



JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

J. Am. Chem. Soc., 1996, 118(24), 5684-5689, DOI:[10.1021/ja960519o](https://doi.org/10.1021/ja960519o)

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1996 American Chemical Society

J5689-1

Table 6. Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

	x	y	z	Biso
Pt1	0.89248 (3)	1/4	0.661690 (13)	1.305 (13)
C1	0.9487 (7)	0.3582 (4)	0.7381 (3)	2.20 (21)
B1	0.9997 (10)	1/4	0.4919 (5)	1.7 (3)
N11	0.8288 (6)	0.3575 (3)	0.57795 (22)	1.64 (15)
N12	0.8948 (5)	0.3439 (3)	0.50807 (22)	1.57 (15)
C13	0.8367 (7)	0.4161 (4)	0.4620 (3)	1.81 (19)
C14	0.7336 (7)	0.4764 (4)	0.5025 (3)	2.15 (19)
C15	0.7297 (6)	0.4378 (3)	0.5740 (3)	1.82 (19)
C16	0.8875 (7)	0.4237 (5)	0.3822 (3)	2.77 (24)
C17	0.6335 (7)	0.4727 (4)	0.6402 (3)	2.56 (22)
N21	1.1395 (7)	1/4	0.6160 (3)	1.64 (24)
N22	1.1535 (7)	1/4	0.5400 (3)	1.47 (23)
C23	1.3155 (9)	1/4	0.5212 (4)	1.7 (3)
C24	1.4062 (9)	1/4	0.5861 (5)	2.3 (4)
C25	1.2930 (9)	1/4	0.6438 (4)	2.3 (3)
C26	1.3755 (9)	1/4	0.4427 (5)	2.3 (3)
C27	1.3297 (12)	1/4	0.7267 (5)	3.7 (4)
H	0.714	1/4	0.683	2.1
H1	1.031	1/4	0.440	2.4
H1a	0.960 (5)	0.3283 (6)	0.7864 (4)	3.0
H1b	0.8621 (24)	0.4070 (16)	0.7394 (16)	3.0
H1c	1.0501 (25)	0.3901 (20)	0.7244 (12)	3.0
H14	0.675	0.534	0.484	2.9
H16a	0.847	0.485	0.362	3.6
H16b	0.843	0.368	0.355	3.6
H16c	1.005	0.422	0.379	3.6
H17a	0.533	0.503	0.624	3.3
H17b	0.697	0.521	0.667	3.3
H17c	0.609	0.417	0.672	3.3
H24	1.524	1/4	0.591	3.1
H26a	1.494	1/4	0.443	3.1
H26b	1.336	0.191	0.417	3.1
H27a	1.229	1/4	0.755	4.5
H27b	1.392	0.191	0.739	4.5

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

J5689-2

Table 7. $u(i,j)$ or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
Pt1	1.824(18)	1.946(17)	1.190(17)	0.0	0.077(12)	0.0
C1	3.4 (3)	3.1 (3)	1.8 (3)	0.21(25)	0.21(24)	-0.01(23)
B1	1.9 (4)	2.4 (4)	2.0 (4)	0.0	0.2 (3)	0.0
N11	2.44(21)	1.76(20)	2.01(22)	-0.11(19)	0.02(18)	-0.66(17)
N12	2.15(21)	2.15(20)	1.66(20)	-0.24(17)	0.10(17)	-0.05(16)
C13	2.5 (3)	1.94(23)	2.4 (3)	-0.46(23)	-0.68(22)	0.40(20)
C14	3.1 (3)	2.00(23)	3.0 (3)	0.19(23)	-0.91(23)	0.24(22)
C15	2.4 (3)	1.78(24)	2.7 (3)	-0.03(20)	-0.67(22)	-0.29(21)
C16	3.6 (3)	4.3 (3)	2.5 (3)	0.0 (3)	-0.84(24)	1.2 (3)
C17	3.4 (3)	3.1 (3)	3.2 (3)	0.98(24)	-0.28(24)	-0.8 (3)
N21	1.8 (3)	2.7 (3)	1.7 (3)	0.0	-0.21(24)	0.0
N22	2.1 (3)	2.1 (3)	1.5 (3)	0.0	0.15(24)	0.0
C23	2.0 (4)	1.9 (3)	2.5 (4)	0.0	0.4 (4)	0.0
C24	1.6 (4)	3.9 (5)	3.2 (5)	0.0	0.0 (3)	0.0
C25	1.7 (4)	5.2 (5)	1.9 (4)	0.0	-0.2 (3)	0.0
C26	2.7 (4)	2.7 (4)	3.1 (5)	0.0	0.6 (3)	0.0
C27	3.3 (5)	8.4 (7)	2.4 (5)	0.0	-0.5 (4)	0.0
H	2.7					
H1	3.1					
H1a	3.8					
H1b	3.8					
H1c	3.8					
H14	3.7					
H16a	4.5					
H16b	4.5					
H16c	4.5					
H17a	4.2					
H17b	4.2					
H17c	4.2					
H24	3.9					
H26a	3.9					
H26b	3.9					
H27a	5.7					
H27b	5.7					

