86B	109.0
H86A	C86	H86B	107.8	C68	C87	H87	119.7
C74	C87	H87	119.7	C67	C88	H88A	109.5
C67	C88	H88B	109.5	C67	C88	H88C	109.5
H88A	C88	H88B	109.5	H88A	C88	H88C	109.5
H88B	C88	H88C	109.5	C65	C90	H90A	109.5
C65	C90	H90B	109.5	C65	C90	H90C	109.5
H90A	C90	H90B	109.5	H90A	C90	H90C	109.5
H90B	C90	H90C	109.5	C84	C91	H91A	109.5
C84	C91	H91B	109.5	C84	C91	H91C	109.5
H91A	C91	H91B	109.5	H91A	C91	H91C	109.5
H91B	C91	H91C	109.5	C72	C92	H92A	108.3
C72	C92	H92B	108.3	C93	C92	H92A	108.3
C93	C92	H92B	108.3	H92A	C92	H92B	107.4
C92	C93	H93A	109.5	C92	C93	H93B	109.5
C92	C93	H93C	109.5	H93A	C93	H93B	109.5
H93A	C93	H93C	109.5	H93B	C93	H93C	109.5

Table 9. Torsion Angles(o)

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

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C33	O1	B83	O2	-0.1(4)	C33	O1	B83	C29	-179.8(2)
B83	O1	C33	C25	32.7(3)	C47	O2	B83	O1	-5.1(4)
C47	O2	B83	C29	174.6(2)	B83	O2	C47	C25	-23.1(3)
C52	O3	B89	O4	6.4(4)	C52	O3	B89	C26	-174.9(2)
B89	O3	C52	C44	-30.8(3)	C56	O4	B89	O3	-4.7(4)
C56	O4	B89	C26	176.6(2)	B89	O4	C56	C44	27.2(3)
C50	O5	C59	C44	162.3(2)	C59	O5	C50	C25	-164.7(2)
C80	O6	B73	O11	-1.6(5)	C80	O6	B73	C45	179.5(3)
B73	O6	C80	C72	-23.0(4)	C69	O7	B85	O8	0.3(5)
C69	O7	B85	C42	178.0(2)	B85	O7	C69	C10	-34.5(4)
C78	O8	B85	O7	6.9(5)	C78	O8	B85	C42	-170.9(3)
B85	O8	C78	C10	20.7(4)	C77	O9	C81	C10	163.0(2)
C81	O9	C77	C72	-168.1(2)		C86	O11	B73	O6 -2.4(5)

C86	O11	B73	C45	176.5(3)	B73	O11	C86	C72	30.4(5)
C69	C10	C78	O8	-51.5(4)	C78	C10	C69	O7	58.6(4)
C69	C10	C81	O9	-53.4(3)	C81	C10	C69	O7	-60.0(4)
C69	C10	C84	C91	-43.3(5)	C84	C10	C69	O7	178.6(3)
C78	C10	C81	O9	-170.6(2)		C81	C10	C78	O8
	67.4(3)								
C78	C10	C84	C91	75.1(4)	C84	C10	C78	O8	-172.6(3)
C81	C10	C84	C91	-164.9(3)		C84	C10	C81	O9
	69.2(4)								
C16	C12	C46	C57	179.1(2)	C46	C12	C16	C20	-57.7(3)
C46	C12	C16	C24	122.4(3)	C16	C12	C68	C87	-178.8(2)
C68	C12	C16	C20	121.4(3)	C68	C12	C16	C24	-58.5(4)
C46	C12	C68	C87	0.3(4)	C68	C12	C46	C57	-0.1(4)
C22	C13	C24	C16	-52.1(4)	C22	C13	C24	C94	126.3(3)
C24	C13	C22	C28	-175.9(2)		C22	C13	C27	C35
	0.4(4)								
C27	C13	C22	C28	-0.0(4)	C24	C13	C27	C35	176.4(2)
C27	C13	C24	C16	132.1(3)	C27	C13	C24	C94	-49.5(3)
C21	C14	C32	C18	52.5(3)	C21	C14	C32	C37	-128.0(3)
C32	C14	C21	C38	178.2(2)	C21	C14	C41	C43	1.9(4)
C41	C14	C21	C38	-2.4(4)	C32	C14	C41	C43	-178.7(2)
C41	C14	C32	C18	-126.9(3)		C41	C14	C32	C37
	52.6(4)								
C18	C15	C34	C42	0.4(4)	C34	C15	C18	C32	177.4(2)
C34	C15	C18	C40	-1.9(4)	C12	C16	C20	C48	120.9(2)
C12	C16	C20	C54	-60.7(3)	C12	C16	C24	C13	-4.6(4)
C12	C16	C24	C94	177.2(2)	C20	C16	C24	C13	175.5(2)
C20	C16	C24	C94	-2.7(4)	C24	C16	C20	C48	-59.2(3)

Table 9. Torsion angles (o) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C24	C16	C20	C54	119.2(3)	C23	C17	C29	C19	1.0(4)
C23	C17	C29	B83	-178.4(2)		C29	C17	C23	C94 -0.5(4)
C15	C18	C32	C14	56.4(3)	C15	C18	C32	C37	-123.1(3)
C15	C18	C40	C49	2.2(4)	C32	C18	C40	C49	-177.0(2)

