Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	Retracted by	DOI	Refcode
trans-Bis{1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato}copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato-κ^2O,O')copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehydo)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato-κ^2O,O')zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato-κ^2O,O')nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
Bis(2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
Bis(2-formylphenolato-κ^2O,O')manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline-κ^2N,N')copper(II) naphthalene-1,5-disulfonate dihydrate	Liu *et al.* (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline-κ^2N,N')nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui *et al.* (2006)	Journal	10.1107/S160053680604565X	HESPEB
Bis(2-formylphenolato-κ^2O,O')iron(II)	Yang *et al.* (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer *et al.* (2007*a*)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer *et al.* (2007*b*)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu *et al.* (2007)	Author	10.1107/S1600536807031121	WIHKEE
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen *et al.* (2007)	Author	10.1107/S1600536807032540	WIHRIP
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li *et al.* (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(methanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O'-cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratolutetium(III)zinc(II)	Sui, Sui *et al.* (2007)	Author	10.1107/S1600536807037737	AFEFOH
catena-Poly[[chloridonickel(II)]-di-μ-chlorido-[chloridonickel(II)]-μ-4,4′-methylenebis(3,5-dimethylpyrazole)-κ^2N^2:$N^{2'}$]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}zinc(II)	Liu *et al.* (2007*a*)	Author	10.1107/S1600536807040640	DIKYUS
trans-Bis(ethylenediamine-κ^2N,N')bis(nitrato-κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[N,N′-(o-Phenylene)bis(picolinamido)-κ^4N,N',N'',N''']cobalt(II)	Liu & Zeng (2007*a*)	Author	10.1107/S1600536807044571	XILFII
[N,N′-(o-Phenylene)dipicolinamide-κ^4N]nickel(II)	Liu & Zeng (2007*b*)	Author	10.1107/S1600536807048386	WINWEW
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)	Liu *et al.* (2007*b*)	Author	10.1107/S1600536807052993	VIQPIV
N-(2-Amino-3-pyridyl)urea monohydrate	Li *et al.* (2007)	Author	10.1107/S1600536807047526	SIMFEA
N-(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime-κ^2N,N')(3,5-dinitro-2-oxidobenzoato-κ^2O^1,O^2)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ-Acetato-tri-μ-ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)]	Liu, Lin *et al.* (2007)	Journal	10.1107/S1600536807059041	HIQQEE

 doi:10.1107/S1600536809054300

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoeuropium(III)zinc(II)	Hu *et al.* (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li *et al.* (2008)	Author	10.1107/S1600536807056309	RISTET
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoterbium(III)zinc(II)	Chen *et al.* (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato-κ^2O^1,O^6)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoholmium(III)zinc(II)	Xiao, Sui *et al.* (2008)	Author	10.1107/S1600536808013743	BIZTUA
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu *et al.* (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid–4,4′-bipyridine (2/1)	Wang *et al.* (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(ethanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O′-samarium(III)zinc(II)	Huang *et al.* (2009)	Journal	10.1107/S1600536809033558	YUCWAV

