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SUPPLEMENTARY MATERIAL

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BELONGING TO THE PAPER

Homo-Arcyriaflavin: The Synthesis of Ring-expanded Arcyriaflavin Analogs

by

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$C_{26}H_{24}N_4O_2 \cdot CH_3OH$ compound **31**

Experimental

Compound **31**

Crystal data

$C_{27}H_{28}N_4O_3$

M_r = 456.53
Kristallsystem: monoclinic
Raumgruppe: $P2_1/n$
a = 10.8085 (7) Å
b = 20.1630 (10) Å
c = 10.9501 (9) Å
a = 90.000 (5) °
b = 103.027 (8) °
g = 90.000 (5) °
V = 2325.0 (3) $Å^3$
Z = 2
D_x = 1.304 Mg m^{-3}
D_m = yes Mg m^{-3}
yes
Mo K a
l = 0.71069 Å
m = 0.087 mm^{-1}
T = 150 (1) K

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0.320 x 0.080 x 0.040 mm
Farbe: dark red

Data collection

Stoe --IPDS, plate distance 73 mm
140 plates, phi increment 1.0 °
Absorption correction: none
11418 measured reflections
4001 independent reflections
1300 observed reflections
Criterion: >2sigma(I) I > 2 s (I)
Rint = 0.1138
$\langle theta \rangle_{max}$ = 25.04 °
h = -12 -> 12
k = -23 -> 23
l = -13 -> 12
intensity variation: 0 %

Refinement

Refinement on F^2
Final R = 0.0451
wR = 0.0694
S = 0.911
4001 reflections
324 parameters
riding atoms (Abstand für die H-Atome frei)
w = calc w=1/' $\langle sigma \rangle^2$ (Fo^2)+$(0.0132P)^2$+0.0000PÂ where
$P=(Fo^2+2Fc^2)/3$
d / s_{max} = -0.001
Extinction correction: none
Atomic scattering factors from International Tables Vol C Tables 4.2.6.8 and 6.1.1.4

Data collection: Stoe --IPDS software version 2.78 (Stoe , 1997)
Cell refinement: Stoe --IPDS software version 2.78 (Stoe , 1997)
Data reduction: Stoe --IPDS software version 2.78 (Stoe , 1997)
Program used to solve structure: SIR-92 (Altomare, 1990) (direkte Methode)
Program used to refine structure: SHELXL-93 (Sheldrick, 1993)
Molecular graphics: PLATON (Speck 1992)
Software used to prepare material for publication

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---------- Table of coordinates ----------

Table. Fractional atomic coordinates and equivalent isotropic thermal parameters (Å ^{2})

U_{eq} = 1/3<Sum>i<Sum>j Uijai*aj* ai.aj.

	x	y	z	U_{eq}
O001	-0.1931 (2)	0.20141 (13)	1.0186 (2)	0.0355 (7)
O002	-0.4985 (3)	0.04761 (12)	0.8678 (3)	0.0376 (7)
N001	-0.0347 (3)	0.17357 (13)	0.6078 (3)	0.0288 (9)
N002	-0.3112 (3)	0.02061 (15)	0.4760 (3)	0.0279 (8)
N003	-0.3627 (3)	0.12954 (15)	0.9652 (3)	0.0279 (8)
N004	-0.1057 (3)	0.0349 (15)	0.2434 (3)	0.0307 (9)
C001	0.0562 (4)	0.1835 (2)	0.7171 (4)	0.0273 (10)
C002	0.1850 (4)	0.1983 (2)	0.7337 (4)	0.0326 (12)
C003	0.2569 (4)	0.2024 (2)	0.8549 (4)	0.0370 (12)
C004	0.2012 (4)	0.1921 (2)	0.9567 (4)	0.0360 (12)
C005	0.0740 (4)	0.1789 (2)	0.9408 (4)	0.0302 (11)
C006	-0.0021 (4)	0.1749 (2)	0.8185 (4)	0.0254 (10)
C007	-0.1337 (4)	0.1579 (2)	0.7658 (3)	0.0231 (9)
C008	-0.2334 (3)	0.1361 (2)	0.8241 (3)	0.0240 (9)
C009	-0.3226 (4)	0.0886 (2)	0.7810 (3)	0.0243 (10)
C010	-0.3332 (3)	0.0479 (2)	0.6703 (3)	0.0236 (10)
C011	-0.3619 (3)	-0.0221 (2)	0.6507 (4)	0.0262 (10)
C012	-0.3909 (3)	-0.0732 (2)	0.7261 (4)	0.0283 (10)
C013	-0.4078 (4)	-0.1366 (2)	0.6765 (4)	0.0355 (11)
C014	-0.3954 (4)	-0.1499 (2)	0.5549 (4)	0.0369 (12)
C015	-0.3646 (3)	-0.1009 (2)	0.4782 (4)	0.0324 (11)
C016	-0.3477 (3)	-0.0370 (2)	0.5297 (4)	0.0269 (10)
C017	-0.3029 (3)	0.0712 (2)	0.5622 (4)	0.0252 (10)
C018	-0.2660 (3)	0.1419 (2)	0.5407 (3)	0.0278 (10)
C019	-0.1483 (4)	0.1576 (2)	0.6372 (4)	0.0251 (10)
C020	-0.2839 (3)	0.0255 (2)	0.3519 (4)	0.0300 (11)
C021	-0.1450 (4)	0.0104 (2)	0.3554 (4)	0.0328 (11)
C022	-0.1784 (4)	0.0025 (2)	0.1295 (4)	0.0423 (13)
C023	0.0313 (4)	0.0197 (2)	0.2576 (4)	0.0449 (13)
C024	-0.2545 (4)	0.1617 (2)	0.9468 (4)	0.0261 (10)
C025	-0.4074 (4)	0.0831 (2)	0.8713 (4)	0.0267 (10)
C026	-0.4173 (4)	0.1409 (2)	0.0735 (4)	0.0408 (12)
C027	0.0431 (4)	0.2015 (2)	0.2891 (4)	0.0493 (14)
O003	-0.0423 (3)	0.1647 (13)	0.3463 (3)	0.0430 (9)