C40	C18	C32	C14	-124.3(3)		C40	C18	C32	C37
	56.2(4)								
C29	C19	C31	C94	0.7(4)	C31	C19	C29	C17	-1.0(4)
C31	C19	C29	B83	178.3(2)	C16	C20	C48	C53	177.0(2)
C16	C20	C54	C60	-176.1(2)		C48	C20	C54	C60
	2.3(4)								
C54	C20	C48	C53	-1.4(4)	C14	C21	C38	C26	1.3(4)
C13	C22	C28	C45	-0.1(4)	C17	C23	C94	C24	177.3(2)
C17	C23	C94	C31	0.1(4)	C13	C24	C94	C23	-43.7(3)
C13	C24	C94	C31	133.4(2)	C16	C24	C94	C23	134.7(3)
C16	C24	C94	C31	-48.2(4)	C33	C25	C47	O2	52.5(3)
C47	C25	C33	O1	-57.5(3)	C33	C25	C50	O5	46.2(3)
C50	C25	C33	O1	59.6(3)	C33	C25	C61	C79	51.2(3)
C61	C25	C33	O1	-178.2(2)		C47	C25	C50	O5
	162.8(2)								
C50	C25	C47	O2	-65.9(3)	C47	C25	C61	C79	-67.5(3)
C61	C25	C47	O2	173.5(2)	C50	C25	C61	C79	173.24(19)
C61	C25	C50	O5	-76.4(3)	C38	C26	C43	C41	-0.9(4)
C43	C26	C38	C21	0.4(4)	C38	C26	B89	O3	171.5(2)
C38	C26	B89	O4	-9.7(4)	B89	C26	C38	C21	-178.5(2)
C43	C26	B89	O3	-7.3(4)	C43	C26	B89	O4	171.5(2)
B89	C26	C43	C41	178.0(2)	C13	C27	C35	C45	-0.8(4)
C22	C28	C45	C35	-0.2(4)	C22	C28	C45	B73	178.0(2)
C17	C29	B83	O1	-170.0(2)		C17	C29	B83	O2
	10.3(4)								
C19	C29	B83	O1	10.7(4)	C19	C29	B83	O2	-169.0(3)
C37	C30	C51	C64	177.3(3)	C51	C30	C37	C32	-127.5(3)
C51	C30	C37	C39	51.4(4)	C37	C30	C55	C70	-178.1(3)
C55	C30	C37	C32	53.0(4)	C55	C30	C37	C39	-128.2(3)
C51	C30	C55	C70	2.3(5)	C55	C30	C51	C64	-3.1(5)
C19	C31	C94	C23	-0.1(4)	C19	C31	C94	C24	-177.2(2)
C14	C32	C37	C30	3.1(4)	C14	C32	C37	C39	-175.7(2)
C18	C32	C37	C30	-177.5(2)		C18	C32	C37	C39
	3.8(4)								
C15	C34	C42	C49	0.8(4)	C15	C34	C42	B85	-178.0(2)
C27	C35	C45	C28	0.7(4)	C27	C35	C45	B73	-177.5(3)
C30	C37	C39	C58	-134.8(3)		C30	C37	C39	C66
	42.0(4)								
C32	C37	C39	C58	44.1(4)	C32	C37	C39	C66	-139.2(3)

Table 9. Torsion angles (o) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C37	C39	C58	C63	176.6(3)	C37	C39	C66	C82	-176.4(3)
C58	C39	C66	C82	0.5(5)	C66	C39	C58	C63	-0.2(5)
C18	C40	C49	C42	-1.0(4)	C14	C41	C43	C26	-0.3(4)
C34	C42	C49	C40	-0.5(4)	C34	C42	B85	O7	-24.3(4)
C34	C42	B85	O8	153.5(3)	C49	C42	B85	O7	157.0(3)
C49	C42	B85	O8	-25.2(5)	B85	C42	C49	C40	178.2(3)
C52	C44	C56	O4	-48.4(3)	C56	C44	C52	O3	50.2(3)
C52	C44	C59	O5	-67.5(3)	C59	C44	C52	O3	-69.3(3)
C52	C44	C65	C90	179.1(2)	C65	C44	C52	O3	168.7(2)
C56	C44	C59	O5	173.6(2)	C59	C44	C56	O4	71.8(3)
C56	C44	C65	C90	-63.3(3)	C65	C44	C56	O4	-165.9(2)
C59	C44	C65	C90	57.7(4)	C65	C44	C59	O5	52.4(3)
C28	C45	B73	O6	2.5(5)	C28	C45	B73	O11	-176.5(3)
C35	C45	B73	O6	-179.4(3)		C35	C45	B73	O11
	1.7(5)								
C12	C46	C57	C74	-0.6(4)	C20	C48	C53	C62	-0.1(4)
C30	C51	C64	C71	1.0(5)	C48	C53	C62	C60	0.7(4)
C20	C54	C60	C62	-1.7(4)	C30	C55	C70	C71	0.5(5)
C46	C57	C74	C87	1.0(5)	C39	C58	C63	C75	-0.7(5)
C54	C60	C62	C53	0.2(5)	C58	C63	C75	C82	1.3(6)
C51	C64	C71	C70	1.9(5)	C39	C66	C82	C75	0.0(6)
C12	C68	C87	C74	0.1(6)	C55	C70	C71	C64	-2.6(6)
C77	C72	C80	O6	-71.6(4)	C80	C72	C77	O9	-173.8(2)
C77	C72	C86	O11	67.6(4)	C86	C72	C77	O9	67.2(3)
C77	C72	C92	C93	-58.3(5)	C92	C72	C77	O9	-52.6(4)
C80	C72	C86	O11	-51.8(4)	C86	C72	C80	O6	48.0(4)
C80	C72	C92	C93	62.4(5)	C92	C72	C80	O6	167.1(3)
C86	C72	C92	C93	-178.6(4)		C92	C72	C86	O11 -171.8(4)
C57	C74	C87	C68	-0.8(6)	C63	C75	C82	C66	-0.9(7)

Table 10. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	O5	3.214(3)	O1	C19	2.973(3)
O1	C47	2.847(3)	O1	C50	2.925(4)
O2	C17	2.904(3)	O2	C33	2.813(3)
O2	C50	2.964(3)	O3	C43	2.975(4)
O3	C56	2.845(4)	O3	C59	3.066(4)
O4	C38	2.928(4)	O4	C52	2.826(4)
O4	C59	3.074(4)	O5	C33	2.756(4)
O5	C52	2.941(4)	O5	C61	3.070(4)
O5	C65	2.821(4)	O5	C90	3.413(5)
O6	C28	2.911(4)	O6	C77	3.059(5)
O6	C86	2.816(5)	O7	O9	3.326(3)
O7	C34	2.936(4)	O7	C78	2.840(5)
O7	C81	2.911(4)	O8	C49	3.036(4)
O8	C69	2.792(4)	O8	C81	3.011(4)
O9	C69	2.803(4)	O9	C84	2.975(5)
O9	C86	2.933(5)	O9	C92	2.801(6)
O9	C93	3.389(7)	O11	C35	2.967(4)
O11	C77	3.025(4)	O11	C80	2.846(4)
C10	B85	2.751(5)	C12	C13	2.982(4)
C12	C22	3.130(4)	C12	C54	3.114(4)
C12	C74	2.797(5)	C13	C23	2.929(4)
C13	C45	2.831(4)	C13	C68	3.225(5)
C14	C15	3.043(4)	C14	C26	2.835(4)
C14	C30	2.961(4)	C14	C55	3.095(4)
C15	C21	3.496(4)	C15	C37	3.567(4)
C15	C49	2.773(5)	C16	C22	3.142(4)
C16	C31	3.135(4)	C17	C31	2.773(4)
C18	C21	3.021(4)	C18	C39	3.005(4)
C18	C42	2.829(4)	C18	C58	3.061(4)
C19	C23	2.782(3)	C20	C31	3.062(4)
C20	C46	3.078(4)	C20	C62	2.802(4)
C20	C94	2.964(4)	C21	C43	2.766(4)
C22	C35	2.780(4)	C22	C68	3.403(5)