References

Chen, Q. (2006). *Acta Cryst.* E**62**, m56–m57.
Chen, J.-R., Sui, Y., Luo, Q.-Y. & Jiang, R.-Q. (2007). *Acta Cryst.* E**63**, m2091–m2092.
Chen, J.-R., Sui, Y., Chen, L., Wen, J.-W. & Yin, L.-Y. (2008). *Acta Cryst.* E**64**, m562–m563.
Han, Z.-Q. (2008). *Acta Cryst.* E**64**, m592.
Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* E**66**, e1–e2.
Hu, R.-H., Sui, Y., Chen, L. & He, C.-M. (2008). *Acta Cryst.* E**64**, m8–m9.
Hu, R.-H., Sui, Y., Fang, X.-N. & Chen, H.-M. (2007). *Acta Cryst.* E**63**, m2039–m2040.
Huang, C.-F. & Chen, H.-L. (2007). *Acta Cryst.* E**63**, m2356–m2357.
Huang, Q., Sui, Y.-H. & Zhang, G.-X. (2009). *Acta Cryst.* E**65**, m1161–m1162.
Li, Y.-G. & Chen, H.-J. (2006). *Acta Cryst.* E**62**, m1038–m1039.
Li, N.-G., Tao, R.-M. & Fu, B.-F. (2007). *Acta Cryst.* E**63**, o4228.
Li, Z., Zhang, X. & Pu, X. (2008). *Acta Cryst.* E**64**, m215.
Liu, J.-T. & Fan, S.-D. (2006). *Acta Cryst.* E**62**, m2507–m2508.
Liu, J.-T., Fan, S.-D. & Li, D.-Q. (2006). *Acta Cryst.* E**62**, m2165–m2166.
Liu, D., Lin, J., Xu, Y., Huang, C. & Li, X. (2007). *Acta Cryst.* E**63**, m3094.
Liu, Y.-Q. & Wen, H.-R. (2007). *Acta Cryst.* E**63**, m2928.
Liu, Y.-Q. & Zeng, X.-R. (2007*a*). *Acta Cryst.* E**63**, m2547.
Liu, Y.-Q. & Zeng, X.-R. (2007*b*). *Acta Cryst.* E**63**, m2684.
Liu, Y.-Q., Zeng, X.-R. & Chen, W.-T. (2007). *Acta Cryst.* E**63**, m2462.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007*a*). *Acta Cryst.* E**63**, m2396.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007*b*). *Acta Cryst.* E**63**, m2854.
Qadeer, G., Rama, N. H. & Chen, W.-T. (2007*a*). *Acta Cryst.* E**63**, o2892.
Qadeer, G., Rama, N. H. & Chen, W.-T. (2007*b*). *Acta Cryst.* E**63**, o2932.
Qiu, X.-Y. (2006). *Acta Cryst.* E**62**, m1190–m1191.
Sui, Y., Fang, X.-N., Hu, P. & Lin, J. (2007). *Acta Cryst.* E**63**, m2135–m2136.
Sui, Y., Fang, X.-N. & Yuan, M.-W. (2007). *Acta Cryst.* E**63**, m2275–m2276.
Sui, Y., Li, X.-F., Huang, G.-S. & Wang, G.-J. (2007). *Acta Cryst.* E**63**, m2093–m2094.
Sui, Y., Sui, Y.-H., Luo, Q.-Y. & Wang, Y.-D. (2007). *Acta Cryst.* E**63**, m2277–m2278.
Sui, Y., Xiao, Y.-A., Fang, X.-N., Zeng, X.-R. & Li, M.-H. (2006). *Acta Cryst.* E**62**, m3205–m3207.
Sui, Y., Zhang, J.-H., Hu, R.-H. & Jiang, R.-Q. (2007). *Acta Cryst.* E**63**, m2256–m2257.
Sui, Y., Zhang, J.-H., Hu, R.-H. & Yin, L.-Y. (2007). *Acta Cryst.* E**63**, m2089–m2090.
Sun, Y.-X. & Gao, G.-Z. (2005). *Acta Cryst.* E**61**, m354–m355.
Wang, Q. & Fang, X.-N. (2006). *Acta Cryst.* E**62**, m1492–m1493.
Wang, S., Yang, T., Li, Z. & Yu, X. (2009). *Acta Cryst.* E**65**, o2198.
Xiao, Y.-A., Fu, X.-K., Sui, Y., Wu, Q. & Xiong, S.-H. (2008). *Acta Cryst.* E**64**, m806–m807.
Xiao, Y.-A., Sui, Y., Yi, X.-G., Wu, J.-H. & Zhang, L.-P. (2008). *Acta Cryst.* E**64**, m804–m805.
Xiong, Z.-Y. & Liu, L.-J. (2005). *Acta Cryst.* E**61**, m863–m864.
Yang, X.-M. (2007). *Acta Cryst.* E**63**, o4453.
Yang, Y.-M., Lu, P.-C., Zhu, T.-T. & Liu, C.-H. (2007). *Acta Cryst.* E**63**, m1613.
Zhang, P. (2004). *Acta Cryst.* E**60**, m1808–m1810.

