Polaron Delocalization in Ladder Macromolecular Systems

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Supplementary Material

Crystal Data and Structure Refinement for 2

Data Collection

A colorless plate crystal of $C_{57}H_{60}N_3O_2$ having approximate dimensions of 0.06 x 0.10 x 0.13 mm was mounted on a glass fiber. All measurements were made on a Nonius KappaCCD diffractometer with graphite monochromated Mo-K̲ radiation.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using ten (1^o in ω, 30s exposure, de-zingered) data frames, corresponded to a primitive triclinic cell with dimensions:

a = 10.3141(3) Å	α= 93.178(2)^o
b = 13.1178(4) Å	β = 94.933(2)^o
c = 17.064(1) Å	γ = 95.508(2)
V = 2284.8(1) Å^3	

For Z = 2 and F.W. = 819.12, the calculated density is 1.19 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be: P_{-1} (#2). Two benzene solvent molecules were observed in the asymmetric unit.

The data were collected at a temperature of -90 ± 1 ^{o}C to a maximum 2θ value of 50.2^o. Five omega scans consisting of 55, 54, 31, 54, and 55 data frames, respectively, were collected with a scan width of 2.0^o and a detector-to-crystal distance, Dx, of 33 mm. Each frame was exposed twice (for the purpose of de-zingering) for 180 s. The data frames were processed and scaled using the DENZO software package. (Z. Otwinowski and W. Minor, "Processing of X-Ray Diffraction Data Collected in Oscillation Mode," Methods in Enzymology, vol. 276: Macromolecular Crystallography, part A, 307-326, 1997, C.W. Carter, Jr. & R.M. Sweet, Eds., Academic Press).

Data Reduction

A total of 8093 reflections was collected. No decay correction was applied. The linear absorption coefficient, μ, for Mo-Kα radiation is 0.7 cm^{-1} and no absorption correction was applied. 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[2]. Most non-hydrogen atoms were refined anisotropically, while C26, C27, C28, C29 and C30 were refined isotropically. Carbon atoms C26-C29 were heavily disordered about two positions. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 4712 observed reflections ($I > 5.00\sigma(I)$) and 550 variable parameters and converged (largest parameter shift was 3.52 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo| - |Fc|| / \Sigma |Fo| = 0.061$$
$$R_w = [(\Sigma w (|Fo| - |Fc|)^2 / \Sigma w Fo^2)]^{1/2} = 0.077$$

The standard deviation of an observation of unit weight[4] was 3.50. The weighting scheme was based on counting statistics and included a factor ($p = 0.020$) to downweight the intense reflections. Plots of $\Sigma w (|Fo| - |Fc|)^2$ versus $|Fo|$, reflection order in data collection, $\sin\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.59 and -0.58 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., & Polidori, G.; *J. Appl. Cryst.,* 27, 435-436 (1994).

(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized $Sw(|F_o|-|F_c|)^2$

where $w = 4F_o^2/2(F_o^2)$

and $s^2(F_o^2) = [S^2(C+R^2B) + (pF_o^2)^2]/Lp^2$

S = Scan rate

C = Total integrated peak count

R = Ratio of scan time to background counting time

B = Total background count

Lp = Lorentz-polarization factor

p = p-factor

(4) Standard deviation of an observation of unit weight:

$[Sw(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$

where N_o = number of observations

N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

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

(7) 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).

(8) 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).

(9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

Experimental Details for 2

A. Crystal Data

Empirical Formula	$C_{57}H_{60}N_3O_2$
Formula Weight	819.12
Crystal Color, Habit	colorless, plate
Crystal Dimensions	0.06 X 0.10 X 0.13 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 10.3141(3)Å b = 13.1178(4) Å c = 17.064(1) Å . = 93.178(2)° . = 94.933(2)° . = 95.508(2)° V = 2284.8(1) Å^3
Space Group	P_{-1} (#2)
Z value	2
Dcalc	1.191 g/cm^3
F000	878.00
μ(MoKα)	0.71 cm^{-1}

B. Intensity Measurements

Diffractometer	Nonius KappaCCD
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated

Take-off Angle	2.8^{o}
Crystal to Detector Distance	33 mm
Temperature	-90.0 ^{o}C
Scan Rate	180 s/frame
Scan Width	2.0^{o}/frame
$2\theta_{max}$	50.2^{o}
No. of Reflections Measured	Total: 8093
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	$1/^2\sigma$(Fo)
p-factor	0.0200
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>5.00σ(I))	4712
No. Variables	550
Reflection/Parameter Ratio	8.57
Residuals: R; Rw	0.061 ; 0.077
Goodness of Fit Indicator	3.50
Max Shift/Error in Final Cycle	3.52
Maximum peak in Final Diff. Map	0.59 e^{-}/Å^3