C23	C27	3.249(4)	C24	C46	3.559(4)
C24	C48	3.158(4)	C24	C54	3.544(4)
C24	C68	3.184(5)	C25	B83	2.752(4)
C27	C28	2.771(4)	C27	C94	2.989(4)

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

atom	atom	distance	atom	atom	distance
C29	C94	2.830(4)	C30	C41	3.114(4)
C30	C66	2.954(5)	C30	C71	2.802(5)
C31	C43	3.567(4)	C31	C48	3.280(4)
C32	C51	3.589(4)	C32	C55	3.127(4)
C32	C58	3.126(4)	C33	C79	3.030(5)
C34	C40	2.781(4)	C37	C40	3.175(4)
C37	C41	3.171(4)	C38	C41	2.783(4)
C39	C40	3.210(4)	C39	C51	3.019(5)
C39	C75	2.801(5)	C40	C58	3.229(5)
C41	C55	3.243(4)	C44	B89	2.814(5)
C46	C87	2.747(7)	C47	C79	3.176(5)
C48	C60	2.769(4)	C48	C94	3.183(4)
C50	B83	3.094(4)	C51	C66	3.285(5)
C51	C70	2.773(4)	C53	C54	2.770(5)
C54	C64	3.592(5)	C55	C64	2.776(5)
C56	C90	3.099(6)	C57	C68	2.763(5)
C58	C82	2.769(6)	C58	C87	3.560(6)
C59	C90	3.077(5)	C59	B89	3.319(5)
C63	C66	2.774(4)	C69	C91	2.964(6)
C72	B73	2.790(5)	C77	C93	3.052(6)
C77	B73	3.254(6)	C78	C91	3.237(6)
C80	C93	3.084(6)	C81	B85	3.115(5)

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H19	2.664	O1	H47B	3.232

O1	H50B	2.727	O1	H52A	3.158
O2	H17	2.570	O2	H33A	3.108
O2	H50A	3.474	O2	H50B	2.534
O3	H19	3.342	O3	H43	2.654
O3	H56A	3.239	O3	H59A	2.718
O4	H38	2.599	O4	H52B	3.184
O4	H59A	2.820	O4	H59B	3.334
O5	H33B	2.431	O5	H52A	2.563
O5	H61A	3.485	O5	H61B	2.713
O5	H65B	2.513	O5	H90B	2.965
O6	H28	2.571	O6	H77A	3.326
O6	H77B	2.801	O6	H86A	3.156
O7	H34	2.623	O7	H78A	3.245
O7	H81A	2.643	O7	H86B	3.571
O8	H49	2.772	O8	H69B	3.065
O8	H81A	2.630	O8	H81B	3.444
O9	H69A	2.466	O9	H84A	2.554
O9	H84B	3.461	O9	H86B	2.561
O9	H92A	2.478	O9	H93A	2.943
O11	H34	3.490	O11	H35	2.648
O11	H77B	2.668	O11	H80B	3.254
N36	H88A	3.048	N36	H88B	3.033
N36	H88C	3.056	C10	H91A	2.865
C10	H91B	2.772	C10	H91C	3.418
C12	H22	2.814	C12	H54	2.939
C12	H57	3.254	C12	H87	3.249
C13	H23	2.686	C13	H28	3.254
C13	H35	3.259	C13	H68	3.010
C14	H15	2.837	C14	H38	3.260
C14	H43	3.257	C14	H55	2.843
C15	H21	3.409	C15	H35	3.429
C15	H40	3.242	C15	H58	3.019
C16	H22	2.974	C16	H31	2.958
C16	H46	2.623	C16	H48	2.679
C16	H54	2.647	C16	H68	2.697
C17	H19	3.248	C18	H21	2.798

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C18	H34	3.255	C18	H49	3.258
C18	H58	2.654	C19	H17	3.246
C19	H43	3.027	C20	H31	2.709
C20	H46	2.901	C20	H53	3.254
C20	H60	3.255	C21	H15	3.431
C21	H41	3.241	C21	H55	3.263
C22	H23	3.271	C22	H27	3.253
C22	H68	3.484	C23	H27	3.175
C23	H31	3.248	C23	H48	3.556
C24	H22	2.696	C24	H23	2.629
C24	H27	2.650	C24	H31	2.704
C24	H48	3.046	C24	H68	3.058
C25	H79A	3.418	C25	H79B	2.789
C25	H79C	2.849	C26	H21	3.270
C26	H41	3.271	C27	H15	3.048
C27	H22	3.254	C27	H23	3.107
C27	H68	3.507	C28	H35	3.239
C29	H23	3.270	C29	H31	3.263
C29	H50B	3.587	C30	H41	2.856
C30	H64	3.263	C30	H66	2.707
C30	H70	3.255	C31	H23	3.250
C31	H27	3.459	C31	H41	3.432
C31	H43	2.876	C31	H48	3.412
C32	H15	2.619	C32	H21	2.626
C32	H40	2.704	C32	H41	2.713
C32	H55	2.984	C32	H58	2.924
C33	H47A	3.309	C33	H47B	2.702
C33	H50A	3.337	C33	H50B	2.805
C33	H52A	3.359	C33	H61A	3.353
C33	H61B	2.786	C33	H79B	3.242
C33	H79C	2.752	C34	H35	3.411
C34	H49	3.244	C35	H15	3.094
C35	H28	3.238	C35	H34	3.401
C37	H40	3.057	C37	H41	3.029
C37	H51	2.637	C37	H55	2.693
C37	H58	2.696	C37	H66	2.638