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Terephthalic acid–4,4′-bipyridine (2/1)

Suwen Wang,[a] Tianyu Yang,[b] Zhongfang Li[a]* and Xianjin Yu[a]

[a]College of Chemical Engineering, Shandong University of Technology, Zibo 255049, People's Republic of China, and [b]The College of Life Sciences, Northwest University, Xi-An 710069, People's Republic of China
Correspondence e-mail: zhfli_sdut@yahoo.cn

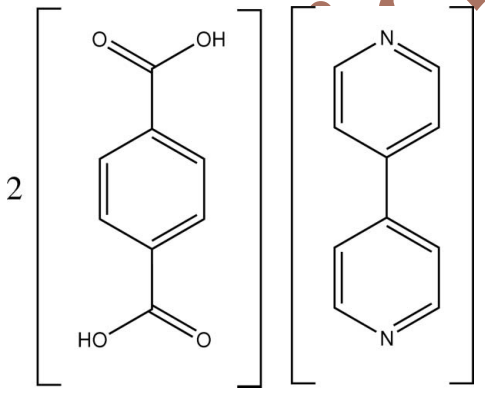
Received 4 August 2009; accepted 15 August 2009

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.054; wR factor = 0.178; data-to-parameter ratio = 11.4.

In the title compound, $2C_8H_6O_4\cdot C_{10}H_8N_2$, the 4,4′-bipyridine molecule is located on an inversion centre. In the crystal structure, strong intermolecular O—H···N hydrogen bonds between the terephthalic acid and 4,4′-bipyridine molecules lead to the formation of chains with graph-set motif $C_2^2(8)$ along the diagonal of the bc plane.

Related literature

For the potential applications of metal-organic frameworks, see: Zhang *et al.* (2007); Zhang *et al.* (2009). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$2C_8H_6O_4\cdot C_{10}H_8N_2$ M_r = 488.44
Monoclinic, $P2_1/n$
a = 7.788 (10) Å
b = 6.814 (8) Å
c = 20.77 (3) Å
β = 92.25 (2)°
V = 1102 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 K
0.27 × 0.19 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.971, T_{max} = 0.980
5164 measured reflections
1930 independent reflections
1192 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.178
S = 1.00
1930 reflections
169 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H2···N1	0.82 (2)	1.78 (2)	2.598 (4)	177.8 (14)

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank the NSFC (grant No. 20776081) and the Natural Science Foundation of Shandong Province (grant No. Y2006B37).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2232).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2001). *SAINT-Plus* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, X. T., Dou, J. M., Wang, D. Q., Zhou, Y., Zhang, Y. X., Li, R. J., Yan, S. S., Ni, Z. H. & Jiang, J. Z. (2007). *Cryst. Growth Des.* **7**, 1699–1705.
Zhang, X. T., Dou, J. M., Wei, P. H., Li, D. C., Li, B., Shi, C. W. & Hu, B. (2009). *Inorg. Chim. Acta*, **362**, 3325–3332.

supporting information

Acta Cryst. (2009). E**65**, o2198 [doi:10.1107/S160053680903236X]

Terephthalic acid–4,4′-bipyridine (2/1)

Suwen Wang, Tianyu Yang, Zhongfang Li and Xianjin Yu

S1. Comment

Design and construction of metal-organic frameworks (MOFs) have attracted considerable attention in recent years, not only for their intriguing structural motifs but also for their potential applications in the areas of catalysis, separation, gas adsorption, molecular recognition, nonlinear optics, and magnetochemistry (Zhang *et al.* (2007); Zhang *et al.* (2009)). The title compound was not the intended product of a reaction to make a MOFs. We report here the crystal and molecular structure of (I). The asymmetric unit of the title compound contains one terephthalic acid molecule and half 4,4′-bipyridine molecule, Fig. 1. The crystal structure is stabilized by strong intermolecular O—H··· N hydrogen bonds between terephthalic acid and 4,4′-bipyridine molecules, this interaction lead to the formation chains $C_2^2(8)$ (Bernstein, *et al.*, 1995) along the diagonal of the bc-plane , Fig 2, Table 1.

