Structural Data

Date: December 6, 2013

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Sample Reference Number:

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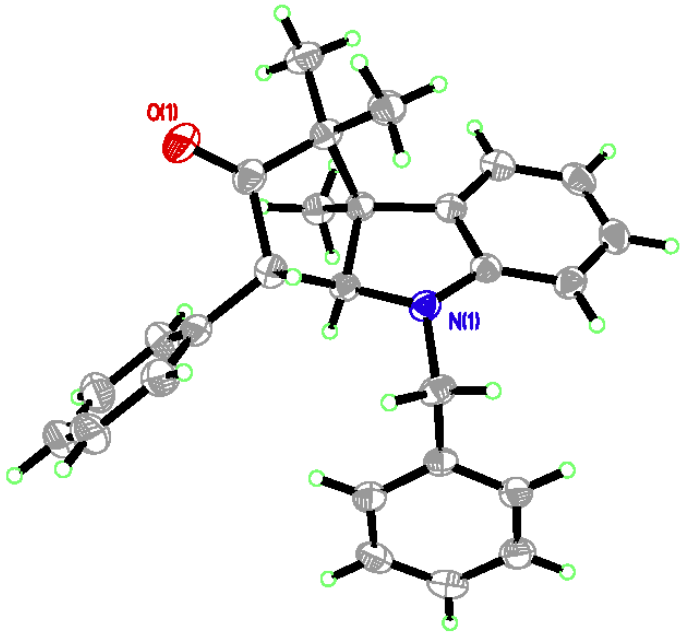


Experimental Section:

A colorless block crystal with dimensions 0.44 x 0.30 x 0.20 mm was mounted on a Nylon loop using very small amount of paratone oil.

Data were collected using a Bruker CCD (charge coupled device) based diffractometer equipped with an Oxford Cryostream low-temperature apparatus operating at 173 K. Data were measured using omega and phi scans of 0.5° per frame for 30 s. The total number of images was based on results from the program COSMO[1] where redundancy was expected to be 4.0 and completeness to 0.83 Å to 100%. Cell parameters were retrieved using APEX II software[2] and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software[3] which corrects for Lp. Scaling and absorption corrections were applied using SADABS[4] multi-scan technique, supplied by George Sheldrick. The structures are solved by the direct method using the SHELXS-97 program and refined by least squares method on F^2, SHELXL-97[5], which are incorporated in OLEX2.[6]

The structure was solved in the space group $P\bar{1}$ (# 2). All non-hydrogen atoms are refined anisotropically. Hydrogens were calculated by geometrical methods and refined as a riding model. All drawings are done at 50% ellipsoids.

Acknowledgement. The CCD based x-ray diffractometer at Michigan State University were upgraded and/or replaced by departmental funds.

References

1. COSMO V1.61, *Software for the CCD Detector Systems for Determining Data Collection Parameters.* Bruker Analytical X-ray Systems, Madison, WI (2009).

2. APEX2 V2010.11-3. Software *for the CCD Detector System*; Bruker Analytical X-ray Systems, Madison, WI (2010).

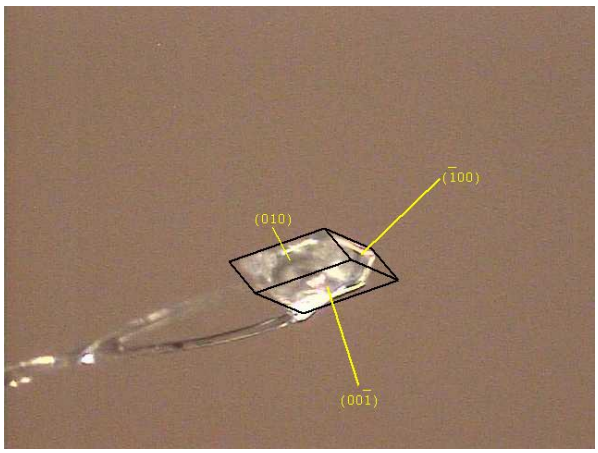
3. SAINT V 7.68A Software *for the Integration of CCD Detector System* Bruker Analytical X-ray Systems, Madison, WI (2010).

4. SADABS V2008/2 Program for absorption corrections using Bruker-AXS CCD based on the method of Robert Blessing; Blessing, R.H. Acta Cryst. A51, 1995, 33-38.

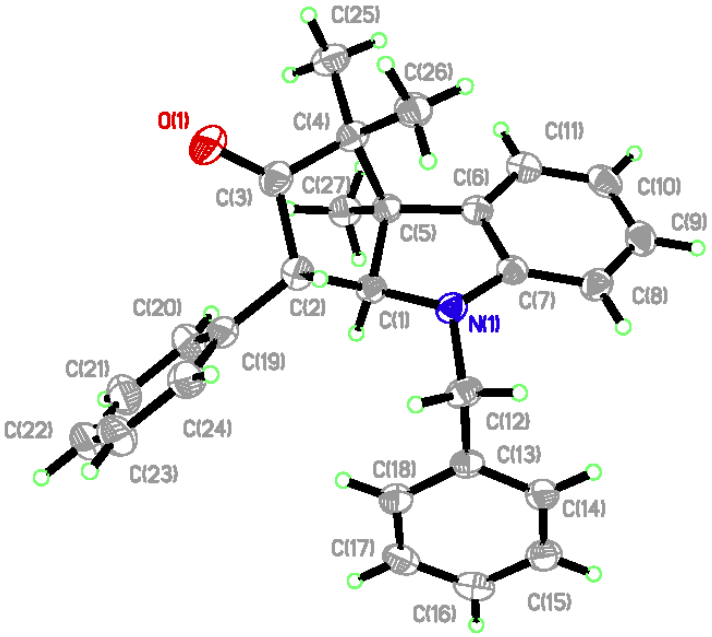
5. Sheldrick, G.M. "A short history of SHELX". *Acta Cryst*. **A64**, 2008, 112-122.

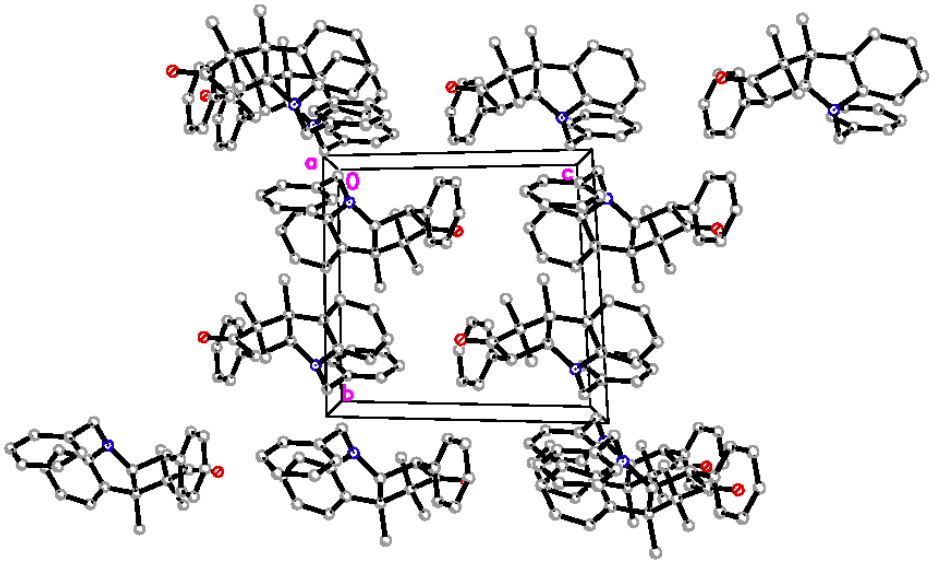
6. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. (2009). 42, 339-341.

[a] Obtained with graphite monochromated Cu Kα (λ = 0.71073) radiation.
[b] $R1 = \sum ||F_o| - |F_c|| / |F_o|$ [c] $wR_2 = \{|[w(F_o^2 - F_c^2)^2.\{\sum[w(F_o^2)^2]\}^{1/2}$.



The following are 50% thermal ellipsoidal drawings of the molecule in the asymmetric cell with various amount of labeling.


C(25)
C(26)
O(1)
C(4)
C(11)
C(6)
C(10)
C(3)
C(27)
C(9)
C(5)
C(20)
C(2)
C(1)
C(7)
C(8)
N(1)
C(21)
C(19)
C(12)
C(22)
C(24)
C(13)
C(18)
C(23)
C(14)
C(17)
C(15)
C(16)



This is a drawing of the packing along the a-axis.

Table 1 Crystal data and structure refinement for jw713a

Identification code	jw713a
Empirical formula	$C_{27}H_{27}NO$
Formula weight	381.50
Temperature/K	173.15
Crystal system	triclinic
Space group	P-1
a/Å	10.0359(18)
b/Å	10.4992(19)
c/Å	10.888(2)
α/°	81.541(2)
β/°	69.756(2)
γ/°	70.441(2)
Volume/Å^3	1013.6(3)
Z	2
ρ_{calc}mg/mm^3	1.250
m/mm^{-1}	0.075
F(000)	408.0
Crystal size/mm^3	0.443 × 0.301 × 0.204
2Θ range for data collection	3.98 to 50.8°
Index ranges	-11 ≤ h ≤ 12, -12 ≤ k ≤ 11, -13 ≤ l ≤ 13
Reflections collected	11104
Independent reflections	3732[R(int) = 0.0371]
Data/restraints/parameters	3732/0/265
Goodness-of-fit on F^2	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0426, wR_2 = 0.0980
Final R indexes [all data]	R_1 = 0.0656, wR_2 = 0.1121
Largest diff. peak/hole / e Å^{-3}	0.24/-0.19

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for jw713a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)

