

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
<i>trans</i> -Bis[1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato]copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato- $\kappa^2 O, O'$)copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehyde)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato- $\kappa^2 O, O'$)zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato- $\kappa^2 O, O'$)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- $\kappa^2 O, O'$)manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline- $\kappa^2 N, N'$)copper(II) naphthalene-1,5-disulfonate dihydrate	Liu <i>et al.</i> (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline- $\kappa^2 N, N'$)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 <i>et al.</i> (2006)	Journal	10.1107/S160053680604565X	HESPEP
Bis(2-formylphenolato- $\kappa^2 O, O'$)iron(II)	Yang <i>et al.</i> (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer <i>et al.</i> (2007a)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer <i>et al.</i> (2007b)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (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 <i>et al.</i> (2007)	Author	10.1107/S1600536807032540	WIHRIP
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li <i>et al.</i> (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1 $\kappa^4 O^1, O^2, O^3, O^4, O^5, O^6, O^7, O^8, O^9, O^{10}, O^{11}, O^{12}, O^{13}, O^{14}, O^{15}, O^{16}, O^{17}, O^{18}, O^{19}, O^{20}, O^{21}, O^{22}, O^{23}, O^{24}, O^{25}, O^{26}, O^{27}, O^{28}, O^{29}, O^{30}, O^{31}, O^{32}, O^{33}, O^{34}, O^{35}, O^{36}, O^{37}, O^{38}, O^{39}, O^{40}, O^{41}, O^{42}, O^{43}, O^{44}, O^{45}, O^{46}, O^{47}, O^{48}, O^{49}, O^{50}, O^{51}, O^{52}, O^{53}, O^{54}, O^{55}, O^{56}, O^{57}, O^{58}, O^{59}, O^{60}, O^{61}, O^{62}, O^{63}, O^{64}, O^{65}, O^{66}, O^{67}, O^{68}, O^{69}, O^{70}, O^{71}, O^{72}, O^{73}, O^{74}, O^{75}, O^{76}, O^{77}, O^{78}, O^{79}, O^{80}, O^{81}, O^{82}, O^{83}, O^{84}, O^{85}, O^{86}, O^{87}, O^{88}, O^{89}, O^{90}, O^{91}, O^{92}, O^{93}, O^{94}, O^{95}, O^{96}, O^{97}, O^{98}, O^{99}, O^{100}, O^{101}, O^{102}, O^{103}, O^{104}, O^{105}, O^{106}, O^{107}, O^{108}, O^{109}, O^{110}, O^{111}, O^{112}, O^{113}, O^{114}, O^{115}, O^{116}, O^{117}, O^{118}, O^{119}, O^{120}, O^{121}, O^{122}, O^{123}, O^{124}, O^{125}, O^{126}, O^{127}, O^{128}, O^{129}, O^{130}, O^{131}, O^{132}, O^{133}, O^{134}, O^{135}, O^{136}, O^{137}, O^{138}, O^{139}, O^{140}, O^{141}, O^{142}, O^{143}, O^{144}, O^{145}, O^{146}, O^{147}, O