Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Retraction of articles by H. Zhong *et al.*

H. Zhong,[a]* S.-H. Duan,[a] Y.-P. Hong,[a] M.-L. Li,[a] Y.-Q. Liu,[a] C.-J. Luo,[a] Q.-Y. Luo,[a] S.-Z. Xiao,[a] H.-L. Xie,[a] Y.-P. Xu,[a] X.-M. Yang,[b,a] X.-R. Zeng[a] and Q. Y. Zhong[c]

[a]College of Chemistry and Chemical Engineering, Provincial Key Laboratory of Coordination Chemistry, Jinggangshan University, Jian 343009, People's Republic of China, [b]Institute of Applied Materials, Jiangxi University of Finance and Economics, Nanchang 330032, People's Republic of China, and [c]Jian Training School, Jian 343000, People's Republic of China
Correspondence e-mail: huazhong06@126.com

Received 20 November 2009; accepted 15 December 2009

A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. 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	DOI	Refcode
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate	Zhong, Zeng, Liu & Luo (2006*a*)	10.1107/S1600536806041122	KERQEE
cis-Dichlorobis(1,10-phenanthroline)cobalt(II)	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
Tris(quinolin-8-olato-κ^2N,O)cobalt(III) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2006*b*)	10.1107/S1600536806050240	MEQHEW
(8-Quinolinol-κ^2N,O)bis(8-quinolinolato-κ^2N,O)nickel(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
(8-Quinolinol-κ^2N,O)-bis(8-quinolinolato-κ^2N,O)zinc(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')nickel(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*a*)	10.1107/S1600536807004102	YEYGOZ
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')zinc(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*b*)	10.1107/S1600536807004096	YEYGUF
Chloridobis(1,10-phenanthroline-$\kappa N,N'$)copper(I) hexahydrate	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)	Zhong, Zeng, Yang & Luo (2007*a*)	10.1107/S1600536807017461	ITCPCO01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)	Zhong, Zeng, Yang & Luo (2007*b*)	10.1107/S160053680701879X	AVUJEG02
Tetrakis(nitrato-κ^2O,O')bis(4-phenylpyridine-κN)cerium(IV)	Zhong, Zeng, Yang & Luo (2007*c*)	10.1107/S1600536807018831	CICDOI
Bis(4,4′-bipyridine-κ^2N,N')tetrakis(nitrato-κ^2O,O')cerium(IV)	Zhong, Zeng, Yang & Luo (2007*d*)	10.1107/S1600536807021502	YIDNEF
(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)	Zhong, Yang, Luo & Xu (2007*a*)	10.1107/S1600536807028061	EDUTUT
(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)	Zhong, Yang, Luo & Xu (2007*b*)	10.1107/S1600536807028693	RIGQEE
(1,10-Phenanthroline-κ^2N,N')tris(phenoxyacetato)-$\kappa O;\kappa O;\kappa O,O'$-neodymium(III)	Zhong, Yang, Luo & Xu (2007*c*)	10.1107/S1600536807030371	UDUMEM
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)nickel(II)	Zhong, Yang, Luo & Xu (2007*d*)	10.1107/S1600536807031613	YEJGOJ01
Bis(2,2′-bipyridyl-κ^2N,N')bis(isothiocyanato-κN)copper(II)	Zhong, Yang, Luo & Xu (2007*e*)	10.1107/S1600536807033181	UFAPOH
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)zinc(II)	Zhong, Yang, Luo & Xu (2007*f*)	10.1107/S1600536807035337	TIGFAR
(1,10-Phenanthroline-κ^2N,N')tris(3-phenylpropanoato-κO)neodymium(III)	Zhong, Yang, Luo & Xu (2007*g*)	10.1107/S1600536807035350	TIGFEV
2-Fluoro-3,5-dinitrobenzamide monohydrate	Zhong, Yang, Xie & Luo (2007*j*)	10.1107/S1600536807038676	VIKGAY
2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*k*)	10.1107/S1600536807039724	KILKIA
1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate	Zhong, Yang, Xie & Luo (2007*l*)	10.1107/S1600536807040779	AFETAH
N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*m*)	10.1107/S160053680704086X	AFINAF
catena-Poly[[bis(μ-anilinoacetato-$\kappa^2O:O'$)bis(μ-anilinoacetato-$\kappa^3O,O':O$)bis[(1,10-phenanthroline-κ^2N,N')samarium(III)]-μ-anilinoacetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*a*)	10.1107/S1600536807043528	PILDAQ
2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate	Zhong, Yang, Xie & Luo (2007*n*)	10.1107/S1600536807045199	XILWIZ
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*b*)	10.1107/S1600536807048489	WIMWEV
Hexaaquacopper(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*c*)	10.1107/S1600536807049525	TOLSCV01