C37	H68	3.568	C38	H43	3.238

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C39	H40	3.006	C39	H51	2.793
C39	H63	3.259	C39	H82	3.256
C40	H15	3.241	C40	H21	3.322
C40	H58	3.076	C41	H15	3.383
C41	H21	3.240	C41	H27	3.590
C41	H31	3.344	C41	H55	3.293
C42	H15	3.266	C42	H40	3.273
C42	H81A	3.559	C43	H31	3.184
C43	H38	3.240	C44	H90A	2.808
C44	H90B	2.795	C44	H90C	3.408
C45	H22	3.267	C45	H27	3.265
C46	H22	3.122	C46	H68	3.221
C46	H74	3.235	C47	H33A	2.664
C47	H33B	3.312	C47	H50A	2.787
C47	H50B	2.533	C47	H61A	2.656
C47	H61B	3.346	C47	H79B	2.853
C47	H79C	3.577	C48	H31	3.198
C48	H46	3.339	C48	H54	3.238
C48	H62	3.253	C49	H34	3.245
C50	H33A	3.344	C50	H33B	2.700
C50	H47A	2.613	C50	H47B	3.316
C50	H59A	2.483	C50	H59B	2.723
C50	H61A	2.723	C50	H61B	2.624
C51	H41	3.264	C51	H54	3.022
C51	H55	3.242	C51	H66	3.136
C51	H68	3.546	C51	H71	3.249
C52	H56A	2.752	C52	H56B	3.311
C52	H59A	2.643	C52	H59B	3.337
C52	H65A	2.634	C52	H65B	2.620
C53	H60	3.231	C54	H31	2.987
C54	H48	3.239	C54	H62	3.248
C54	H64	3.252	C55	H41	3.281

C55	H51	3.242	C55	H66	3.337
C55	H71	3.251	C56	H52A	3.315
C56	H52B	2.734	C56	H59A	2.731
C56	H59B	2.636	C56	H65A	2.669
C56	H65B	3.342	C56	H90A	2.789

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C56	H90B	3.423	C57	H87	3.214
C58	H40	3.321	C58	H51	3.485
C58	H66	3.243	C58	H68	3.363
C58	H75	3.244	C58	H87	2.792
C59	H50A	2.700	C59	H50B	2.492
C59	H52A	2.621	C59	H52B	3.326
C59	H56A	3.321	C59	H56B	2.597
C59	H65A	3.355	C59	H65B	2.739
C59	H90A	3.387	C59	H90B	2.755
C60	H53	3.231	C60	H64	3.466
C61	H33A	2.698	C61	H33B	2.724
C61	H47A	2.748	C61	H47B	2.652
C61	H50A	2.598	C61	H50B	3.343
C62	H48	3.248	C62	H54	3.244
C63	H82	3.233	C63	H87	2.859
C64	H54	2.799	C64	H60	3.463
C64	H70	3.235	C65	H52A	2.721
C65	H52B	2.551	C65	H56A	2.577
C65	H56B	2.784	C65	H59A	3.368
C65	H59B	2.787	C66	H51	3.151
C66	H58	3.243	C66	H75	3.247
C68	H22	3.359	C68	H46	3.219
C68	H51	3.151	C68	H54	3.387
C68	H58	3.507	C68	H74	3.247
C69	H78A	2.693	C69	H78B	3.286
C69	H81A	2.732	C69	H81B	3.324
C69	H84A	2.845	C69	H84B	3.332
C69	H86B	3.472	C69	H91A	2.727

C69	H91B	3.090	C70	H64	3.237
C71	H51	3.245	C71	H55	3.248
C72	H93A	2.800	C72	H93B	2.773
C72	H93C	3.393	C74	H46	3.226
C74	H68	3.243	C75	H58	3.239
C75	H66	3.245	C77	H80A	2.584
C77	H80B	3.312	C77	H81A	2.486
C77	H81B	2.717	C77	H86A	3.329
C77	H86B	2.629	C77	H92A	2.712

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C77	H92B	3.342	C77	H93A	2.746
C77	H93B	3.335	C78	H69A	3.294
C78	H69B	2.632	C78	H81A	2.614
C78	H81B	2.753	C78	H84A	3.327
C78	H84B	2.592	C78	H91B	2.924
C79	H33A	2.664	C79	H33B	3.269
C79	H47A	3.545	C79	H47B	2.796
C80	H77A	2.628	C80	H77B	2.719
C80	H86A	2.723	C80	H86B	3.310
C80	H92A	3.331	C80	H92B	2.674
C80	H93A	3.435	C80	H93B	2.758
C81	H69A	2.674	C81	H69B	3.327
C81	H77A	2.684	C81	H77B	2.523
C81	H78A	3.332	C81	H78B	2.631
C81	H84A	2.556	C81	H84B	2.777
C82	H63	3.235	C84	H69A	2.713
C84	H69B	2.693	C84	H78A	2.633
C84	H78B	2.742	C84	H81A	3.348
C84	H81B	2.630	C86	H77A	3.337
C86	H77B	2.639	C86	H80A	3.307
C86	H80B	2.751	C86	H92A	2.630
C86	H92B	2.651	C87	H51	3.473
C87	H57	3.218	C87	H58	3.413
C90	H56A	3.192	C90	H56B	2.862

C90	H59B	2.818	C91	H69A	3.149
C91	H69B	2.603	C91	H78A	2.870
C92	H77A	2.765	C92	H77B	3.354
C92	H80A	2.770	C92	H80B	2.582
C92	H86A	2.594	C92	H86B	2.716
C93	H77A	2.791	C93	H80A	2.845
C93	H80B	3.189	C94	H17	3.253
C94	H19	3.262	C94	H27	2.792
C94	H48	3.006	B73	H28	2.708
B73	H35	2.732	B73	H77B	2.755
B73	H80A	3.157	B73	H80B	2.921
B73	H86A	2.856	B73	H86B	3.168
B83	H17	2.699	B83	H19	2.744

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
B83	H33A	2.832	B83	H33B	3.172
B83	H47A	3.153	B83	H47B	2.913
B83	H50B	2.576	B85	H34	2.690
B85	H49	2.763	B85	H69A	3.168
B85	H69B	2.812	B85	H78A	2.935
B85	H78B	3.150	B85	H81A	2.579
B89	H38	2.718	B89	H43	2.734
B89	H52A	3.179	B89	H52B	2.860
B89	H56A	2.885	B89	H56B	3.163
B89	H59A	2.840	H15	H21	3.579
H15	H27	2.745	H15	H34	2.308
H15	H35	2.818	H15	H41	3.510
H15	H58	3.331	H17	H23	2.305
H19	H31	2.304	H19	H43	2.786
H21	H38	2.315	H21	H40	3.439
H21	H55	3.529	H22	H23	3.548
H22	H28	2.302	H22	H46	3.304
H23	H27	3.286	H27	H35	2.303
H27	H41	3.379	H31	H41	2.836
H31	H43	2.500	H31	H48	3.568