^{148}, O^{149}, O^{150}, O^{151}, O^{152}, O^{153}, O^{154}, O^{155}, O^{156}, O^{157}, O^{158}, O^{159}, O^{160}, O^{161}, O^{162}, O^{163}, O^{164}, O^{165}, O^{166}, O^{167}, O^{168}, O^{169}, O^{170}, O^{171}, O^{172}, O^{173}, O^{174}, O^{175}, O^{176}, O^{177}, O^{178}, O^{179}, O^{180}, O^{181}, O^{182}, O^{183}, O^{184}, O^{185}, O^{186}, O^{187}, O^{188}, O^{189}, O^{190}, O^{191}, O^{192}, O^{193}, O^{194}, O^{195}, O^{196}, O^{197}, O^{198}, O^{199}, O^{200}, O^{201}, O^{202}, O^{203}, O^{204}, O^{205}, O^{206}, O^{207}, O^{208}, O^{209}, O^{210}, O^{211}, O^{212}, O^{213}, O^{214}, O^{215}, O^{216}, O^{217}, O^{218}, O^{219}, O^{220}, O^{221}, O^{222}, O^{223}, O^{224}, O^{225}, O^{226}, O^{227}, O^{228}, O^{229}, O^{230}, O^{231}, O^{232}, O^{233}, O^{234}, O^{235}, O^{236}, O^{237}, O^{238}, O^{239}, O^{240}, O^{241}, O^{242}, O^{243}, O^{244}, O^{245}, O^{246}, O^{247}, O^{248}, O^{249}, O^{250}, O^{251}, O^{252}, O^{253}, O^{254}, O^{255}, O^{256}, O^{257}, O^{258}, O^{259}, O^{260}, O^{261}, O^{262}, O^{263}, O^{264}, O^{265}, O^{266}, O^{267}, O^{268}, O^{269}, O^{270}, O^{271}, O^{272}, O^{273}, O^{274}, O^{275}, O^{276}, O^{277}, O^{278}, O^{279}, O^{280}, O^{281}, O^{282}, O^{283}, O^{284}, O^{285}, O^{286}, O^{287}, O^{288}, O^{289}, O^{290}, O^{291}, O^{292}, O^{293}, O^{294}, O^{295}, O^{296}, O^{297}, O^{298}, O^{299}, O^{300}, O^{301}, O^{302}, O^{303}, O^{304}, O^{305}, O^{306}, O^{307}, O^{308}, O^{309}, O^{310}, O^{311}, O^{312}, O^{313}, O^{314}, O^{315}, O^{316}, O^{317}, O^{318}, O^{319}, O^{320}, O^{321}, O^{322}, O^{323}, O^{324}, O^{325}, O^{326}, O^{327}, O^{328}, O^{329}, O^{330}, O^{331}, O^{332}, O^{333}, O^{334}, O^{335}, O^{336}, O^{337}, O^{338}, O^{339}, O^{340}, O^{341}, O^{342}, O^{343}, O^{344}, O^{345}, O^{346}, O^{347}, O^{348}, O^{349}, O^{350}, O^{351}, O^{352}, O^{353}, O^{354}, O^{355}, O^{356}, O^{357}, O^{358}, O^{359}, O^{360}, O^{361}, O^{362}, O^{363}, O^{364}, O^{365}, O^{366}, O^{367}, O^{368}, O^{369}, O^{370}, O^{371}, O^{372}, O^{373}, O^{374}, O^{375}, O^{376}, O^{377}, O^{378}, O^{379}, O^{380}, O^{381}, O^{382}, O^{383}, O^{384}, O^{385}, O^{386}, O^{387}, O^{388}, O^{389}, O^{390}, O^{391}, O^{392}, O^{393}, O^{394}, O^{395}, O^{396}, O^{397}, O^{398}, O^{399}, O^{400}, O^{401}, O^{402}, O^{403}, O^{404}, O^{405}, O^{406}, O^{407}, O^{408}, O^{409}, O^{410}, O^{411}, O^{412}, O^{413}, O^{414}, O^{415}, O^{416}, O^{417}, O^{418}, O^{419}, O^{420}, O^{421}, O^{422}, O^{423}, O^{424}, O^{425}, O^{426}, O^{427}, O^{428}, O^{429}, O^{430}, O^{431}, O^{432