Table 1 (continued)

Title	Reference	DOI	Refcode
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*d*)	10.1107/S1600536807051240	GIMZEI
Hexaaquachromium(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*e*)	10.1107/S1600536807051227	GIMZIM
Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*f*)	10.1107/S1600536807052051	QUKQES01
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*g*)	10.1107/S1600536807053494	NIQLAB
Hexaaquanickel(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007*a*)	10.1107/S1600536807054372	HIPZOW
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*h*)	10.1107/S160053680705622X	XIRGOV
Hexaaquazinc(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007*b*)	10.1107/S1600536807056498	XIRJEO
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*i*)	10.1107/S1600536807058540	HIQJOH
Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
catena-Poly[[(1,10-phenanthroline-κ^2N,N')praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-[(1,10-phenanthroline-κ^2N,N')-praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-di-μ-phenoxyacetato-$\kappa^3O,O':O;\kappa^3O:O,O'$]	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

References

Zhong, H., Xie, H.-L. & Luo, C.-J. (2007). *Acta Cryst.* E**63**, m3054.
Zhong, H., Yang, X.-M., Duan, S.-H. & Hong, Y.-P. (2007). *Acta Cryst.* E**63**, m3142–m3143.
Zhong, H., Yang, X.-M., Luo, C.-J. & Li, M.-L. (2007). *Acta Cryst.* E**63**, m3160–m3161.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*a*). *Acta Cryst.* E**63**, m1885–m1886.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*b*). *Acta Cryst.* E**63**, m1909.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*c*). *Acta Cryst.* E**63**, m2019.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*d*). *Acta Cryst.* E**63**, m2062.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*e*). *Acta Cryst.* E**63**, m2141.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*f*). *Acta Cryst.* E**63**, m2208.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*g*). *Acta Cryst.* E**63**, m2209–m2210.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2008). *Acta Cryst.* E**64**, m317–m318.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*a*). *Acta Cryst.* E**63**, m2508–m2509.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*b*). *Acta Cryst.* E**63**, m2680–m2681.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*c*). *Acta Cryst.* E**63**, m2724–m2725.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*d*). *Acta Cryst.* E**63**, m2772–m2773.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*e*). *Acta Cryst.* E**63**, m2774.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*f*). *Acta Cryst.* E**63**, m2825.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*g*). *Acta Cryst.* E**63**, m2895–m2896.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*h*). *Acta Cryst.* E**63**, m2979.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*i*). *Acta Cryst.* E**63**, m3053.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*j*). *Acta Cryst.* E**63**, o3780.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*k*). *Acta Cryst.* E**63**, o3831.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*l*). *Acta Cryst.* E**63**, o3881.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*m*). *Acta Cryst.* E**63**, o3882.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*n*). *Acta Cryst.* E**63**, o4191.
Zhong, H., Zeng, X.-R., Liu, Y.-Q. & Luo, Q.-Y. (2006*a*). *Acta Cryst.* E**62**, m2925–m2927.
Zhong, H., Zeng, X.-R., Liu, Y.-Q. & Luo, Q.-Y. (2006*b*). *Acta Cryst.* E**62**, m3557–m3559.
Zhong, H., Zeng, X.-R., Liu, Y.-Q. & Luo, Q.-Y. (2007). *Acta Cryst.* E**63**, m187–m189.
Zhong, H., Zeng, X.-R. & Luo, Q.-Y. (2006). *Acta Cryst.* E**62**, m3330–m3332.
Zhong, H., Zeng, X.-R. & Luo, Q.-Y. (2007). *Acta Cryst.* E**63**, m221–m223.
Zhong, H., Zeng, X.-R., Luo, Q.-Y., Li, M.-L. & Xiao, S.-Z. (2007). *Acta Cryst.* E**63**, m492–m494.
Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007*a*). *Acta Cryst.* E**63**, m1379.
Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007*b*). *Acta Cryst.* E**63**, m1445.
Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007*c*). *Acta Cryst.* E**63**, m1455.
Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007*d*). *Acta Cryst.* E**63**, m1592–m1593.
Zhong, H., Zeng, X.-R., Yang, X.-M., Luo, Q.-Y. & Li, M.-L. (2007*a*). *Acta Cryst.* E**63**, m639–m641.
Zhong, H., Zeng, X.-R., Yang, X.-M., Luo, Q.-Y. & Li, M.-L. (2007*b*). *Acta Cryst.* E**63**, m642–m644.
Zhong, H., Zeng, X.-R., Yang, X.-M., Luo, Q.-Y. & Xiao, S.-Z. (2007). *Acta Cryst.* E**63**, m826–m828.
Zhong, H., Zeng, X.-R., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007). *Acta Cryst.* E**63**, m1868–m1869.
Zhong, H., Zhong, Q. Y., Xie, H.-L. & Luo, C.-J. (2007*a*). *Acta Cryst.* E**63**, m2913–m2914.
Zhong, H., Zhong, Q.-Y., Xie, H.-L. & Luo, C.-J. (2007*b*). *Acta Cryst.* E**63**, m2990.