O1	7534.3(14)	7161.4(15)	4993.1(12)	48.5(4)
N1	4692.6(14)	8320.1(13)	9258.9(12)	24.0(3)
C1	5044.0(17)	7345.5(16)	8268.0(14)	22.7(4)
C2	5305.5(17)	7965.0(17)	6860.3(15)	26.0(4)
C3	6969.6(18)	7258.8(17)	6163.0(16)	28.9(4)
C4	7776.5(17)	6717.4(17)	7179.8(15)	26.0(4)
C5	6539.1(17)	6272.3(16)	8330.0(15)	22.6(4)
C6	6514.8(17)	6467.3(16)	9685.4(15)	23.0(4)
C7	5385.7(17)	7653.2(16)	10190.6(15)	22.4(4)
C8	5120.2(18)	8034.8(18)	11443.3(15)	28.2(4)
C9	5987.2(19)	7213.4(19)	12179.2(16)	32.4(4)
C10	7104.5(19)	6042.1(19)	11687.4(16)	32.7(4)
C11	7373.4(18)	5669.4(18)	10429.7(16)	29.1(4)
C12	3220.8(17)	9341.8(16)	9613.4(16)	27.4(4)
C13	1911.2(17)	8827.7(16)	10379.2(15)	24.3(4)
C14	1325.1(18)	8914.2(17)	11733.9(16)	28.9(4)
C15	118.5(18)	8464.1(18)	12441.6(17)	34.1(4)
C16	-532.1(19)	7923.8(18)	11807.2(18)	34.5(5)
C17	22.2(19)	7845.9(18)	10463.7(18)	34.3(4)
C18	1231.3(18)	8301.0(17)	9750.7(17)	30.8(4)
C19	4268.7(17)	7887.6(18)	6164.8(15)	27.2(4)
C20	4072(2)	6661.8(19)	6067.8(17)	34.0(4)
C21	3119(2)	6584(2)	5443.2(17)	39.0(5)
C22	2341(2)	7732(2)	4900.2(18)	42.4(5)
C23	2514(2)	8959(2)	4990.9(18)	44.1(5)
C24	3474.7(19)	9041.1(19)	5620.0(16)	34.5(4)
C25	9239.3(19)	5593.5(19)	6679.3(17)	36.4(5)
C26	8117.0(19)	7916.6(18)	7525.2(17)	31.7(4)
C27	6567.8(19)	4848.1(16)	8156.5(16)	28.9(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for jw713a. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	37.3(7)	75.9(11)	23.5(7)	-0.1(6)	-3.6(6)	-13.1(7)
N1	23.3(7)	22.0(8)	24.0(7)	-2.5(6)	-6.3(6)	-3.8(6)
C1	21.7(8)	21.9(9)	22.8(8)	0.3(7)	-6.9(7)	-5.4(7)

C2	28.4(9)	23.1(9)	25.7(9)	0.7(7)	-9.3(7)	-6.9(7)
C3	31.2(9)	30.3(10)	23.9(9)	0.8(7)	-4.6(7)	-13.0(8)
C4	24.3(8)	27.4(10)	24.1(8)	-1.3(7)	-4.0(7)	-8.6(7)
C5	21.5(8)	20.6(9)	23.8(8)	-1.6(7)	-6.1(7)	-4.8(7)
C6	22.9(8)	22.0(9)	24.6(8)	2.1(7)	-6.3(7)	-10.2(7)
C7	21.2(8)	24.3(9)	22.8(8)	2.7(7)	-6.1(7)	-10.5(7)
C8	27.0(9)	30.8(10)	26.1(9)	-3.7(7)	-3.5(7)	-11.9(8)
C9	34.4(10)	45.7(12)	23.8(9)	2.1(8)	-9.5(8)	-21.9(9)
C10	31.3(9)	40.8(11)	31.3(10)	9.7(8)	-16.1(8)	-15.8(9)
C11	26.8(9)	27.9(10)	32.5(9)	4.4(8)	-10.5(7)	-9.5(8)
C12	24.7(9)	21.3(9)	29.3(9)	-1.7(7)	-5.4(7)	-1.3(7)
C13	21.0(8)	17.0(9)	30.0(9)	-1.9(7)	-8.2(7)	0.8(7)
C14	25.0(9)	28.8(10)	32.2(9)	-5.1(7)	-8.8(7)	-6.3(7)
C15	26.6(9)	39.6(11)	30.9(9)	-0.2(8)	-7.3(8)	-6.0(8)
C16	23.1(9)	33.0(11)	44.8(11)	4.1(8)	-11.1(8)	-7.3(8)
C17	27.5(9)	29.5(10)	49.8(11)	-5.8(8)	-19.0(9)	-4.9(8)
C18	26.4(9)	30.8(10)	31.0(9)	-4.5(8)	-10.6(8)	-0.6(8)
C19	24.0(8)	33.8(10)	20.7(8)	0.8(7)	-5.3(7)	-7.5(8)
C20	36.6(10)	35.0(11)	34.1(10)	3.6(8)	-17.9(8)	-10.7(8)
C21	42.3(11)	46.2(13)	34.8(10)	1.1(9)	-17.2(9)	-17.5(10)
C22	35.2(10)	63.8(15)	31.4(10)	2.2(10)	-16.0(8)	-15.4(10)
C23	39.1(11)	50.9(14)	37.5(11)	9.2(10)	-20.2(9)	-3.9(10)
C24	32.6(10)	36.1(11)	30.4(9)	4.3(8)	-9.7(8)	-7.7(8)
C25	26.1(9)	38.7(11)	35.4(10)	-4.4(8)	-2.6(8)	-4.8(8)
C26	30.8(9)	34.2(11)	31.9(9)	2.2(8)	-8.0(8)	-15.8(8)
C27	29.5(9)	24.2(10)	31.8(9)	-1.4(7)	-9.0(8)	-7.3(7)

Table 4 Bond Lengths for jw713a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C3	1.2059(19)	C8	C9	1.385(2)
N1	C1	1.468(2)	C9	C10	1.383(2)
N1	C7	1.399(2)	C10	C11	1.390(2)
N1	C12	1.4655(19)	C12	C13	1.516(2)
C1	C2	1.544(2)	C13	C14	1.390(2)
C1	C5	1.562(2)	C13	C18	1.388(2)
C2	C3	1.541(2)	C14	C15	1.383(2)

C2	C19	1.511(2)	C15	C16	1.379(2)
C3	C4	1.527(2)	C16	C17	1.378(2)
C4	C5	1.571(2)	C17	C18	1.389(2)
C4	C25	1.523(2)	C19	C20	1.390(2)
C4	C26	1.536(2)	C19	C24	1.387(2)
C5	C6	1.510(2)	C20	C21	1.379(3)
C5	C27	1.524(2)	C21	C22	1.375(3)
C6	C7	1.401(2)	C22	C23	1.378(3)
C6	C11	1.379(2)	C23	C24	1.392(3)
C7	C8	1.389(2)			

Table 5 Bond Angles for jw713a.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C7	N1	C1	107.90(12)	C11	C6	C7	120.14(15)
C7	N1	C12	122.33(12)	N1	C7	C6	110.39(13)
C12	N1	C1	118.67(13)	C8	C7	N1	129.19(15)
N1	C1	C2	113.67(13)	C8	C7	C6	120.40(15)
N1	C1	C5	104.62(12)	C9	C8	C7	118.56(16)
C2	C1	C5	107.96(12)	C10	C9	C8	121.40(16)
C3	C2	C1	103.57(13)	C9	C10	C11	119.84(16)
C19	C2	C1	116.20(14)	C6	C11	C10	119.66(16)
C19	C2	C3	114.41(13)	N1	C12	C13	116.13(13)
O1	C3	C2	124.67(16)	C14	C13	C12	120.63(15)
O1	C3	C4	125.86(15)	C18	C13	C12	121.27(14)
C4	C3	C2	109.47(13)	C18	C13	C14	118.07(15)
C3	C4	C5	100.82(12)	C15	C14	C13	121.16(16)
C3	C4	C26	106.43(14)	C16	C15	C14	120.18(16)
C25	C4	C3	113.30(14)	C17	C16	C15	119.45(16)
C25	C4	C5	114.77(14)	C16	C17	C18	120.46(17)
C25	C4	C26	108.56(14)	C13	C18	C17	120.67(16)
C26	C4	C5	112.56(13)	C20	C19	C2	120.90(16)
C1	C5	C4	104.38(12)	C24	C19	C2	120.84(17)
C6	C5	C1	101.42(12)	C24	C19	C20	118.25(17)
C6	C5	C4	114.74(13)	C21	C20	C19	121.24(18)
C6	C5	C27	112.62(13)	C22	C21	C20	120.1(2)
C27	C5	C1	111.49(13)	C21	C22	C23	119.55(18)

C27	C5	C4	111.43(12)	C22	C23	C24	120.47(18)
C7	C6	C5	109.61(14)	C19	C24	C23	120.33(19)
C11	C6	C5	130.23(15)				

Table 6 Torsion Angles for jw713a.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
O1	C3	C4	C5	-144.46(18)	C5	C6	C11	C10	-177.71(16)
O1	C3	C4	C25	-21.3(3)	C6	C7	C8	C9	-0.5(2)
O1	C3	C4	C26	97.9(2)	C7	N1	C1	C2	-142.50(13)
N1	C1	C2	C3	113.72(14)	C7	N1	C1	C5	-24.96(16)
N1	C1	C2	C19	-119.94(15)	C7	N1	C12	C13	-69.5(2)
N1	C1	C5	C4	-97.82(14)	C7	C6	C11	C10	0.5(2)
N1	C1	C5	C6	21.69(15)	C7	C8	C9	C10	0.5(2)
N1	C1	C5	C27	141.77(13)	C8	C9	C10	C11	-0.1(3)
N1	C7	C8	C9	-178.36(15)	C9	C10	C11	C6	-0.5(2)
N1	C12	C13	C14	98.32(18)	C11	C6	C7	N1	178.20(14)
N1	C12	C13	C18	-83.87(19)	C11	C6	C7	C8	-0.1(2)
C1	N1	C7	C6	18.22(17)	C12	N1	C1	C2	72.71(17)
C1	N1	C7	C8	-163.71(16)	C12	N1	C1	C5	-169.75(12)
C1	N1	C12	C13	70.05(19)	C12	N1	C7	C6	161.45(14)
C1	C2	C3	O1	158.56(17)	C12	N1	C7	C8	-20.5(2)
C1	C2	C3	C4	-21.75(17)	C12	C13	C14	C15	179.18(15)
C1	C2	C19	C20	-53.0(2)	C12	C13	C18	C17	-179.35(15)
C1	C2	C19	C24	126.23(16)	C13	C14	C15	C16	-0.3(3)
C1	C5	C6	C7	-11.78(16)	C14	C13	C18	C17	-1.5(2)
C1	C5	C6	C11	166.61(16)	C14	C15	C16	C17	-0.5(3)
C2	C1	C5	C4	23.57(16)	C15	C16	C17	C18	0.3(3)
C2	C1	C5	C6	143.07(13)	C16	C17	C18	C13	0.7(3)
C2	C1	C5	C27	-96.84(15)	C18	C13	C14	C15	1.3(2)
C2	C3	C4	C5	35.86(16)	C19	C2	C3	O1	31.1(2)
C2	C3	C4	C25	159.01(14)	C19	C2	C3	C4	-149.22(14)
C2	C3	C4	C26	-81.77(15)	C19	C20	C21	C22	0.0(3)
C2	C19	C20	C21	179.51(15)	C20	C19	C24	C23	-0.2(2)
C2	C19	C24	C23	-179.49(15)	C20	C21	C22	C23	-0.3(3)
C3	C2	C19	C20	67.7(2)	C21	C22	C23	C24	0.4(3)
C3	C2	C19	C24	-113.07(17)	C22	C23	C24	C19	-0.1(3)

C3	C4	C5	C1	-35.20(15)	C24	C19	C20	C21	0.3(2)
C3	C4	C5	C6	-145.27(14)	C25	C4	C5	C1	-157.32(14)
C3	C4	C5	C27	85.26(15)	C25	C4	C5	C6	92.61(17)
C4	C5	C6	C7	100.06(15)	C25	C4	C5	C27	-36.87(19)
C4	C5	C6	C11	-81.6(2)	C26	C4	C5	C1	77.84(16)
C5	C1	C2	C3	-1.87(17)	C26	C4	C5	C6	-32.23(19)
C5	C1	C2	C19	124.47(15)	C26	C4	C5	C27	-161.71(14)
C5	C6	C7	N1	-3.22(18)	C27	C5	C6	C7	-131.06(14)
C5	C6	C7	C8	178.52(14)	C27	C5	C6	C11	47.3(2)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for jw713a.