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 C(25)  -0.1793(4)  0.4460(4)   0.4047(3)   0.088(2)    Uij ? ?
 C(26a) -0.289(1)   0.520(1)    0.4181(8)   0.113(4)    Uij ? ?
 C(26b) -0.247(2)   0.557(2)    0.409(1)    0.112(6)    Uij ? ?
 C(27a) -0.286(1)   0.567(1)    0.4890(9)   0.175(5)    Uij ? ?
 C(27b) -0.205(2)   0.613(2)    0.432(1)    0.124(8)    Uij ? ?
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C(28b)	-0.371(2)	0.687(1)	0.422(1)	0.157(6)	Uij ? ?
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C(29b)	-0.416(2)	0.704(1)	0.4901(9)	0.113(5)	Uij ? ?
C(30)	-0.4927(5)	0.7883(4)	0.5092(3)	0.102(2)	Uij ? ?
C(31)	0.3217(3)	0.2176(2)	0.2083(2)	0.0331(9)	Uij ? ?
C(32)	0.3844(3)	0.2803(2)	0.2715(2)	0.0379(10)	Uij ? ?
C(33)	0.5152(3)	0.3137(2)	0.2703(2)	0.039(1)	Uij ? ?
C(34)	0.5868(3)	0.2854(2)	0.2091(2)	0.0346(9)	Uij ? ?
C(35)	0.5233(3)	0.2244(2)	0.1452(2)	0.0301(9)	Uij ? ?
C(36)	0.3907(3)	0.1921(2)	0.1450(2)	0.0304(9)	Uij ? ?
C(37)	0.6965(3)	0.2533(2)	0.0534(2)	0.0297(9)	Uij ? ?
C(38)	0.7080(3)	0.3602(2)	0.0633(2)	0.0334(9)	Uij ? ?
C(39)	0.8126(3)	0.4154(2)	0.0342(2)	0.0346(9)	Uij ? ?
C(40)	0.9036(3)	0.3684(2)	-0.0058(2)	0.0347(9)	Uij ? ?
C(41)	0.8919(3)	0.2617(2)	-0.0172(2)	0.0308(9)	Uij ? ?
C(42)	0.7899(3)	0.2053(2)	0.0154(2)	0.0310(9)	Uij ? ?
C(43)	0.5455(3)	0.0948(2)	0.0393(2)	0.0284(9)	Uij ? ?
C(44)	0.5344(3)	0.0066(2)	0.0801(2)	0.0312(9)	Uij ? ?
C(45)	0.4896(3)	-0.0874(2)	0.0415(2)	0.0324(9)	Uij ? ?
C(46)	0.9389(4)	0.0761(4)	0.6512(2)	0.067(1)	Uij ? ?
C(47)	0.8229(4)	0.0301(3)	0.6143(3)	0.071(2)	Uij ? ?
C(48)	0.7906(5)	0.0427(4)	0.5360(3)	0.083(2)	Uij ? ?
C(49)	0.8757(5)	0.1009(4)	0.4940(3)	0.083(2)	Uij ? ?
C(50)	0.9906(5)	0.1464(4)	0.5311(3)	0.079(2)	Uij ? ?
C(51)	1.0227(4)	0.1344(3)	0.6099(3)	0.070(1)	Uij ? ?
C(52)	0.2831(4)	0.0925(3)	0.7585(2)	0.060(1)	Uij ? ?
C(53)	0.2539(4)	-0.0089(3)	0.7349(2)	0.059(1)	Uij ? ?
C(54)	0.3408(4)	-0.0602(3)	0.6956(2)	0.057(1)	Uij ? ?
C(55)	0.4572(4)	-0.0087(3)	0.6788(2)	0.062(1)	Uij ? ?
C(56)	0.4854(4)	0.0935(3)	0.7024(2)	0.064(1)	Uij ? ?
C(57)	0.3980(4)	0.1443(3)	0.7418(2)	0.058(1)	Uij ? ?
H(1)	-0.0403	0.1131	0.1325	0.0444	Uij ? ?
H(2)	-0.1080	-0.0481	0.0700	0.0441	Uij ? ?
H(3)	0.2362	-0.1475	0.1463	0.0390	Uij ? ?
H(4)	0.3063	0.0140	0.2066	0.0412	Uij ? ?
H(5)	-0.0203	-0.2942	0.1914	0.0443	Uij ? ?
H(6)	-0.2081	-0.3830	0.2293	0.0431	Uij ? ?
H(7)	-0.4024	-0.3392	0.0196	0.0422	Uij ? ?
H(8)	-0.2108	-0.2540	-0.0195	0.0408	Uij ? ?
H(9)	-0.5817	-0.3670	0.1037	0.0488	Uij ? ?
H(10)	-0.5413	-0.4648	0.0607	0.0488	Uij ? ?
H(11)	-0.7288	-0.5046	0.1221	0.0566	Uij ? ?
H(12)	-0.6158	-0.5632	0.1570	0.0566	Uij ? ?
H(13)	-0.7205	-0.5080	0.2586	0.0651	Uij ? ?
H(14)	-0.5856	-0.4432	0.2645	0.0651	Uij ? ?
H(15)	-0.6817	-0.3106	0.2121	0.0837	Uij ? ?
H(16)	-0.8166	-0.3754	0.2053	0.0837	Uij ? ?
H(17)	-0.6787	-0.3090	0.3496	0.0978	Uij ? ?
H(18)	-0.7918	-0.2527	0.3120	0.0978	Uij ? ?
H(19)	-0.9403	-0.3812	0.3343	0.1107	Uij ? ?
H(20)	-0.8536	-0.3540	0.4129	0.1107	Uij ? ?
H(21)	-0.8318	-0.4498	0.3600	0.1107	Uij ? ?
H(22)	0.0757	0.1739	0.3389	0.0503	Uij ? ?

