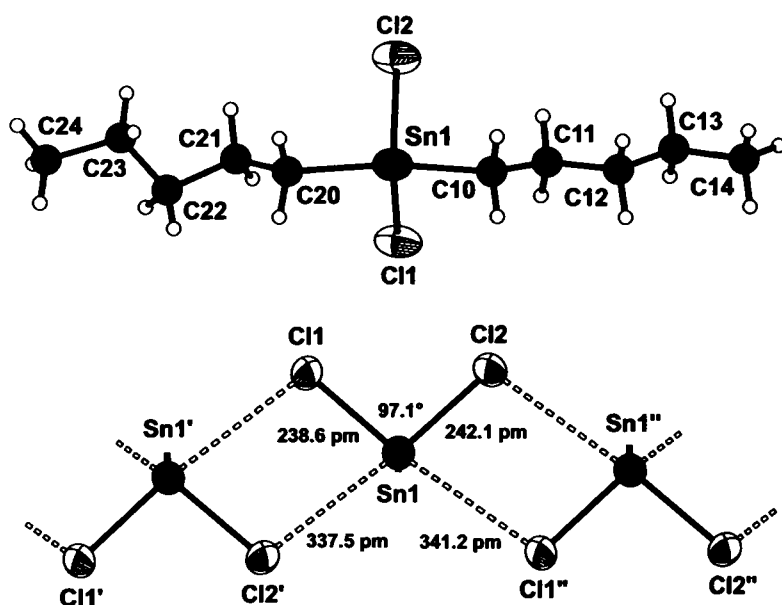


Crystal structure of dichloro-bis(*n*-pentyl)tin(IV), $\text{Sn}(\text{C}_5\text{H}_{11})_2\text{Cl}_2$, *tin-halide compounds – part VI*

H. Reuter* and M. Izaaryene

Universität Osnabrück, Institut für Chemie, Barbarastr. 7, 49069 Osnabrück, Germany

Received July 31, 2006, accepted and available on-line September 13, 2006; CCDC no. 1267/1861



Abstract

$\text{C}_{10}\text{H}_{22}\text{Cl}_2\text{Sn}$, orthorhombic, $P2_12_12_1$ (no. 19),
 $a = 6.5566(6)$ Å, $b = 9.068(1)$ Å, $c = 25.316(2)$ Å,
 $V = 1505.2$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.062$, $wR_{\text{ref}}(F^2) = 0.167$,
 $T = 258$ K.

Source of material

The title compound was synthesized according to published procedure [1]. Suitable single crystals were grown from the melt.

Experimental details

Because of the high flexibility of the *n*-pentyl rest high anisotropic thermal parameters resulted for all carbon atoms. Because this effect distorted some of the bond lengths and angles all carbon atoms were refined isotropically in addition to a common carbon-carbon bond length. Moreover, the most prominent disordering of side chain 2 was taken into account by a second position of the methylene groups C22, C23 and the methyl group C24 with side occupancy factors for both conformations of 0.75 and 0.25, respectively.

Discussion

Diorganotin dichlorides are versatile tools for the preparation of other organotin compounds. The most interesting structural features of their solid state structures result from the intermolecular interaction of the polar molecules which show in solutions of non complexing solvents a tetrahedral coordination of the tin atom. In the title compound (figure, top) this intermolecular interaction

leads to an antiparallel orientation of the dipole moments of the individual R_2SnCl_2 molecules thus forming linear chains along the *b* axis (figure, bottom).

Among the dialkyltin dichlorides, R_2SnCl_2 , those with unbranched chains ($\text{R} = \text{Me}$ [2], Et [3], Bu [4]) adopt the same arrangement as the title compound with its unbranched *n*-pentyl rest. Probably as a result of this interaction, there are significant angular distortions in the individual molecules as well as changes of the tin-chlorine bond lengths. Angular distortions from tetrahedral values are best described with respect to the C–Sn–C and Cl–Sn–Cl angles which are widened and reduced, respectively. The corresponding values are $139.6(5)^\circ/97.1(2)^\circ$ in the title compound and $142.2^\circ/98.6^\circ$ ($\text{R} = \text{Me}$), $133.8^\circ/96.0^\circ$ ($\text{R} = \text{Et}$) and $132.1^\circ/97.2^\circ$ ($\text{R} = \text{Bu}$). On the other hand intramolecular tin-chlorine bond lengths depend from the extend of the intermolecular interaction which is best described by the intermolecular tin...chlorine distances. The actual values are $242.1(4)$ pm/ $238.6(4)$ pm (average value 240.4 pm) for the intramolecular bonds and 341.2 pm/ 337.5 pm (average value 339.4 pm) for the intermolecular distances. The corresponding average values of the other compounds are 238.9 pm/ 343.3 pm ($\text{R} = \text{Me}$), 238.6 pm/ 346.2 pm ($\text{R} = \text{Et}$), and 238.1 pm/ 352.9 pm ($\text{R} = \text{Bu}$). There is a direct correlation between both bond lengths: the shorter the intermolecular contact the longer the intramolecular bonds. Dialkyltin dichlorides with branched alkyl groups adopt a somewhat different type of structure ($\text{R} = \text{Pr}$ [5]) or represent monomeric molecules in solid state ($\text{R} = \text{Bu}$ [5]). In Bu_2SnCl_2 there is no intermolecular contact shorter than 460 pm. In this case the average intramolecular tin-chlorine bond length is 233.5 pm, and the values of the angles C–Sn–C and Cl–Sn–Cl are 101.9° and 133.1° , respectively.

* Correspondence author (e-mail: hreuter@uos.de)

Table 1. Data collection and handling.

Crystal:	colorless transparent needle, size 0.12 × 0.13 × 0.15 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	20.18 cm ⁻¹
Diffractometer, scan mode:	Siemens P4, $\omega/2\theta$
$2\theta_{\max}$:	41.96°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	1860, 1554
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1461
$N(\text{param})_{\text{refined}}$:	73
Programs:	SHELXS-97 [6], SHELXL-97 [7], DIAMOND [8], SHELXTL [9]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	Occ.	x	y	z	U_{iso}
C(10)	4a		0.595(2)	0.362(2)	0.8271(6)	0.071(4)
H(101)	4a		0.5346	0.4485	0.8435	0.20(3)
H(102)	4a		0.5357	0.2755	0.8432	0.20
C(11)	4a		0.822(2)	0.363(2)	0.8371(5)	0.080(5)
H(111)	4a		0.8828	0.2792	0.8193	0.20
H(112)	4a		0.8801	0.4519	0.8220	0.20
C(12)	4a		0.874(2)	0.356(2)	0.8949(5)	0.087(5)
H(121)	4a		0.8351	0.2606	0.9087	0.20
H(122)	4a		0.7953	0.4305	0.9136	0.20
C(13)	4a		1.097(2)	0.381(3)	0.9053(7)	0.108(7)
H(131)	4a		1.1769	0.3087	0.8862	0.20
H(132)	4a		1.1361	0.4785	0.8927	0.20

Table 2. Continued.

Atom	Site	Occ.	x	y	z	U_{iso}
C(14)	4a		1.142(5)	0.370(3)	0.9635(7)	0.16(1)
H(141)	4a		1.2848	0.3861	0.9694	0.20
H(142)	4a		1.1053	0.2734	0.9758	0.20
H(143)	4a		1.0644	0.4427	0.9823	0.20
C(20)	4a		0.269(2)	0.361(2)	0.6943(4)	0.079(5)
H(201)	4a		0.1914	0.2716	0.7010	0.20
H(202)	4a		0.1817	0.4438	0.7032	0.20
C(21)	4a		0.316(1)	0.368(2)	0.6362(4)	0.14(1)
H(211)	4a		0.4381	0.3108	0.6290	0.20
H(212)	4a		0.3436	0.4697	0.6263	0.20
C(22A)	4a	0.75	0.1422(8)	0.310(1)	0.6036(4)	0.18(1)
H(22A)	4a	0.75	0.1957	0.2589	0.5729	0.20
H(22A)	4a	0.75	0.0649	0.2392	0.6243	0.20
C(23A)	4a	0.75	0.003(5)	0.432(2)	0.586(1)	0.22(2)
H(23A)	4a	0.75	0.0844	0.5179	0.5764	0.20
H(23A)	4a	0.75	-0.0857	0.4603	0.6149	0.20
C(24)	4a		-0.124(3)	0.386(3)	0.5393(8)	0.22(2)
H(24A)	4a	0.75	-0.2100	0.4664	0.5287	0.20
H(24A)	4a	0.75	-0.2067	0.303	0.5489	0.20
H(24A)	4a	0.75	-0.0360	0.3592	0.5105	0.20
C(22B)	4a	0.25	0.1422(8)	0.310(1)	0.6036(4)	0.18
H(22B)	4a	0.25	0.1796	0.2149	0.5888	0.20
H(22B)	4a	0.25	0.0240	0.2954	0.6261	0.20
C(23B)	4a	0.25	0.088(5)	0.414(4)	0.560(1)	0.22
H(23B)	4a	0.25	0.1853	0.4028	0.5309	0.20
H(23B)	4a	0.25	0.0978	0.5151	0.5723	0.20
H(24B)	4a	0.25	-0.1555	0.4557	0.5120	0.20
H(24B)	4a	0.25	-0.2198	0.3966	0.5677	0.20
H(24B)	4a	0.25	-0.1317	0.2878	0.5253	0.20