Atom	***x***	***y***	***z***	**U(eq)**
H1	4240	6908	8497	27
H2	5183	8943	6909	31
H8	4361	8841	11788	34
H9	5810	7460	13040	39
H10	7687	5493	12208	39
H11	8145	4869	10085	35
H12A	3045	9806	8798	33
H12B	3241	10026	10137	33
H14	1761	9289	12181	35
H15	-263	8528	13367	41
H16	-1356	7608	12293	41
H17	-425	7478	10022	41
H18	1596	8251	8824	37
H20	4604	5862	6439	41
H21	3000	5736	5388	47
H22	1688	7679	4466	51
H23	1974	9754	4621	53
H24	3587	9892	5677	41
H25A	9055	4865	6357	55
H25B	9661	5237	7394	55
H25C	9944	5954	5965	55
H26A	8567	7635	8228	48
H26B	7189	8661	7818	48

H26C	8812	8218	6750	48
H27A	7449	4189	8325	43
H27B	6607	4767	7259	43
H27C	5665	4672	8774	43

Crystal structure determination of [jw713a]

Crystal Data. $C_{27}H_{27}NO$, M =381.50, triclinic, a = 10.0359(18) Å, b = 10.4992(19) Å, c = 10.888(2) Å, α = 81.541(2)°, β = 69.756(2)°, γ = 70.441(2)°, V = 1013.6(3) Å^3, T = 173.15, space group P-1 (no. 2), Z = 2, μ(MoKα) = 0.075, 11104 reflections measured, 3732 unique (R_{int} = 0.0371) which were used in all calculations. The final wR_2 was 0.1121 (all data) and R_1 was 0.0426 (>2sigma(I)).

Structural Data

Date: December 6, 2013

Submitter: Hui Li, Jimmy Wu

Sample Reference Number: Oct 2012

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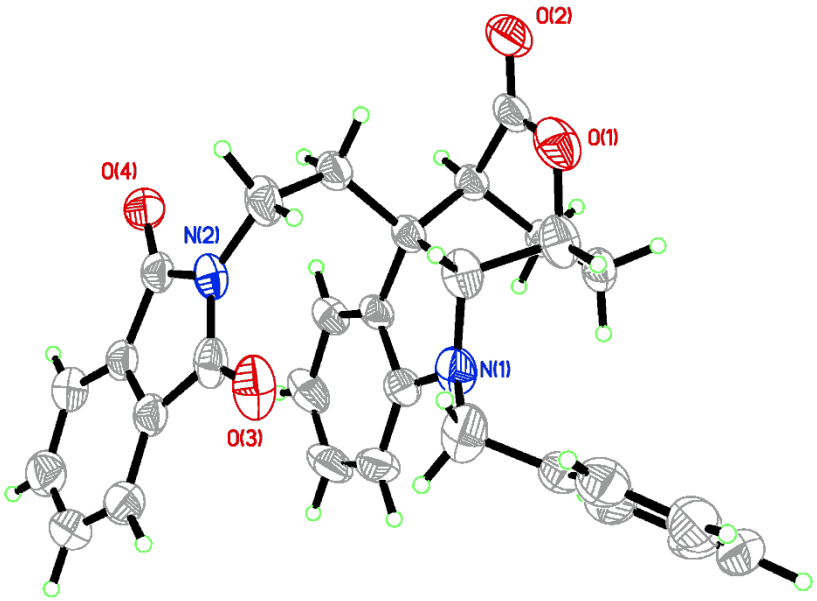


Experimental Section:

A yellow plate crystal with dimensions 0.38 x 0.24 x 0.11 mm was mounted on a Nylon loop using very small amount of paratone oil.

Data were collected using a Bruker CCD (charge coupled device) based diffractometer equipped with an Oxford Cryostream low-temperature apparatus operating at 173 K. Data were measured using omega and phi scans of 1.0° per frame for 30 s. The total number of images was based on results from the program COSMO[1] where redundancy was expected to be 4.0 and completeness to 0.83 Å to 100%. Cell parameters were retrieved using APEX II software[2] and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software[3] which corrects for Lp. Scaling and absorption corrections were applied using SADABS[4] multi-scan technique, supplied by George Sheldrick. The structures are solved by the direct method using the SHELXS-97 program and refined by least squares method on F^2, SHELXL-97[5], which are incorporated in OLEX2.[6]

The structure was solved in the space group $P\bar{1}$ (# 2). All non-hydrogen atoms are refined anisotropically. Hydrogens were calculated by geometrical methods and refined as a riding model. All drawings are done at 50% ellipsoids.

Acknowledgement. The CCD based x-ray diffractometer at Michigan State University were upgraded and/or replaced by departmental funds.

References

1. COSMO V1.61, *Software for the CCD Detector Systems for Determining Data Collection Parameters.* Bruker Analytical X-ray Systems, Madison, WI (2009).

2. APEX2 V2010.11-3. Software *for the CCD Detector System*; Bruker Analytical X-ray Systems, Madison, WI (2010).

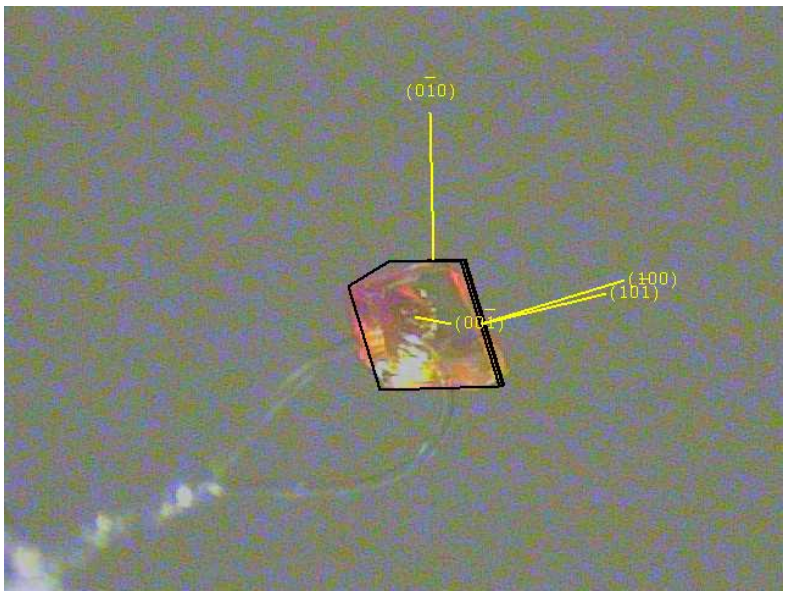
3. SAINT V 7.68A Software *for the Integration of CCD Detector System* Bruker Analytical X-ray Systems, Madison, WI (2010).

4. SADABS V2008/2 Program for absorption corrections using Bruker-AXS CCD based on the method of Robert Blessing; Blessing, R.H. Acta Cryst. A51, 1995, 33-38.

5. Sheldrick, G.M. "A short history of SHELX". *Acta Cryst*. **A64**, 2008, 112-122.

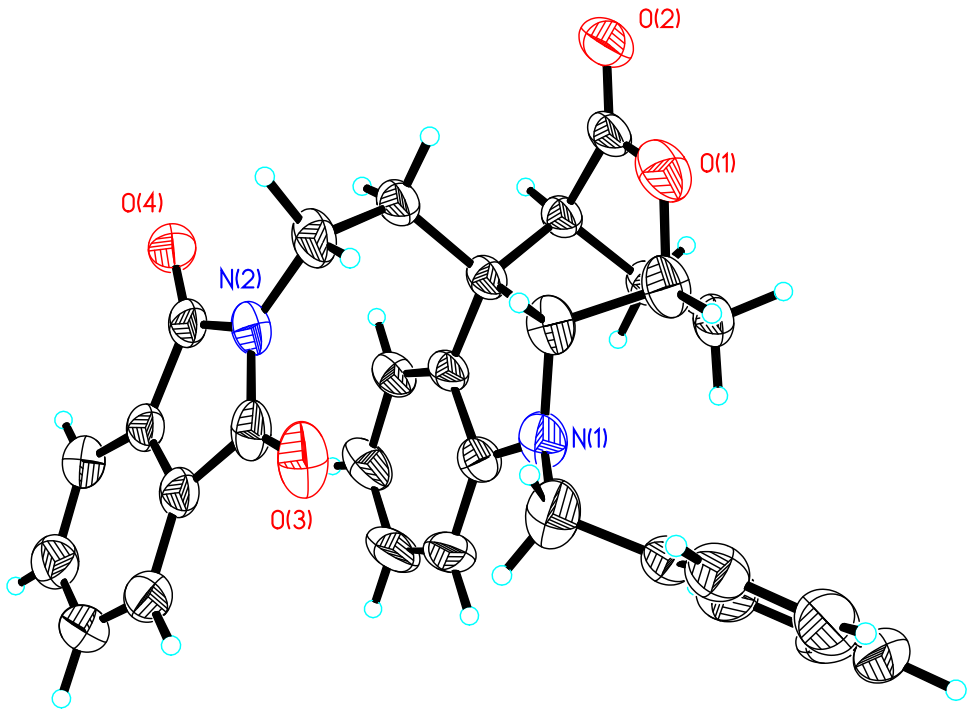
6. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. (2009). 42, 339-341.