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 H(26)  -0.2125     0.3789      0.4158      0.1060      Uij ? ?
 H(27)  -0.1031     0.4676      0.4393      0.1060      Uij ? ?
 H(28b) -0.2720     0.5767      0.3817      0.1179      Uij ? ?
 H(28a) -0.2026     0.5427      0.4431      0.0641      Uij ? ?
 H(29b) -0.3447     0.5658      0.3927      0.0641      Uij ? ?
 H(29a) -0.3698     0.4863      0.4013      0.1179      Uij ? ?
 H(30)  -0.2925     0.5125      0.5250      0.2131      Uij ? ?
 H(31)  -0.2086     0.6091      0.5022      0.2131      Uij ? ?
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 H(33)  -0.4508     0.6302      0.5506      0.1511      Uij ? ?
 H(34)  -0.2829     0.7323      0.5396      0.1752      Uij ? ?
 H(35)  -0.3142     0.7256      0.4488      0.1752      Uij ? ?
 H(36)  -0.4698     0.8591      0.5026      0.1218      Uij ? ?
 H(37)  -0.5614     0.7624      0.4705      0.1218      Uij ? ?
 H(38)  -0.5208     0.7804      0.5602      0.1218      Uij ? ?
 H(39)  0.3379      0.2999      0.3147      0.0453      Uij ? ?
 H(40)  0.5575      0.3575      0.3130      0.0474      Uij ? ?
 H(41)  0.6775      0.3071      0.2107      0.0415      Uij ? ?
 H(42)  0.3467      0.1520      0.1008      0.0364      Uij ? ?
 H(43)  0.6453      0.3945      0.0896      0.0401      Uij ? ?
 H(44)  0.8220      0.4882      0.0420      0.0416      Uij ? ?
 H(45)  0.9739      0.4085      -0.0255     0.0417      Uij ? ?
 H(46)  0.7845      0.1324      0.0115      0.0371      Uij ? ?
 H(47)  0.5576      0.0106      0.1354      0.0374      Uij ? ?
 H(48)  0.4827      -0.1487     0.0709      0.0390      Uij ? ?
 H(49)  0.9610      0.0674      0.7055      0.0801      Uij ? ?
 H(50)  0.7647      -0.0104     0.6431      0.0850      Uij ? ?
 H(51)  0.7098      0.0112      0.5108      0.0999      Uij ? ?
 H(52)  0.8542      0.1094      0.4397      0.1005      Uij ? ?
 H(53)  1.0492      0.1868      0.5023      0.0942      Uij ? ?
 H(54)  1.1029      0.1665      0.6354      0.0844      Uij ? ?
 H(55)  0.2232      0.1272      0.7866      0.0725      Uij ? ?
 H(56)  0.1732      -0.0439     0.7458      0.0710      Uij ? ?
 H(57)  0.3210      -0.1311     0.6799      0.0690      Uij ? ?
 H(58)  0.5176      -0.0436     0.6511      0.0741      Uij ? ?
 H(59)  0.5657      0.1290      0.6913      0.0765      Uij ? ?
 H(60)  0.4173      0.2152      0.7575      0.0693      Uij ? ?

