Crystal structure of 5,11,17,23-tetrakis-cyanomethyl 25,26,27,28-tetrahydroxycalix[4]arene, $C_{36}H_{28}N_4O_4$, a test case on microcrystals using synchrotron radiation

M. Lecouvey, A. Neuman and T. Prangé*

Université Paris-Nord (UMR 7033 CNRS), UFR-SMBH, Chimie Structurale et Spectroscopie Biomoléculaire, 74 rue M. Cachin, F-93017 Bobigny Cedex, France.

Received April 23, 2002, accepted and available on-line August 14, 2002; CCDC-No. 1267/853

[4]calixarenes, a single crystal analysis was attempted on the title compound using a synchrotron source.

In the title compound, the *para* cyano groups at rings labeled (B) and (D) are in two different orientations each (upper figure). These disorders are mutually exclusive: a molecule with cyano groups in one orientation faces another equivalent molecule and vice-versa for the second disordered orientation.

At the temperature of measurement (100 K), the four phenolic hydrogens are clearly visible and strongly H-bonded to a neighboring phenol oxygen in a circular way that stabilizes the "cone" conformation and also breaks the *m* symmetry observed at room temperature. This is illustrated in the lower figure.

Table 1. Data collection and handling.

Crystal:	yellowish plate, size 0.01 × 0.02 × 0.05 mm
Wavelength:	synchrotron radiation (0.96200 Å)
μ :	0.88 cm ⁻¹
Diffraction, scan mode:	MARResearch MAR345; 100 frames, $\Delta\phi = 4^\circ$, 2 min/ $^\circ$
$2\theta_{\max}$:	56.28°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	9883, 2561
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2561
$N(\text{param})_{\text{refined}}$:	464
Programs:	SHELXS-86 [4], SHELXL-97 [5]

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

Atom	Site	Occ.	x	y	z	U_{iso}
H(1A)	2i		0.351(4)	0.291(1)	0.651(3)	0.088
H(3A)	2i		0.7170	0.4225	0.4797	0.085
H(5A)	2i		0.8011	0.6445	0.7056	0.084
H(71A)	2i		0.9054	0.5886	0.4823	0.109
H(72A)	2i		0.8894	0.6849	0.5385	0.109
H(10A)	2i		0.4440	0.5278	0.7714	0.079
H(11A)	2i		0.5978	0.6309	0.7934	0.079
H(1B)	2i		0.334(4)	0.143(3)	0.712(1)	0.087
H(3B)	2i		0.6978	-0.0124	0.6965	0.073
H(5B)	2i		0.6978	0.1963	0.4880	0.072
H(71B)	2i	0.50	0.8578	0.0002	0.5857	0.161
H(72B)	2i	0.50	0.9617	0.1156	0.6365	0.161
H(73B)	2i	0.50	0.8334	0.0574	0.4864	0.051
H(74B)	2i	0.50	0.9610	0.1266	0.5895	0.051
H(10B)	2i		0.4737	0.2696	0.4319	0.084
H(11B)	2i		0.3471	0.2523	0.4935	0.084
H(1C)	2i		0.377(4)	0.223(1)	0.870(3)	0.088
H(3C)	2i		0.8015	0.2058	1.1444	0.084
H(5C)	2i		0.7173	-0.0198	0.9219	0.086
H(71C)	2i		0.8909	0.0387	1.1850	0.107
H(72C)	2i		0.9062	-0.0174	1.0884	0.107
H(10C)	2i		0.3468	-0.0064	0.7519	0.083
H(11C)	2i		0.4730	-0.0682	0.7691	0.083
H(1D)	2i		0.388(4)	0.372(3)	0.804(2)	0.085
H(3D)	2i		0.8522	0.6471	0.9382	0.075
H(5D)	2i		0.8516	0.4382	1.1471	0.075
H(71D)	2i	0.50	1.1271	0.5963	1.1438	0.086
H(72D)	2i	0.50	1.0809	0.6910	1.0889	0.086
H(73D)	2i	0.50	1.0760	0.5918	1.1938	0.107
H(74D)	2i	0.50	1.1254	0.6477	1.1008	0.107
H(10D)	2i		0.5974	0.2933	1.1308	0.080
H(11D)	2i		0.4438	0.2708	1.0277	0.080