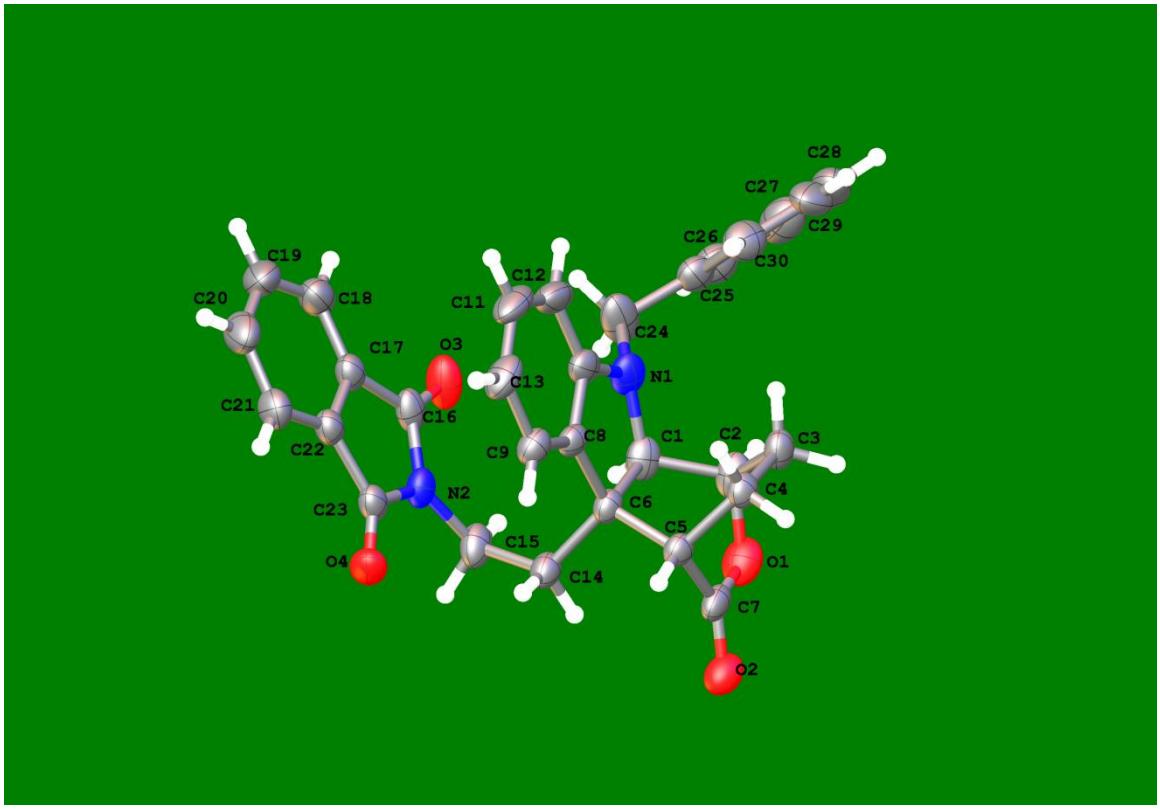
[a] Obtained with graphite monochromated Cu Kα (λ = 1.54178Å) radiation.
[b] $R1 = \sum ||F_o| - |F_c|| / |F_o|$ [c] $wR_2 = \{|[w(F_o^2 - F_c^2)^2.\{\sum[w(F_o^2)^2]\}^{1/2}$.

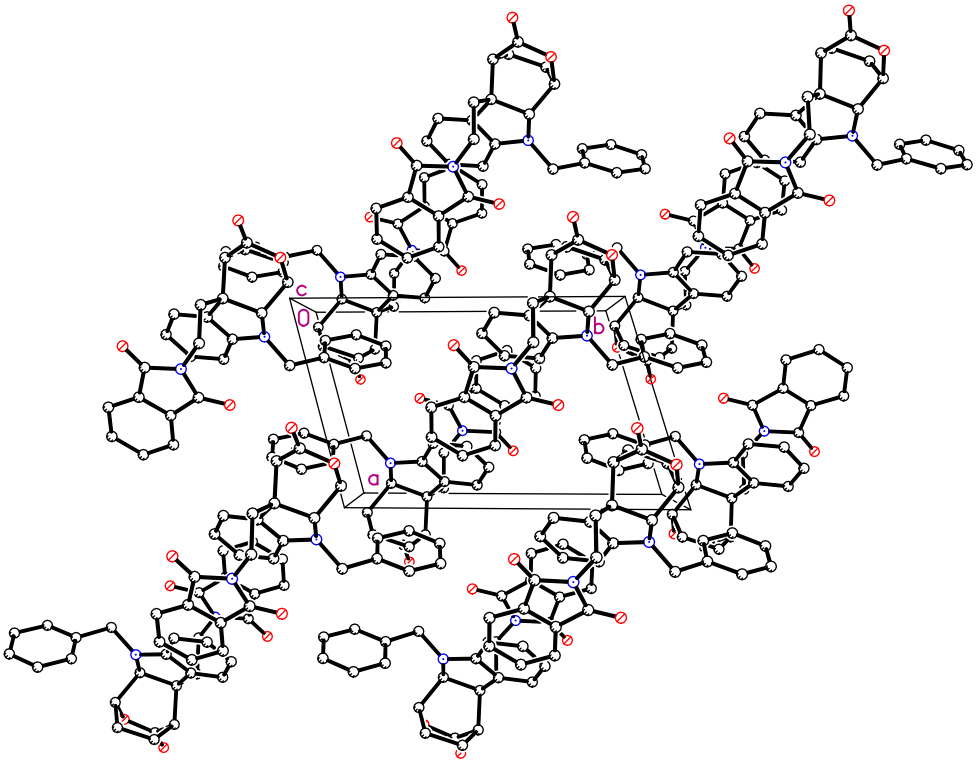


The following are 50% thermal ellipsoidal drawings of the molecule in the asymmetric cell with

various amount of labeling.




C28
C27
C29
C26
C30
C19
C12
C25
C20
C18
C11
C24
C17
O3
N1
C13
C21
C16
C8
C1
C2
C3
C22
C9
C4
N2
C6
C23
C5
C15
O1
O4
C14
C7
O2


c
b
a

This is a drawing of the packing along the c-axis.

Table 1. Crystal data and structure refinement for jw412_0m.

Identification code	jw412_0m	
Empirical formula	C60 H52 N4 O8	
Formula weight	957.06	
Temperature	446.15 K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.24560(10) Å	α= 83.0987(6)°.
	b = 12.3627(2) Å	β= 73.8045(7)°.
	c = 12.7774(2) Å	γ= 72.8974(8)°.
Volume	1194.47(3) $Å^3$	
Z	1	
Density (calculated)	1.330 Mg/m^3	
Absorption coefficient	0.716 mm^{-1}	
F(000)	504	
Crystal size	0.336 x 0.279 x 0.106 mm^3	
Theta range for data collection	3.61 to 67.84°.	
Index ranges	-9<=h<=9, -14<=k<=14, -15<=l<=15	
Reflections collected	15251	
Independent reflections	4199 [R(int) = 0.0311]	
Completeness to theta = 67.84°	96.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7530 and 0.6725	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4199 / 0 / 429	
Goodness-of-fit on F^2	1.480	
Final R indices [I>2sigma(I)]	R1 = 0.0534, wR2 = 0.1717	
R indices (all data)	R1 = 0.0582, wR2 = 0.1780	
Largest diff. peak and hole	0.728 and -0.242 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jw412_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	-2045(2)	10016(1)	9648(1)	54(1)
O(2)	-3763(2)	9126(1)	10833(1)	56(1)
O(3)	5173(2)	7157(1)	8279(2)	56(1)
O(4)	2313(2)	4537(1)	9988(1)	50(1)
N(1)	1747(2)	8684(1)	7412(2)	46(1)
N(2)	3417(2)	6055(1)	9298(1)	39(1)
C(1)	617(2)	8896(2)	8517(2)	41(1)
C(2)	-927(3)	9958(2)	8537(2)	46(1)
C(3)	-2020(3)	9913(2)	7771(2)	41(1)
C(4)	-2656(2)	8844(1)	8060(1)	34(1)
C(5)	-2130(2)	8253(1)	9093(1)	32(1)
C(6)	-99(2)	7841(1)	8895(1)	31(1)
C(7)	-2770(2)	9132(2)	9948(1)	41(1)
C(8)	761(2)	7091(1)	7920(1)	31(1)
C(9)	599(2)	6046(2)	7777(1)	38(1)
C(10)	1582(3)	5496(2)	6813(2)	51(1)
C(11)	2687(3)	6004(2)	6031(2)	58(1)
C(12)	2835(3)	7068(2)	6159(2)	54(1)
C(13)	1848(2)	7619(2)	7117(1)	39(1)
C(14)	297(2)	7236(2)	9964(1)	40(1)
C(15)	2187(3)	6906(2)	10058(2)	47(1)
C(16)	4805(2)	6268(2)	8469(2)	41(1)
C(17)	5694(2)	5184(1)	7897(1)	37(1)
C(18)	7165(3)	4915(2)	7037(2)	53(1)
C(19)	7685(3)	3824(2)	6669(2)	60(1)
C(20)	6756(3)	3040(2)	7148(2)	56(1)
C(21)	5289(3)	3306(2)	8027(2)	44(1)
C(22)	4788(2)	4400(1)	8388(1)	35(1)
C(23)	3341(2)	4947(1)	9319(1)	37(1)
C(24)	3188(3)	9211(2)	7024(2)	61(1)
C(25)	2765(2)	10311(2)	6364(2)	42(1)
C(26)	3335(3)	11209(2)	6536(2)	53(1)
C(27)	3032(4)	12203(2)	5910(3)	70(1)

C(28)	2135(4)	12316(2)	5121(3)	80(1)
C(29)	1535(4)	11451(3)	4968(2)	71(1)
C(30)	1856(3)	10443(2)	5572(2)	55(1)

Table 3. Bond lengths [Å] and angles [°] for jw412_0m.