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)

H. Zhong,* H.-L. Xie and C.-J. Luo

College of Chemistry & Chemical Engineering, Provincial Key Laboratory of Coordination Chemistry, Jinggangshan University, Jian 343009, People's Republic of China
Correspondence e-mail: huazhong06@126.com

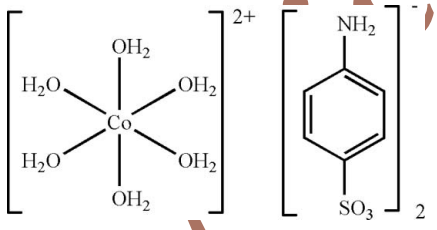
Received 8 November 2007; accepted 13 November 2007

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; R factor = 0.029; wR factor = 0.072; data-to-parameter ratio = 13.8.

The asymmetric unit of the title compound, $[Co(H_2O)_6](C_6H_6NO_3S)_2$, contains one half-cation and one anion; the Co atom lies on an inversion centre. In the crystal structure, intermolecular O—H···O and O—H···S hydrogen bonds result in the formation of a supramolecular network. The conformation of the anion is stabilized by an intramolecular C—H···O hydrogen-bonding interaction.

Related literature

For a related structure, see: Zhong *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Co(H_2O)_6](C_6H_6NO_3S)_2$
M_r = 511.38
Monoclinic, $P2_1/n$
a = 7.110 (2) Å
b = 6.1905 (17) Å
c = 24.9016 (11) Å
β = 91.005 (4)°
V = 1095.9 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.03 mm^{-1}
T = 273 (2) K
0.51 × 0.39 × 0.19 mm

Data collection

Bruker APEX-II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.623, T_{max} = 0.829
6730 measured reflections
2164 independent reflections
1869 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.072
S = 1.01
2164 reflections
157 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.0690 (17)	Co1—O3	2.0456 (17)
Co1—O2	1.9872 (16)		
O1—Co1—O1^{i}	180	O2—Co1—O2^{i}	180
O1—Co1—O2	90.33 (8)	O2—Co1—O3^{i}	89.20 (8)
O1^{i}—Co1—O2	89.67 (8)	O2^{i}—Co1—O3^{i}	90.80 (8)
O1^{i}—Co1—O3	86.58 (10)	O3^{i}—Co1—O3	180
O1—Co1—O3	93.42 (10)		

Symmetry code: (i) $-x+1, -y, -z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O5	0.93	2.57	2.910 (3)	102
O1—H1*B*···S1^{ii}	0.827 (17)	3.080 (17)	3.863 (2)	159 (2)
O1—H1*A*···O4^{iii}	0.790 (16)	1.953 (17)	2.738 (2)	173 (3)
O1—H1*B*···O5^{ii}	0.827 (17)	2.008 (18)	2.832 (3)	174 (3)
O2—H2*A*···O4^{ii}	0.842 (17)	1.973 (18)	2.807 (2)	171 (3)
O2—H2*B*···O6^{iv}	0.845 (17)	1.935 (18)	2.764 (2)	167 (3)
O3—H3*A*···S1^{v}	0.784 (17)	3.17 (2)	3.890 (2)	155 (2)
O3—H3*B*···O5^{iv}	0.831 (17)	1.976 (18)	2.801 (2)	172 (3)
O3—H3*A*···O6^{v}	0.784 (17)	1.960 (17)	2.742 (2)	174 (3)