---------- Table of bonds ----------

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O001 --- C024	1.211 (4)	C011 --- C012	1.401 (5)
O002 --- C025	1.211 (4)	C011 --- C016	1.401 (5)
N001 --- C019	1.376 (4)	C012 --- C013	1.385 (5)
N001 --- C001	1.381 (4)	C012 --- H012	1.000 (4)
N001 --- H001	0.820 (4)	C013 --- C014	1.394 (5)
N002 --- C017	1.379 (5)	C013 --- H013	0.970 (4)
N002 --- C016	1.398 (5)	C014 --- C015	1.385 (5)
N002 --- C020	1.457 (5)	C014 --- H014	0.890 (4)
N003 --- C024	1.391 (4)	C015 --- C016	1.401 (5)
N003 --- C025	1.394 (4)	C015 --- H015	1.000 (4)
N003 --- C026	1.456 (5)	C017 --- C018	1.512 (5)
N004 --- C022	1.468 (4)	C018 --- C019	1.493 (4)
N004 --- C021	1.470 (5)	C018 --- H01A	1.030 (2)
N004 --- C023	1.485 (4)	C018 --- H01B	1.030 (2)
C001 --- C002	1.396 (5)	C020 --- C021	1.524 (5)
C001 --- C006	1.406 (5)	C020 --- H02A	0.990 (2)
C002 --- C003	1.381 (5)	C020 --- H02B	0.990 (2)
C002 --- H002	0.860 (4)	C021 --- H02C	0.960 (2)
C003 --- C004	1.397 (5)	C021 --- H02D	0.960 (2)
C003 --- H003	0.970 (4)	C022 --- H02E	0.970 (2)
C004 --- C005	1.373 (5)	C022 --- H02F	0.970 (2)
C004 --- H004	0.950 (4)	C022 --- H02G	0.970 (2)
C005 --- C006	1.406 (5)	C023 --- H02H	0.990 (2)
C005 --- H005	0.900 (4)	C023 --- H02I	0.990 (2)
C006 --- C007	1.450 (5)	C023 --- H02J	0.990 (2)
C007 --- C019	1.382 (5)	C026 --- H02K	0.870 (2)
C007 --- C008	1.439 (5)	C026 --- H02L	0.870 (2)
C008 --- C009	1.365 (5)	C026 --- H02M	0.870 (2)
C008 --- C024	1.504 (5)	C027 --- O003	1.434 (5)
C009 --- C010	1.447 (5)	C027 --- H02N	1.010 (2)
C009 --- C025	1.496 (5)	C027 --- H02O	1.010 (2)
C010 --- C017	1.379 (5)	C027 --- H02P	1.010 (2)
C010 --- C011	1.450 (5)	O003 --- H00A	0.820 (4)