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

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1A)	2i		0.3786(3)	0.3564(2)	0.6632(2)	0.087(2)	0.060(1)	0.066(1)	0.030(1)	0.010(1)	-0.003(1)
C(1A)	2i		0.5170(4)	0.4169(2)	0.6413(2)	0.078(2)	0.054(2)	0.048(2)	0.032(2)	0.007(2)	0.007(2)
C(2A)	2i		0.5581(4)	0.3788(2)	0.5605(2)	0.088(2)	0.062(2)	0.042(2)	0.044(2)	0.004(2)	0.007(1)
C(3A)	2i		0.6888(5)	0.4455(3)	0.5344(2)	0.100(3)	0.073(2)	0.051(2)	0.050(2)	0.019(2)	0.013(2)
C(4A)	2i		0.7788(4)	0.5448(3)	0.5863(2)	0.088(2)	0.075(2)	0.053(2)	0.039(2)	0.014(2)	0.019(2)
C(5A)	2i		0.7385(4)	0.5782(2)	0.6688(2)	0.091(2)	0.057(2)	0.057(2)	0.033(2)	0.010(2)	0.013(2)
C(6A)	2i		0.6073(4)	0.5155(2)	0.6982(2)	0.089(2)	0.054(2)	0.044(2)	0.040(2)	0.006(2)	0.008(1)
C(7A)	2i		0.9120(5)	0.6190(3)	0.5495(3)	0.099(3)	0.098(3)	0.073(2)	0.040(2)	0.017(2)	0.024(2)
C(8A)	2i		1.0752(6)	0.6409(4)	0.6203(3)	0.102(3)	0.149(4)	0.052(2)	0.052(3)	0.029(2)	0.023(2)
N(9A)	2i		1.2076(6)	0.6595(5)	0.6764(3)	0.116(3)	0.281(6)	0.076(2)	0.069(4)	0.028(2)	0.048(3)
C(10A)	2i		0.5637(4)	0.5546(2)	0.7877(2)	0.089(2)	0.048(2)	0.060(2)	0.034(2)	0.013(2)	0.003(1)
O(1B)	2i		0.3311(3)	0.1503(2)	0.6490(2)	0.073(2)	0.070(1)	0.065(1)	0.021(1)	0.013(1)	-0.008(1)
C(1B)	2i		0.4643(4)	0.1311(2)	0.6309(2)	0.064(2)	0.045(2)	0.053(2)	0.016(2)	0.008(2)	-0.012(1)
C(2B)	2i		0.5272(4)	0.0575(2)	0.6853(2)	0.075(2)	0.035(2)	0.056(2)	0.012(1)	0.018(2)	-0.008(1)
C(3B)	2i		0.6545(4)	0.0373(2)	0.6617(2)	0.083(2)	0.040(2)	0.053(2)	0.023(2)	0.014(2)	-0.001(1)
C(4B)	2i		0.7197(4)	0.0883(2)	0.5883(2)	0.075(2)	0.044(2)	0.049(2)	0.020(2)	0.014(2)	-0.005(1)
C(5B)	2i		0.6545(4)	0.1616(2)	0.5376(2)	0.084(2)	0.046(2)	0.045(2)	0.020(2)	0.015(2)	-0.000(1)
C(6B)	2i		0.5273(4)	0.1855(2)	0.5576(2)	0.074(2)	0.049(2)	0.043(2)	0.022(2)	0.006(2)	-0.007(1)
C(7B)	2i	0.50	0.867(3)	0.073(2)	0.578(2)	0.21(2)	0.10(2)	0.14(2)	0.05(1)	0.11(1)	0.02(1)
C(8B)	2i	0.50	0.9065(9)	0.0983(5)	0.4818(7)	0.081(5)	0.048(4)	0.074(5)	0.028(3)	0.020(4)	0.004(4)
N(9B)	2i	0.50	0.9407(9)	0.1256(5)	0.4098(6)	0.123(6)	0.077(4)	0.097(5)	0.039(4)	0.044(4)	0.017(4)
C(7B')	2i	0.50	0.862(1)	0.065(1)	0.562(1)	0.040(5)	0.039(6)	0.042(5)	0.021(4)	-0.004(5)	-0.010(4)
C(8B')	2i	0.50	0.9041(9)	-0.0179(6)	0.5968(5)	0.082(5)	0.073(5)	0.061(4)	0.024(4)	0.028(3)	-0.008(4)
N(9B')	2i	0.50	0.9398(9)	-0.0912(6)	0.6256(5)	0.119(5)	0.096(5)	0.093(4)	0.057(4)	0.036(4)	0.010(4)
C(10B)	2i		0.4639(4)	0.2696(2)	0.5017(2)	0.098(2)	0.069(2)	0.043(2)	0.042(2)	0.008(2)	-0.001(1)
O(1C)	2i		0.3782(3)	0.1620(2)	0.8553(2)	0.088(2)	0.051(1)	0.078(1)	0.015(1)	0.030(1)	-0.003(1)
C(1C)	2i		0.5181(4)	0.1410(2)	0.9166(2)	0.077(2)	0.043(2)	0.062(2)	0.013(2)	0.029(2)	0.009(1)
C(2C)	2i		0.6078(4)	0.1983(2)	1.0158(2)	0.088(2)	0.042(2)	0.057(2)	0.009(2)	0.031(2)	0.007(1)
C(3C)	2i		0.7387(4)	0.1689(2)	1.0783(2)	0.093(2)	0.049(2)	0.060(2)	0.013(2)	0.027(2)	0.012(1)
C(4C)	2i		0.7783(4)	0.0864(2)	1.0451(3)	0.090(2)	0.049(2)	0.082(2)	0.020(2)	0.037(2)	0.020(2)
C(5C)	2i		0.6885(4)	0.0344(2)	0.9451(3)	0.101(3)	0.043(2)	0.079(2)	0.021(2)	0.044(2)	0.010(2)
C(6C)	2i		0.5576(4)	0.0603(2)	0.8787(2)	0.089(2)	0.038(2)	0.068(2)	0.010(2)	0.037(2)	0.008(1)