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn(1)	4a	0.5271(1)	0.3634(1)	0.74548(5)	0.0362(5)	0.0496(6)	0.0994(8)	0.0031(4)	0.0006(5)	0.0025(7)
Cl(1)	4a	0.7318(6)	0.1672(4)	0.7118(2)	0.048(2)	0.048(2)	0.124(3)	0.002(2)	0.016(2)	-0.004(2)
Cl(2)	4a	0.7313(6)	0.5646(5)	0.7116(2)	0.044(2)	0.055(2)	0.130(4)	-0.005(2)	0.017(2)	0.005(3)

References

- Schumann, H.; Schumann, I.: Gmelin Handbuch der Anorganischen Chemie, Sn, Zinn-Organische Verbindungen, Teil 6, Diorganozinndichloride, Organozintrichloride, 8. Aufl., Springer, Berlin, 1979, S. 108.
- Reuter, H.; Pawlak, R.: Zinnhalogenverbindungen. III. Neuere Daten zur Kristall- und Molekülstruktur von Dimethylzinndichlorid, Me₂SnCl₂. Z. Kristallogr. **216** (2001) 56–59.
- Alcock, N. W.; Sawyer, J. F.: Secondary Bonding. Part 2. Crystal and Molecular Structures of Diethyltin Dichloride, Dibromide, and Di-iodide. J. Chem. Soc., Dalton Trans. (1977) 1090–1095.
- Sawyer, J. F.: Dibutyltin dichloride. Acta Crystallogr. **C44** (1988) 633–636.
- Dakternieks, D.; Jurkschat, K.; Tiekink, E. R. T.: Crystal and molecular structures of diisopropyltin dichloride and di-*tert*-butyltin dichloride. Main Group Metal Chem. **17** (1994) 471–480.
- Sheldrick, G. M.: SHELXS-97. Program for the Solution of Crystal Structures. University of Göttingen, Germany, 1997.
- Sheldrick, G. M.: SHELXL-97. Program for the Refinement of Crystal Structures. University of Göttingen, Germany, 1997.
- Brandenburg, K.: DIAMOND. Visual Crystal Structure Information System. Version 2.1c. Crystal Impact, Bonn, Germany 1999.
- Sheldrick, G. M.: SHELXTL. Structure Determination Software Suite. Version 5.1. Bruker AXS, Madison, Wisconsin, USA 1995.

Instructions to Contributors

General

It is understood that contributions which are submitted to **Zeitschrift für Kristallographie – New Crystal Structures** have not, nor will be simultaneously submitted or published elsewhere unless otherwise agreed. With the acceptance of the file for publication the publishers acquire full and exclusive copyright for all languages and for all countries.

The journal contains two kinds of New Crystal Structure publications (NCS):

- (i) results of determinations of hitherto unknown crystal structures with a short discussion of determination procedure, crystal structure, and/or structure-property relations (routine determinations and structures);
- (ii) refinements of previously published crystal structures which result in crystallographic data of higher quality in comparison with previously published ones.

Each publication should contain information about one structure only. For strongly related structures (e.g. isotopes), two (exceptionally more) data sets can be included in one publication. Both, single crystal and powder data are acceptable.

Paper charge

The correspondence author is asked to pay EUR 161 (+ 16 % VAT) for each publication and should indicate his agreement clearly in the item `_publ_contact_letter` of the CIF-file.

Submission

Data files (CIF format), plot files shall be delivered via e-mail to:

e-mail: zkrist@oldenbourg.de

Samples of CIF-files can be downloaded from:

<ftp://ftp.oldenbourg.de/pub/download/frei/ncs>

For any question please ask the Technical Editor (e-mail: zkrist@oldenbourg.de) or the Managing Editor Prof. Yuri Grin (e-mail: grin@cpfs.mpg.de).

Text part

The text part of the publication should be written in English and must be positioned in the following items:

`_publ_section_exptl_prep`
`_publ_section_experimental`
`_publ_section_comment`

It is expected, that the item `_publ_section_exptl_prep` contains information about the source of the material and/or synthesis conditions, the item `_publ_section_experimental` contains information about non-routine details of the diffraction experiment and the item `_publ_section_comment` should include crystal structure description and discussion. Special details of the experiments (chemical analysis data, melting points, spectroscopic results) can be included in the text if they are absolutely necessary for the interpretation of the crystallographic data. These data will be available on-line in the CIF-file ([www.zkristallogr.de/Zeitschrift für Kristallographie - New Crystal Structures/news](http://www.zkristallogr.de/Zeitschrift_für_Kristallographie-New_Crystal_Structures/news)).

Overall volume of the text part should not exceed 2800 characters (40 lines 70 characters each).

References

References in the text should read:

Arabic number in square brackets $\Rightarrow$ [5].

References have to be ordered according to the mentioning in the text parts (see items order in the "Text part").

The software used should also be referenced and the references should be added at the end of the reference list. The authors are asked to complete data items in the `_computing` category of the CIF format containing details about the computer programs used in the crystal structure solution, refinement and analysis.

All references must be positioned in the item `_publ_section_references` and have to follow the standard rules of citation:

Journal publications:

Fitch, A. N.; Cockcroft, J. H. K.: The structure of solid carbon tetrafluoride. *Z. Kristallogr.* **203** (1993) 29–39.

Books:

Hausühl, S.: *Kristallphysik*. Physik-Verlag, Verlag Chemie, Weinheim 1983.

Articles in multi-author book publications:

Thompson, J. B.; Waldbaum, D. R.; Hovis, G. L.: Thermodynamic properties related to ordering in end member alkali feldspar. In: *The Feldspars* (Eds. W. S. MacKenzie, J. Zussman), p. 218–248. Manchester University Press 1974.

Figures

Figures can be accepted in the following format: PostScript (PS, EPS), BitMap (BMP), Windows Metafile (WMF), HPGL or TIF. The files containing figures should be submitted together with CIF-files per e-mail.

For reasons of quality the submitted figures should have the final size (85 mm wide). Letters and numbers may not be smaller than 2 mm.

Usually, only one figure is allowed for one structure. No figure caption will be printed.

International System of Units/IUPAC

The International System of Units (SI, *Système International d'Unités*) is to be used wherever possible (especially the temperature values should be given in K). Unit cell parameters and distances should be given in Å. The nomenclature should follow the IUPAC rules.

Please make sure, that you

- do not use word processors for editing CIF-files. At least the saving must be done in ASCII format.
- do not use LaTeX conventions for the text part.
- do not use non standard characters from the second half of the ASCII table (ä, Å, ç, Ç). In this case, the CIF convention should be applied (ä = "a, Å = "a); ask the editorial office for examples.

- do not write text lines longer than 80 characters.
- do not use tabs as separators in the CIF file.
- do not add or change information in the CIF items which contradicts their definition in CIF format.
- do not use word processors for preparing the plots and sending plots as WORD documents.
- do not send Bitmaps files without paying attention to the resolution of the lines and curves in the figure.
- do not forget atom labels in the figure(s) or use different labels in the figure(s) and the tables.
- do not forget to show the orientation of the unit cell (axes).

Proofs

Proofs will be sent only once to the author explicitly marked as correspondence author. Corrections are to be restricted to typographical errors. Any other changes involve time-consuming and expensive work, and the costs will be charged to the author (s).

Offprints

Thirty offprints of each article will be provided. Unless otherwise specified they will be sent to the correspondence author. Additional copies can be ordered upon return of the proofs. They will be charged according to the relevant price list.

The pdf-files of all publications are available from (www.zkristallogr.de/Zeitschrift für Kristallographie - New Crystal Structures/news).

Depositing of Data

The authors are asked to keep structure factor lists for one year after publication in case they are requested.

After the publication has been accepted, the submitted data will be deposited with the Fachinformationszentrum Karlsruhe (FIZ) or the Cambridge Crystallographic Data Centre (CCDC). Both databases provide the publisher with a deposition number which will be included in the contribution in *Zeitschrift für Kristallographie – New Crystal Structures*.

