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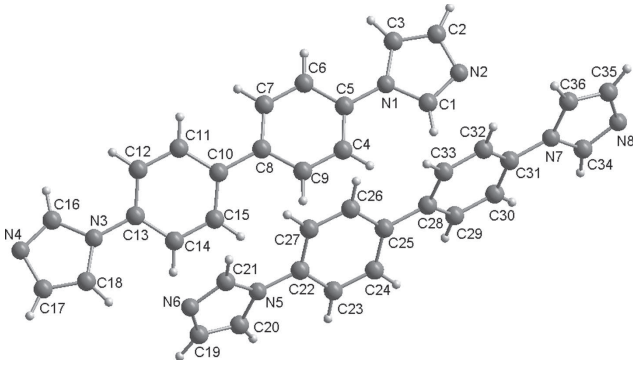
Crystal structure of 4,4′-di(1*H*-imidazol-1-yl)-1,1′-biphenyl, $C_{36}H_{28}N_8$



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Abstract

$C_{36}H_{28}N_8$, triclinic, $P\bar{1}$, $a = 10.5381(10)$ Å, $b = 11.2172(11)$ Å, $c = 14.0925(13)$ Å, $\alpha = 73.912(3)°$, $\beta = 68.626(3)°$, $\gamma = 62.739(3)°$, $V = 1366.7(2)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0593$, $wR_{ref}(F^2) = 0.1429$, $T = 293(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $Co(NO_3)_2{\cdot}6H_2O$ (0.1 mmol, 29 mg), 4,4′-di(1H-imidazol-1-yl)-1,1′-biphenyl (0.1 mmol, 52 mg), 4,4′-bipyridine (0.1 mmol, 31.2 mg), KOH (0.1 mmol, 5.6 mg) and H_2O (8 mL) were placed in a Teflon-lined stainless steel vessel, heated to 413 K for four days, and then cooled to room temperature over 24 h. Colourless block-shaped crystals of the educt 4,4′-di(1*H*-imidazol-1-yl)-1,1′-biphenyl were obtained.

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Table 1: Data collection and handling.

Crystal:	Colorless blocks size 0.45 × 0.38 × 0.28 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.9 cm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω
$2\theta_{max}$, completeness:	51°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	18335, 5071, 0.034
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3252
$N(param)_{refined}$:	400
Programs:	Bruker programs [1], SHELX [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
N1	0.3476(2)	0.4127(2)	−0.10100(15)	0.0376(5)
N2[a]	0.4138(3)	0.2653(3)	−0.2042(2)	0.0539(7)
C2A[a]	0.4138(3)	0.2653(3)	−0.2042(2)	0.0539(7)
H2A[a]	0.4169	0.1979	−0.2324	0.065*
N3	−0.2245(2)	0.9672(2)	0.47656(15)	0.0382(5)
N4[a]	−0.2976(3)	1.1224(3)	0.5748(2)	0.0545(7)
C17A[a]	−0.2976(3)	1.1224(3)	0.5748(2)	0.0545(7)
H17A[a]	−0.3033	1.1929	0.6009	0.065*
N5	−0.2273(2)	0.4766(2)	0.47222(15)	0.0386(5)
N6[a]	−0.2844(3)	0.5713(3)	0.60843(19)	0.0545(7)
C19A[b]	−0.2844(3)	0.5713(3)	0.60843(19)	0.0545(7)
H19A[b]	−0.2821	0.5899	0.6629	0.065*
N7	0.3497(2)	−0.0913(2)	−0.09719(15)	0.0370(5)
N8[a]	0.4035(3)	−0.1810(3)	−0.23536(19)	0.0536(7)
C35A[a]	0.4035(3)	−0.1810(3)	−0.23536(19)	0.0536(7)
H35A[a]	0.3953	−0.2002	−0.2925	0.064*
C1	0.3190(3)	0.3153(3)	−0.1196(2)	0.0498(7)
H1	0.2427	0.2882	−0.0779	0.060*
C2[a]	0.5085(3)	0.3326(3)	−0.2437(2)	0.0560(7)
H2[a]	0.5869	0.3185	−0.3036	0.067*
N2A[a]	0.5085(3)	0.3326(3)	−0.2437(2)	0.0560(7)
C3	0.4673(3)	0.4207(3)	−0.1806(2)	0.0469(7)
H3	0.5126	0.4788	−0.1892	0.056*
C4	0.1476(3)	0.4700(3)	0.0571(2)	0.0439(7)
H4	0.1181	0.4061	0.0519	0.053*
C5	0.2680(3)	0.4892(2)	−0.01641(18)	0.0337(6)
C6	0.3097(3)	0.5837(3)	−0.00651(19)	0.0394(6)
H6	0.3913	0.5975	−0.0550	0.047*
C7	0.2315(3)	0.6580(3)	0.07477(19)	0.0383(6)
H7	0.2615	0.7216	0.0796	0.046*
C8	0.1095(3)	0.6411(2)	0.14962(18)	0.0326(6)