S2. Experimental

A mixture of terephthalic acid (1 mmoL), 4,4′-bipyridine (1 mmoL, 0.156 g), and iron trichloride (1 mmoL, 0.162 g) in 10 ml distilled water sealed in a 25 ml Teflon-lined stainless steel autoclave was kept at 433 K for three days. Colorless crystals suitable for the X-ray experiment were obtained. Anal. Calc. for $C_{26}H_{20}N_2O_8$: C 63.88, H 4.09, N 5.73%; Found: C 63.70, H 3.98, N 5.62%.

S3. Refinement

The H2 atom was refined isotropically. All other H atoms were placed in calculated positions with C—H = 0.93 and O1—H1 = 0.80 Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.5(O).

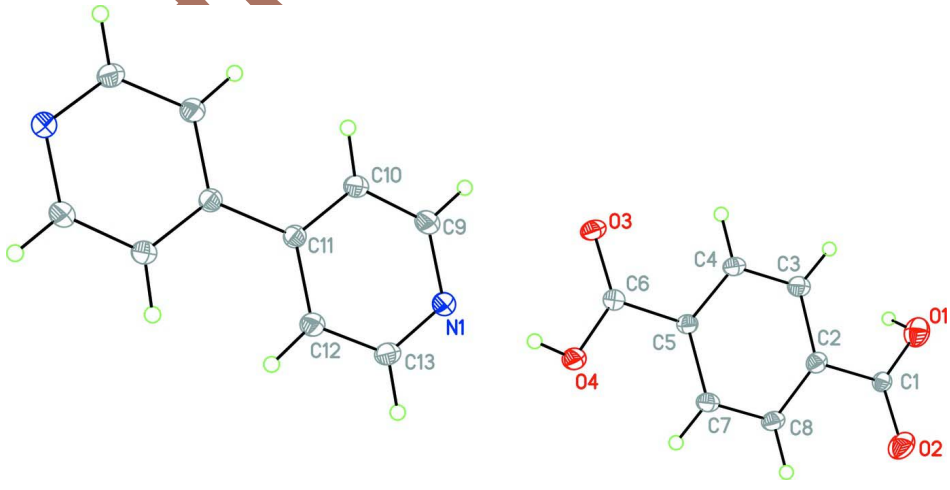


Figure 1

A view of the structure of (I), showing the atomic numbering scheme and 30% probability displacement ellipsoids.