Symmetry codes: (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, -y, -z+1$; (iv) $-x, -y+1, -z+1$; (v) $-x, -y, -z+1$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

We thank the Science and Technology Program of Jinggangshan University for financial support of this work (grant No. 2007).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2478).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2005). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SAINT* and *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Zhong, H., Zhong, Q. Y., Xie, H.-L. & Luo, C.-J. (2007). *Acta Cryst.* E**63**, m2913–m2914.

supplementary materials

Acta Cryst. (2007). E**63**, m3054 [**doi:10.1107/S1600536807058527**]

Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)

H. Zhong, H.-L. Xie and C.-J. Luo

Comment

The crystal structure of hexaaquanickel(II) bis(4-aminobenzenesulfonate), (II), has previously been reported (Zhong *et al.*, 2007). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with that of (II). We report herein the crystal structure of (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The title compound, $[Co(H_2O)_6](C_6H_6NO_3S)_2$, contains one half-cation and one anion; the Co atom lies on an inversion centre, as in (II).

In the crystal structure, intermolecular O—H···O and O—H···S hydrogen bonds (Fig. 2 and Table 2) result in the formation of a supramolecular network structure. The conformation of the anion is stabilized by an intramolecular C—H···O hydrogen-bonding interaction., as in (II).

The both compounds, (I) and (II), are isostructural.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Europium (III) nitrate pentahydrate (213.9 mg, 0.5 mmol), cobalt nitrate hexahydrate (145.9 mg, 0.5 mmol), *p*-aminobenzenesulfonic acid (346.4 mg, 2 mmol), ammonia (0.5 mol/l, 4 ml) and distilled water (8 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 453 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colourless solution was decanted from small pink crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H atoms (for H_2O) were located in difference syntheses and refined isotropically. The H atoms were positioned geometrically, with N—H = 0.86 Å (for NH_2) and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Figures

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): $-x + 3/2, y + 1/2, -z + 1/2$].

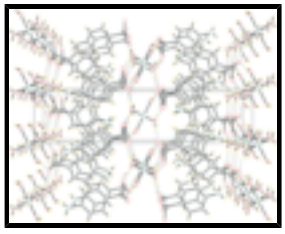


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)

Crystal data

$[Co(H_2O)_6](C_6H_6NO_3S)_2$
$M_r = 511.38$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.110$ (2) Å
$b = 6.1905$ (17) Å
$c = 24.9016$ (11) Å
$\beta = 91.005$ (4)°
$V = 1095.9$ (5) Å^3
$Z = 2$
$F_{000} = 530$
$D_x = 1.550$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 5606 reflections
$\theta = 2.2$–26.5°
$\mu = 1.03$ mm^{-1}
$T = 273$ (2) K
Prism, pink
0.51 × 0.39 × 0.19 mm

Data collection

Bruker APEX-II area-detector diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
$T = 273(2)$ K
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.623$, $T_{max} = 0.829$
6730 measured reflections
2164 independent reflections
1869 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 26.4$°
$\theta_{min} = 3.0$°
$h = -8 \rightarrow 8$
$k = -7 \rightarrow 7$
$l = -31 \rightarrow 30$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.072$
$S = 1.01$
2164 reflections
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
$w = 1/[\sigma^2(F_o^2) + (0.0305P)^2 + 0.444P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}

157 parameters
9 restraints
Primary atom site location: structure-invariant direct methods