}, O^{433}, O^{434}, O^{435}, O^{436}, O^{437}, O^{438}, O^{439}, O^{440}, O^{441}, O^{442}, O^{443}, O^{444}, O^{445}, O^{446}, O^{447}, O^{448}, O^{449}, O^{450}, O^{451}, O^{452}, O^{453}, O^{454}, O^{455}, O^{456}, O^{457}, O^{458}, O^{459}, O^{460}, O^{461}, O^{462}, O^{463}, O^{464}, O^{465}, O^{466}, O^{467}, O^{468}, O^{469}, O^{470}, O^{471}, O^{472}, O^{473}, O^{474}, O^{475}, O^{476}, O^{477}, O^{478}, O^{479}, O^{480}, O^{481}, O^{482}, O^{483}, O^{484}, O^{485}, O^{486}, O^{487}, O^{488}, O^{489}, O^{490}, O^{491}, O^{492}, O^{493}, O^{494}, O^{495}, O^{496}, O^{497}, O^{498}, O^{499}, O^{500}, O^{501}, O^{502}, O^{503}, O^{504}, O^{505}, O^{506}, O^{507}, O^{508}, O^{509}, O^{510}, O^{511}, O^{512}, O^{513}, O^{514}, O^{515}, O^{516}, O^{517}, O^{518}, O^{519}, O^{520}, O^{521}, O^{522}, O^{523}, O^{524}, O^{525}, O^{526}, O^{527}, O^{528}, O^{529}, O^{530}, O^{531}, O^{532}, O^{533}, O^{534}, O^{535}, O^{536}, O^{537}, O^{538}, O^{539}, O^{540}, O^{541}, O^{542}, O^{543}, O^{544}, O^{545}, O^{546}, O^{547}, O^{548}, O^{549}, O^{550}, O^{551}, O^{552}, O^{553}, O^{554}, O^{555}, O^{556}, O^{557}, O^{558}, O^{559}, O^{560}, O^{561}, O^{562}, O^{563}, O^{564}, O^{565}, O^{566}, O^{567}, O^{568}, O^{569}, O^{570}, O^{571}, O^{572}, O^{573}, O^{574}, O^{575}, O^{576}, O^{577}, O^{578}, O^{579}, O^{580}, O^{581}, O^{582}, O^{583}, O^{584}, O^{585}, O^{586}, O^{587}, O^{588}, O^{589}, O^{590}, O^{591}, O^{592}, O^{593}, O^{594}, O^{595}, O^{596}, O^{597}, O^{598}, O^{599}, O^{600}, O^{601}, O^{602}, O^{603}, O^{604}, O^{605}, O^{606}, O^{607}, O^{608}, O^{609}, O^{610}, O^{611}, O^{612}, O^{613}, O^{614}, O^{615}, O^{616}, O^{617}, O^{618}, O^{619}, O^{620}, O^{621}, O^{622}, O^{623}, O^{624}, O^{625}, O^{626}, O^{627}, O^{628}, O^{629}, O^{630}, O^{631}, O^{632}, O^{633}, O^{634}, O^{635}, O^{636}, O^{637}, O^{638}, O^{639}, O^{640}, O^{641}, O^{642}, O^{643}, O^{644}, O^{645}, O^{646}, O^{647}, O^{648}, O^{649}, O^{650}, O^{651}, O^{652}, O^{653}, O^{654}, O^{655}, O^{656}, O^{657}, O^{658}, O^{659}, O^{660}, O^{661}, O^{662}, O^{663}, O^{664}, O^{665}, O^{666}, O^{667}, O^{668}, O^{669}, O^{670}, O^{671}, O^{672}, O^{673}, O^{674}, O^{675}, O^{676}, O^{677}, O^{678}, O^{679}, O^{680}, O^{681}, O^{682}, O^{683}, O^{684}, O^{685}, O^{686}, O^{687}, O^{688}, O^{689}, O^{690}, O^{691}, O^{692}, O^{693}, O^{694}, O^{695}, O^{696}, O^{697}, O^{698}, O^{699}, O^{700}, O^{701}, O^{702}, O^{703}, O^{704}, O^{705}, O^{706}, O^{707}, O^{708}, O^{709}, O^{710}, O^{711}, O^{712}, O^{713}, O^{714}, O^{715}, O^{716}, O^