Author Index of Volume 221 Issues 1-3

- Akhtar, H., 305, 307
 Alami, M., 381
 Al-Harrasi, A., 12, 131
 Al-Resayes, S., 275
 An, Z., 372
 Arfan, M., 305
 Arif, A. M., 289, 291, 293
 Babizhetskyy, V., 1, 259
 Balalaie, S., 337, 339
 Balireddi, S., 20, 23
 Balliano, T. L., 49
 Basta, R., 289
 Bee, K., 15
 Bekaert, A., 45, 309, 381
 Beyer, C., 393
 Bildstein, B., 301, 303
 BlöB, S. P., 209
 Bogdanovic, G. A., 345
 Bolte, M., 219
 Brion, J. D., 45, 309, 381
 Brüdgam, I., 12, 131, 213, 278
 Buchta, M., 97
 Budnyk, S., 238
 Burkhardt, U., 109, 255
 Cai, T.-J., 231, 287, 335, 421
 Cai, X.-Q., 37
 Cao, F.-Q., 395
 Cao, P., 403
 Capriati, V., 398
 Caracelli, I., 159, 167
 Cardoso-Gil, R., 255, 261
 Čejka, J., 97
 Cella, R., 167
 Cerqueira Jr., C. R., 165, 311
 Chang, Y., 105
 Chen, F., 47
 Chen, X.-L., 171
 Cheng, H.-J., 197
 Cheng, M.-Q., 299, 369
 Cheng, X.-L., 105
 Chowdhury, M. A., 213
 Chruszcz, M., 359
 Cioletti, A. G., 49
 Clemente, J., 15
 Costa, M. M. R., 157
 Criado, A., 157
 Cuocci, C., 398
 Cussigh, O., 159
 Cymborowski, M., 359
 Dashjav, E., 267
 De Simone, C. A., 49, 233, 357
 Decurtins, S., 135
 Deeken, S., 93
 Deiseroth, H.-J., 119
 Demchyna, R., 109
 Deng, Q., 231, 287, 335, 421
 Deng, Y.-H., 316
 DiMuzio, S. J., 15
 Ding, J.-C., 57, 59, 83
 DiSalvo, F. J., 271
 Dobosz, M., 151
 Domingues, N. L. C., 161, 163
 Dong, J.-C., 332, 383
 Dou, Y.-L., 25, 181, 183, 185
 Doyle, C. R., 359
 Du, Z.-X., 313
 Dunstan, P. O., 159
 Eichele, K., 275
 Ernst, R. D., 289, 291, 293
 Fan, R., 183
 Feng, J.-N., 343
 Feng, W.-J., 375
 Feng, X., 296, 313
 Feng, Y.-L., 173
 Fettouhi, M., 221
 Florio, S., 398
 Frederick, J., 15
 Frey, W., 43, 87, 89, 215, 217, 347, 349
 Fu, F., 195, 391
 Fucci, A., 15
 Fukuda, Y., 123, 126, 129
 Galanski, M., 226
 Galdino, S. L., 357
 Gao, H.-W., 332, 383
 García-Granda, S., 241
 García-Hernández, Z., 419
 Gautier-Luneau, I., 243, 245, 247, 249
 Gawlicka-Chruszcz, A., 359
 Giorgi, M., 75
 Gjikaj, M., 121
 Glatz, G., 411
 Göbel, S., 257
 Góger, S., 75
 Gordon, L., 15
 Goulart, M. O. F., 49
 Grin, Yu., 238, 261, 263, 265
 Grüner, D., 269
 Gu, S.-J., 200
 Guarda, V. L. M., 357
 Guérin, R., 259
 Gulla, M., 89, 215, 217
 Guo, H., 321
 Guo, H.-M., 352
 Guo, J.-X., 195
 Guo, J.-Y., 229, 281
 Guo, S., 393
 Guo, W.-F., 27
 Ha, K., 363, 365, 367
 Haarmann, F., 257
 Han, M.-L., 313
 Han, X., 296
 Han, X.-Q., 73
 Harper, A., 15
 Hartl, H., 12, 131, 213, 278
 Harvey, B. G., 291
 Haug, E., 43
 Haukka, M., 226
 Hauptmann, R., 393
 Haussühl, E., 35, 77
 He, D.-P., 25
 He, Y., 105
 He, Y.-H., 142
 Herberhold, M., 419
 Hinrichs, F., 121
 Hoffmann, S., 251, 253
 Holthouse, B., 91
 Horn, E., 123, 126, 129
 Hou, Y.-Q., 51
 Hu, M.-L., 37, 39, 47, 375
 Hu, X.-J., 203, 327, 329
 Huang, S.-J., 273
 Humberto, M. M. S., 233
 Hunter, A. D., 15
 Hušák, M., 97
 Hwang, I.-C., 363, 365, 367
 Iqbal, R., 305, 307
 Irrgang, T., 20, 23, 93, 95, 283, 411, 413, 415, 419
 Isab, A. A., 221
 Izaaryene, M., 423
 Jäger, V., 87, 89, 215, 217, 347, 349
 Jansen, M., 206, 209
 Jegorov, A., 97
 Jégou, A., 87
 Jiang, W.-J., 231, 287, 335, 421
 Jiménez, A., 241
 Jin, Q.-H., 332, 383
 Jin, Z.-M., 375
 Jing, L.-H., 200
 Ju, Y.-L., 7, 9
 Kaizer, J., 75
 Kaluderovic, G. N., 345
 Kantelehnner, W., 43
 Karthikeyan, S., 20, 23, 95
 Kasmar, A., 15
 Kasmar, C., 15
 Keller, H.-L., 377, 379
 Kelly, P. F., 226
 Kempe, R., 20, 23, 93, 95, 153, 283, 411, 413, 415, 419
 Keppler, B. K., 226
 Khan, G. S., 153
 Kim, T. H., 367
 Kniep, R., 251, 253, 267
 Koizumi, R., 123
 Kollmann, T., 393
 Kong, F.-Y., 341
 Kopacka, H., 301, 303
 Koziol, A. E., 151
 Kratochvíl, B., 97
 Kreiner, G., 267, 269
 Królikowska, M., 155
 Kuhn, P., 31
 Kukushkin, V. Yu., 226
 Kulsomphob, V., 293
 Kuz'ma, Yu. B., 238
 Kuzma, M., 97
 Labat, G., 135
 Lamenha, G. S., 233
 Lan, K., 171
 Laurent, M., 68, 71
 Laus, G., 103
 Le Bras, G., 381
 Lee, Y. B., 367
 Lei, X.-X., 37
 Leithe-Jasper, A., 255
 Lemoine, P., 45, 309, 381
 Li, C., 323
 Li, D.-S., 85, 195, 391
 Li, J., 51, 85, 319
 Li, M.-F., 41
 Li, P., 179
 Li, P.-G., 391
 Li, P.-Z., 332, 383
 Li, T.-B., 55
 Li, T.-H., 169
 Li, X., 5, 7, 9
 Li, Y., 203, 327, 329
 Li, Z.-F., 211
 Lima, F. S., 161, 163
 Lin, H., 173
 Liu, C.-H., 401, 403, 405, 407, 409
 Liu, H.-Q., 185
 Liu, J.-K., 203, 327, 329
 Liu, L.-H., 229
 Liu, M.-C., 57, 59, 83
 Liu, S.-X., 135
 Liu, W.-J., 323
 Liu, W.-L., 223
 Liu, X.-F., 223