H31	H54	3.257	H33A	H47A	3.568
H33A	H47B	2.540	H33A	H61A	3.550
H33A	H61B	3.075	H33A	H79A	3.589
H33A	H79B	2.748	H33A	H79C	2.233
H33B	H47B	3.583	H33B	H50A	3.523
H33B	H50B	3.140	H33B	H52A	2.743
H33B	H61B	2.628	H33B	H65B	3.335
H33B	H79C	2.847	H34	H35	2.781
H40	H49	2.317	H40	H58	3.421
H41	H43	2.310	H41	H51	3.553
H41	H54	3.569	H41	H55	3.571
H41	H68	3.375	H46	H48	3.354
H46	H57	2.314	H47A	H50A	2.583
H47A	H50B	2.673	H47A	H61A	2.520
H47A	H61B	3.569	H47A	H79B	3.213
H47B	H50B	3.467	H47B	H61A	2.830
H47B	H61B	3.566	H47B	H79B	2.229

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H47B	H79C	3.192	H48	H53	2.318
H50A	H59A	2.873	H50A	H59B	2.692
H50A	H61A	2.455	H50A	H61B	2.698
H50B	H59A	2.203	H50B	H59B	2.923
H50B	H61A	3.515	H50B	H61B	3.556
H51	H54	2.932	H51	H64	2.321
H51	H66	3.248	H51	H68	2.911
H51	H87	3.469	H52A	H59A	2.799
H52A	H59B	3.541	H52A	H65A	3.011
H52A	H65B	2.506	H52B	H56A	2.656
H52B	H59A	3.563	H52B	H65A	2.340
H52B	H65B	2.736	H53	H62	2.318
H54	H60	2.312	H54	H64	2.526
H54	H68	3.445	H55	H66	3.575
H55	H70	2.316	H56A	H59B	3.473
H56A	H65A	2.372	H56A	H65B	3.467

H56A	H90A	2.788	H56B	H59A	2.909
H56B	H59B	2.365	H56B	H65A	3.077
H56B	H90A	2.368	H56B	H90B	3.063
H57	H74	2.303	H58	H63	2.315
H58	H68	2.927	H58	H87	2.737
H59A	H65B	3.583	H59B	H65B	3.127
H59B	H90A	3.001	H59B	H90B	2.317
H60	H62	2.315	H60	H64	2.966
H60	H71	3.523	H61A	H79A	2.306
H61A	H79B	2.375	H61A	H79C	2.823
H61B	H79A	2.353	H61B	H79B	2.824
H61B	H79C	2.327	H63	H75	2.312
H63	H87	2.860	H64	H71	2.314
H65A	H90A	2.348	H65A	H90B	2.827
H65A	H90C	2.339	H65B	H90A	2.826
H65B	H90B	2.359	H65B	H90C	2.328
H66	H82	2.309	H68	H87	2.313
H69A	H78A	3.568	H69A	H81A	3.041
H69A	H81B	3.532	H69A	H84A	2.697
H69A	H86B	2.698	H69A	H91A	2.714
H69A	H91B	3.523	H69A	H92A	3.582

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H69B	H78A	2.518	H69B	H78B	3.539
H69B	H84A	3.159	H69B	H84B	3.501
H69B	H91A	2.272	H69B	H91B	2.551
H69B	H91C	3.550	H70	H71	2.321
H74	H87	2.312	H75	H82	2.319
H77A	H80A	2.355	H77A	H80B	3.468
H77A	H81A	2.848	H77A	H81B	2.665
H77A	H86B	3.547	H77A	H92A	3.096
H77A	H93A	2.311	H77A	H93B	2.943
H77B	H80A	2.896	H77B	H81A	2.237
H77B	H81B	2.957	H77B	H86A	3.558
H77B	H86B	2.814	H77B	H92A	3.560

H78A	H81A	3.537	H78A	H81B	3.583
H78A	H84A	3.558	H78A	H84B	2.719
H78A	H91A	3.363	H78A	H91B	2.305
H78B	H81A	2.777	H78B	H81B	2.533
H78B	H84A	3.521	H78B	H84B	2.467
H78B	H91B	3.366	H80A	H92B	3.075
H80A	H93A	3.077	H80A	H93B	2.327
H80B	H86A	2.648	H80B	H92A	3.469
H80B	H92B	2.389	H80B	H93B	2.778
H81A	H84A	3.493	H81A	H84B	3.595
H81B	H84A	2.667	H81B	H84B	2.559
H84A	H91A	2.316	H84A	H91B	2.825
H84A	H91C	2.369	H84A	H92A	3.432
H84B	H91A	2.822	H84B	H91B	2.391
H84B	H91C	2.295	H86A	H92A	2.786
H86A	H92B	2.387	H86B	H92A	2.495
H86B	H92B	3.001	H92A	H93A	2.322
H92A	H93B	2.810	H92A	H93C	2.323
H92B	H93A	2.809	H92B	H93B	2.344
H92B	H93C	2.301			

Table 12. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	C741	3.483(5)	O2	O42	3.525(3)
O2	N363	3.581(5)	O2	C673	3.444(5)
O3	N36	3.515(4)	O4	O22	3.525(3)
O4	N36	3.349(4)	O4	C472	3.377(3)
O6	C534	3.466(4)	O6	C715	3.269(4)
O8	C644	3.452(5)	N36	O26	3.581(5)
N36	O3	3.515(4)	N36	O4	3.349(4)
N36	C476	3.489(5)	N36	C52	3.548(5)
N36	C56	3.422(5)	N36	C937	3.560(6)
N36	B89	3.350(4)	C29	C883	3.592(6)
C47	O42	3.377(3)	C47	N363	3.489(5)
C52	N36	3.548(5)	C53	O61	3.466(4)
C56	N36	3.422(5)	C57	C675	3.571(5)

C64	O81	3.452(5)	C67	O26	3.444(5)
C67	C578	3.571(5)	C67	B836	3.427(5)
C67	B89	3.379(5)	C70	C88	3.499(6)
C71	O68	3.269(4)	C74	O14	3.483(5)
C88	C296	3.592(6)	C88	C70	3.499(6)
C88	B836	3.553(6)	C93	N369	3.560(6)
B83	C673	3.427(5)	B83	C883	3.553(6)
B89	N36	3.350(4)	B89	C67	3.379(5)