O(1)-C(2)	1.458(3)
O(1)-C(7)	1.362(3)
O(2)-C(7)	1.198(2)
O(3)-C(16)	1.204(2)
O(4)-C(23)	1.204(2)
N(1)-C(1)	1.464(3)
N(1)-C(13)	1.384(3)
N(1)-C(24)	1.461(2)
N(2)-C(15)	1.465(2)
N(2)-C(16)	1.391(3)
N(2)-C(23)	1.386(2)
C(1)-C(2)	1.533(3)
C(1)-C(6)	1.558(2)
C(2)-C(3)	1.519(3)
C(3)-C(4)	1.530(2)
C(4)-C(5)	1.538(2)
C(5)-C(6)	1.555(2)
C(5)-C(7)	1.510(2)
C(6)-C(8)	1.5202(19)
C(6)-C(14)	1.547(2)
C(8)-C(9)	1.375(2)
C(8)-C(13)	1.397(2)
C(9)-C(10)	1.400(2)
C(10)-C(11)	1.379(4)
C(11)-C(12)	1.389(4)
C(12)-C(13)	1.395(3)
C(14)-C(15)	1.526(3)
C(16)-C(17)	1.492(3)
C(17)-C(18)	1.377(3)
C(17)-C(22)	1.382(2)
C(18)-C(19)	1.387(4)
C(19)-C(20)	1.390(4)
C(20)-C(21)	1.389(3)
C(21)-C(22)	1.388(3)
C(22)-C(23)	1.491(2)
C(24)-C(25)	1.513(3)

C(25)-C(26)	1.388(3)
C(25)-C(30)	1.387(3)
C(26)-C(27)	1.381(4)
C(27)-C(28)	1.380(5)
C(28)-C(29)	1.358(5)
C(29)-C(30)	1.381(4)

C(7)-O(1)-C(2)	113.20(13)
C(13)-N(1)-C(1)	110.00(14)
C(13)-N(1)-C(24)	123.09(19)
C(24)-N(1)-C(1)	118.81(19)
C(16)-N(2)-C(15)	123.67(16)
C(23)-N(2)-C(15)	124.30(17)
C(23)-N(2)-C(16)	112.03(15)
N(1)-C(1)-C(2)	111.55(16)
N(1)-C(1)-C(6)	106.19(13)
C(2)-C(1)-C(6)	109.32(14)
O(1)-C(2)-C(1)	106.51(16)
O(1)-C(2)-C(3)	108.14(16)
C(3)-C(2)-C(1)	113.00(15)
C(2)-C(3)-C(4)	108.75(14)
C(3)-C(4)-C(5)	109.32(13)
C(4)-C(5)-C(6)	111.25(13)
C(7)-C(5)-C(4)	107.16(13)
C(7)-C(5)-C(6)	106.12(13)
C(5)-C(6)-C(1)	107.37(13)
C(8)-C(6)-C(1)	102.68(13)
C(8)-C(6)-C(5)	111.99(12)
C(8)-C(6)-C(14)	112.65(13)
C(14)-C(6)-C(1)	114.70(13)
C(14)-C(6)-C(5)	107.41(13)
O(1)-C(7)-C(5)	113.09(15)
O(2)-C(7)-O(1)	118.20(16)
O(2)-C(7)-C(5)	128.68(19)
C(9)-C(8)-C(6)	129.13(15)
C(9)-C(8)-C(13)	121.54(15)
C(13)-C(8)-C(6)	109.32(14)
C(8)-C(9)-C(10)	118.72(17)

C(11)-C(10)-C(9)	119.80(19)
C(10)-C(11)-C(12)	121.89(17)
C(11)-C(12)-C(13)	118.28(18)
N(1)-C(13)-C(8)	111.68(16)
N(1)-C(13)-C(12)	128.58(18)
C(12)-C(13)-C(8)	119.74(18)
C(15)-C(14)-C(6)	118.42(16)
N(2)-C(15)-C(14)	114.68(14)
O(3)-C(16)-N(2)	125.48(19)
O(3)-C(16)-C(17)	128.76(19)
N(2)-C(16)-C(17)	105.76(14)
C(18)-C(17)-C(16)	130.04(17)
C(18)-C(17)-C(22)	121.76(18)
C(22)-C(17)-C(16)	108.20(15)
C(17)-C(18)-C(19)	117.0(2)
C(18)-C(19)-C(20)	121.3(2)
C(21)-C(20)-C(19)	121.6(2)
C(22)-C(21)-C(20)	116.40(18)
C(17)-C(22)-C(21)	121.84(17)
C(17)-C(22)-C(23)	107.73(15)
C(21)-C(22)-C(23)	130.40(16)
O(4)-C(23)-N(2)	124.98(18)
O(4)-C(23)-C(22)	128.80(16)
N(2)-C(23)-C(22)	106.20(14)
N(1)-C(24)-C(25)	114.59(17)
C(26)-C(25)-C(24)	119.21(19)
C(30)-C(25)-C(24)	122.05(19)
C(30)-C(25)-C(26)	118.7(2)
C(27)-C(26)-C(25)	120.2(2)
C(28)-C(27)-C(26)	120.2(3)
C(29)-C(28)-C(27)	119.8(2)
C(28)-C(29)-C(30)	120.7(3)
C(29)-C(30)-C(25)	120.3(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for jw412_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	57(1)	45(1)	61(1)	-22(1)	-20(1)	-3(1)
O(2)	50(1)	62(1)	43(1)	-15(1)	-11(1)	6(1)
O(3)	45(1)	38(1)	94(1)	9(1)	-32(1)	-16(1)
O(4)	39(1)	50(1)	50(1)	11(1)	-4(1)	-9(1)
N(1)	27(1)	45(1)	64(1)	7(1)	-12(1)	-12(1)
N(2)	30(1)	36(1)	48(1)	-1(1)	-17(1)	-1(1)
C(1)	35(1)	40(1)	56(1)	-4(1)	-22(1)	-11(1)
C(2)	44(1)	33(1)	66(1)	-8(1)	-20(1)	-9(1)
C(3)	33(1)	36(1)	51(1)	2(1)	-14(1)	-3(1)
C(4)	29(1)	36(1)	36(1)	-4(1)	-13(1)	-4(1)
C(5)	26(1)	35(1)	33(1)	-5(1)	-8(1)	-3(1)
C(6)	25(1)	34(1)	34(1)	-6(1)	-11(1)	-2(1)
C(7)	32(1)	48(1)	36(1)	-11(1)	-13(1)	9(1)
C(8)	21(1)	39(1)	32(1)	-5(1)	-8(1)	-3(1)
C(9)	29(1)	41(1)	43(1)	-9(1)	-10(1)	-4(1)
C(10)	40(1)	54(1)	55(1)	-24(1)	-15(1)	4(1)
C(11)	39(1)	82(2)	37(1)	-21(1)	-6(1)	10(1)
C(12)	31(1)	76(1)	38(1)	2(1)	0(1)	-1(1)
C(13)	22(1)	50(1)	40(1)	3(1)	-10(1)	-5(1)
C(14)	33(1)	45(1)	35(1)	-7(1)	-12(1)	4(1)
C(15)	43(1)	47(1)	49(1)	-10(1)	-26(1)	5(1)
C(16)	31(1)	38(1)	59(1)	8(1)	-25(1)	-9(1)
C(17)	28(1)	39(1)	45(1)	8(1)	-14(1)	-7(1)
C(18)	36(1)	60(1)	54(1)	16(1)	-10(1)	-10(1)
C(19)	46(1)	67(1)	45(1)	2(1)	-2(1)	5(1)
C(20)	63(1)	48(1)	47(1)	-5(1)	-15(1)	2(1)
C(21)	46(1)	37(1)	49(1)	2(1)	-18(1)	-7(1)
C(22)	30(1)	36(1)	39(1)	5(1)	-14(1)	-6(1)
C(23)	28(1)	39(1)	41(1)	5(1)	-14(1)	-4(1)
C(24)	33(1)	62(1)	91(2)	26(1)	-25(1)	-21(1)
C(25)	29(1)	49(1)	46(1)	2(1)	-6(1)	-12(1)
C(26)	42(1)	57(1)	57(1)	-4(1)	-7(1)	-17(1)
C(27)	60(2)	47(1)	90(2)	-2(1)	7(1)	-17(1)

C(28)	56(2)	66(2)	78(2)	31(1)	13(1)	0(1)
C(29)	57(1)	100(2)	37(1)	15(1)	-5(1)	-6(1)
C(30)	48(1)	70(1)	48(1)	-5(1)	-13(1)	-14(1)

Table 5. Torsion angles [°] for jw412_0m.

O(1)-C(2)-C(3)-C(4)	-61.50(18)
O(3)-C(16)-C(17)-C(18)	1.9(3)
O(3)-C(16)-C(17)-C(22)	-178.79(18)
N(1)-C(1)-C(2)-O(1)	174.33(13)
N(1)-C(1)-C(2)-C(3)	55.7(2)
N(1)-C(1)-C(6)-C(5)	-117.44(14)
N(1)-C(1)-C(6)-C(8)	0.75(16)
N(1)-C(1)-C(6)-C(14)	123.29(15)
N(1)-C(24)-C(25)-C(26)	138.2(2)
N(1)-C(24)-C(25)-C(30)	-43.3(3)
N(2)-C(16)-C(17)-C(18)	-178.05(18)
N(2)-C(16)-C(17)-C(22)	1.25(18)
C(1)-N(1)-C(13)-C(8)	4.0(2)
C(1)-N(1)-C(13)-C(12)	-177.09(18)
C(1)-N(1)-C(24)-C(25)	-95.8(3)
C(1)-C(2)-C(3)-C(4)	56.1(2)
C(1)-C(6)-C(8)-C(9)	-179.20(16)
C(1)-C(6)-C(8)-C(13)	1.54(16)
C(1)-C(6)-C(14)-C(15)	-51.5(2)
C(2)-O(1)-C(7)-O(2)	-177.26(17)
C(2)-O(1)-C(7)-C(5)	4.6(2)
C(2)-C(1)-C(6)-C(5)	3.03(18)
C(2)-C(1)-C(6)-C(8)	121.22(15)
C(2)-C(1)-C(6)-C(14)	-116.24(16)
C(2)-C(3)-C(4)-C(5)	5.7(2)
C(3)-C(4)-C(5)-C(6)	-63.63(17)
C(3)-C(4)-C(5)-C(7)	51.95(18)
C(4)-C(5)-C(6)-C(1)	57.50(16)
C(4)-C(5)-C(6)-C(8)	-54.48(17)
C(4)-C(5)-C(6)-C(14)	-178.66(12)
C(4)-C(5)-C(7)-O(1)	-60.85(18)
C(4)-C(5)-C(7)-O(2)	121.3(2)
C(5)-C(6)-C(8)-C(9)	-64.3(2)
C(5)-C(6)-C(8)-C(13)	116.43(15)
C(5)-C(6)-C(14)-C(15)	-170.70(14)
C(6)-C(1)-C(2)-O(1)	57.19(17)