- Liu, Z.-H., 179, 189
 Long, Y.-F., 231, 287, 335, 421
 Loosli, C., 135
 Lorch, M., 219
 Louati, A., 31
 Lu, Y., 197
 Lü, Z.-X., 145
 Luisi, R., 398
 Lukachuk, M., 3
 Luo, Y.-H., 327, 329
 Ma, J.-Y., 53
 Ma, L.-F., 299, 369
 Ma, P.-T., 235, 319
 Ma, Z.-C., 65
 Maganhi, S., 165
 Maisel, H., 411
 Maliszewska-Guz, A., 151
 Malta, V. R. S., 49, 233
 Mao, X.-B., 169
 Mao, Z.-H., 200
 Marchand-Brynaert, J., 68, 71
 Matos Gomes, E., 157
 Matt, D., 31
 Mattausch, H., 1, 3
 Mazur, L., 151
 McKay, S. E., 91
 Menezes, P. W., 251, 253
 Minor, W., 359
 Miyamoto, K., 123, 126, 129
 Mondino, M. G., 161, 163
 Nasiri, H. R., 219
 Neels, A., 135
 Niu, J.-Y., 235
 Noor, A., 153, 283, 415
 Nuss, H., 206
 Nuss, J., 209
 Odoko, M., 395
 Okabe, N., 395
 Oldag, T., 377, 379
 Olivato, P. R., 161, 163, 165, 311
 Oliveira da Silva, R., 311
 Oloumi, Z., 337, 339
 Ormeci, A., 269
 Oryshchyn, S., 259
 Pan, X.-F., 53
 Peng, Z.-S., 231, 287, 335, 421
 Pereira, M. A., 49
 Peyrat, J.-F., 381
 Phanon, D., 243, 245, 247, 249
 Pitta, I. R., 357
 Pitucha, M., 151
 Polomsky, S., 15
 Porto, K. R. A., 233
 Prieto, M., 241
 Prots, Yu., 109, 112, 115, 238, 251, 253, 257, 263, 265
 Qadeer, S., 153, 305, 307
 Qi, G.-C., 391
 Qin, D.-B., 200
 Rahmani, H., 133
 Rama, N. H., 153
 Ramlau, R., 255
 Reckeweg, O., 271
 Réglie, M., 75
 Reis, A. K. C. A., 161, 163
 Reißig, H.-U., 12, 131, 213, 278
 Ren, F.-J., 229, 281
 Reuter, H., 423
 Richter, K. W., 112, 115
 Rittner, R., 161, 163
 Rodrigues, A., 311
 Rodrigues, V. H., 157
 Rodríguez, J. D., 241
 Rominger, F., 337, 339
 Sabo, T. J., 345
 Salomone, A., 398
 Samareh Afsari, H., 133
 Sant'Ana, A. E. G., 233
 Scaffidi-Domianello, Yu. Yu., 226
 Schmalz, T., 95
 Schmidt, M., 263
 Schneider, J. J., 393
 Schnelle, W., 109, 263, 267
 Schottenberger, H., 103
 Schreuer, J., 35, 77
 Schwalbe, H., 219
 Schwarz, U., 109
 Sedmera, P., 97
 Shan, Y.-K., 41
 Shao, J., 405
 Shaw, D., 87
 She, J.-B., 25, 181, 183, 185
 She, X.-G., 53
 Shi, J., 176
 Shi, X., 145
 Shi, X.-Y., 148
 Shi, Y.-C., 197
 Shiva, S., 347, 349
 Sichevych, O., 261, 263, 265
 Simmons, A., 15
 Simon, A., 1, 3
 Skrzypczak, A., 155
 Smallsreed, D., 15
 Song, Q.-B., 169, 285
 Sörgel, S., 278
 Spannenberg, A., 413
 Speier, G., 75
 Stefani, H. A., 167
 Steiner, G., 301, 303
 Stoyko, S., 259
 Strasser, C. E., 103
 Su, H., 173
 Sun, J., 273
 Tai, X.-S., 341
 Tang, L., 85, 195
 Tinant, B., 68, 71
 Torre-Fernández, L., 241
 Toupet, L., 31
 Trindade, A. C., 159
 Tu, S.-J., 343
 Underwood, T., 15
 Velasquez, N., 49
 Vinhato, E., 165, 311
 Viossat, B., 45, 309, 381
 von Schnering, H. G., 257
 Wagner, F. R., 267
 Wang, A.-Q., 321
 Wang, C., 51
 Wang, C.-C., 385, 388
 Wang, F.-W., 325
 Wang, G.-X., 101, 187, 211
 Wang, H., 375
 Wang, J.-J., 85
 Wang, J.-P., 235, 319
 Wang, J.-W., 85, 195
 Wang, L.-Y., 296, 299, 369
 Wang, P., 107, 211
 Wang, Q.-L., 391
 Wang, R.-J., 203, 327, 329
 Wang, R.-S., 372
 Wang, S.-F., 409
 Wang, W.-D., 375
 Wang, X.-L., 361
 Wang, X.-Q., 27, 55
 Wang, Y., 395
 Wang, Y.-H., 352
 Wang, Y.-L., 27
 Warad, I., 275
 Wazeer, M. I. M., 221
 Wei, D.-Y., 273
 Wei, J.-F., 148
 Wei, Y.-J., 325
 Wen, Y.-H., 142
 Werz, D. B., 337, 339
 Wheeler, K. A., 91
 Wiehl, L., 35, 77
 Wong, W.-Y., 305, 307
 Wrackmeyer, B., 419
 Wu, H.-Y., 57, 59, 83
 Wu, M.-H., 323
 Wu, R.-F., 229, 281
 Wu, T., 281
 Wu, T.-X., 53
 Wu, Y., 321
 Wujec, M., 151
 Wurst, K., 103, 301, 303
 Xin, X.-L., 332, 383
 Xiong, J., 37, 39
 Xu, D., 27, 55
 Xu, S.-P., 401, 403, 405, 407, 409
 Xu, W., 107
 Yang, H.-J., 203, 327, 329
 Yang, L., 229, 281, 332, 383
 Yang, X.-H., 323
 Yang, X.-J., 316
 Yang, Y.-L., 316
 Yin, M.-H., 181
 Yin, P., 39
 Yu, L., 319
 Yu, W., 229, 281
 Yu, W.-T., 27, 55
 Yu, Y.-Y., 63
 Yuan, J.-X., 37, 39
 Yue, G.-R., 73
 Zaidi, J. H., 307
 Zaiss, T., 119
 Zareef, M., 305, 307
 Zeller, M., 15
 Zhang, B.-S., 191, 352, 355
 Zhang, F.-X., 51
 Zhang, G.-F., 181, 183, 185
 Zhang, G.-H., 27, 55
 Zhang, G.-L., 223
 Zhang, H., 203, 327, 329
 Zhang, H.-X., 200
 Zhang, J., 285
 Zhang, J.-G., 229, 281
 Zhang, L.-J., 57, 83
 Zhang, M.-L., 195
 Zhang, Q.-W., 101, 187
 Zhang, T.-L., 229, 281
 Zhang, T.-T., 7, 9
 Zhang, W.-J., 189
 Zhang, X.-L., 80
 Zhang, X.-Q., 80
 Zhang, Z.-T., 80, 176
 Zhao, G.-L., 145
 Zhao, L.-F., 29
 Zhao, M.-G., 61
 Zhao, S.-M., 185
 Zheng, Y.-Q., 107, 273
 Zhou, C.-H., 85
 Zhou, R., 197
 Zhou, Y.-Z., 343
 Zhu, C.-H., 407
 Zhu, H.-J., 343
 Zhu, Y., 401
 Zimmerman, M. D., 359
 Zonouzi, A., 133
 Zou, W.-D., 323
 Zukerman-Schpector, J., 159, 161, 163, 165, 167, 311

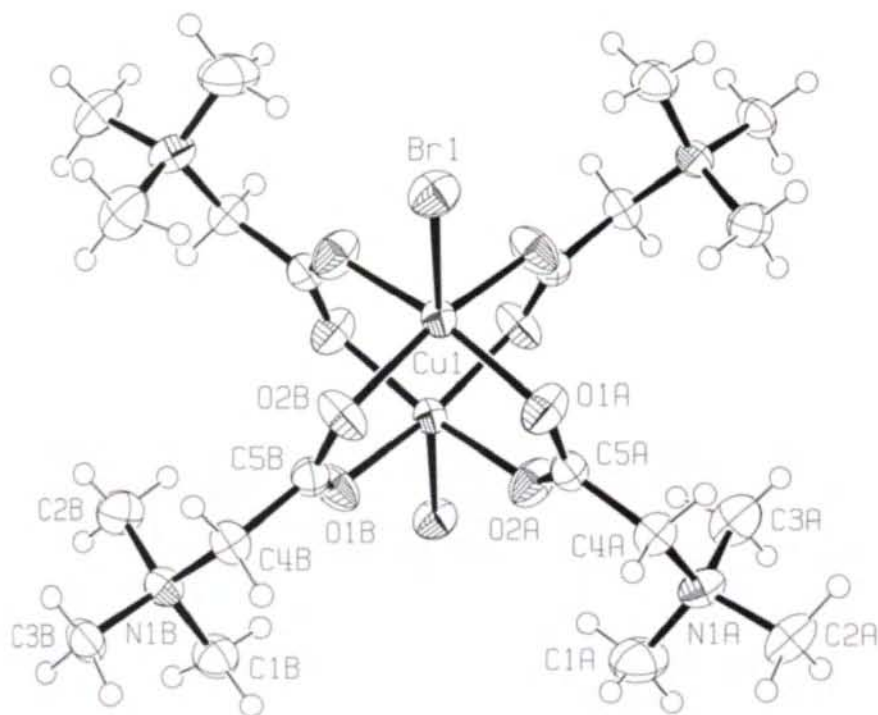
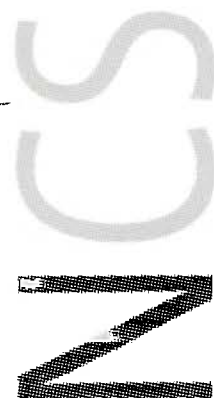
Formulae Index of Volume 221 Issues 1-3