{717}, O^{718}, O^{719}, O^{720}, O^{721}, O^{722}, O^{723}, O^{724}, O^{725}, O^{726}, O^{727}, O^{728}, O^{729}, O^{730}, O^{731}, O^{732}, O^{733}, O^{734}, O^{735}, O^{736}, O^{737}, O^{738}, O^{739}, O^{740}, O^{741}, O^{742}, O^{743}, O^{744}, O^{745}, O^{746}, O^{747}, O^{748}, O^{749}, O^{750}, O^{751}, O^{752}, O^{753}, O^{754}, O^{755}, O^{756}, O^{757}, O^{758}, O^{759}, O^{760}, O^{761}, O^{762}, O^{763}, O^{764}, O^{765}, O^{766}, O^{767}, O^{768}, O^{769}, O^{770}, O^{771}, O^{772}, O^{773}, O^{774}, O^{775}, O^{776}, O^{777}, O^{778}, O^{779}, O^{780}, O^{781}, O^{782}, O^{783}, O^{784}, O^{785}, O^{786}, O^{787}, O^{788}, O^{789}, O^{790}, O^{791}, O^{792}, O^{793}, O^{794}, O^{795}, O^{796}, O^{797}, O^{798}, O^{799}, O^{800}, O^{801}, O^{802}, O^{803}, O^{804}, O^{805}, O^{806}, O^{807}, O^{808}, O^{809}, O^{810}, O^{811}, O^{812}, O^{813}, O^{814}, O^{815}, O^{816}, O^{817}, O^{818}, O^{819}, O^{820}, O^{821}, O^{822}, O^{823}, O^{824}, O^{825}, O^{826}, O^{827}, O^{828}, O^{829}, O^{830}, O^{831}, O^{832}, O^{833}, O^{834}, O^{835}, O^{836}, O^{837}, O^{838}, O^{839}, O^{840}, O^{841}, O^{842}, O^{843}, O^{844}, O^{845}, O^{846}, O^{847}, O^{848}, O^{849}, O^{850}, O^{851}, O^{852}, O^{853}, O^{854}, O^{855}, O^{856}, O^{857}, O^{858}, O^{859}, O^{860}, O^{861}, O^{862}, O^{863}, O^{864}, O^{865}, O^{866}, O^{867}, O^{868}, O^{869}, O^{870}, O^{871}, O^{872}, O^{873}, O^{874}, O^{875}, O^{876}, O^{877}, O^{878}, O^{879}, O^{880}, O^{881}, O^{882}, O^{883}, O^{884}, O^{885}, O^{886}, O^{887}, O^{888}, O^{889}, O^{890}, O^{891}, O^{892}, O^{893}, O^{894}, O^{895}, O^{896}, O^{897}, O^{898}, O^{899}, O^{900}, O^{901}, O^{902}, O^{903}, O^{904}, O^{905}, O^{906}, O^{907}, O^{908}, O^{909}, O^{910}, O^{911}, O^{912}, O^{913}, O^{914}, O^{915}, O^{916}, O^{917}, O^{918}, O^{919}, O^{920}, O^{921}, O^{922}, O^{923}, O^{924}, O^{925}, O^{926}, O^{927}, O^{928}, O^{929}, O^{930}, O^{931}, O^{932}, O^{933}, O^{934}, O^{935}, O^{936}, O^{937}, O^{938}, O^{939}, O^{940}, O^{941}, O^{942}, O^{943}, O^{944}, O^{945}, O^{946}, O^{947}, O^{948}, O^{949}, O^{950}, O^{951}, O^{952}, O^{953}, O^{954}, O^{955}, O^{956}, O^{957}, O^{958}, O^{959}, O^{960}, O^{961}, O^{962}, O^{963}, O^{964}, O^{965}, O^{966}, O^{967}, O^{968}, O^{969}, O^{970}, O^{971}, O^{972}, O^{973}, O^{974}, O^{975}, O^{976}, O^{977}, O^{978}, O^{979}, O^{980}, O^{981}, O^{982}, O^{983}, O^{984}, O^{985}, O^{986}, O^{987}, O^{988}, O^{989}, O^{990}, O^{991}, O^{992}, O^{993}, O^{994}, O^{995}, O^{996}, O^{997}, O^{998}, O^{999}, O^{1000}$				