C(6)-C(1)-C(2)-C(3)	-61.4(2)
C(6)-C(5)-C(7)-O(1)	58.09(18)
C(6)-C(5)-C(7)-O(2)	-119.8(2)
C(6)-C(8)-C(9)-C(10)	-177.73(16)
C(6)-C(8)-C(13)-N(1)	-3.49(19)
C(6)-C(8)-C(13)-C(12)	177.52(15)
C(6)-C(14)-C(15)-N(2)	-64.8(2)
C(7)-O(1)-C(2)-C(1)	-64.17(18)
C(7)-O(1)-C(2)-C(3)	57.6(2)
C(7)-C(5)-C(6)-C(1)	-58.72(16)
C(7)-C(5)-C(6)-C(8)	-170.70(13)
C(7)-C(5)-C(6)-C(14)	65.12(17)
C(8)-C(6)-C(14)-C(15)	65.5(2)
C(8)-C(9)-C(10)-C(11)	0.1(3)
C(9)-C(8)-C(13)-N(1)	177.19(15)
C(9)-C(8)-C(13)-C(12)	-1.8(3)
C(9)-C(10)-C(11)-C(12)	-1.3(3)
C(10)-C(11)-C(12)-C(13)	1.0(3)
C(11)-C(12)-C(13)-N(1)	-178.23(18)
C(11)-C(12)-C(13)-C(8)	0.6(3)
C(13)-N(1)-C(1)-C(2)	-121.86(16)
C(13)-N(1)-C(1)-C(6)	-2.85(18)
C(13)-N(1)-C(24)-C(25)	118.7(2)
C(13)-C(8)-C(9)-C(10)	1.4(3)
C(14)-C(6)-C(8)-C(9)	56.9(2)
C(14)-C(6)-C(8)-C(13)	-122.37(16)
C(15)-N(2)-C(16)-O(3)	0.5(3)
C(15)-N(2)-C(16)-C(17)	-179.53(14)
C(15)-N(2)-C(23)-O(4)	-3.5(3)
C(15)-N(2)-C(23)-C(22)	178.06(14)
C(16)-N(2)-C(15)-C(14)	114.9(2)
C(16)-N(2)-C(23)-O(4)	176.41(16)
C(16)-N(2)-C(23)-C(22)	-2.07(18)
C(16)-C(17)-C(18)-C(19)	-179.65(19)
C(16)-C(17)-C(22)-C(21)	179.27(16)
C(16)-C(17)-C(22)-C(23)	-2.47(17)
C(17)-C(18)-C(19)-C(20)	0.1(3)
C(17)-C(22)-C(23)-O(4)	-175.59(18)

C(17)-C(22)-C(23)-N(2)	2.81(18)
C(18)-C(17)-C(22)-C(21)	-1.4(3)
C(18)-C(17)-C(22)-C(23)	176.90(16)
C(18)-C(19)-C(20)-C(21)	-1.2(4)
C(19)-C(20)-C(21)-C(22)	1.0(3)
C(20)-C(21)-C(22)-C(17)	0.3(3)
C(20)-C(21)-C(22)-C(23)	-177.55(18)
C(21)-C(22)-C(23)-O(4)	2.5(3)
C(21)-C(22)-C(23)-N(2)	-179.13(17)
C(22)-C(17)-C(18)-C(19)	1.1(3)
C(23)-N(2)-C(15)-C(14)	-65.2(2)
C(23)-N(2)-C(16)-O(3)	-179.36(16)
C(23)-N(2)-C(16)-C(17)	0.59(18)
C(24)-N(1)-C(1)-C(2)	88.45(19)
C(24)-N(1)-C(1)-C(6)	-152.53(16)
C(24)-N(1)-C(13)-C(8)	152.17(18)
C(24)-N(1)-C(13)-C(12)	-28.9(3)
C(24)-C(25)-C(26)-C(27)	177.1(2)
C(24)-C(25)-C(30)-C(29)	-178.3(2)
C(25)-C(26)-C(27)-C(28)	1.1(4)
C(26)-C(25)-C(30)-C(29)	0.2(3)
C(26)-C(27)-C(28)-C(29)	0.6(4)
C(27)-C(28)-C(29)-C(30)	-1.9(4)
C(28)-C(29)-C(30)-C(25)	1.5(4)
C(30)-C(25)-C(26)-C(27)	-1.4(3)

Symmetry transformations used to generate equivalent atoms:

Structural Data

Date: December 6, 2013

Submitter: Hui Li

Sample Reference Number:

Center Crystallographic for Research
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Department of Chemistry
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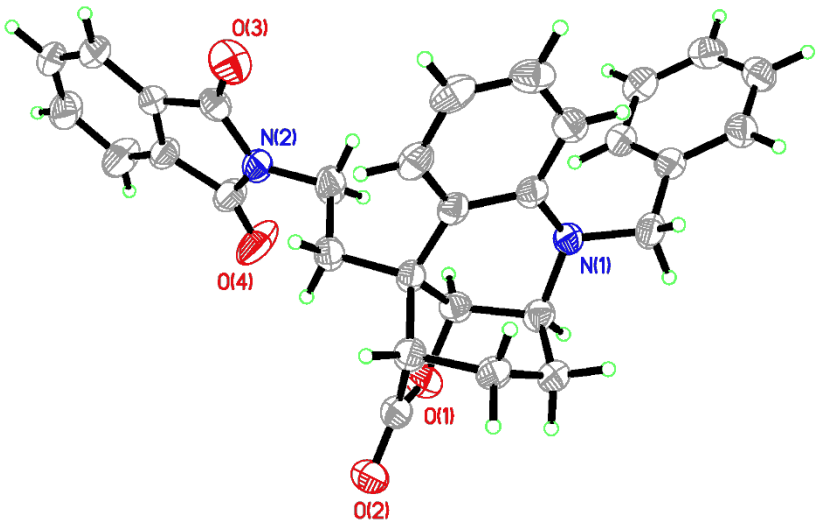


Experimental Section:

A colorless block crystal with dimensions 0.37 x 0.26 x 0.24 mm was mounted on a glass fiber using very small amount of paratone oil.

Data were collected using a Bruker CCD (charge coupled device) based diffractometer equipped with an Oxford Cryostream low-temperature apparatus operating at 173 K. Data were measured using omega and phi scans of 0.5° per frame for 10 s. The total number of images was based on results from the program COSMO[1] where redundancy was expected to be 4.0 and completeness to 0.83 Å to 100%. Cell parameters were retrieved using APEX II software[2] and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software[3] which corrects for Lp. Scaling and absorption corrections were applied using SADABS[4] multi-scan technique, supplied by George Sheldrick. The structures are solved by the direct method using the SHELXS-97 program and refined by least squares method on F^2, SHELXL-97[5], which are incorporated in OLEX2.[6]

The structure was solved in the space group $P2_1/n$(# 14). All non-hydrogen atoms are refined anisotropically. Hydrogens were calculated by geometrical methods and refined as a riding model. All drawings are done at 50% ellipsoids.

Acknowledgement. The CCD based x-ray diffractometer at Michigan State University were upgraded and/or replaced by departmental funds.

References

1. COSMO V1.61, *Software for the CCD Detector Systems for Determining Data Collection Parameters.* Bruker Analytical X-ray Systems, Madison, WI (2009).

2. APEX2 V2010.11-3. Software *for the CCD Detector System*; Bruker Analytical X-ray Systems, Madison, WI (2010).

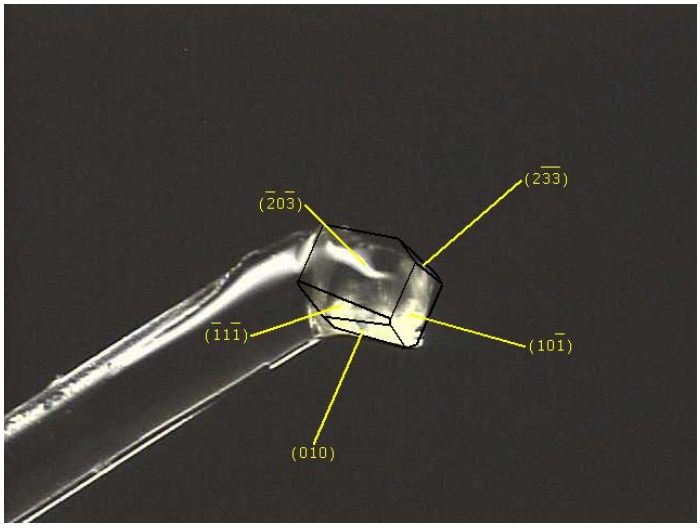
3. SAINT V 7.68A Software *for the Integration of CCD Detector System* Bruker Analytical X-ray Systems, Madison, WI (2010).

4. SADABS V2008/2 Program for absorption corrections using Bruker-AXS CCD based on the method of Robert Blessing; Blessing, R.H. Acta Cryst. A51, 1995, 33-38.

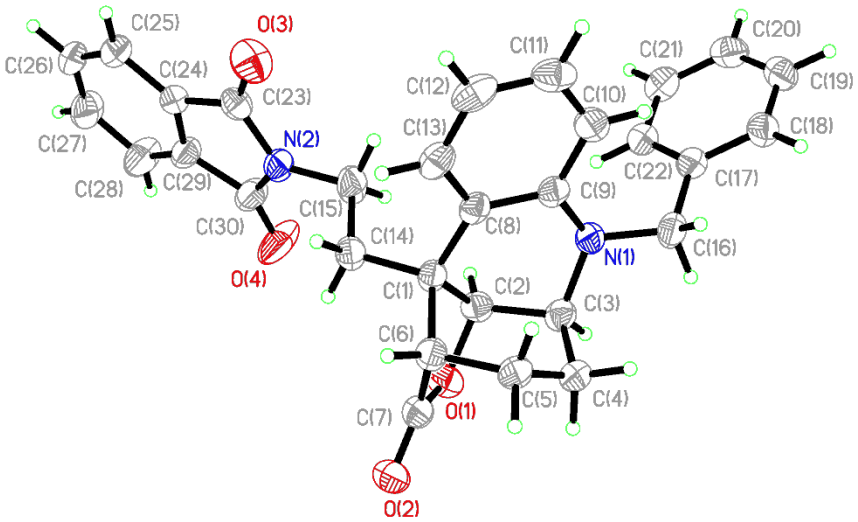
5. Sheldrick, G.M. "A short history of SHELX". *Acta Cryst*. **A64**, 2008, 112-122.

6. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. (2009). 42, 339-341.

[a] Obtained with graphite monochromated Cu Kα (λ = 0.71073) radiation.
[b] $R1 = \sum ||F_o| - |F_c|| / |F_o|$ [c] $wR_2 = \{|[w(F_o^2 - F_c^2)^2.\{\sum[w(F_o^2)^2]\}^{1/2}$.



The following are 50% thermal ellipsoidal drawings of the molecule in the asymmetric cell with various amount of labeling.


C(25)
O(3)
C(26)
C(24)
C(23)
C(27)
N(2)
C(28)
C(29)
C(30)
O(4)
C(15)
C(14)
C(1)
C(2)
C(3)
C(6)
C(7)
O(1)
C(5)
C(4)
O(2)
C(11)
C(12)
C(10)
C(13)
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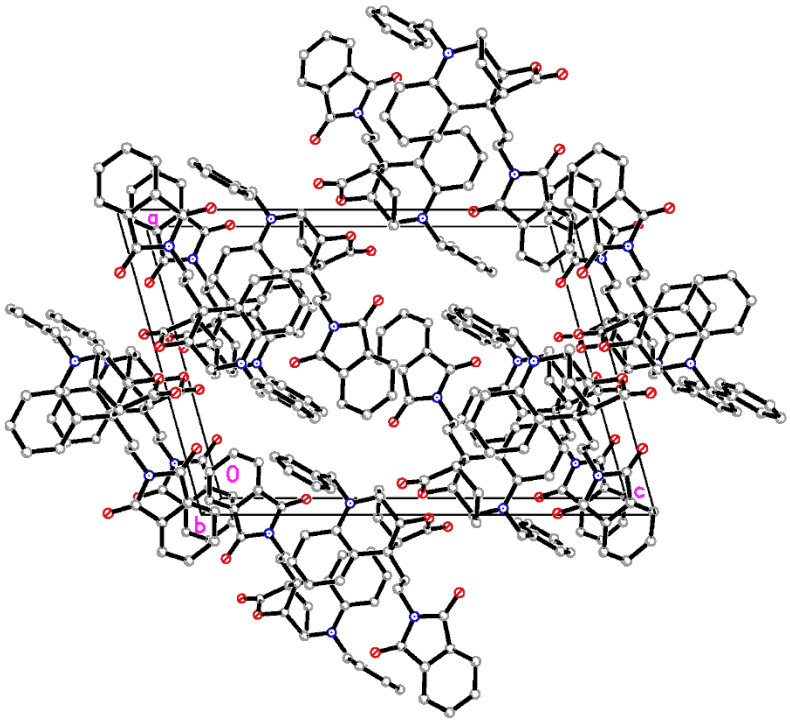
C(19)
C(18)
C(22)
C(17)
C(16)



This is a drawing of the packing along the b-axis.

Table 1 Crystal data and structure refinement for jw512

Identification code	JW512
Empirical formula	$C_{30}H_{26}N_2O_4$
Formula weight	478.53
Temperature/K	173.15
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.0202(8)
b/Å	10.2694(7)
c/Å	18.7419(12)
α/°	90.00
β/°	105.5710(10)
γ/°	90.00
Volume/Å^3	2414.0(3)
Z	4
ρ_{calc}mg/mm^3	1.317
m/mm^{-1}	0.088
F(000)	1008.0
Crystal size/mm^3	0.366 × 0.26 × 0.242
2Θ range for data collection	4.42 to 50.76°
Index ranges	-15 ≤ h ≤ 15, -12 ≤ k ≤ 12, -22 ≤ l ≤ 22
Reflections collected	19250
Independent reflections	4414[R(int) = 0.0293]
Data/restraints/parameters	4414/0/325
Goodness-of-fit on F^2	1.024
Final R indexes [I>=2σ (I)]	R_1 = 0.0405, wR_2 = 0.0929
Final R indexes [all data]	R_1 = 0.0535, wR_2 = 0.0999
Largest diff. peak/hole / e Å^{-3}	0.30/-0.17

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for jw51. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O2	962.4(11)	8644.4(13)	4610.6(7)	51.6(4)
O1	532.1(10)	6722.6(11)	5007.7(6)	40.3(3)
O3	5008.8(11)	4178.3(13)	7114.3(7)	51.6(3)
O4	2884.4(11)	3518.9(18)	4784.1(8)	72.9(5)
N1	-39.2(10)	5869.9(13)	6770.4(7)	32.5(3)
C1	1716.1(12)	6668.0(14)	6207.2(9)	29.5(3)
C14	2683.2(13)	6093.9(15)	5987(1)	34.8(4)
N2	3761.9(11)	4097.4(13)	5974.7(8)	35.0(3)
C23	4755.0(13)	3864.8(15)	6471.3(9)	33.2(4)
C20	-1364.5(14)	1871.6(18)	7878.5(10)	44.3(5)
C19	-1786.1(14)	2945.3(18)	8139.6(9)	40.7(4)
C18	-1646.5(13)	4171.6(18)	7875.0(9)	38.7(4)
C17	-1088.9(13)	4338.8(17)	7345.0(9)	36.0(4)
C16	-979.2(13)	5707.2(17)	7040.8(10)	38.9(4)
C3	-242.9(13)	6471.1(15)	6037.3(9)	32.9(4)
C2	677.7(13)	6098.1(15)	5726.4(9)	32.7(4)
C15	2860.4(15)	4663.0(16)	6193.7(11)	43.7(4)
C30	3675.6(14)	3515.7(19)	5296.5(10)	43.0(4)
C29	4726.9(13)	2892.1(18)	5351.1(9)	37.8(4)
C28	5078.2(16)	2150(2)	4852.8(10)	56.2(6)
C27	6112.1(16)	1669(2)	5075.7(11)	51.7(5)
C4	-398.1(13)	7958.1(16)	6028.5(10)	36.0(4)
C5	646.2(13)	8724.8(15)	6251.7(9)	34.9(4)
C6	1504.8(13)	8095.9(15)	5935.1(9)	33.8(4)
C7	1014.9(14)	7912.1(17)	5118.1(10)	38.6(4)
C8	1817.9(12)	6510.0(14)	7029.4(9)	29.5(3)
C13	2769.1(13)	6792.4(16)	7549.1(10)	36.7(4)
C12	2898.0(15)	6646.7(16)	8299.3(10)	43.3(4)
C11	2048.5(15)	6194.1(16)	8539.9(10)	42.1(4)
C10	1082.9(14)	5926.7(15)	8043.1(9)	36.6(4)
C9	938.2(13)	6105.5(14)	7279.6(9)	29.6(3)
C24	5377.0(12)	3129.4(15)	6047.8(9)	30.9(4)
C26	6760.8(14)	1929.9(19)	5762.3(11)	46.5(5)
C25	6407.6(14)	2672.3(19)	6263.7(10)	42.8(4)
C22	-686.9(14)	3246.7(17)	7075.3(10)	40.5(4)

C21	-817.6(14)	2017.4(18)	7344.7(10)	43.3(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for jw51. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O2	61.2(9)	49.6(8)	52.7(8)	19.7(7)	30.4(7)	17.1(7)
O1	47.5(7)	40.2(7)	33.8(6)	1.7(5)	12.1(5)	-0.6(6)
O3	62.6(9)	54.6(8)	39.7(8)	-13.9(6)	17.1(6)	-7.1(7)
O4	38.8(8)	118.4(14)	51.8(9)	-13.9(9)	-4.9(7)	30.9(8)
N1	27.6(7)	31.6(7)	39.9(8)	6.5(6)	11.7(6)	-0.8(6)
C1	27.0(8)	24.4(8)	38.8(9)	1.4(7)	12.0(7)	0.5(6)
C14	35.2(9)	28.1(8)	45.3(10)	2.3(7)	17.9(8)	1.6(7)
N2	35.3(8)	31.5(7)	42.2(8)	1.5(6)	17.3(6)	8.5(6)
C23	39.1(10)	28.1(8)	34.2(9)	-0.1(7)	13.2(7)	-3.8(7)
C20	37.7(10)	41.5(10)	48.9(11)	11.4(8)	3.1(8)	-9.2(8)
C19	32.8(9)	53.7(11)	34.2(9)	3.3(8)	6.4(7)	-10.9(8)
C18	34.6(9)	44.9(10)	37.0(9)	0.6(8)	10.5(7)	-0.3(8)
C17	29.9(9)	40.3(9)	37.8(9)	6.4(7)	8.9(7)	1.6(7)
C16	30.5(9)	40.8(10)	49.1(10)	3.0(8)	16.9(8)	4.4(7)
C3	27.0(8)	33.5(9)	36.4(9)	0.9(7)	5.6(7)	-1.9(7)
C2	35.5(9)	27.4(8)	35.4(9)	1.1(7)	10.1(7)	0.3(7)
C15	46.8(11)	31.6(9)	62.4(12)	4.7(8)	31.7(9)	9.1(8)
C30	33.7(10)	55.8(12)	37.9(10)	0.3(8)	6.9(8)	12.0(8)
C29	30.9(9)	49.8(10)	32.5(9)	-0.2(8)	8.1(7)	9.3(8)
C28	43.4(11)	87.4(16)	35(1)	-14.6(10)	5.6(8)	18.0(11)
C27	46.6(12)	65.9(13)	47.9(12)	-3.7(10)	22.1(10)	16.9(10)
C4	32.2(9)	35.7(9)	41.3(10)	7.1(7)	11.7(7)	6.7(7)
C5	38.7(9)	25.6(8)	42.1(9)	2.2(7)	13.6(8)	6.7(7)
C6	32.0(9)	24.3(8)	47.3(10)	3.7(7)	14.7(8)	0.0(7)
C7	40.1(10)	35.8(9)	45.4(10)	8.2(8)	20.9(8)	10.5(8)
C8	29.3(8)	21.2(7)	38.6(9)	-0.7(6)	10.2(7)	3.9(6)
C13	31.1(9)	30.0(9)	47(1)	-3.2(7)	7.0(8)	3.1(7)
C12	39.7(10)	32.8(9)	48.8(11)	-7.1(8)	-3.3(8)	7.7(8)
C11	58.1(12)	30.3(9)	35.0(9)	-0.1(7)	7.5(9)	11.2(8)
C10	44.2(10)	27.5(8)	41.1(10)	2.7(7)	16.5(8)	6.1(7)
C9	32.5(9)	20.1(7)	37.5(9)	1.2(6)	11.6(7)	5.2(6)
C24	29.0(8)	33.4(9)	30.4(8)	2.6(7)	8.1(7)	0.2(7)
C26	30.7(10)	61.3(12)	50.3(11)	11.9(9)	16.0(8)	13.6(9)
C25	29.4(9)	58.4(12)	37.8(10)	6.0(9)	4.2(7)	1.1(8)