- Ag₉AlS₆, 119
 Al₂₃Co₁₀Si₈, 112
 Al_{42.51}Co_{19.49}Si_{12.49}, 115
 Al_{43.14}Co_{18.86}Si_{11.86}, 115
 As₂Ca₂H₁₃NaO₁₄, 241
 BHKO₉P₂Sc, 251
 BHO₉P₂RbSc, 253
 B₂C₅Pr₅, 1
 Ba_{0.73}Eu_{0.27}Ge₃Pt, 109
 BaGe₃Pt, 109
 BiH₄I₃O₁₁, 243
 Br₁₄K₂Mo₆, 107
 CMo₂PrSi₂, 267
 C₃H₃CuN₂, 377
 C₄H₇BF₃KS₂, 167
 C₅H₃N₃O₅, 183
 C₆H₅FN₂O₄, 57
 C₆H₇N₃O, 307
 C₆H₈BrN₃O₂, 49
 C₆H₉N₅Pd, 379
 C₆H₁₂Br₂N₄S₂Zn, 221
 C₆H₁₆Cl₄NOTa, 209
 C₇H₇BrN₂O, 305
 C₇H₇CuNO₆, 35
 C₇H_{12.5}Br_{1.5}NO, 215
 C₇H₂₂ClMnN₄O₄, 405
 C_{7.5}H_{12.5}B₅N_{1.5}O₁₀, 189
 C₈H₈FN₃O₅, 37
 C₈H₁₂N₆S₂, 151
 C₈H₁₃ClN₄O₇, 375
 C₈H₁₈Cl₄N₂O₄Pt, 345
 C₈H₂₅Br₂N₃NiO₃, 129
 C₉H₁₀N₄O₄, 59
 C₉H₁₁O_{4.5}, 187
 C₉H₁₄BrNO, 89
 C₉H₁₄CuN₆O₅S, 195
 C₁₀H₈O₂, 337
 C₁₀H₁₃NO₁₀, 229
 C₁₀H₁₅I₃O, 393
 C₁₀H₁₆N₆NiO₁₆, 61
 C₁₀H₂₂Cl₂Sn, 423
 C₁₀H₂₆B₂₀Se₄, 419
 C₁₁H₉ClN₂OS, 43
 C₁₁H₉FN₂O₂, 83
 C₁₁H₁₂BrNO, 217
 C₁₁H₁₄Cl₄CuN₂O, 53
 C₁₁H₁₄N₂O₅S, 161
 C₁₂H₁₀CuMoN₂O₅, 335
 C₁₂H₁₀F₂N₂O₃, 359
 C₁₂H₁₄Cl₅FeN₈, 47
 C₁₂H₁₄N₂O₃S, 357
 C₁₂H₁₄O₂S, 311
 C₁₂H₁₄O₇, 153
 C₁₂H₁₆K_{1.67}O₁₅Rb_{0.33}, 157
 C₁₂H₁₉N₂O₆V, 343
 C₁₃H₁₆N₂OS, 367
 C₁₄H₁₁N₅O₇, 29
 C₁₄H₁₅N₃O₃, 341
 C₁₄H₁₆BrCuN₃O₄, 383
 C₁₄H₁₈CdN₂O₇, 395
 C₁₄H₂₁IN₂O₆, 87
 C₁₅H₁₂O, 323
 C₁₅H₁₇BrO₅, 278
 C₁₅H₂₆Dy₂O₁₈, 273
 C₁₅H₃₃Cl₄CoMnN₃O₆, 77
 C₁₅H₃₃Cl₄MnN₃O₆Zn, 77
 C₁₆H₁₄N₂O₄Pb, 299
 C₁₆H₁₆BNO₆, 179
 C₁₆H₂₁NO₅S, 165
 C₁₆H₂₂V, 289
 C₁₆H₂₈N₈O₈S₂, 281
 C₁₇H₁₆N₂O₂, 349
 C₁₇H₁₆N₈S₂, 185
 C₁₇H₁₉FN₄O₆, 39
 C₁₇H₂₃N₃O₇, 133
 C_{17.5}H₂₁Cl₂NO₂PtS₂, 226
 C₁₈H₁₅CdN₂O₅, 421
 C₁₈H₁₅N₃O, 211
 C₁₈H₁₆ClNO₂S, 163
 C₁₈H₁₇ClN₂O₂, 347
 C₁₈H₁₈N₂O₆Zn, 287
 C₁₈H₂₀CuN₄O₇, 369
 C₁₈H₂₀N₂, 233
 C₁₈H₂₁NO₈S, 105
 C₁₈H₂₆B₂F₈N₁₂Ni₂O₂, 403
 C₁₈H₂₆Cl₂Co₂N₁₂O₁₀, 401
 C₁₈H₂₇Al₄Cl₄N₃O₁₃, 309
 C₁₈H₃₀Cu₃O₂₄, 101
 C₁₈H₄₉Cl₄IN₆Ni₃O, 123
 C₁₈H₄₉Cl₄I₃N₆Ni₃O, 126
 C₁₉H₁₇BrClNO, 321
 C₁₉H₁₇O₂P, 171
 C₁₉H₂₁NO₄, 361
 C₁₉H₂₂FeN₅O₂S, 296
 C₁₉H₂₃NO₂, 398
 C₁₉H₂₅NO, 145
 C_{19.5}H₂₆N₂O_{1.5}, 219
 C₂₀H₁₄O₄, 339
 C₂₀H₁₈Br₂CoN₂O₂, 325
 C₂₀H₁₈CuN₄O₆, 73
 C₂₀H₂₀HgN₂S₁₀, 27
 C₂₀H₂₂N₈S₂, 25
 C₂₀H₂₈ClMnN₂O₇, 363
 C₂₀H₃₀F₂Ti, 206
 C₂₀H₃₉ClN₂O₂, 155
 C₂₀H₄₄Cl₂Mn₂N₈O₁₂, 407
 C₂₁H₃₀ClMnN₂O₇, 365
 C₂₂H₂₀CoF₆PRu, 103
 C₂₂H₃₀N₃P, 411
 C₂₂H₄₆N₂₄O₁₆, 313
 C₂₂H₄₉NO₅Si₂, 131
 C₂₃H₂₄O₁₁, 80
 C₂₃H₂₇NO₃, 68, 71
 C₂₃H₂₇NO₄, 213
 C₂₃H₂₈CoN₃O₄, 409
 C₂₄H₁₄Cu₂N₄O₂, 319
 C₂₄H₁₆AgN₅O₃, 391
 C₂₄H₁₆F₂N₂O₄Pb, 355
 C₂₄H₂₆Cl₂CrN, 303
 C₂₄H₂₇N₃O₃, 285
 C₂₄H₃₂N₂O₂, 63
 C₂₄H₃₈Zr, 291
 C₂₅H₁₃N₇O₂, 91
 C₂₅H₂₂N₄NiO₇, 85
 C₂₅H₄₂AuNS₁₀, 55
 C₂₆H₂₃N₃O₃, 169
 C₂₆H₃₂Mo₈N₄O₂₆, 388
 C₂₆H₄₂N₄RuSi₂, 93
 C₂₇H₁₉CdClN₄O₂, 231
 C₂₈H₂₃MnN₂O₅, 51
 C₂₈H₂₈N₂NiO₄, 159
 C₂₈H₂₈N₄O₈S₂, 200
 C₂₈H₄₆Br₂Cu₂N₈O₄, 181
 C₂₈H₄₉NO₅Si₂, 12
 C₂₉H₂₀O₇, 176
 C₃₀H₂₄Br₄O₄, 327
 C₃₀H₃₆N₄O₁₄U₂, 45
 C₃₂H₂₆Fe₂O₄, 197
 C₃₂H₄₈Cl₂Cr₂N₈O₂Si₄, 413
 C₃₃H₂₈N₂O₂, 65
 C₃₃H₄₄Cl₂N₂O₂P₂Ru, 275
 C₃₄H₅₃N₃Zr, 293
 C₃₅H₂₂BF₁₅N₂, 283
 C₃₆H₂₆Cu₂N₄O_{6.5}Pb, 352
 C₃₆H₃₀Cl₄O₂P₂Ti, 41
 C₃₆H₃₂N₄P₂Pt, 95
 C₃₆H₄₂N₈, 23
 C₃₆H₆₀N₈Si₄Zr, 415
 C₃₈H₂₉Cl₂N₄O_{6.5}Pb, 352
 C₃₉H₄₄O₁₂P₂W, 148
 C_{39.33}H₄₂Cl₄Cu₂N₆O_{8.67}, 75
 C₄₀H₃₅Cl₂Cu₂N₃P₂, 332
 C₄₀H₄₈BaF₂N₆O₁₅, 372
 C₄₃H₄₂N₈O, 20
 C₄₄H₄₂N₂O₁₂, 381
 C₄₄H₅₀Cl₂N₆Pd, 301
 C₄₈H₆₄Br₂N₂O₆, 203
 C₄₈H₆₆N₂O₆, 329
 C₄₉H₄₀O₅, 31
 C₄₉H₆₂N₂O₁₄, 97
 C₅₄H₄₈Cl₄CuN₄O₈, 15
 C₅₄H₄₈Cl₄N₄NiO₈, 15
 C₅₄H₅₀Cl₄N₄O₈, 15
 C₆₀H₇₂Cl₄Cu₄N₁₂O₂₈, 223
 C₆₂H₆₄Cu₂I₂O₄P₄, 316
 C₆₆H₄₀Cl₆La₂N₄O₁₂, 191
 C₆₆H₄₀Dy₂F₆N₄O₁₂, 7
 C₆₆H₄₀F₆N₄Nd₂O₁₂, 5
 C₇₂H₆₄Cu₆N₁₂O₃₅, 142
 C₇₈H₇₀N₄O₁₂Sm₂, 9
 C₈₁H₇₄DyN₁₇O₂, 135
 C₈₁H₇₅N₁₇O_{2.50}Tb, 135
 C₉₂H₁₄₀Cl₆Cu₂N₆O₃₈, 173
 Cr_{1.02}NbNi_{0.98}, 269
 EuGa₂, 261
 EuGe₃Pt, 109
 Eu₂Ga₃Ir, 263
 Eu_{2.88}Ga_{8.36}, 265
 Ga_{8.45}Sr_{2.85}, 257
 Gd₃P₄Pd₇, 238
 Gd₄GeI₆, 3
 H₄I₃InO₁₁, 247
 H₄I₃O₁₁Yb, 245
 H₆I₃InO₁₂, 249
 H₂₄MgN₂O₈P₂S₆, 121
 H₁₁₄MnNa₆Nb₁₂O₉₂, 235
 I₂OSr₂, 271
 Ni₄₂P_{30.34}Y₂₀, 259
 P₄Pd₇Tb₃, 238
 Rh₇Sb₆Yb₄, 255