---------- Table of angles ----------

C019 --- N001 --- C001	109.2 (3)
C019 --- N001 --- H001	125.4 (2)
C001 --- N001 --- H001	125.4 (2)
C017 --- N002 --- C016	107.9 (3)
C017 --- N002 --- C020	126.3 (3)
C016 --- N002 --- C020	125.7 (3)
C024 --- N003 --- C025	111.6 (3)
C024 --- N003 --- C026	123.6 (3)
C025 --- N003 --- C026	124.7 (3)
C022 --- N004 --- C021	111.1 (3)
C022 --- N004 --- C023	109.1 (3)
C021 --- N004 --- C023	108.2 (3)
N001 --- C001 --- C002	129.6 (4)
N001 --- C001 --- C006	108.0 (3)
C002 --- C001 --- C006	122.4 (4)
C003 --- C002 --- C001	117.8 (4)
C003 --- C002 --- H002	121.1 (3)
C001 --- C002 --- H002	121.1 (3)
C002 --- C003 --- C004	120.5 (4)
C002 --- C003 --- H003	119.7 (3)
C004 --- C003 --- H003	119.7 (2)
C005 --- C004 --- C003	121.8 (4)
C005 --- C004 --- H004	119.1 (3)
C003 --- C004 --- H004	119.1 (2)
C004 --- C005 --- C006	119.1 (4)
C004 --- C005 --- H005	120.4 (3)
C006 --- C005 --- H005	120.4 (2)
C001 --- C006 --- C005	118.3 (4)
C001 --- C006 --- C007	106.8 (3)
C005 --- C006 --- C007	134.7 (4)
C019 --- C007 --- C008	121.8 (3)
C019 --- C007 --- C006	106.4 (4)
C008 --- C007 --- C006	131.3 (3)
C009 --- C008 --- C007	127.0 (4)
C009 --- C008 --- C024	108.2 (3)
C007 --- C008 --- C024	124.8 (3)
C008 --- C009 --- C010	127.1 (4)
C008 --- C009 --- C025	108.3 (3)
C010 --- C009 --- C025	124.5 (3)
C017 --- C010 --- C009	122.4 (3)
C017 --- C010 --- C011	106.8 (3)
C009 --- C010 --- C011	130.5 (4)
C012 --- C011 --- C016	119.1 (3)
C012 --- C011 --- C010	134.3 (4)
C016 --- C011 --- C010	106.5 (3)
C013 --- C012 --- C011	118.4 (4)
C013 --- C012 --- H012	120.8 (3)
C011 --- C012 --- H012	120.8 (2)
C012 --- C013 --- C014	121.3 (4)

C012 --- C013 --- H013	119.3 (3)
C014 --- C013 --- H013	119.3 (3)
C015 --- C014 --- C013	122.0 (4)
C015 --- C014 --- H014	119.0 (2)
C013 --- C014 --- H014	119.0 (3)
C014 --- C015 --- C016	116.1 (4)
C014 --- C015 --- H015	122.0 (2)
C016 --- C015 --- H015	122.0 (3)
C015 --- C016 --- N002	128.2 (4)
C015 --- C016 --- C011	123.1 (4)
N002 --- C016 --- C011	108.7 (3)
N002 --- C017 --- C010	110.1 (3)
N002 --- C017 --- C018	124.7 (4)
C010 --- C017 --- C018	125.2 (3)
C019 --- C018 --- C017	107.6 (3)
C019 --- C018 --- H01A	110.2 (2)
C017 --- C018 --- H01A	110.2 (2)
C019 --- C018 --- H01B	110.2 (2)
C017 --- C018 --- H01B	110.2 (2)
H01A --- C018 --- H01B	108.5
N001 --- C019 --- C007	109.6 (3)
N001 --- C019 --- C018	123.2 (3)
C007 --- C019 --- C018	127.3 (4)
N002 --- C020 --- C021	111.6 (3)
N002 --- C020 --- H02A	109.3 (2)
C021 --- C020 --- H02A	109.3 (2)
N002 --- C020 --- H02B	109.3 (2)
C021 --- C020 --- H02B	109.3 (2)
H02A --- C020 --- H02B	108.0
N004 --- C021 --- C020	112.3 (3)
N004 --- C021 --- H02C	109.1 (2)
C020 --- C021 --- H02C	109.1 (2)
N004 --- C021 --- H02D	109.1 (2)
C020 --- C021 --- H02D	109.1 (2)
H02C --- C021 --- H02D	107.9
N004 --- C022 --- H02E	109.5 (2)
N004 --- C022 --- H02F	109.5 (2)
H02E --- C022 --- H02F	109.5
N004 --- C022 --- H02G	109.5 (2)
H02E --- C022 --- H02G	109.5
H02F --- C022 --- H02G	109.5
N004 --- C023 --- H02H	109.5 (2)
N004 --- C023 --- H02I	109.5 (2)
H02H --- C023 --- H02I	109.5
N004 --- C023 --- H02J	109.5 (2)
H02H --- C023 --- H02J	109.5
H02I --- C023 --- H02J	109.5
O001 --- C024 --- N003	124.7 (4)
O001 --- C024 --- C008	129.5 (4)
N003 --- C024 --- C008	105.8 (3)

O002 --- C025 --- N003	124.4 (4)
O002 --- C025 --- C009	129.6 (4)
N003 --- C025 --- C009	106.0 (3)
N003 --- C026 --- H02K	109.5 (2)
N003 --- C026 --- H02L	109.5 (2)
H02K --- C026 --- H02L	109.5
N003 --- C026 --- H02M	109.5 (2)
H02K --- C026 --- H02M	109.5
H02L --- C026 --- H02M	109.5
O003 --- C027 --- H02N	109.5 (2)
O003 --- C027 --- H02O	109.5 (2)
H02N --- C027 --- H02O	109.5
O003 --- C027 --- H02P	109.5 (2)
H02N --- C027 --- H02P	109.5
H02O --- C027 --- H02P	109.5
C027 --- O003 --- H00A	109.5 (2)

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, and complete geometry
have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 00000 (00 pp.).
Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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