Symmetry Operators:

(1)	X,-Y+2,Z+1	(2)	-X+1,-Y+1,-Z+1
(3)	X-1,Y,Z	(4)	X,-Y+2,Z
(5)	X-1,-Y+2,Z	(6)	X+1,Y,Z
(7)	X+1,Y,Z+1	(8)	X+1,-Y+2,Z+1
(9)	X-1,Y,Z-1		

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H741	2.600	O1	H88A2	3.455
O2	H382	3.314	O2	H56B3	3.165
O2	H59A3	3.457	O2	H59B3	3.207
O3	H751	3.239	O4	H47A3	2.548
O4	H47B4	3.052	O5	H91C5	3.351
O6	H492	3.056	O6	H536	3.023
O6	H717	2.978	O7	H69A8	3.555
O8	H606	3.473	O8	H646	2.586
O8	H80B4	2.876	O11	H91A8	3.050
O11	H91B8	3.514	N36	H33A4	2.858
N36	H47B4	2.737	N36	H52B	2.907
N36	H56A	2.767	N36	H579	2.923
N36	H79B4	3.323	N36	H821	3.249
N36	H93A10	3.244	N36	H93C10	3.008
C12	H81B1	3.502	C15	H61A3	3.469
C15	H626	3.556	C15	H79A3	3.116

C17	H212	3.333	C17	H552	3.559
C17	H56B3	3.593	C17	H59B3	3.076
C17	H88A2	3.401	C17	H88C2	3.220
C17	H90B3	3.430	C19	H741	3.477
C19	H88A2	3.469	C20	H77A1	3.449
C21	H174	2.976	C21	H234	3.488
C21	H61A3	3.169	C21	H88C	3.422
C21	H90A11	3.469	C22	H402	3.022
C23	H212	3.461	C23	H552	3.219
C23	H90B3	3.306	C26	H47A3	3.107
C26	H61A3	3.557	C26	H88C	2.985
C27	H90B3	3.329	C28	H402	2.979
C28	H492	3.340	C28	H536	2.921
C28	H626	3.535	C28	H717	3.351
C29	H59B3	3.414	C29	H88A2	3.002
C29	H88C2	3.423	C33	H741	3.318
C33	H84A5	3.428	C33	H84B5	3.326
C33	H91C5	3.242	C34	H606	3.377
C34	H626	3.405	C34	H79A3	2.782
C35	H626	3.491	C35	H90B3	3.269
C35	H90C3	3.388	C38	H174	3.035

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C38	H47A3	2.882	C38	H56B11	3.353
C38	H61A3	3.124	C38	H88C	3.010
C40	H284	3.580	C42	H606	3.065
C42	H79A3	3.338	C43	H751	3.429
C43	H88C	3.369	C45	H492	3.580
C45	H536	3.246	C45	H626	3.208
C45	H90C3	3.544	C46	H662	3.548
C46	H77A1	2.990	C46	H81B1	2.924
C46	H822	3.439	C46	H93A1	3.414
C47	H383	3.332	C47	H56A2	3.278
C48	H552	3.597	C48	H702	3.454
C48	H77A1	3.339	C48	H77B1	3.391

C49	H606	3.397	C49	H716	3.259
C50	H59A3	3.293	C53	H281	3.473
C53	H702	3.308	C53	H77B1	3.045
C54	H631	3.531	C54	H77B1	3.545
C54	H81A1	3.031	C54	H81B1	3.367
C55	H484	2.871	C55	H88B	3.578
C55	H88C	3.281	C56	H3811	3.326
C56	H47A3	3.523	C56	H47B4	3.005
C56	H79B4	3.336	C57	H81B1	3.004
C57	H822	3.448	C57	H88A7	3.399
C57	H93A1	3.301	C58	H606	3.477
C59	H50B3	3.340	C60	H581	3.429
C60	H631	2.959	C60	H77B1	3.233
C60	H81A1	2.888	C61	H91C5	3.287
C62	H581	3.327	C62	H631	3.373
C62	H77B1	2.971	C62	H81A1	3.546
C63	H606	3.370	C64	H78B1	3.302
C64	H80A9	3.207	C64	H80B9	3.556
C65	H91C5	3.556	C66	H224	3.254
C66	H464	3.563	C67	H33A4	3.303
C67	H47B4	3.250	C67	H52B	3.584
C67	H579	2.914	C67	H751	3.280
C67	H821	3.020	C69	H69A8	3.014
C69	H86B8	3.302	C70	H289	3.417
C70	H484	2.994	C70	H534	3.126

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C70	H88B	2.992	C70	H88C	3.340
C71	H289	3.124	C71	H491	3.521
C71	H80A9	3.329	C74	H88A7	3.224
C75	H88B6	2.857	C77	H466	3.198
C78	H646	3.037	C78	H80B4	3.154
C79	H343	3.574	C79	H56A2	3.396
C79	H84A5	3.474	C79	H91C5	3.556
C82	H224	3.597	C82	H88B6	3.004

C82	H93B9	3.557	C84	H33A12	3.491
C84	H33B12	3.053	C84	H79C12	3.304
C86	H69B8	3.191	C86	H91A8	3.107
C86	H91B8	3.441	C88	H55	3.418
C88	H579	3.464	C88	H70	2.868
C88	H751	3.102	C88	H821	3.272
C90	H2111	3.488	C90	H233	3.530
C91	H33B12	3.116	C91	H61B12	3.392
C91	H65B12	3.176	C91	H79C12	3.391
C91	H86A8	3.586	C91	H86B8	3.330
C93	H52B13	3.536	C93	H576	3.549
C93	H827	3.409	B73	H492	3.441
B73	H536	3.339	B73	H626	3.582
B83	H59B3	3.580	B83	H741	3.446
B83	H88A2	3.130	B83	H88C2	3.562
B85	H606	3.384	B89	H47A3	3.040
B89	H88C	3.557	H15	H61A3	3.072
H15	H61B3	3.419	H15	H79A3	3.295
H17	C212	2.976	H17	C382	3.035
H17	H212	2.657	H17	H382	2.754
H17	H56B3	2.805	H17	H59B3	2.868
H17	H88A2	3.600	H17	H88C2	3.052
H17	H90A3	3.159	H17	H90B3	3.249
H19	H741	2.934	H21	C174	3.333
H21	C234	3.461	H21	C9011	3.488
H21	H174	2.657	H21	H234	2.922
H21	H56B11	3.216	H21	H61A3	3.390
H21	H90A11	2.588	H22	C662	3.254
H22	C822	3.597	H22	H402	3.030