Zeitschrift für Kristallographie

**NEW CRYSTAL
STRUCTURES**

1741-1192



Volume 221 4/2006

Zeitschrift für Kristallographie – New Crystal Structures

International journal for structural, physical, and chemical aspects of crystalline materials

Zeitschrift für Kristallographie – New Crystal Structures offers a place for researchers to present

- (i) results of determinations of hitherto unknown crystal structures which do not justify detailed discussion of determination procedure, crystal structure, and/or structure-property relations (routine determinations and structures),
- (ii) refinement of previously published crystal structures which do not require a new description or discussion.

New Crystal Structures (NCS) have to be submitted as CIF-file to: zkrist@oldenbourg.de

Oldenbourg Wissenschaftsverlag
Lektorat MINT
Kristin Berber-Nerlinger
Postfach 80 13 60
81613 München
oldenbourg.de

Tel.: 49/89/4 50 51–3 24
Telefax: 49/89/4 50 51–2 92
E-mail: berber@oldenbourg.de
zkristallogr.de

Editor in chief:
Professor Walter Steurer
ETH Hönggerberg HCI G 511
Laboratorium für Kristallographie
Wolfgang-Pauli-Straße 10, 8093 Zürich, Switzerland
e-mail: Walter.Steurer@mat.ethz.ch; Fax: +41-1-6 32 11 33

Managing Editor:
Professor Yuri Grin
Max-Planck-Institut für Chemische Physik fester Stoffe
Nöthnitzer Str. 40, 01187 Dresden, Germany
e-mail: grin@cpfs.mpg.de; Fax: +49-3 51-46 46-33 40

Technical Editor:
Dr. Gernot Zahn
e-mail: zkrist@oldenbourg.de

For detailed information please see the **Instructions to Contributors**. They are printed in Issue 1 and 3 of each Volume and are available at: zkristallogr.de

© Copyright 2006 by Oldenbourg Wissenschaftsverlag GmbH, D-81671 München.

All rights reserved (including translation and storage by electronic means). No part of this issue may be reproduced in any form – by photoprint, microfilm, or any other means – nor transmitted or translated into a machine language without written permission from the publisher.

The journal has been registered with the Copyright Clearance Center (CCC), 27 Congress Street, Salem, MA 01970, U.S.A., under the fee code 1433-7266. Registered names, trademarks, etc. used in this journal, even when not marked as such, are not to be considered unprotected by law.

Z. Kristallogr. NCS 221 (2006)
ISSN 1433-7266
Oldenbourg Wissenschaftsverlag, München

Subscription information

Volume 221: 4 issues will appear in 2006

Annual subscription prices: EUR 278.— + postage:

EUR 19.— (Germany), EUR 27.— (elsewhere).

Single issue: EUR 84.— + postage.

For EU countries all prices are including 7% VAT, for all other countries they are gross prices.

Orders can either be placed with your bookdealer or sent directly to the publisher.

Cancellation of subscription

The publisher must be notified not later than three months before the end of the calendar year.

Setting and printing

Druckhaus „Thomas Müntzer“ GmbH, Bad Langensalza

Front cover, with the friendly assistance of Dr. Leonore Wiehl: Crystal structure of tetrakis(μ -betaine-O,O')-dibromo-dicopper(II) dibromide dihydrate, $[\text{Cu}_2\{(\text{CH}_3)_3\text{-NCH}_2\text{COO}\}_4\text{Br}_2]\text{Br}_2 \cdot 2 \text{H}_2\text{O}$, with a propeller-shaped dinuclear copper complex (cf. figure of L. Wiehl *et al.*, this issue pp. 527–528).

Zeitschrift für Kristallographie New Crystal Structures

Volume 221 • Issue 4 • 2006

Inorganic Crystal Structures

R. Gumeniuk, H. Borrmann and A. Leithe-Jasper
Refinement of the crystal structures of trinickel boron, Ni_3B , and tripalladium boron, Pd_3B 425

R. Demchyna, Yu. Prots, U. Burkhardt, U. Schwarz and Yu. Grin
Crystal structure of hafnium palladium gallium, HfPdGa .. 427

P. W. Menezes, S. Hoffmann, Yu. Prots and R. Kniep
Crystal structure of calcium nickel(II) (monohydrogen-monophosphate-dihydrogenmonoborate-monophosphate), $\text{CaNi}[\text{BP}_2\text{O}_7(\text{OH})_3]$ 429

H. B. Tanh Jeazet, P. W. Menezes, S. Hoffmann, Yu. Prots and R. Kniep
Crystal structures of lead(II) cobalt(II) (monophosphate-hydrogenmonoborate-monophosphate), $\text{PbCo}[\text{BP}_2\text{O}_8(\text{OH})]$, and lead(II) zinc(II) (monophosphate-hydrogenmonoborate-monophosphate), $\text{PbZn}[\text{BP}_2\text{O}_8(\text{OH})]$ 431

V. Smetana, V. Babizhetskyy, C. Hoch and A. Simon
Refinement of the crystal structure of barium tetralithium, BaLi_4 434

M. Zelinska, J.-Y. Pivan, S. Oryshchyn, O. Zhak, M. Potel, O. Tougait and H. Noel
Crystal structure of erbium palladium phosphor (3:20:6), $\text{Er}_3\text{Pd}_{20}\text{P}_6$ 435

C. Ehrhardt and M. Gjikaj
Crystal structure of strontium hexathiodiphosphate(IV) decahydrate, $\text{Sr}_2[\text{P}_2\text{S}_6] \cdot 10\text{H}_2\text{O}$ 437

Organic and Metalorganic Crystal Structures

J.-X. Guo, F. Fu, D.-S. Li, J. Li, L. Tang and G.-C. Qi
Crystal structure of tetraaqua-bis(4-(5-tetrazolato)pyridyl-*N*)zinc(II) dihydrate, $\text{Zn}(\text{H}_2\text{O})_4(\text{C}_6\text{H}_4\text{N}_5)_2 \cdot 2\text{H}_2\text{O}$ 439

L. Tang, D.-S. Li, F. Fu, J. Li, X.-Z. Zhao and J.-W. Wang
Crystal structure of tetraaqua-bis(3-(3-acrylato)pyridyl-*N*)zinc(II), $\text{Zn}(\text{H}_2\text{O})_4(\text{C}_8\text{H}_6\text{O}_2\text{N})_2$ 441

L. Chen
Crystal structure of bis(pyridin-2-yl)disulfide hydrotriiodide, $[\text{C}_{10}\text{H}_9\text{N}_2\text{S}_2][\text{I}_3]$ 443