Anisotropic Temperature Factors are of the form

$$\text{Temp} = -2\pi^2 (h^2 u_{11}^* a^* a^* + \dots + 2hk u_{12}^* a^* b^* + \dots)$$

J5689-3

Table 8. Complete list of bond lengths.

Pt(1) - C(1)	2.048(5)	C(13) - C(14)	1.372(8)
Pt(1) - C(1) a	2.048(5)	C(13) - C(16)	1.495(8)
Pt(1) - N(11)	2.145(4)	C(14) - C(15)	1.385(7)
Pt(1) - N(11) a	2.145(4)	C(15) - C(17)	1.497(8)
Pt(1) - N(21)	2.169(6)	N(21) - N(22)	1.371(8)
B(1) - N(12)	1.546(6)	N(21) - C(25)	1.344(9)
B(1) - N(12) a	1.546(6)	N(22) - C(23)	1.359(10)
B(1) - N(22)	1.520(10)	C(23) - C(24)	1.379(11)
N(11) - N(12)	1.377(6)	C(23) - C(26)	1.493(11)
N(11) - C(15)	1.346(6)	C(24) - C(25)	1.387(11)
N(12) - C(13)	1.357(6)	C(25) - C(27)	1.520(12)

Table 9. Complete list of bond angles.

C(1) - Pt(1) - C(1) a	90.07(21)	N(12) - C(13) - C(16)	122.4(5)
C(1) - Pt(1) - N(11)	92.85(18)	C(14) - C(13) - C(16)	129.6(5)
C(1) - Pt(1) - N(11) a	177.05(18)	C(13) - C(14) - C(15)	106.6(4)
C(1) - Pt(1) - N(21)	92.70(19)	N(11) - C(15) - C(14)	109.5(4)
C(1) a - Pt(1) - N(11)	177.05(18)	N(11) - C(15) - C(17)	121.3(5)
C(1) a - Pt(1) - N(11) a	92.85(18)	C(14) - C(15) - C(17)	129.2(5)
C(1) a - Pt(1) - N(21)	92.70(19)	Pt(1) - N(21) - N(22)	117.0(4)
N(11) - Pt(1) - N(11) a	84.24(14)	Pt(1) - N(21) - C(25)	136.0(5)
N(11) - Pt(1) - N(21)	87.60(17)	N(22) - N(21) - C(25)	107.0(6)
N(11) a - Pt(1) - N(21)	87.60(17)	B(1) - N(22) - N(21)	119.9(6)
N(12) - B(1) - N(12) a	108.8(5)	B(1) - N(22) - C(23)	131.0(6)
N(12) - B(1) - N(22)	110.3(4)	N(21) - N(22) - C(23)	109.1(6)
N(12) a - B(1) - N(22)	110.3(4)	N(22) - C(23) - C(24)	108.0(6)
Pt(1) - N(11) - N(12)	117.2(3)	N(22) - C(23) - C(26)	123.4(7)
Pt(1) - N(11) - C(15)	135.9(3)	C(24) - C(23) - C(26)	128.6(7)
N(12) - N(11) - C(15)	106.9(4)	C(23) - C(24) - C(25)	106.0(6)
B(1) - N(12) - N(11)	119.6(4)	N(21) - C(25) - C(24)	109.8(7)
B(1) - N(12) - C(13)	131.0(5)	N(21) - C(25) - C(27)	123.1(7)
N(11) - N(12) - C(13)	109.0(4)	C(24) - C(25) - C(27)	127.0(7)
N(12) - C(13) - C(14)	108.0(4)		