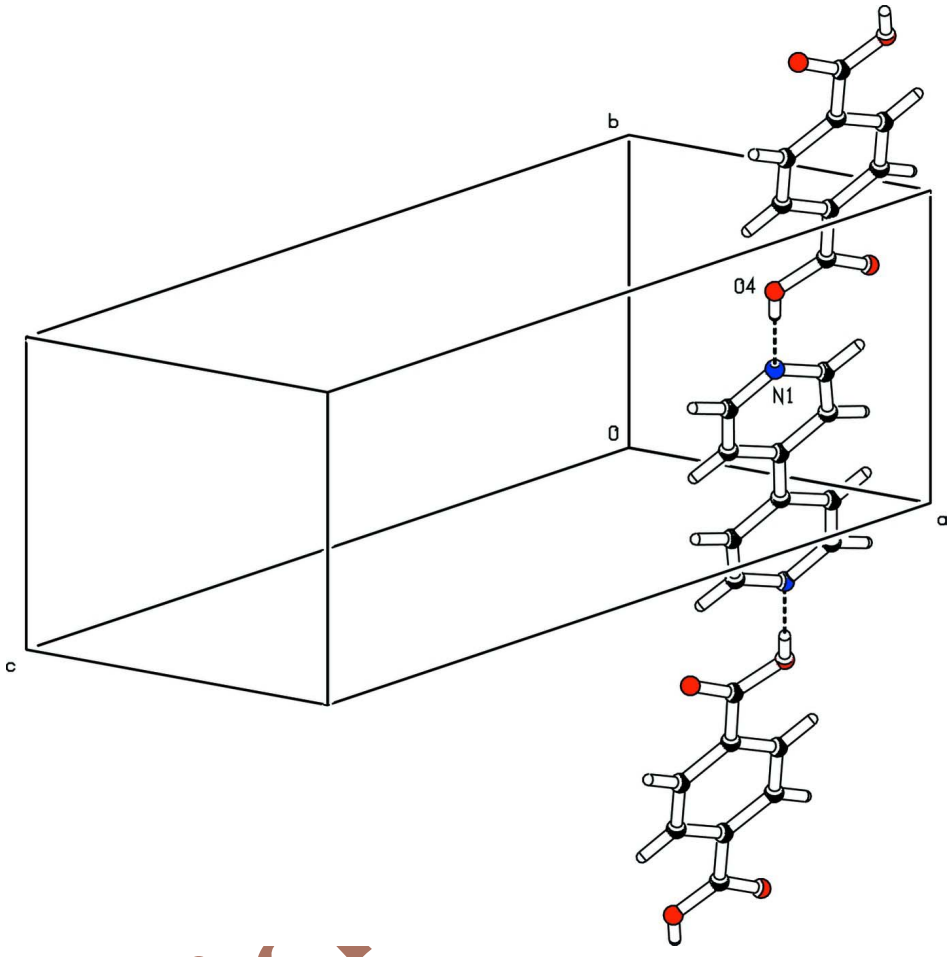


Figure 2

Packing diagram of (I). Dotted lines show hydrogen bonding.

terephthalic acid–4,4′-bipyridine (2/1)

Crystal data

$2C_8H_6O_4{\cdot}C_{10}H_8N_2$
$M_r = 488.44$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.788\ (10)$ Å
$b = 6.814\ (8)$ Å
$c = 20.77\ (3)$ Å
$\beta = 92.25\ (2)°$
$V = 1102\ (2)$ Å^3
$Z = 2$

$F(000) = 508$
$D_x = 1.473$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1066 reflections
$\theta = 2.8–23.0°$
$\mu = 0.11$ mm^{-1}
$T = 296$ K
Block, colorless
0.27 × 0.19 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.971, T_{max} = 0.980
5164 measured reflections
1930 independent reflections
1192 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −9→9
k = −8→6
l = −24→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.178
S = 1.00
1930 reflections
169 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.098P)^2 + 0.1551P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	1.1228 (3)	1.5441 (4)	0.21096 (13)	0.0521 (7)
C2	1.0571 (3)	1.3616 (4)	0.18496 (13)	0.0568 (7)
C3	1.0878 (4)	1.3136 (4)	0.12209 (14)	0.0652 (8)
H3	1.1497	1.3981	0.0966	0.078*
C4	1.0260 (3)	1.1400 (4)	0.09756 (13)	0.0615 (7)
H4	1.0458	1.1057	0.0552	0.074*
C5	0.9345 (3)	1.0161 (4)	0.13570 (12)	0.0531 (7)
C6	0.8676 (3)	0.8295 (4)	0.10696 (13)	0.0594 (7)
C7	0.9048 (3)	1.0691 (4)	0.19886 (13)	0.0616 (8)
H7	0.8420	0.9859	0.2245	0.074*
C8	0.9666 (3)	1.2420 (4)	0.22379 (13)	0.0615 (7)
H8	0.9475	1.2771	0.2662	0.074*
C9	0.6969 (4)	0.3813 (4)	0.02420 (16)	0.0782 (9)
H9	0.7712	0.4676	0.0046	0.094*
C10	0.6398 (4)	0.2208 (4)	−0.00991 (15)	0.0758 (9)