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
 O(1)   0.030(1)    0.043(1)    0.048(1)    -0.002(1)   0.007(1)    0.008(1)
 O(2)   0.051(2)    0.052(2)    0.074(2)    0.021(1)    0.011(1)    -0.022(1)
 N(1)   0.034(2)    0.025(2)    0.052(2)    -0.003(1)   0.016(1)    -0.006(1)
 N(2)   0.032(2)    0.033(2)    0.060(2)    -0.005(1)   0.016(1)    -0.016(1)
 N(3)   0.034(1)    0.027(2)    0.036(2)    -0.004(1)   0.011(1)    -0.006(1)
```

```
 C(1)   0.033(2)    0.027(2)    0.037(2)    -0.001(1)   0.012(2)    -0.004(1)
 C(2)   0.035(2)    0.027(2)    0.049(2)    0.004(1)    0.010(2)    -0.002(2)
 C(3)   0.030(2)    0.032(2)    0.047(2)    0.000(2)    0.005(2)    -0.004(2)
 C(4)   0.033(2)    0.027(2)    0.039(2)    -0.002(1)   0.013(2)    0.000(1)
 C(5)   0.036(2)    0.026(2)    0.037(2)    0.006(1)    0.012(2)    0.002(1)
 C(6)   0.032(2)    0.036(2)    0.035(2)    0.001(2)    0.006(1)    0.001(2)
 C(7)   0.030(2)    0.023(2)    0.043(2)    0.002(1)    0.010(2)    -0.004(1)
 C(8)   0.029(2)    0.038(2)    0.044(2)    0.005(1)    0.003(2)    -0.002(2)
 C(9)   0.038(2)    0.034(2)    0.037(2)    0.004(2)    0.007(2)    0.005(2)
 C(10)  0.030(2)    0.024(2)    0.044(2)    0.001(1)    0.009(2)    0.001(2)
 C(11)  0.033(2)    0.030(2)    0.042(2)    0.001(1)    0.004(2)    -0.001(2)
 C(12)  0.038(2)    0.028(2)    0.036(2)    0.001(1)    0.006(2)    0.001(1)
 C(13)  0.033(2)    0.040(2)    0.048(2)    -0.002(2)   0.005(2)    0.001(2)
 C(14)  0.034(2)    0.051(2)    0.057(2)    -0.001(2)   0.010(2)    0.006(2)
 C(15)  0.042(2)    0.057(3)    0.064(3)    0.002(2)    0.009(2)    0.004(2)
 C(16)  0.077(3)    0.053(3)    0.081(3)    0.014(2)    0.017(2)    -0.006(2)
 C(17)  0.071(3)    0.066(3)    0.108(4)    0.006(2)    0.022(3)    -0.017(3)
 C(18)  0.116(4)    0.072(3)    0.091(4)    0.005(3)    0.030(3)    -0.005(3)
 C(19)  0.031(2)    0.029(2)    0.041(2)    -0.002(1)   0.010(2)    -0.011(2)
 C(20)  0.045(2)    0.037(2)    0.048(2)    0.012(2)    0.014(2)    0.005(2)
 C(21)  0.048(2)    0.050(2)    0.043(2)    0.011(2)    0.017(2)    -0.002(2)
 C(22)  0.032(2)    0.036(2)    0.052(2)    0.005(2)    0.002(2)    -0.014(2)
 C(23)  0.050(2)    0.036(2)    0.050(2)    0.008(2)    -0.001(2)   0.001(2)
 C(24)  0.047(2)    0.038(2)    0.038(2)    0.002(2)    0.008(2)    -0.002(2)
 C(25)  0.077(3)    0.104(4)    0.087(4)    0.044(3)    0.020(3)    -0.042(3)
 C(31)  0.031(2)    0.027(2)    0.040(2)    -0.001(1)   0.008(2)    -0.003(2)
 C(32)  0.042(2)    0.035(2)    0.037(2)    0.000(2)    0.014(2)    -0.007(2)
 C(33)  0.044(2)    0.035(2)    0.037(2)    -0.001(2)   0.003(2)    -0.010(2)
 C(34)  0.032(2)    0.034(2)    0.036(2)    -0.001(1)   0.002(2)    -0.002(2)
 C(35)  0.033(2)    0.024(2)    0.034(2)    0.003(1)    0.008(1)    -0.002(1)