Table 1 (continued)

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

References

- Chen, Q. (2006). *Acta Cryst.* **E62**, m56–m57.
- Chen, J.-R., Sui, Y., Luo, Q.-Y. & Jiang, R.-Q. (2007). *Acta Cryst.* **E63**, m2091–m2092.
- Chen, J.-R., Sui, Y., Wen, J.-W. & Yin, L.-Y. (2008). *Acta Cryst.* **E64**, m562–m563.
- Han, Z.-Q. (2008). *Acta Cryst.* **E64**, m592.
- Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* **E66**, e1–e2.
- Hu, R.-H., Sui, Y., Chen, L. & He, C.-M. (2008). *Acta Cryst.* **E64**, m8–m9.
- Hu, R.-H., Sui, Y., Fang, X.-N. & Chen, H.-M. (2007). *Acta Cryst.* **E63**, m2039–m2040.
- Huang, C.-F. & Chen, H.-L. (2007). *Acta Cryst.* **E63**, m2356–m2357.
- Huang, Q., Sui, Y.-H. & Zhang, G.-X. (2009). *Acta Cryst.* **E65**, m1161–m1162.
- Li, Y.-G. & Chen, H.-J. (2006). *Acta Cryst.* **E62**, m1038–m1039.
- Li, N.-G., Tao, R.-M. & Fu, B.-F. (2007). *Acta Cryst.* **E63**, o4228.
- Li, Z., Zhang, X. & Pu, X. (2008). *Acta Cryst.* **E64**, m215.
- Liu, J.-T. & Fan, S.-D. (2006). *Acta Cryst.* **E62**, m2507–m2508.
- Liu, J.-T., Fan, S.-D. & Li, D.-Q. (2006). *Acta Cryst.* **E62**, m2165–m2166.
- Liu, D., Lin, J., Xu, Y., Huang, C. & Li, X. (2007). *Acta Cryst.* **E63**, m3094.
- Liu, Y.-Q. & Wen, H.-R. (2007). *Acta Cryst.* **E63**, m2928.
- Liu, Y.-Q. & Zeng, X.-R. (2007a). *Acta Cryst.* **E63**, m2547.
- Liu, Y.-Q. & Zeng, X.-R. (2007b). *Acta Cryst.* **E63**, m2684.
- Liu, Y.-Q., Zeng, X.-R. & Chen, W.-T. (2007). *Acta Cryst.* **E63**, m2462.
- Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007a). *Acta Cryst.* **E63**, m2396.
- Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007b). *Acta Cryst.* **E63**, m2854.
- Qadeer, G., Rama, N. H. & Chen, W.-T. (2007a). *Acta Cryst.* **E63**, o2892.
- Qadeer, G., Rama, N. H. & Chen, W.-T. (2007b). *Acta Cryst.* **E63**, o2932.
- Qiu, X.-Y. (2006). *Acta Cryst.* **E62**, m1190–m1191.
- Sui, Y., Fang, X.-N., Hu, P. & Lin, J. (2007). *Acta Cryst.* **E63**, m2135–m2136.
- Sui, Y., Fang, X.-N. & Yuan, M.-W. (2007). *Acta Cryst.* **E63**, m2275–m2276.
- Sui, Y., Li, X.-F., Huang, G.-S. & Wang, G.-J. (2007). *Acta Cryst.* **E63**, m2093–m2094.
- Sui, Y., Sui, Y.-H., Luo, Q.-Y. & Wang, Y.-D. (2007). *Acta Cryst.* **E63**, m2277–m2278.
- Sui, Y., Xiao, Y.-A., Fang, X.-N., Zeng, X.-R. & Li, M.-H. (2006). *Acta Cryst.* **E62**, m3205–m3207.
- Sui, Y., Zhang, J.-H., Hu, R.-H. & Jiang, R.-Q. (2007). *Acta Cryst.* **E63**, m2256–m2257.
- Sui, Y., Zhang, J.-H., Hu, R.-H. & Yin, L.-Y. (2007). *Acta Cryst.* **E63**, m2089–m2090.
- Sun, Y.-X. & Gao, G.-Z. (2005). *Acta Cryst.* **E61**, m354–m355.
- Wang, Q. & Fang, Z.-N. (2006). *Acta Cryst.* **E62**, m1492–m1493.
- Wang, S., Yang, T., Li, Z. & Yu, X. (2009). *Acta Cryst.* **E65**, o2198.
- Xiao, Y.-A., Fu, X.-K., Sui, Y., Wu, Q. & Xiong, S.-H. (2008). *Acta Cryst.* **E64**, m806–m807.
- Xiao, Y.-A., Sui, Y., Yi, X.-G., Wu, J.-H. & Zhang, L.-P. (2008). *Acta Cryst.* **E64**, m804–m805.
- Xiong, Z.-Y. & Liu, L.-J. (2005). *Acta Cryst.* **E61**, m863–m864.
- Yang, X.-M. (2007). *Acta Cryst.* **E63**, o4453.
- Yang, Y.-M., Lu, P.-C., Zhu, T.-T. & Liu, C.-H. (2007). *Acta Cryst.* **E63**, m1613.
- Zhang, P. (2004). *Acta Cryst.* **E60**, m1808–m1810.