C22	35.8(10)	42.8(10)	44.9(10)	8.1(8)	14.1(8)	5.8(8)
C21	36.3(10)	38.4(10)	53.0(11)	0.1(8)	7.9(8)	1.4(8)

Table 4 Bond Lengths for jw51.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O2	C7	1.200(2)	C17	C16	1.538(2)
O1	C2	1.4577(19)	C17	C22	1.389(2)
O1	C7	1.364(2)	C3	C2	1.516(2)
O3	C23	1.2047(19)	C3	C4	1.540(2)
O4	C30	1.205(2)	C30	C29	1.490(2)
N1	C16	1.454(2)	C29	C28	1.376(2)
N1	C3	1.464(2)	C29	C24	1.374(2)
N1	C9	1.392(2)	C28	C27	1.388(3)
C1	C14	1.543(2)	C27	C26	1.363(3)
C1	C2	1.526(2)	C4	C5	1.529(2)
C1	C6	1.553(2)	C5	C6	1.541(2)
C1	C8	1.520(2)	C6	C7	1.504(2)
C14	C15	1.521(2)	C8	C13	1.385(2)
N2	C23	1.396(2)	C8	C9	1.412(2)
N2	C15	1.464(2)	C13	C12	1.379(2)
N2	C30	1.382(2)	C12	C11	1.382(3)
C23	C24	1.484(2)	C11	C10	1.376(3)
C20	C19	1.379(3)	C10	C9	1.404(2)
C20	C21	1.383(3)	C24	C25	1.376(2)
C19	C18	1.383(2)	C26	C25	1.381(3)
C18	C17	1.389(2)	C22	C21	1.387(2)

Table 5 Bond Angles for jw51.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C7	O1	C2	108.27(12)	O4	C30	C29	128.99(17)
C16	N1	C3	114.71(13)	N2	C30	C29	106.04(14)
C9	N1	C16	118.77(14)	C28	C29	C30	131.18(16)
C9	N1	C3	118.17(12)	C24	C29	C30	108.03(14)
C14	C1	C6	111.00(12)	C24	C29	C28	120.75(16)
C2	C1	C14	110.65(13)	C29	C28	C27	117.70(17)
C2	C1	C6	96.75(12)	C26	C27	C28	121.30(17)
C8	C1	C14	112.02(13)	C5	C4	C3	113.78(13)
C8	C1	C2	112.34(13)	C4	C5	C6	111.26(13)
C8	C1	C6	113.17(13)	C5	C6	C1	110.62(13)
C15	C14	C1	112.32(13)	C7	C6	C1	101.84(13)
C23	N2	C15	123.36(14)	C7	C6	C5	106.94(13)
C30	N2	C23	111.81(13)	O2	C7	O1	121.01(17)
C30	N2	C15	123.80(15)	O2	C7	C6	130.29(17)
O3	C23	N2	125.27(15)	O1	C7	C6	108.60(13)
O3	C23	C24	128.95(16)	C13	C8	C1	120.59(14)
N2	C23	C24	105.74(13)	C13	C8	C9	118.69(15)
C19	C20	C21	120.10(17)	C9	C8	C1	120.70(14)
C20	C19	C18	119.86(16)	C12	C13	C8	122.37(16)
C19	C18	C17	120.86(17)	C13	C12	C11	118.70(16)
C18	C17	C16	119.76(15)	C10	C11	C12	120.80(17)
C22	C17	C18	118.72(16)	C11	C10	C9	120.77(16)
C22	C17	C16	121.44(15)	N1	C9	C8	119.84(14)
N1	C16	C17	113.87(13)	N1	C9	C10	121.59(14)
N1	C3	C2	106.94(13)	C10	C9	C8	118.56(15)
N1	C3	C4	114.73(14)	C29	C24	C23	108.25(14)
C2	C3	C4	111.20(13)	C29	C24	C25	121.49(15)
O1	C2	C1	104.58(12)	C25	C24	C23	130.21(15)
O1	C2	C3	108.90(13)	C27	C26	C25	121.04(17)
C3	C2	C1	110.05(13)	C24	C25	C26	117.70(17)
N2	C15	C14	112.97(14)	C21	C22	C17	120.50(16)
O4	C30	N2	124.96(16)	C20	C21	C22	119.94(17)

Table 6 Torsion Angles for jw51.

A	B	C	D	Angle/˚
O3	C23	C24	C29	174.22(17)
O3	C23	C24	C25	-3.4(3)
O4	C30	C29	C28	-1.1(4)
O4	C30	C29	C24	-178.8(2)
N1	C3	C2	O1	-177.60(12)
N1	C3	C2	C1	-63.51(16)
N1	C3	C4	C5	80.86(17)
C1	C14	C15	N2	178.82(14)
C1	C6	C7	O2	-156.94(18)
C1	C6	C7	O1	26.84(16)
C1	C8	C13	C12	-179.18(14)
C1	C8	C9	N1	-1.1(2)
C1	C8	C9	C10	177.64(13)
C14	C1	C2	O1	-73.66(15)
C14	C1	C2	C3	169.52(13)
C14	C1	C6	C5	-171.85(14)
C14	C1	C6	C7	74.76(16)
C14	C1	C8	C13	45.20(19)
C14	C1	C8	C9	-136.46(14)
N2	C23	C24	C29	-3.55(18)
N2	C23	C24	C25	178.82(17)
N2	C30	C29	C28	177.7(2)
N2	C30	C29	C24	0.0(2)
C23	N2	C15	C14	102.81(19)
C23	N2	C30	O4	176.5(2)
C23	N2	C30	C29	-2.4(2)
C23	C24	C25	C26	175.50(17)
C20	C19	C18	C17	0.3(3)
C19	C20	C21	C22	0.4(3)
C19	C18	C17	C16	177.88(16)
C19	C18	C17	C22	1.0(3)
C18	C17	C16	N1	153.82(16)
C18	C17	C22	C21	-1.6(3)
C17	C22	C21	C20	0.9(3)
C16	N1	C3	C2	-158.62(13)
C16	N1	C3	C4	77.57(17)
C16	N1	C9	C8	-167.99(14)
C16	N1	C9	C10	13.3(2)

C16	C17	C22	C21	-178.40(16)
C3	N1	C16	C17	131.71(15)
C3	N1	C9	C8	-21.4(2)
C3	N1	C9	C10	159.86(14)
C3	C4	C5	C6	38.84(19)
C2	O1	C7	O2	-176.44(15)
C2	O1	C7	C6	0.20(17)
C2	C1	C14	C15	-69.42(18)
C2	C1	C6	C5	72.94(15)
C2	C1	C6	C7	-40.44(14)
C2	C1	C8	C13	170.48(14)
C2	C1	C8	C9	-11.18(19)
C2	C3	C4	C5	-40.65(19)
C15	N2	C23	O3	-5.5(3)
C15	N2	C23	C24	172.40(14)
C15	N2	C30	O4	7.8(3)
C15	N2	C30	C29	-171.05(15)
C30	N2	C23	O3	-174.23(17)
C30	N2	C23	C24	3.64(18)
C30	N2	C15	C14	-89.8(2)
C30	C29	C28	C27	-178.3(2)
C30	C29	C24	C23	2.18(19)
C30	C29	C24	C25	-179.93(16)
C29	C28	C27	C26	-0.4(3)
C29	C24	C25	C26	-1.9(3)
C28	C29	C24	C23	-175.78(18)
C28	C29	C24	C25	2.1(3)
C28	C27	C26	C25	0.6(3)
C27	C26	C25	C24	0.5(3)
C4	C3	C2	O1	-51.64(17)
C4	C3	C2	C1	62.45(17)
C4	C5	C6	C1	-58.32(18)
C4	C5	C6	C7	51.78(17)
C5	C6	C7	O2	87.0(2)
C5	C6	C7	O1	-89.26(15)
C6	C1	C14	C15	-175.63(15)
C6	C1	C2	O1	41.82(14)
C6	C1	C2	C3	-75.00(14)
C6	C1	C8	C13	-81.21(17)
C6	C1	C8	C9	97.13(16)

C7	O1	C2	C1	-28.02(16)
C7	O1	C2	C3	89.59(15)
C8	C1	C14	C15	56.79(19)
C8	C1	C2	O1	160.31(12)
C8	C1	C2	C3	43.49(17)
C8	C1	C6	C5	-44.90(18)
C8	C1	C6	C7	-158.29(13)
C8	C13	C12	C11	0.4(2)
C13	C8	C9	N1	177.24(13)
C13	C8	C9	C10	-4.0(2)
C13	C12	C11	C10	-1.7(2)
C12	C11	C10	C9	0.1(2)
C11	C10	C9	N1	-178.45(14)
C11	C10	C9	C8	2.8(2)
C9	N1	C16	C17	-80.58(18)
C9	N1	C3	C2	53.47(18)
C9	N1	C3	C4	-70.34(18)
C9	C8	C13	C12	2.4(2)
C24	C29	C28	C27	-0.9(3)
C22	C17	C16	N1	-29.4(2)
C21	C20	C19	C18	-1.0(3)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for jw51.

Atom	*x*	*y*	*z*	U(eq)
H14A	2570	6190	5446	42
H14B	3330	6593	6237	42
H20	-1450	1030	8066	53
H19	-2172	2843	8500	49
H18	-1936	4909	8058	46
H16A	-1621	5895	6631	47
H16B	-953	6353	7437	47
H3	-907	6075	5713	39
H2	730	5131	5684	39
H15A	2987	4571	6736	52
H15B	2206	4169	5953	52
H28	4629	1972	4373	67
H27	6372	1149	4743	62
H4A	-802	8228	5524	43
H4B	-832	8185	6371	43
H5A	906	8758	6799	42
H5B	516	9629	6067	42
H6	2174	8624	6041	41
H13	3354	7098	7383	44
H12	3558	6853	8644	52
H11	2132	6066	9054	51
H10	508	5618	8219	44
H26	7467	1596	5898	56
H25	6861	2861	6741	51
H22	-320	3342	6704	49
H21	-532	1276	7163	52