 C(36)  0.033(2)    0.025(2)    0.032(2)    0.001(1)    0.002(1)    -0.004(1)
 C(37)  0.029(2)    0.028(2)    0.030(2)    -0.001(1)   0.004(1)    -0.003(1)
 C(38)  0.035(2)    0.025(2)    0.040(2)    0.003(1)    0.006(2)    -0.002(1)
 C(39)  0.039(2)    0.021(2)    0.044(2)    0.001(1)    0.010(2)    -0.002(1)
 C(40)  0.033(2)    0.028(2)    0.042(2)    -0.003(1)   0.009(2)    0.000(2)
 C(41)  0.033(2)    0.024(2)    0.035(2)    0.000(1)    0.006(1)    -0.002(1)
 C(42)  0.035(2)    0.022(2)    0.036(2)    0.002(1)    0.005(2)    -0.001(1)
 C(43)  0.025(2)    0.026(2)    0.034(2)    -0.002(1)   0.006(1)    -0.004(1)
 C(44)  0.033(2)    0.030(2)    0.030(2)    0.002(1)    0.002(1)    -0.003(1)
 C(45)  0.036(2)    0.025(2)    0.037(2)    0.001(1)    0.009(1)    0.002(1)
 C(46)  0.066(3)    0.087(3)    0.054(3)    0.024(2)    0.014(2)    0.016(2)
 C(47)  0.058(3)    0.078(3)    0.081(3)    0.016(2)    0.014(3)    0.020(3)
 C(48)  0.075(3)    0.079(4)    0.091(4)    0.006(3)    -0.017(3)   0.012(3)
 C(49)  0.104(4)    0.083(4)    0.061(3)    0.004(3)    -0.010(3)   0.021(3)
 C(50)  0.081(3)    0.091(4)    0.064(3)    0.002(3)    0.004(3)    0.026(3)
 C(51)  0.066(3)    0.085(3)    0.061(3)    0.006(2)    0.000(2)    0.021(2)
 C(52)  0.058(3)    0.069(3)    0.058(3)    0.025(2)    0.004(2)    0.003(2)
 C(53)  0.047(2)    0.071(3)    0.061(3)    0.006(2)    0.002(2)    0.009(2)
 C(54)  0.062(3)    0.047(2)    0.059(3)    0.009(2)    -0.014(2)   -0.004(2)
 C(55)  0.051(3)    0.073(3)    0.061(3)    0.017(2)    0.005(2)    -0.014(2)
 C(56)  0.059(3)    0.068(3)    0.063(3)    -0.004(2)   0.012(2)    0.000(2)
 C(57)  0.071(3)    0.046(2)    0.057(3)    0.014(2)    0.001(2)    0.002(2)
#-------------------------------------------------------------------------
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_refine_ls_structure_factor_coef       F
_refine_ls_matrix_type                 full
_refine_ls_weighting_scheme            sigma
_refine_ls_hydrogen_treatment          noref
_refine_ls_extinction_method           none
_refine_ls_extinction_coef             ?
_refine_ls_abs_structure_details       ?
_refine_ls_abs_structure_Flack         ?
_refine_ls_number_reflns               4712
_refine_ls_number_parameters           550
_refine_ls_number_restraints           0
_refine_ls_number_constraints          ?
_refine_ls_R_factor_all                ?
_refine_ls_R_factor_obs                0.0606
_refine_ls_wR_factor_all               ?
_refine_ls_wR_factor_obs               0.0775
_refine_ls_goodness_of_fit_all         ?
_refine_ls_goodness_of_fit_obs         3.501
_refine_ls_shift/esd_max               3.5215
_refine_ls_shift/esd_mean              ?
_refine_diff_density_min               -0.58
_refine_diff_density_max               0.59