Tetraaqua(1,10-phenanthroline- κ^2N,N')copper(II)
naphthalene-1,5-disulfonate dihydrateJu-Tao Liu,^{a*} Sheng-Di Fan^a and
De-Qian Li^b^aSchool of Life Sciences, Dalian Nationalities University, Dalian 116600, People's Republic of China, and ^bChangchun Institute of Applied Chemistry, Academia Sinica, Changchun 130022, People's Republic of ChinaCorrespondence e-mail:
jutaoliu@yahoo.com.cn

Key indicators

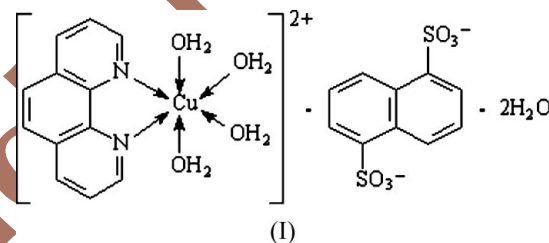
Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(C-C) = 0.005$ Å
 R factor = 0.040
 wR factor = 0.116
Data-to-parameter ratio = 13.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title structure, $[Cu(C_{12}H_8N_2)(H_2O)_4](C_{10}H_6S_2O_6) \cdot 2H_2O$, the cation lies on a crystallographic twofold rotation axis and the anion lies on a centre of inversion. The Cu^{II} atom is coordinated by two N atoms of a 1,10-phenanthroline ligand and four O atoms from four water ligands in a distorted octahedral geometry. The unique Cu—O distances are 2.054 (2) and 2.088 (2) Å and the Cu—N distance is 2.073 (2) Å. In the crystal structure, a three-dimensional supramolecular framework is constructed by extensive intermolecular O—H...O hydrogen bonds.

Received 2 August 2006
Accepted 4 August 2006

Comment

The structures of some tetraaqua(1,10-phenanthroline)metal ionic complexes (Zhang *et al.*, 1999; Cherni *et al.*, 1999) with different anions have been reported. As a multifunctional ligand, naphthalene-1,5-disulfonate often forms ionic compounds (Cai *et al.*, 2001; Piguet *et al.*, 1989) with other metal complex cations. Here we report the crystal structure of the title naphthalene-1,5-disulfonate ionic complex, (I).