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Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
C9	0.0703(3)	0.5443(3)	0.1383(2)	0.0428(7)
H9	−0.0104	0.5293	0.1870	0.051*
C10	0.0230(3)	0.7244(2)	0.23539(18)	0.0336(6)
C11	0.0822(3)	0.7926(3)	0.2638(2)	0.0452(7)
H11	0.1788	0.7849	0.2287	0.054*
C12	0.0024(3)	0.8715(3)	0.3425(2)	0.0471(7)
H12	0.0457	0.9153	0.3599	0.057*
C13	−0.1413(3)	0.8855(2)	0.39547(18)	0.0342(6)
C14	−0.2026(3)	0.8188(3)	0.36907(19)	0.0429(6)
H14	−0.2995	0.8272	0.4042	0.051*
C15	−0.1214(3)	0.7393(3)	0.29078(19)	0.0420(6)
H15	−0.1647	0.6943	0.2746	0.050*
C16	−0.1988(3)	1.0677(3)	0.4925(2)	0.0503(7)
H16	−0.1219	1.0940	0.4510	0.060*
C17[a]	−0.3921(3)	1.0541(3)	0.6151(2)	0.0558(7)
H17[a]	−0.4725	1.0705	0.6737	0.067*
N4A[a]	−0.3921(3)	1.0541(3)	0.6151(2)	0.0558(7)
C18	−0.3465(3)	0.9613(3)	0.5548(2)	0.0456(7)
H18	−0.3904	0.9019	0.5642	0.055*
C19[a]	−0.408(5)	0.635(5)	0.575(4)	0.054(3)
H19[a]	−0.4980	0.7018	0.6045	0.065*
N6A[a]	−0.402(4)	0.634(4)	0.559(3)	0.054(3)
C20	−0.3686(3)	0.5767(3)	0.4838(2)	0.0476(7)
H20	−0.4281	0.6022	0.4405	0.057*
C21	−0.1822(3)	0.4789(3)	0.5506(2)	0.0510(7)
H21	−0.0899	0.4217	0.5616	0.061*
C22	−0.1459(3)	0.3912(2)	0.39377(18)	0.0347(6)
C23	−0.2170(3)	0.3755(3)	0.3362(2)	0.0430(7)
H23	−0.3197	0.4201	0.3496	0.052*
C24	−0.1377(3)	0.2946(3)	0.25887(19)	0.0422(6)
H24	−0.1880	0.2870	0.2201	0.051*
C25	0.0160(3)	0.2238(2)	0.23724(18)	0.0340(6)
C26	0.0846(3)	0.2390(3)	0.29771(19)	0.0400(6)
H26	0.1869	0.1923	0.2861	0.048*
C27	0.0067(3)	0.3206(3)	0.37431(19)	0.0412(6)
H27	0.0566	0.3284	0.4132	0.049*
C28	0.1019(3)	0.1408(2)	0.15159(18)	0.0328(6)
C29	0.0464(3)	0.1597(3)	0.07090(19)	0.0402(6)
H29	−0.0483	0.2257	0.0714	0.048*
C30	0.1254(3)	0.0848(3)	−0.01010(19)	0.0409(6)
H30	0.0835	0.1005	−0.0624	0.049*
C31	0.2669(3)	−0.0134(2)	−0.01367(18)	0.0334(6)
C32	0.3247(3)	−0.0345(3)	0.06552(19)	0.0420(6)
H32	0.4197	−0.1002	0.0644	0.050*
C33	0.2441(3)	0.0403(3)	0.14659(19)	0.0404(6)

Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
H33	0.2858	0.0231	0.1994	0.048*
C34	0.3004(3)	−0.0949(3)	−0.1731(2)	0.0508(7)
H34	0.2048	−0.0423	−0.1796	0.061*
C35[a]	0.5289(3)	−0.2389(3)	−0.1992(2)	0.0580(7)
H35[a]	0.6203	−0.3044	−0.2281	0.070*
N8A[a]	0.5289(3)	−0.2389(3)	−0.1992(2)	0.0580(7)
C36	0.4946(3)	−0.1838(3)	−0.1157(2)	0.0451(7)
H36	0.5584	−0.2046	−0.0766	0.054*

[a]Occupancy: 0.5; [b]Occupancy: 0.4.

Experimental details

The hydrogen atoms were assigned with isotropic displacement factors $U_{iso}(H) = 1.2U_{eq}$ (N and imidazol C), or $U_{iso}(H) = 1.5U_{eq}$ (methyl C) and included in the final refinement by using geometrical restraints, with C–H = 0.93 Å (imidazol) or C–H = 0.96 Å (methyl), and N–H = 0.86 Å.

Discussion

4,4′-Bipyridine and its derivatives are important building modules of N-containing heterocyclic ring compounds which, provide supramolecular recognition sites for N—H···O, C—H···O, C—H···π and π–π interactions to construct supramolecular architectures.

The asymmetric unit of the title structure contains two 4,4′-di(1*H*-imidazol-1-yl)-1,1′-biphenyl molecules. In the imidazol ring the C21—N6 bond lengths is 1.318(3) Å, and the C34—N8 bond lengths is 1.318(3) Å, which are shorter than the single bond value. The dihedral angles between four rings in each of the two crystallographically molecules are small. Consequently, they are both approximately flat. On the other hand, the two crystallographically independent molecules are packed with an angle of roughly 60° to each other.

References

1. Bruker. APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA, 2009.
2. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112–122.