$\Delta\rho_{min} = -0.25$ e Å^{-3}
Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	0.0000	0.0000	0.03904 (12)
S1	−0.01463 (7)	0.60843 (8)	0.90518 (2)	0.04647 (15)
O1	0.7236 (3)	−0.1026 (3)	0.04780 (9)	0.0786 (6)
O2	0.5086 (3)	0.2884 (3)	0.03500 (7)	0.0603 (4)
O3	0.3031 (3)	−0.1035 (3)	0.05312 (9)	0.0796 (6)
O4	0.1552 (2)	0.5138 (2)	0.93055 (7)	0.0599 (4)
O5	−0.0146 (2)	0.8390 (2)	0.90902 (7)	0.0584 (4)
O6	−0.1924 (2)	0.5169 (2)	0.92380 (7)	0.0604 (4)
N1	0.0301 (5)	0.3770 (7)	0.67180 (12)	0.1339 (13)
H1AA	0.0032	0.4707	0.6474	0.161*
H1BB	0.0673	0.2500	0.6629	0.161*
C1	−0.0035 (3)	0.5452 (4)	0.83690 (9)	0.0506 (5)
C2	−0.0538 (4)	0.6917 (5)	0.79840 (11)	0.0691 (7)
H2	−0.0932	0.8294	0.8081	0.083*
C3	−0.0458 (4)	0.6342 (6)	0.74494 (11)	0.0801 (8)
H3	−0.0813	0.7344	0.7188	0.096*
C4	0.0125 (4)	0.4347 (6)	0.72937 (11)	0.0725 (7)
C5	0.0607 (4)	0.2900 (5)	0.76906 (11)	0.0765 (8)
H5	0.0998	0.1521	0.7595	0.092*
C6	0.0527 (4)	0.3427 (4)	0.82191 (10)	0.0654 (6)
H6	0.0855	0.2412	0.8480	0.078*
H1A	0.755 (3)	−0.224 (3)	0.0515 (11)	0.071 (8)*
H2A	0.608 (3)	0.340 (5)	0.0485 (12)	0.095 (11)*
H3A	0.278 (4)	−0.224 (3)	0.0590 (11)	0.077 (9)*
H1B	0.811 (3)	−0.023 (3)	0.0581 (12)	0.079 (9)*
H2B	0.418 (3)	0.340 (5)	0.0524 (11)	0.096 (11)*
H3B	0.212 (3)	−0.027 (4)	0.0615 (13)	0.089 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0496 (2)	0.0268 (2)	0.0507 (2)	0.00076 (14)	0.00183 (14)	0.00170 (15)
S1	0.0485 (3)	0.0343 (3)	0.0567 (3)	0.0006 (2)	0.0030 (2)	−0.0004 (2)
O1	0.0800 (13)	0.0383 (10)	0.1157 (16)	0.0055 (9)	−0.0434 (11)	0.0001 (10)
O2	0.0558 (9)	0.0415 (9)	0.0836 (12)	−0.0008 (7)	0.0051 (9)	−0.0138 (8)
O3	0.0875 (13)	0.0375 (10)	0.1156 (16)	0.0007 (9)	0.0521 (12)	0.0059 (10)
O4	0.0676 (10)	0.0444 (9)	0.0674 (10)	0.0052 (7)	−0.0115 (8)	−0.0026 (7)
O5	0.0633 (9)	0.0349 (8)	0.0772 (10)	0.0000 (7)	0.0057 (8)	−0.0016 (7)
O6	0.0649 (10)	0.0434 (9)	0.0736 (10)	−0.0041 (7)	0.0177 (8)	−0.0022 (7)
N1	0.140 (3)	0.190 (4)	0.0716 (18)	0.007 (3)	0.0108 (17)	−0.012 (2)
C1	0.0461 (11)	0.0467 (12)	0.0591 (12)	−0.0006 (9)	0.0015 (9)	0.0040 (10)
C2	0.0734 (15)	0.0650 (17)	0.0691 (16)	0.0113 (13)	0.0055 (12)	0.0130 (13)
C3	0.0765 (17)	0.098 (2)	0.0656 (16)	0.0088 (16)	0.0003 (13)	0.0245 (16)
C4	0.0611 (15)	0.097 (2)	0.0593 (15)	−0.0067 (14)	0.0024 (12)	−0.0012 (14)
C5	0.0886 (19)	0.0746 (19)	0.0665 (16)	0.0056 (15)	0.0039 (13)	−0.0151 (14)
C6	0.0834 (17)	0.0534 (14)	0.0593 (13)	0.0107 (12)	−0.0002 (12)	−0.0029 (11)

Geometric parameters (Å, °)