The structure of (I) is shown in Fig. 1. The cation lies on a crystallographic twofold rotation axis which runs through the Cu^{II} atom and bisects the plane of the 1,10-phenanthroline ligand. The anion has a center of symmetry located at the centre of the naphthalene unit. In the cation, the coordination geometry at the Cu^{II} atom is distorted octahedral, with an N_2O_4 environment consisting of two N atoms of a 1,10-phenanthroline ligand and four O atoms from four water ligands. Selected bond distances and angles are listed in Table 1. In the crystal structure, a three-dimensional supramolecular framework of cations, anions and uncoordinated water molecules (Fig. 2) is formed *via* intermolecular O—H...O hydrogen-bond interactions (Table 2).

Experimental

A mixture of $Cu(NO_3)_2 \cdot 3H_2O$ (43 mg, 0.2 mmol), 1,10-phenanthroline (37 mg, 0.2 mmol) and disodium naphthalene-1,5-disulfonate (67 mg, 0.2 mmol) in water (15 ml) was placed in a Teflon-lined stainless steel Parr bomb that was heated at 433 K for 48 h. The bomb

was then cooled to room temperature over a period of 24 h. Blue crystals were isolated in about 15% yield based on Cu.

Crystal data

[Cu(C₁₂H₈N₂)(H₂O)₄](C₁₀H₆O₆S₂)·2H₂O
M_r = 638.11
 Monoclinic, *C*2/*c*
a = 20.562 (3) Å
b = 12.4311 (19) Å
c = 12.5373 (18) Å
 β = 124.576 (2)°
V = 2638.6 (7) Å³
Z = 4
D_x = 1.606 Mg m⁻³
 Mo *K*α radiation
 μ = 1.05 mm⁻¹
T = 294 (2) K
 Block, blue
 0.24 × 0.22 × 0.22 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 1998)
T_{min} = 0.676, *T_{max}* = 0.790
 7258 measured reflections
 2676 independent reflections
 2166 reflections with *I* > 2σ(*I*)
R_{int} = 0.030
 θ_{max} = 26.4°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.040
wR (*F*²) = 0.116
S = 1.03
 2676 reflections
 195 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0621P)^2 + 4.912P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.88 e Å⁻³
 Δρ_{min} = -0.57 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—N1	2.073 (2)	Cu1—O2W	2.054 (2)
Cu1—O1W	2.088 (2)		
N1 ⁱ —Cu1—N1	79.75 (13)	O2W—Cu1—N1 ⁱ	170.24 (11)
N1 ⁱ —Cu1—O1W	95.99 (8)	O2W—Cu1—O1W	88.83 (9)
N1—Cu1—O1W	88.31 (8)	O2W ⁱⁱ —Cu1—O1W	87.45 (9)
O1W—Cu1—O1W ⁱ	174.40 (11)	O2W—Cu1—O2W ⁱ	96.74 (18)
O2W—Cu1—N1	91.95 (11)		

Symmetry code: (i) -x + 1, y, -z + ½.

Table 2

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
O1W—H1WA...O2	0.84 (5)	1.90 (3)	2.726 (3)	169 (3)
O1W—H1WB...O1 ⁱⁱ	0.85 (5)	1.96 (3)	2.805 (3)	178 (3)
O2W—H2WB...O3W	0.84 (5)	1.85 (5)	2.683 (4)	170 (4)
O2W—H2WA...O3 ⁱⁱ	0.84 (5)	1.94 (4)	2.760 (3)	165 (4)
O3W—H3WA...O1 ⁱⁱⁱ	0.85 (5)	2.42 (6)	2.915 (5)	118 (5)
O3W—H3WA...O1W ⁱ	0.85 (5)	2.59 (4)	3.299 (4)	142 (6)
O3W—H3WB...O3 ^{iv}	0.85 (5)	2.01 (8)	2.837 (4)	166 (6)

Symmetry codes: (i) -x + 1, y, -z + ½; (ii) -x + ¾, -y + ¾, -z + 1; (iii) x - ½, -y + ¾, z - ½; (iv) x - ½, y + ½, z.