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H22	H662	3.102	H23	C212	3.488
H23	C903	3.530	H23	H212	2.922
H23	H402	3.242	H23	H552	3.102
H23	H90A3	3.263	H23	H90B3	3.024

H27	H90B3	3.339	H28	C402	3.580
H28	C536	3.473	H28	C707	3.417
H28	C717	3.124	H28	H402	2.953
H28	H492	2.991	H28	H536	2.599
H28	H707	3.015	H28	H717	2.450
H31	H631	3.263	H33A	N362	2.858
H33A	C672	3.303	H33A	C845	3.491
H33A	H571	3.030	H33A	H741	3.202
H33A	H84A5	2.972	H33A	H84B5	3.200
H33A	H91C5	3.434	H33B	C845	3.053
H33B	C915	3.116	H33B	H741	3.451
H33B	H84A5	2.960	H33B	H84B5	2.613
H33B	H91C5	2.413	H34	C793	3.574
H34	H61B3	3.487	H34	H626	3.374
H34	H79A3	2.761	H35	H61B3	3.092
H35	H90B3	3.249	H35	H90C3	3.393
H38	O24	3.314	H38	C473	3.332
H38	C5611	3.326	H38	H174	2.754
H38	H47A3	2.540	H38	H47B3	3.273
H38	H56A11	3.430	H38	H56B11	2.567
H38	H61A3	3.338	H38	H88C	3.298
H40	C224	3.022	H40	C284	2.979
H40	H224	3.030	H40	H234	3.242
H40	H284	2.953	H43	H751	3.003
H46	C662	3.563	H46	C771	3.198
H46	H662	2.905	H46	H77A1	2.279
H46	H81B1	3.029	H46	H822	3.095
H46	H93A1	2.852	H47A	O43	2.548
H47A	C263	3.107	H47A	C383	2.882
H47A	C563	3.523	H47A	B893	3.040
H47A	H383	2.540	H47A	H56A2	3.452
H47A	H56B3	3.393	H47A	H59A3	3.346
H47B	O42	3.052	H47B	N362	2.737

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance

H47B	C562	3.005	H47B	C672	3.250
H47B	H383	3.273	H47B	H56A2	2.360
H47B	H56B2	3.213	H48	C552	2.871
H48	C702	2.994	H48	H552	2.712
H48	H662	3.456	H48	H702	2.920
H48	H77A1	3.589	H49	O64	3.056
H49	C284	3.340	H49	C454	3.580
H49	C716	3.521	H49	B734	3.441
H49	H284	2.991	H49	H646	3.487
H49	H716	2.725	H49	H80B4	3.443
H50A	H59A3	3.097	H50B	C593	3.340
H50B	H50B3	3.092	H50B	H59A3	2.611
H50B	H59B3	3.222	H51	H78B1	3.369
H52B	N36	2.907	H52B	C67	3.584
H52B	C9310	3.536	H52B	H93B10	3.581
H52B	H93C10	2.714	H53	O61	3.023
H53	C281	2.921	H53	C451	3.246
H53	C702	3.126	H53	B731	3.339
H53	H281	2.599	H53	H702	2.625
H53	H77B1	3.397	H54	H81A1	3.106
H54	H81B1	3.221	H55	C174	3.559
H55	C234	3.219	H55	C484	3.597
H55	C88	3.418	H55	H234	3.102
H55	H484	2.712	H55	H88A	3.499
H55	H88B	3.448	H55	H88C	2.801
H56A	N36	2.767	H56A	C474	3.278
H56A	C794	3.396	H56A	H3811	3.430
H56A	H47A4	3.452	H56A	H47B4	2.360
H56A	H79B4	2.437	H56B	O23	3.165
H56B	C173	3.593	H56B	C3811	3.353
H56B	H173	2.805	H56B	H2111	3.216
H56B	H3811	2.567	H56B	H47A3	3.393
H56B	H47B4	3.213	H56B	H79B4	3.459
H57	N367	2.923	H57	C677	2.914
H57	C887	3.464	H57	C931	3.549
H57	H33A6	3.030	H57	H77A1	3.501
H57	H81B1	3.167	H57	H822	3.110

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H57	H88A7	3.227	H57	H88B7	3.592
H57	H93A1	2.633	H58	C606	3.429
H58	C626	3.327	H58	H606	3.029
H58	H626	2.841	H59A	O23	3.457
H59A	C503	3.293	H59A	H47A3	3.346
H59A	H50A3	3.097	H59A	H50B3	2.611
H59B	O23	3.207	H59B	C173	3.076
H59B	C293	3.414	H59B	B833	3.580
H59B	H173	2.868	H59B	H50B3	3.222
H60	O81	3.473	H60	C341	3.377
H60	C421	3.065	H60	C491	3.397
H60	C581	3.477	H60	C631	3.370
H60	B851	3.384	H60	H581	3.029
H60	H631	2.818	H60	H81A1	2.893
H61A	C153	3.469	H61A	C213	3.169
H61A	C263	3.557	H61A	C383	3.124
H61A	H153	3.072	H61A	H213	3.390
H61A	H383	3.338	H61B	C915	3.392
H61B	H153	3.419	H61B	H343	3.487
H61B	H353	3.092	H61B	H91A5	3.460
H61B	H91C5	2.568	H62	C151	3.556
H62	C281	3.535	H62	C341	3.405
H62	C351	3.491	H62	C451	3.208
H62	B731	3.582	H62	H341	3.374
H62	H581	2.841	H62	H631	3.516
H62	H77B1	3.296	H63	C546	3.531
H63	C606	2.959	H63	C626	3.373
H63	H316	3.263	H63	H606	2.818
H63	H626	3.516	H64	O81	2.586
H64	C781	3.037	H64	H491	3.487
H64	H78B1	2.542	H64	H80A9	3.337
H64	H80B9	3.270	H64	H81A1	3.518
H65A	H79B4	3.279	H65A	H93C10	2.882
H65B	C915	3.176	H65B	H91B5	2.893
H65B	H91C5	2.591	H66	C464	3.548