#------------------------------------------------------------------------------
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_geom_special_details                  ?
loop_
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_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
    O(1)      C(10)     1.374(3)   ? ? yes
    O(1)      C(13)     1.435(4)   ? ? yes
    O(2)      C(22)     1.367(4)   ? ? yes
    O(2)      C(25)     1.406(5)   ? ? yes
    N(1)      C(4)      1.434(4)   ? ? yes
    N(1)      C(7)      1.441(4)   ? ? yes
    N(1)      C(41)     1.401(4)   ? ? yes
    N(2)      C(1)      1.421(4)   ? ? yes
    N(2)      C(19)     1.431(4)   ? ? yes
    N(2)      C(31)     1.420(4)   ? ? yes
    N(3)      C(35)     1.419(4)   ? ? yes
    N(3)      C(37)     1.421(4)   ? ? yes
    N(3)      C(43)     1.436(4)   ? ? yes
    C(1)      C(2)      1.386(4)   ? ? yes
    C(1)      C(6)      1.396(4)   ? ? yes
    C(2)      C(3)      1.390(4)   ? ? yes
    C(3)      C(4)      1.381(4)   ? ? yes
    C(4)      C(5)      1.390(4)   ? ? yes
    C(5)      C(6)      1.384(4)   ? ? yes
    C(7)      C(8)      1.385(4)   ? ? yes
    C(7)      C(12)     1.381(4)   ? ? yes
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C(8)	C(9)	1.379(4)	?	?	yes
C(9)	C(10)	1.379(4)	?	?	yes
C(10)	C(11)	1.390(4)	?	?	yes
C(11)	C(12)	1.393(4)	?	?	yes
C(13)	C(14)	1.502(4)	?	?	yes
C(14)	C(15)	1.508(5)	?	?	yes
C(15)	C(16)	1.485(5)	?	?	yes
C(16)	C(17)	1.538(6)	?	?	yes
C(17)	C(18)	1.487(6)	?	?	yes
C(19)	C(20)	1.370(4)	?	?	yes
C(19)	C(24)	1.379(4)	?	?	yes
C(20)	C(21)	1.384(4)	?	?	yes
C(21)	C(22)	1.383(5)	?	?	yes
C(22)	C(23)	1.377(5)	?	?	yes
C(23)	C(24)	1.379(5)	?	?	yes
C(25)	C(26a)	1.59(1)	?	?	yes
C(25)	C(26b)	1.68(2)	?	?	yes
C(26a)	C(26b)	0.65(2)	?	?	yes
C(26a)	C(27a)	1.32(2)	?	?	yes
C(26a)	C(27b)	1.42(3)	?	?	yes
C(26b)	C(27a)	1.46(2)	?	?	yes
C(26b)	C(27b)	0.87(2)	?	?	yes
C(27a)	C(27b)	1.45(2)	?	?	yes
C(27a)	C(28a)	1.72(2)	?	?	yes
C(28b)	C(28a)	1.60(2)	?	?	yes
C(28b)	C(29a)	1.33(2)	?	?	yes
C(28b)	C(29b)	1.30(2)	?	?	yes
C(28a)	C(29a)	1.23(2)	?	?	yes
C(28a)	C(29b)	0.90(2)	?	?	yes
C(29a)	C(29b)	0.72(2)	?	?	yes
C(29a)	C(30)	1.85(2)	?	?	yes
C(29b)	C(30)	1.46(2)	?	?	yes
C(31)	C(32)	1.392(4)	?	?	yes
C(31)	C(36)	1.387(4)	?	?	yes
C(32)	C(33)	1.380(4)	?	?	yes
C(33)	C(34)	1.384(4)	?	?	yes
C(34)	C(35)	1.393(4)	?	?	yes
C(35)	C(36)	1.392(4)	?	?	yes
C(37)	C(38)	1.395(4)	?	?	yes
C(37)	C(42)	1.387(4)	?	?	yes
C(38)	C(39)	1.385(4)	?	?	yes
C(39)	C(40)	1.379(4)	?	?	yes
C(40)	C(41)	1.395(4)	?	?	yes
C(41)	C(42)	1.401(4)	?	?	yes
C(43)	C(44)	1.383(4)	?	?	yes
C(43)	C(45)	1.392(4)	?	?	yes
C(44)	C(45)	1.385(4)	?	?	yes
C(46)	C(47)	1.372(6)	?	?	yes
C(46)	C(51)	1.366(5)	?	?	yes
C(47)	C(48)	1.371(6)	?	?	yes
C(48)	C(49)	1.380(6)	?	?	yes
C(49)	C(50)	1.362(6)	?	?	yes
C(50)	C(51)	1.378(6)	?	?	yes
C(52)	C(53)	1.366(5)	?	?	yes