X.-Y. Shi and J.-F. Wei
Crystal structure of diaqua-bis((*E*)-4-hydroxy-3-((2-hydroxyethylimino)-methyl)-5-(morpholinomethyl)-benzenesulfonato)dycopper(II) diperchlorate hexahydrate, $[\text{Cu}_2(\text{H}_2\text{O})_2(\text{C}_{14}\text{H}_{19}\text{N}_2\text{O}_3\text{SO}_3)_2][\text{ClO}_4]_2 \cdot 6\text{H}_2\text{O}$ 445

W.-K. Dong, J.-H. Feng and X.-Q. Yang
Crystal structure of 4,4'-dibromo-2,2'-((1,3-propylene)-dioxibis(nitrilomethylidyne)diphenol, $\text{C}_{16}\text{H}_{16}\text{Br}_2\text{N}_2\text{O}_4$... 447

Y.-Z. Zhou, X.-M. Zhang and J.-N. Feng
Crystal structure of 2-aminoethylammonium (2-oxyacetophenone benzoylhydrazonato)dioxovanadate(V), $[\text{H}_2\text{N}(\text{CH}_2)_2\text{NH}_3][\text{VO}_2(\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_3)]$ 449

L. Zhu, L.-H. Zhang, B.-Y. Liu and Z. An
Crystal structure of diaquabis(1,10-phenanthroline)-nickel(II) sulfate hydrate (1:5:6), $[\text{Ni}(\text{H}_2\text{O})_2(\text{C}_{12}\text{H}_8\text{N}_2)_2][\text{SO}_4] \cdot 5.6\text{H}_2\text{O}$ 451

G.-X. Wang and Q.-W. Zhang
Crystal structure of bis(5-ammonioisophthalic acid) sulfate dihydrate, $(\text{C}_8\text{H}_8\text{NO}_4)_2[\text{SO}_4] \cdot 2\text{H}_2\text{O}$ 453

S. Ricken, F. Koç, M. Schürmann, H. Preut and P. Eilbracht
Crystal structure of *N,N,N',N',N'',N'''*-hexakis(2-methylallyl)-[1,3,5]-triazin-2,4,6-triamine, $\text{C}_{27}\text{H}_{42}\text{N}_6$ 455

L.-F. Ma, F. Zhong and G.-Y. Zhang
Crystal structure of tetraaqua-*cis*-bis(*N*-2-nitrobenzenesulfonylglycinato)manganese(II), $\text{Mn}(\text{H}_2\text{O})_4(\text{C}_8\text{H}_7\text{N}_2\text{O}_6\text{S})_2$... 457

X. Feng, Y.-F. Wang, L.-Y. Wang
Crystal structure of (μ -4,4'-bipyridine-*N,N'*)bis(*N,N'*-ethylene-bis(salicylaldimino))dizinc(II) methanol disolvate, $\text{Zn}_2(\text{C}_{10}\text{H}_8\text{N}_2)(\text{C}_{16}\text{H}_{14}\text{N}_2\text{O}_2)_2 \cdot 2\text{CH}_3\text{OH}$ 460

R. J. Abdel-Jalil, W. Voelter, C. Maichle-Mössmer, Y. Baqi and H.-J. Machulla
Crystal structure of 2-(3-acetyl-1-(4-bromophenyl)-5-((*R*)-4-chlorophenyl)-1,2,4-triazolo-4-yl)-2-deoxy-1,3,4,6-tetraacetyl- β -D-glucose, $\text{C}_{30}\text{H}_{31}\text{BrClN}_3\text{O}_{10}$ 463

A.-R. Song, I.-C. Hwang and K. Ha
Crystal structures of dichloro((1,2,5,6- η)-1,3,5,7-cyclooctatetraene)platinum(II), $\text{PtCl}_2(\text{C}_8\text{H}_8)$, and diiodo((1,2,5,6- η)-1,3,5,7-cyclooctatetraene)platinum(II), $\text{PtI}_2(\text{C}_8\text{H}_8)$ 465

I.-C. Hwang and K. Ha
Crystal structure of aqua(*N,N,N',N'*-tetrakis(2-pyridylmethyl)-1,2-diaminocyclohexane)manganese(II) dibromide tetrahydrate, $[\text{Mn}\{\text{C}_6\text{H}_{10}\text{N}_2(\text{C}_6\text{H}_6\text{N})_4\}(\text{H}_2\text{O})]\text{Br}_2 \cdot 4\text{H}_2\text{O}$ 468

- A.-R. Song, I.-C. Hwang and K. Ha
Refinement of the crystal structure of μ -((1,2,5,6- η :3,4,7,8- η)-1,3,5,7-cyclooctatetraene)bis(dimethylplatinum(II)), [Pt(CH₃)₂]₂(C₈H₈), at 243 K. 471
- M.-L. Zhang, H.-J. Bai, F.-G. Xin and Z.-L. Wang
Crystal structure of *N,N'*-bis(2-hydroxy-3-methoxybenzyl)oxalamide, C₁₈H₂₀N₂O₆ 473
- X.-X. Lei, Z.-F. Chen, L.-X. Zhang and A.-J. Zhang
Crystal structure of 3-(1-naphthylmethyl)-6-phenyl-7H-1,2,4-triazolo[3,4-*b*][1,3,4]-thiadiazine, C₂₁H₁₆N₄S 475
- Z.-Z. He, X.-X. Lei, Y. Zhou, J.-Z. Sun and A.-J. Zhang
Crystal structure of stigmasta-4,25-diene-3 β ,6 β -diol, C₂₉H₄₈O₂. 477
- N. T. Tzvetkov, B. Neumann, H.-G. Stammer and J. Mattay
Crystal structure of (7a'SR)-7a'-prop-2-ynyl-1',2',4',6',7',7a'-hexahydrospiro[1,3-dioxolan-2,5'-indene], C₁₄H₁₈O₂. 479
- N. T. Tzvetkov, B. Neumann, H.-G. Stammer and J. Mattay
Crystal structure of (1aSR,3aRS,7aSR)-3a-but-2-ynyl-1a,2,3,3a,4,5-hexahydro-1H-cyclopropa[*c*]inden-6(7H)-one, C₁₄H₁₈O 481
- C.-H. Zhang, M.-S. Chen and D.-Z. Kuang
Crystal structure of tetra(4-methylpyridine)copper(II) diperchlorate, [Cu(C₆H₇N)₄][ClO₄]₂ 483
- H.-W. Lin
Crystal structure of *trans*-bis(*N*-cyclohexyl-3-methoxy-salicylideneiminato)cobalt(II), Co(C₁₄H₁₈NO₂)₂. 485
- J. Fahrig, J. Sieler and B. Schulze
Crystal structure of *rac-cis-N*-(2,4-dinitrophenyl)-3,4-diphenyl-5H-1,2-oxathiol-5-amine 2-oxide, C₂₁H₁₅N₃O₆S, *sultim and sultam structures - part 4* 487
- Q.-Y. Du, J.-G. Wang, J.-H. Qin and F.-Y. Ju
Crystal structure of 2-(μ -2-oxyphenyl)-1-(2-(μ -2-oxybenzyl)aminoethyl)-3-(2-(2-oxybenzyl)-bis(aminoethyl))-imidazolidine-dicopper(II) nitrate trihydrate, [Cu₂(C₂₉H₃₂N₅O₃)] [NO₃] · 3H₂O. 489
- T. Lei, G.-Y. Wang, Z.-H. Li, S. Lin and X.-N. Fang
Crystal structure of bis(tetrakis(trimethylsilylmethyl)-(μ -hydroxy)(*p*-nitrobenzoato)(μ^3 -oxo)ditin(IV)), [Sn₂O(OH)(NO₂C₆H₄COO)]{(CH₃)₃SiCH₂)}₄ 492
- T. Zhou, L. Zhao and J.-X. Guo
Crystal structure of bis(lomefloxacin) 1,4-benzenedicarboxylate dihydrate, (C₁₇H₁₉F₂N₃O₃)₂[C₈H₆O₄] · 2H₂O. 495
- G. S. Khan, N. H. Rama, G. Qadeer, A. Noor and R. Kempe
Crystal structure of methyl 2-(2-formyl-3,4,5-trimethoxyphenyl)acetate, C₁₃H₁₆O₆ 497
- Z.-X. Du, M.-L. Han, J.-G. Wang and J.-H. Qin
Crystal structure of melaminium dipicrylamine hydrate, [C₃N₃H(NH₂)₃][N{C₆H₂(NO₂)₃}₂] · H₂O 499
- P.-H. Wen and Q. Feng
Crystal structure of (*N*¹*E,N*²*E*)-*N*^{1,N}²-bis(5-hydroxymethyl-2-methyl-3-oxopyridinio-4-ylmethylene)ethane-1,2-diamine-nickel(II) dihydrochloride, [Ni(C₁₈H₂₂N₄O₄)]Cl₂ 501
- D.-P. Zhou and D.-Q. Bi
Re-determination of the crystal structure of *catena*-(μ -oxo)(μ -molybdate(VI))bis(dioxo(1,10-phenanthroline)-molybdenum(VI)), [Mo(O)₂(C₁₂H₈N₂)]₂(O)(MoO₄) 503
- H.-T. Wang, X.-X. Lei, L.-X. Zhang and C.-Y. Zhang
Crystal structure of 3'-formyl-benzo-15-crown-5, C₁₅H₂₀O₆. 505
- H.-M. Guo and B.-S. Zhang
Crystal structure of bis(2,2'-bipyridine-*N,N'*)carbonatocobalt(III) hydrogencarbonate tetrahydrate, [Co(C₁₀H₈N₂)₂(CO₃)] [HCO₃] · 5H₂O 507
- B.-S. Zhang
Crystal structure of diaquabis(1,10-phenanthroline- κ^2N,N')sodium chloride, [Na(H₂O)₂(C₁₂H₈N₂)₂]Cl 509
- B.-S. Zhang
Crystal structure of bis(1,10-phenanthroline-*N,N'*)-bis(2-bromobenzoato)lead(II) hydrate (1:2.5), [Pb(C₇H₄O₂Br)₂(C₁₂H₈N₂)₂] · 2.5H₂O. 511
- F. Chen and G.-Q. Xiang
Crystal structure of 1,2-bis(pyridin-1-ium-4-yl)ethylene bis(5-fluorouracil-1-acetate), (C₁₂H₁₂N₂)[C₆H₄FN₂O₄]₂ 514
- A. Tomas, P. Retailleau, B. Viossat, T. Prangé and P. Lemoine
Crystal structure of bis(3,5-diisopropylsalicylato)(neocuproine)cadmium(II), Cd(C₁₃H₁₇O₃)₂(C₁₄H₁₂N₂) 517
- L.-Z. Li, B.-Q. Jing, L.-W. Li and T. Xu
Crystal structure of (1,10-phenanthroline- κ^2N,N')oxo-(*N*-salicylideneisoleucinato- κ^3O,N,O')vanadium(IV), VO(C₁₂H₈N₂)(C₁₃H₁₅NO₃) 520
- N. Wang and Y.-L. Pu
Crystal structure of bis(4-bromo-2-((3-methylamino-propylimino)methyl)phenolato)cobalt(II) dinitrate, [Co(C₁₁H₁₅BrN₂O)₂][NO₃]₂. 523
- J. Schreuer, L. Wiehl, A. Wagner and P. Hofmann
Crystal structure of bis(hydrogenbetaine) tetrachlorocuprate(II) monohydrate, [(CH₃)₃NCH₂COOH]₂[CuCl₄] · H₂O. 525
- L. Wiehl, J. Schreuer and A. Stojic
Crystal structure of tetrakis(μ -betaine-*O,O'*)dibromodicopper(II) dibromide dihydrate, [Cu₂{(CH₃)₃NCH₂COO}₄Br₂]₂ · 2H₂O, with a propeller-shaped dinuclear copper complex 527
- J. Schreuer, L. Wiehl, J. Biehler and P. Hofmann
Crystal structure of tetrakis(μ -betaine-*O,O'*)dibromodicopper(II) tetrabromocuprate(II) monohydrate, [Cu₂{(CH₃)₃NCH₂COO}₄Br₂][CuBr₄] · H₂O, with a propeller-shaped dinuclear copper complex 529