H10	0.6744	0.2015	−0.0518	0.091*
C11	0.5323 (3)	0.0887 (3)	0.01718 (13)	0.0519 (7)
C12	0.4889 (3)	0.1285 (4)	0.07984 (14)	0.0655 (8)
H12	0.4178	0.0426	0.1012	0.079*
C13	0.5501 (4)	0.2936 (4)	0.11059 (14)	0.0688 (8)
H13	0.5178	0.3167	0.1525	0.083*
N1	0.6518 (3)	0.4205 (3)	0.08396 (11)	0.0632 (7)
O1	1.2080 (3)	1.6465 (4)	0.17755 (14)	0.0971 (8)
O2	1.0894 (3)	1.5957 (3)	0.26370 (13)	0.1001 (8)
O3	0.9023 (3)	0.7783 (3)	0.05288 (10)	0.0876 (7)
O4	0.7709 (3)	0.7296 (3)	0.14372 (10)	0.0740 (6)
H1	1.2411	1.7424	0.1966	0.146*
H2	0.732 (3)	0.634 (3)	0.1242 (13)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0583 (16)	0.0482 (15)	0.0498 (16)	−0.0067 (12)	0.0016 (13)	−0.0059 (13)
C2	0.0580 (16)	0.0590 (16)	0.0531 (16)	0.0056 (12)	−0.0013 (13)	−0.0056 (13)
C3	0.0746 (18)	0.0663 (17)	0.0554 (17)	−0.0053 (14)	0.0115 (14)	−0.0004 (14)
C4	0.0753 (18)	0.0649 (17)	0.0452 (16)	−0.0029 (14)	0.0132 (13)	−0.0048 (13)
C5	0.0594 (15)	0.0560 (15)	0.0439 (15)	0.0040 (12)	0.0033 (12)	−0.0003 (12)
C6	0.0703 (17)	0.0568 (15)	0.0515 (17)	−0.0001 (13)	0.0079 (14)	0.0009 (13)
C7	0.0730 (18)	0.0671 (17)	0.0454 (16)	−0.0052 (13)	0.0106 (13)	0.0006 (13)
C8	0.0702 (17)	0.0695 (18)	0.0451 (15)	0.0023 (14)	0.0052 (13)	−0.0081 (13)
C9	0.103 (2)	0.0695 (19)	0.064 (2)	−0.0242 (17)	0.0162 (18)	0.0023 (16)
C10	0.106 (2)	0.0689 (18)	0.0530 (18)	−0.0249 (17)	0.0161 (17)	−0.0045 (15)
C11	0.0536 (15)	0.0519 (14)	0.0501 (15)	0.0024 (11)	−0.0001 (12)	0.0001 (12)
C12	0.0717 (18)	0.0655 (17)	0.0603 (18)	−0.0128 (14)	0.0139 (15)	−0.0041 (14)
C13	0.0780 (19)	0.0737 (19)	0.0556 (18)	−0.0069 (15)	0.0138 (15)	−0.0087 (15)
N1	0.0732 (15)	0.0586 (14)	0.0579 (15)	−0.0049 (11)	0.0043 (12)	0.0007 (11)
O1	0.1010 (18)	0.0836 (17)	0.105 (2)	−0.0092 (14)	−0.0137 (17)	−0.0178 (15)
O2	0.1216 (19)	0.0888 (16)	0.0897 (19)	−0.0073 (13)	0.0038 (15)	−0.0325 (14)
O3	0.1339 (18)	0.0751 (14)	0.0559 (13)	−0.0234 (12)	0.0306 (12)	−0.0190 (11)
O4	0.0982 (15)	0.0655 (13)	0.0594 (13)	−0.0208 (11)	0.0183 (11)	−0.0096 (10)

Geometric parameters (Å, º)