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    C(52)     C(57)     1.368(5)   ? ? yes
    C(53)     C(54)     1.370(5)   ? ? yes
    C(54)     C(55)     1.380(5)   ? ? yes
    C(55)     C(56)     1.374(6)   ? ? yes
    C(56)     C(57)     1.370(5)   ? ? yes
#------------------------------------------------------------------------------
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loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
   C(10)     O(1)      C(13)     118.3(2)   ? ? ? yes
   C(22)     O(2)      C(25)     118.3(3)   ? ? ? yes
   C(4)      N(1)      C(7)      116.2(2)   ? ? ? yes
   C(4)      N(1)      C(41)     120.4(2)   ? ? ? yes
   C(7)      N(1)      C(41)     120.6(2)   ? ? ? yes
   C(1)      N(2)      C(19)     120.1(2)   ? ? ? yes
   C(1)      N(2)      C(31)     119.8(2)   ? ? ? yes
   C(19)     N(2)      C(31)     119.9(2)   ? ? ? yes
   C(35)     N(3)      C(37)     122.6(2)   ? ? ? yes
   C(35)     N(3)      C(43)     118.3(2)   ? ? ? yes
   C(37)     N(3)      C(43)     119.1(2)   ? ? ? yes
   N(2)      C(1)      C(2)      121.7(3)   ? ? ? yes
   N(2)      C(1)      C(6)      119.5(3)   ? ? ? yes
   C(2)      C(1)      C(6)      118.8(3)   ? ? ? yes
   C(1)      C(2)      C(3)      120.5(3)   ? ? ? yes
   C(2)      C(3)      C(4)      120.7(3)   ? ? ? yes
   N(1)      C(4)      C(3)      120.6(3)   ? ? ? yes
   N(1)      C(4)      C(5)      120.6(3)   ? ? ? yes
   C(3)      C(4)      C(5)      118.8(3)   ? ? ? yes
   C(4)      C(5)      C(6)      120.7(3)   ? ? ? yes
   C(1)      C(6)      C(5)      120.3(3)   ? ? ? yes
   N(1)      C(7)      C(8)      120.3(3)   ? ? ? yes
   N(1)      C(7)      C(12)     120.4(3)   ? ? ? yes
   C(8)      C(7)      C(12)     119.2(3)   ? ? ? yes
   C(7)      C(8)      C(9)      120.4(3)   ? ? ? yes
   C(8)      C(9)      C(10)     120.4(3)   ? ? ? yes
   O(1)      C(10)     C(9)      115.3(3)   ? ? ? yes
   O(1)      C(10)     C(11)     124.6(3)   ? ? ? yes
   C(9)      C(10)     C(11)     120.1(3)   ? ? ? yes
   C(10)     C(11)     C(12)     119.0(3)   ? ? ? yes
   C(7)      C(12)     C(11)     120.9(3)   ? ? ? yes
   O(1)      C(13)     C(14)     107.8(3)   ? ? ? yes
   C(13)     C(14)     C(15)     115.5(3)   ? ? ? yes
   C(14)     C(15)     C(16)     113.5(3)   ? ? ? yes
   C(15)     C(16)     C(17)     115.3(4)   ? ? ? yes
   C(16)     C(17)     C(18)     115.7(4)   ? ? ? yes
   N(2)      C(19)     C(20)     120.6(3)   ? ? ? yes
   N(2)      C(19)     C(24)     120.3(3)   ? ? ? yes
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C(20)	C(19)	C(24)	119.1(3)	? ? ? yes
C(19)	C(20)	C(21)	120.9(3)	? ? ? yes
C(20)	C(21)	C(22)	119.9(3)	? ? ? yes
O(2)	C(22)	C(21)	124.5(3)	? ? ? yes
O(2)	C(22)	C(23)	116.2(3)	? ? ? yes
C(21)	C(22)	C(23)	119.3(3)	? ? ? yes
C(22)	C(23)	C(24)	120.3(3)	? ? ? yes
C(19)	C(24)	C(23)	120.6(3)	? ? ? yes
O(2)	C(25)	C(26a)	109.6(6)	? ? ? yes
O(2)	C(25)	C(26b)	97.9(7)	? ? ? yes
C(26a)	C(25)	C(26b)	22.8(7)	? ? ? yes
C(25)	C(26a)	C(26b)	86(2)	? ? ? yes
C(25)	C(26a)	C(27a)	116(1)	? ? ? yes
C(25)	C(26a)	C(27b)	97(1)	? ? ? yes
C(26b)	C(26a)	C(27a)	88(2)	? ? ? yes
C(26b)	C(26a)	C(27b)	24(2)	? ? ? yes
C(27a)	C(26a)	C(27b)	63(1)	? ? ? yes
C(25)	C(26b)	C(26a)	70(2)	? ? ? yes
C(25)	C(26b)	C(27a)	104(1)	? ? ? yes
C(25)	C(26b)	C(27b)	121(2)	? ? ? yes
C(26a)	C(26b)	C(27a)	64(2)	? ? ? yes
C(26a)	C(26b)	C(27b)	136(3)	? ? ? yes
C(27a)	C(26b)	C(27b)	72(2)	? ? ? yes
C(26a)	C(27a)	C(26b)	26.4(9)	? ? ? yes
C(26a)	C(27a)	C(27b)	61(1)	? ? ? yes
C(26a)	C(27a)	C(28a)	113(1)	? ? ? yes
C(26b)	C(27a)	C(27b)	34(1)	? ? ? yes
C(26b)	C(27a)	C(28a)	115(1)	? ? ? yes
C(27b)	C(27a)	C(28a)	109(1)	? ? ? yes
C(26a)	C(27b)	C(26b)	18(1)	? ? ? yes
C(26a)	C(27b)	C(27a)	54(1)	? ? ? yes
C(26b)	C(27b)	C(27a)	72(2)	? ? ? yes
C(28a)	C(28b)	C(29a)	48(1)	? ? ? yes
C(28a)	C(28b)	C(29b)	34.0(9)	? ? ? yes
C(29a)	C(28b)	C(29b)	31.5(10)	? ? ? yes
C(27a)	C(28a)	C(28b)	82(1)	? ? ? yes
C(27a)	C(28a)	C(29a)	92(1)	? ? ? yes
C(27a)	C(28a)	C(29b)	123(1)	? ? ? yes
C(28b)	C(28a)	C(29a)	54(1)	? ? ? yes
C(28b)	C(28a)	C(29b)	53(1)	? ? ? yes
C(29a)	C(28a)	C(29b)	35(1)	? ? ? yes
C(28b)	C(29a)	C(28a)	77(1)	? ? ? yes
C(28b)	C(29a)	C(29b)	71(2)	? ? ? yes
C(28b)	C(29a)	C(30)	99(1)	? ? ? yes
C(28a)	C(29a)	C(29b)	46(1)	? ? ? yes
C(28a)	C(29a)	C(30)	89(1)	? ? ? yes
C(29b)	C(29a)	C(30)	47(2)	? ? ? yes
C(28b)	C(29b)	C(28a)	91(1)	? ? ? yes
C(28b)	C(29b)	C(29a)	76(2)	? ? ? yes
C(28b)	C(29b)	C(30)	124(1)	? ? ? yes
C(28a)	C(29b)	C(29a)	98(2)	? ? ? yes
C(28a)	C(29b)	C(30)	136(2)	? ? ? yes
C(29a)	C(29b)	C(30)	111(2)	? ? ? yes
C(29a)	C(30)	C(29b)	21.2(9)	? ? ? yes