Water H atoms were located in a difference map and were refined with an O—H distance restraint of 0.85 (1) Å. H atoms bound to C atoms were placed in calculated positions (C—H = 0.93 Å) and refined in the riding-model approximation, *U*_{iso}(H) = 1.2*U*_{eq}(C,O).

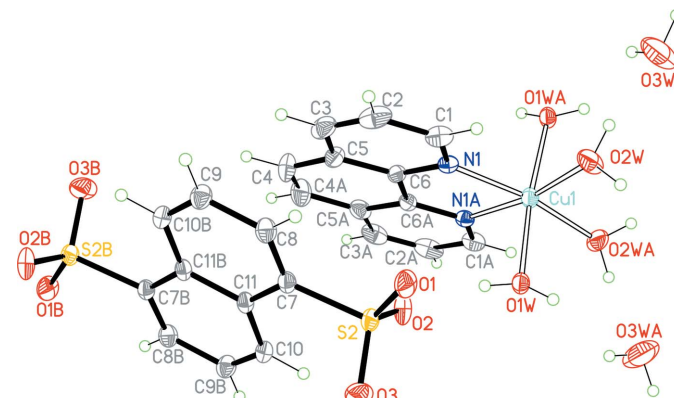


Figure 1

The asymmetric unit of (I), showing displacement ellipsoids at the 30% probability level. [Symmetry codes: (A) 1 - x, y, ½ - z; (B) ¾ - x, ½ - y, 1 - z.]

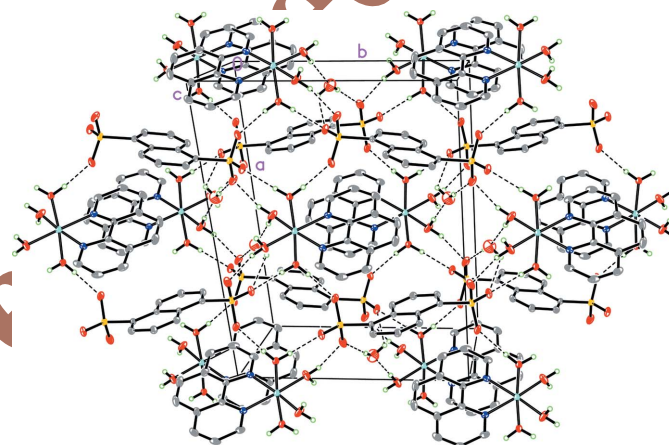


Figure 2

The structure of (I), with hydrogen bonds indicated by dashed lines.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97; molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

The authors thank Dalian Nationalities University and Academia Sinica for supporting this work.

References

Bruker (1998). SMART (Version 5.051), SAINT (Version 5.01), SADABS (Version 2.03) and SHELXTL (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
 Cai, J., Chen, C.-H., Liao, C.-Z., Yao, J.-H., Hu, X.-P. & Chen, X.-M. (2001). *J. Chem. Soc. Dalton Trans.* pp. 1137–1142.
 Cherni, S. N., Driss, A. & Jouini, T. (1999). *Acta Cryst.* **C55**, 1248–1250.
 Piguet, C., Bernardinelli, G. & Williams, A. F. (1989). *Inorg. Chem.* **28**, 2920–2925.
 Sheldrick, G. M. (1997). SHELXL97 and SHELXS97. University of Göttingen, Germany.
 Zhang, C., Yu, K., Wu, D. & Zhao, C. (1999). *Acta Cryst.* **C55**, 1815–1817.