Co1—O1	2.0690 (17)	O3—H3B	0.831 (17)
Co1—O2	1.9872 (16)	N1—C4	1.485 (4)
Co1—O3	2.0456 (17)	N1—H1AA	0.8600
Co1—O2^{i}	1.9872 (16)	N1—H1BB	0.8600
Co1—O3^{i}	2.0456 (17)	C1—C2	1.363 (3)
Co1—O1^{i}	2.0690 (17)	C1—C6	1.369 (3)
S1—O5	1.4307 (16)	C2—C3	1.380 (4)
S1—O6	1.4676 (17)	C2—H2	0.9300
S1—O4	1.4740 (17)	C3—C4	1.361 (4)
S1—C1	1.748 (2)	C3—H3	0.9300
O1—H1A	0.790 (16)	C4—C5	1.373 (4)
O1—H1B	0.827 (17)	C5—C6	1.358 (4)
O2—H2A	0.842 (17)	C5—H5	0.9300
O2—H2B	0.845 (17)	C6—H6	0.9300
O3—H3A	0.784 (17)		
O1—Co1—O1^{i}	180.00 (14)	H2A—O2—H2B	107 (2)
O1—Co1—O2	90.33 (8)	Co1—O3—H3A	125 (2)
O1^{i}—Co1—O2	89.67 (8)	Co1—O3—H3B	122 (2)
O1^{i}—Co1—O3	86.58 (10)	H3A—O3—H3B	109 (2)
O1—Co1—O3	93.42 (10)	C4—N1—H1AA	120.0
O2—Co1—O2^{i}	180.00 (10)	C4—N1—H1BB	120.0
O2—Co1—O3^{i}	89.20 (8)	H1AA—N1—H1BB	120.0
O2^{i}—Co1—O3^{i}	90.80 (8)	C2—C1—C6	119.5 (2)
O3^{i}—Co1—O3	180.00 (10)	C2—C1—S1	121.28 (19)
O2—Co1—O3	90.80 (8)	C6—C1—S1	119.25 (17)

O2^{i}—Co1—O3	89.20 (8)	C1—C2—C3	119.5 (3)
O1—Co1—O2^{i}	89.67 (8)	C1—C2—H2	120.3
O1^{i}—Co1—O2^{i}	90.33 (8)	C3—C2—H2	120.3
O1^{i}—Co1—O3^{i}	93.42 (10)	C4—C3—C2	121.8 (3)
O1—Co1—O3^{i}	86.58 (10)	C4—C3—H3	119.1
O5—S1—O6	111.29 (10)	C2—C3—H3	119.1
O5—S1—O4	111.62 (10)	C3—C4—C5	117.4 (3)
O6—S1—O4	114.49 (10)	C3—C4—N1	121.6 (3)
O5—S1—C1	106.78 (10)	C5—C4—N1	120.9 (3)
O6—S1—C1	105.95 (10)	C6—C5—C4	121.8 (3)
O4—S1—C1	106.10 (10)	C6—C5—H5	119.1
Co1—O1—H1A	124.8 (18)	C4—C5—H5	119.1
Co1—O1—H1B	124.0 (19)	C5—C6—C1	120.1 (2)
H1A—O1—H1B	109 (2)	C5—C6—H6	119.9
Co1—O2—H2A	122 (2)	C1—C6—H6	119.9
Co1—O2—H2B	123 (2)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O5	0.93	2.57	2.910 (3)	102
O1—H1B···S1^{ii}	0.827 (17)	3.080 (17)	3.863 (2)	159 (2)
O1—H1A···O4^{iii}	0.790 (16)	1.953 (17)	2.738 (2)	173 (3)
O1—H1B···O5^{ii}	0.827 (17)	2.008 (18)	2.832 (3)	174 (3)
O2—H2A···O4^{ii}	0.842 (17)	1.973 (18)	2.807 (2)	171 (3)
O2—H2B···O6^{iv}	0.845 (17)	1.935 (18)	2.764 (2)	167 (3)
O3—H3A···S1^{v}	0.784 (17)	3.17 (2)	3.890 (2)	155 (2)
O3—H3B···O5^{iv}	0.831 (17)	1.976 (18)	2.801 (2)	172 (3)
O3—H3A···O6^{v}	0.784 (17)	1.960 (17)	2.742 (2)	174 (3)

Symmetry codes: (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*, −*z*+1; (iv) −*x*, −*y*+1, −*z*+1; (v) −*x*, −*y*, −*z*+1.

Fig. 1

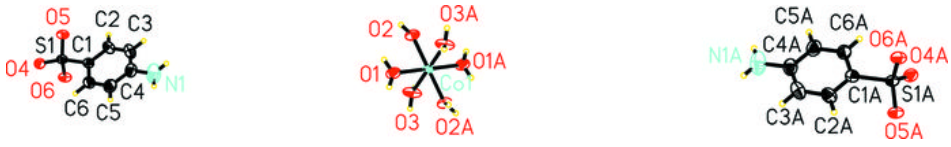


Fig. 2