A. G. Hatzidimitriou, M. Kapnisti and G. Voutsas
Crystal structure of bis((pyridyl)amino-iodobenzeno)-
disulfatodicopper(II) methanol disolvate,
 $\text{Cu}_2(\text{C}_{16}\text{H}_{12}\text{IN}_3)_2(\text{SO}_4)_2 \cdot 2\text{CH}_3\text{OH}$ 532

X.-G. Zhang, X.-H. Zhang and P. Zhong
Crystal structure of 1-(2,6-dichloro-4-(trifluoromethyl)-
phenyl)-5-((3-bromophenyl)methyleneimino)-
1*H*-pyrazole-3-carbonitrile, $\text{C}_{18}\text{H}_8\text{BrCl}_2\text{F}_3\text{N}_4$ 535

J. Zukerman-Schpector, D. C. S. Coelho, C. M. A. Tanaka
and A. J. Marsaioli
Crystal structure of 2-chloro-2-(chloromethyl)-5-
(1-hydroxy-isopropyl)-cyclohexane-1-ol, $\text{C}_{10}\text{H}_{18}\text{Cl}_2\text{O}_2$... 537

F.-Y. Tang, J.-B. She, J.-Z. Li, G.-F. Zhang and G. Zahn
Crystal structure of 4-oxo-3,5-dinitropyridine-*N*-hydroxide
monohydrate, $\text{C}_5\text{NH}_2(\text{NO}_2)_2\text{O}(\text{OH}) \cdot \text{H}_2\text{O}$ 539

A. Aydin, Y. DüNDAR, M. Akkurt, O. Büyükgüngör and
M. F. Sahin
Crystal structure of methyl (6-(2-fluorobenzoyl)-5-chloro-
2-benzoxazolinon-3-yl)-acetate, $\text{C}_{17}\text{H}_{11}\text{ClFNO}_5$ 541

X.-F. Zheng, X.-S. Wan, W. Liu, C.-Y. Niu and C.-H. Kou
Crystal structure of bis(2,5-bis(2-pyridyl)-1,3,4-thiadiazole)-
bis(perchlorato)copper(II), $\text{Cu}(\text{C}_{12}\text{H}_8\text{N}_4\text{S})_2(\text{ClO}_4)_2$ 543

A. Gawlicka-Chruszcz, H. Zheng, M. Hyacinth,
M. Cymborowski, M. Sabat and W. Minor
Crystal structure of 2,6-dichlorobenzaldehyde,
 $\text{C}_7\text{H}_4\text{Cl}_2\text{O}$ 545

A. M. Dietel, T. Irrgang, S. Karthikeyan and R. Kempe
Crystal structure of 2-(2,6-diisopropyl-phenylamino)-
6-(2,4,6-triisopropyl-phenyl)-pyridinium (2-(2,6-
diisopropyl-phenylamido)-6-(2,4,6-triisopropyl-phenyl)-
pyridinium)-(μ -chloro)-di(μ -oxo)-tetrachloro-
tetrahydrofuran-dichromate(IV) pentane solvate,
 $(\text{C}_{32}\text{H}_{45}\text{N}_2)[(\text{C}_{32}\text{H}_{44}\text{N}_2)\text{Cl}_5\text{Cr}_2\text{O}_2(\text{C}_4\text{H}_8\text{O})] \cdot \text{C}_5\text{H}_{12}$ 547

P. Kuhn, D. Matt, L. Ricard and A. Louati
Crystal structure of 5-acetyl-25,27-dipropoxy-26,28-
acetyloxy-calix[4]arene ethyl acetate hemisolvate,
 $\text{C}_{40}\text{H}_{42}\text{O}_7 \cdot \frac{1}{2}\text{C}_4\text{H}_8\text{O}_2$, *partial cone* 551

W.-K. Dong, J.-G. Duan, H.-L. Wu, J.-Y. Shi and T.-Z. Yu
Crystal structure of 2,2'-((1,4-butylene)dioxybis(nitrilo-
methylidene))dinaphthol, $\text{C}_{26}\text{H}_{24}\text{N}_2\text{O}_4$ 555

A. Zonouzi, H. Rahmani, A. Kamali and A. Jahangiri
Crystal structure of dimethyl 2-(*tert*-butylamino)-5-benzoyl-
6-phenyl-4*H*-pyran-3,4-dicarboxylate, $\text{C}_{26}\text{H}_{27}\text{NO}_6$ 557

A. Zonouzi, H. Rahmani, H. Samareh Afsari and
P. Saranjampour
Crystal structure of dimethyl 7-(cyclohexylamino)2,3,4,5-
tetrahydro-1,3-dimethyl-2,4-dioxo-1*H*-pyrano[2,3-*d*]-
pyrimidine-5,6-dicarboxylate, $\text{C}_{19}\text{H}_{25}\text{N}_3\text{O}_7$ 559

Author Index Formulae Index

Further details of the structure determination can be accessed at
the relevant database:

Data with CSD numbers can be obtained from the Fachinfor-
mationszentrum Karlsruhe, Gesellschaft für wissenschaftlich-tech-
nische Information mbH, D-76344 Eggenstein-Leopoldshafen,
Germany (e-mail: docdel@fiz-karlsruhe.de).

Data with CCDC numbers can be obtained from the Cambridge
Crystallographic Data Centre (CCDC), 12 Union Road,
Cambridge CB2 1EZ, UK, (fax: +44-(0)1223-33 60 33 or e-mail:
deposit@chemcrys.cam.ac.uk).