C1—O2	1.189 (3)	C8—H8	0.9300
C1—O1	1.202 (4)	C9—N1	1.330 (4)
C1—C2	1.441 (4)	C9—C10	1.368 (4)
C2—C8	1.362 (4)	C9—H9	0.9300
C2—C3	1.376 (4)	C10—C11	1.366 (4)
C3—C4	1.368 (4)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.384 (4)
C4—C5	1.375 (3)	C11—C11^{i}	1.482 (5)
C4—H4	0.9300	C12—C13	1.370 (4)
C5—C7	1.389 (4)	C12—H12	0.9300

C5—C6	1.491 (4)	C13—N1	1.309 (3)
C6—O3	1.217 (3)	C13—H13	0.9300
C6—O4	1.288 (3)	O1—H1	0.8000
C7—C8	1.367 (4)	O4—H2	0.82 (2)
C7—H7	0.9300		

O2—C1—O1	120.4 (3)	C2—C8—C7	118.3 (3)
O2—C1—C2	120.9 (3)	C2—C8—H8	120.9
O1—C1—C2	118.7 (3)	C7—C8—H8	120.8
O2—C1—H1	94.0	N1—C9—C10	123.4 (3)
C2—C1—H1	145.0	N1—C9—H9	118.3
C8—C2—C3	122.2 (3)	C10—C9—H9	118.3
C8—C2—C1	118.6 (3)	C11—C10—C9	120.4 (3)
C3—C2—C1	119.2 (3)	C11—C10—H10	119.8
C4—C3—C2	119.2 (3)	C9—C10—H10	119.8
C4—C3—H3	120.4	C10—C11—C12	115.8 (2)
C2—C3—H3	120.4	C10—C11—C11^{i}	122.8 (3)
C3—C4—C5	119.9 (3)	C12—C11—C11^{i}	121.4 (3)
C3—C4—H4	120.0	C13—C12—C11	120.4 (3)
C5—C4—H4	120.0	C13—C12—H12	119.8
C4—C5—C7	119.6 (3)	C11—C12—H12	119.8
C4—C5—C6	118.3 (2)	N1—C13—C12	123.4 (3)
C7—C5—C6	122.1 (2)	N1—C13—H13	118.3
O3—C6—O4	123.5 (3)	C12—C13—H13	118.3
O3—C6—C5	121.8 (2)	C13—N1—C9	116.6 (2)
O4—C6—C5	114.6 (2)	C13—N1—H2	123.3 (10)
C8—C7—C5	120.8 (2)	C9—N1—H2	120.1 (10)
C8—C7—H7	119.6	C1—O1—H1	111.00
C5—C7—H7	119.6	C6—O4—H2	110 (2)

C13—N1—C9—C10	1.7 (5)	C1—C2—C3—C4	179.7 (2)
N1—C9—C10—C11	−0.9 (5)	C2—C3—C4—C5	−0.2 (4)
C9—C10—C11—C12	−0.6 (4)	C3—C4—C5—C7	0.4 (4)
C9—C10—C11—C11^{i}	−179.2 (3)	C3—C4—C5—C6	179.4 (2)
C10—C11—C12—C13	1.3 (4)	C4—C5—C6—O3	5.4 (4)
C11^{i}—C11—C12—C13	179.9 (3)	C7—C5—C6—O3	−175.6 (3)
C9—N1—C13—C12	−1.0 (4)	C4—C5—C6—O4	−174.3 (2)
C11—C12—C13—N1	−0.5 (4)	C7—C5—C6—O4	4.7 (4)
O2—C1—C2—C8	−5.1 (4)	C4—C5—C7—C8	−0.5 (4)
O1—C1—C2—C8	177.3 (3)	C6—C5—C7—C8	−179.5 (2)
O2—C1—C2—C3	175.2 (3)	C3—C2—C8—C7	−0.2 (4)
O1—C1—C2—C3	−2.6 (4)	C1—C2—C8—C7	−179.8 (2)
C8—C2—C3—C4	0.1 (4)	C5—C7—C8—C2	0.4 (4)

Symmetry code: (i) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H2···N1	0.82 (2)	1.78 (2)	2.598 (4)	178 (1)