H66	H224	3.102	H66	H464	2.905
H66	H484	3.456	H66	H93B9	3.530

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H69A	O78	3.555	H69A	C698	3.014
H69A	H69A8	2.390	H69A	H69B8	2.882
H69A	H86B8	3.371	H69A	H91A8	3.507
H69B	C868	3.191	H69B	H69A8	2.882
H69B	H86A8	3.084	H69B	H86B8	2.438
H69B	H92A8	3.579	H70	C484	3.454
H70	C534	3.308	H70	C88	2.868
H70	H289	3.015	H70	H484	2.920
H70	H534	2.625	H70	H88A	2.879
H70	H88B	2.350	H70	H88C	2.919
H71	O69	2.978	H71	C289	3.351
H71	C491	3.259	H71	H289	2.450
H71	H491	2.725	H71	H80A9	3.555
H74	O16	2.600	H74	C196	3.477
H74	C336	3.318	H74	B836	3.446
H74	H196	2.934	H74	H33A6	3.202
H74	H33B6	3.451	H74	H88A7	2.924
H75	O36	3.239	H75	C436	3.429
H75	C676	3.280	H75	C886	3.102
H75	H436	3.003	H75	H88B6	2.402
H75	H88C6	3.328	H77A	C206	3.449
H77A	C466	2.990	H77A	C486	3.339
H77A	H466	2.279	H77A	H486	3.589
H77A	H576	3.501	H77B	C486	3.391
H77B	C536	3.045	H77B	C546	3.545
H77B	C606	3.233	H77B	C626	2.971
H77B	H536	3.397	H77B	H626	3.296
H78A	H80B4	2.826	H78A	H92B4	3.205
H78B	C646	3.302	H78B	H516	3.369
H78B	H646	2.542	H78B	H80B4	3.190
H79A	C153	3.116	H79A	C343	2.782

H79A	C423	3.338	H79A	H153	3.295
H79A	H343	2.761	H79B	N362	3.323
H79B	C562	3.336	H79B	H56A2	2.437
H79B	H56B2	3.459	H79B	H65A2	3.279
H79B	H90A2	3.407	H79C	C845	3.304
H79C	C915	3.391	H79C	H84A5	2.538

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H79C	H91A5	3.333	H79C	H91C5	3.029
H79C	H92A5	3.559	H80A	C647	3.207
H80A	C717	3.329	H80A	H647	3.337
H80A	H717	3.555	H80B	O82	2.876
H80B	C647	3.556	H80B	C782	3.154
H80B	H492	3.443	H80B	H647	3.270
H80B	H78A2	2.826	H80B	H78B2	3.190
H81A	C546	3.031	H81A	C606	2.888
H81A	C626	3.546	H81A	H546	3.106
H81A	H606	2.893	H81A	H646	3.518
H81B	C126	3.502	H81B	C466	2.924
H81B	C546	3.367	H81B	C576	3.004
H81B	H466	3.029	H81B	H546	3.221
H81B	H576	3.167	H82	N366	3.249
H82	C464	3.439	H82	C574	3.448
H82	C676	3.020	H82	C886	3.272
H82	C939	3.409	H82	H464	3.095
H82	H574	3.110	H82	H88B6	2.673
H82	H93A9	3.049	H82	H93B9	3.105
H82	H93C9	3.539	H84A	C3312	3.428
H84A	C7912	3.474	H84A	H33A12	2.972
H84A	H33B12	2.960	H84A	H79C12	2.538
H84B	C3312	3.326	H84B	H33A12	3.200
H84B	H33B12	2.613	H86A	C918	3.586
H86A	H69B8	3.084	H86A	H91A8	3.200
H86A	H91B8	3.073	H86B	C698	3.302
H86B	C918	3.330	H86B	H69A8	3.371

H86B	H69B8	2.438	H86B	H91A8	2.596
H86B	H91B8	3.220	H88A	O14	3.455
H88A	C174	3.401	H88A	C194	3.469
H88A	C294	3.002	H88A	C579	3.399
H88A	C749	3.224	H88A	B834	3.130
H88A	H174	3.600	H88A	H55	3.499
H88A	H579	3.227	H88A	H70	2.879
H88A	H749	2.924	H88B	C55	3.578
H88B	C70	2.992	H88B	C751	2.857
H88B	C821	3.004	H88B	H55	3.448

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H88B	H579	3.592	H88B	H70	2.350
H88B	H751	2.402	H88B	H821	2.673
H88C	C174	3.220	H88C	C21	3.422
H88C	C26	2.985	H88C	C294	3.423
H88C	C38	3.010	H88C	C43	3.369
H88C	C55	3.281	H88C	C70	3.340
H88C	B834	3.562	H88C	B89	3.557
H88C	H174	3.052	H88C	H38	3.298
H88C	H55	2.801	H88C	H70	2.919
H88C	H751	3.328	H90A	C2111	3.469
H90A	H173	3.159	H90A	H2111	2.588
H90A	H233	3.263	H90A	H79B4	3.407
H90B	C173	3.430	H90B	C233	3.306
H90B	C273	3.329	H90B	C353	3.269
H90B	H173	3.249	H90B	H233	3.024
H90B	H273	3.339	H90B	H353	3.249
H90C	C353	3.388	H90C	C453	3.544
H90C	H353	3.393	H91A	O118	3.050
H91A	C868	3.107	H91A	H61B12	3.460
H91A	H69A8	3.507	H91A	H79C12	3.333
H91A	H86A8	3.200	H91A	H86B8	2.596
H91B	O118	3.514	H91B	C868	3.441
H91B	H65B12	2.893	H91B	H86A8	3.073

H91B	H86B8	3.220	H91C	O512	3.351
H91C	C3312	3.242	H91C	C6112	3.287
H91C	C6512	3.556	H91C	C7912	3.556
H91C	H33A12	3.434	H91C	H33B12	2.413
H91C	H61B12	2.568	H91C	H65B12	2.591
H91C	H79C12	3.029	H92A	H69B8	3.579
H92A	H79C12	3.559	H92B	H78A2	3.205
H93A	N3613	3.244	H93A	C466	3.414
H93A	C576	3.301	H93A	H466	2.852
H93A	H576	2.633	H93A	H827	3.049
H93B	C827	3.557	H93B	H52B13	3.581
H93B	H667	3.530	H93B	H827	3.105
H93C	N3613	3.008	H93C	H52B13	2.714
H93C	H65A13	2.882	H93C	H827	3.539

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance

Symmetry Operators:

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