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   N(2)      C(31)     C(32)     120.4(3)   ? ? ? yes
   N(2)      C(31)     C(36)     120.1(3)   ? ? ? yes
   C(32)     C(31)     C(36)     119.6(3)   ? ? ? yes
   C(31)     C(32)     C(33)     118.9(3)   ? ? ? yes
   C(32)     C(33)     C(34)     122.3(3)   ? ? ? yes
   C(33)     C(34)     C(35)     118.8(3)   ? ? ? yes
   N(3)      C(35)     C(34)     122.0(2)   ? ? ? yes
   N(3)      C(35)     C(36)     118.6(3)   ? ? ? yes
   C(34)     C(35)     C(36)     119.4(3)   ? ? ? yes
   C(31)     C(36)     C(35)     121.0(3)   ? ? ? yes
   N(3)      C(37)     C(38)     121.7(3)   ? ? ? yes
   N(3)      C(37)     C(42)     118.8(3)   ? ? ? yes
   C(38)     C(37)     C(42)     119.5(3)   ? ? ? yes
   C(37)     C(38)     C(39)     118.7(3)   ? ? ? yes
   C(38)     C(39)     C(40)     122.2(3)   ? ? ? yes
   C(39)     C(40)     C(41)     119.6(3)   ? ? ? yes
   N(1)      C(41)     C(40)     121.7(3)   ? ? ? yes
   N(1)      C(41)     C(42)     119.9(3)   ? ? ? yes
   C(40)     C(41)     C(42)     118.3(3)   ? ? ? yes
   C(37)     C(42)     C(41)     121.5(3)   ? ? ? yes
   N(3)      C(43)     C(44)     120.2(3)   ? ? ? yes
   N(3)      C(43)     C(45)     121.0(3)   ? ? ? yes
   C(44)     C(43)     C(45)     118.7(3)   ? ? ? yes
   C(43)     C(44)     C(45)     120.9(3)   ? ? ? yes
   C(43)     C(45)     C(44)     120.4(3)   ? ? ? yes
   C(47)     C(46)     C(51)     119.9(4)   ? ? ? yes
   C(46)     C(47)     C(48)     120.2(4)   ? ? ? yes
   C(47)     C(48)     C(49)     119.9(4)   ? ? ? yes
   C(48)     C(49)     C(50)     119.6(4)   ? ? ? yes
   C(49)     C(50)     C(51)     120.5(4)   ? ? ? yes
   C(46)     C(51)     C(50)     119.8(4)   ? ? ? yes
   C(53)     C(52)     C(57)     120.5(4)   ? ? ? yes
   C(52)     C(53)     C(54)     120.1(4)   ? ? ? yes
   C(53)     C(54)     C(55)     119.7(4)   ? ? ? yes
   C(54)     C(55)     C(56)     119.7(4)   ? ? ? yes
   C(55)     C(56)     C(57)     120.3(4)   ? ? ? yes
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