Table 3. Continued.

Atom	Site	Occ.	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(7C)	2i		0.9130(5)	0.0499(3)	1.1191(3)	0.100(3)	0.065(2)	0.102(3)	0.024(2)	0.035(2)	0.022(2)
C(8C)	2i		1.0757(6)	0.1200(3)	1.1408(4)	0.103(3)	0.047(2)	0.148(3)	0.032(2)	0.043(3)	0.022(2)
N(9C)	2i		1.2080(6)	0.1767(3)	1.1599(5)	0.121(3)	0.068(2)	0.288(6)	0.034(2)	0.063(4)	0.045(3)
C(10C)	2i		0.4636(4)	0.0017(2)	0.7692(2)	0.096(2)	0.038(2)	0.074(2)	0.014(2)	0.037(2)	0.000(1)
O(1D)	2i		0.4104(3)	0.3656(2)	0.8667(2)	0.078(2)	0.068(1)	0.060(1)	0.023(1)	0.014(1)	-0.007(1)
C(1D)	2i		0.5696(4)	0.4267(2)	0.9266(2)	0.065(2)	0.046(2)	0.049(2)	0.018(2)	0.009(2)	-0.011(1)
C(2D)	2i		0.6457(4)	0.5209(2)	0.8928(2)	0.077(2)	0.041(2)	0.051(2)	0.024(2)	0.017(2)	-0.002(1)
C(3D)	2i		0.7993(4)	0.5832(2)	0.9585(2)	0.082(2)	0.041(2)	0.061(2)	0.019(2)	0.020(2)	0.001(1)
C(4D)	2i		0.8773(4)	0.5536(2)	1.0538(2)	0.074(2)	0.051(2)	0.054(2)	0.022(2)	0.014(2)	-0.004(2)
C(5D)	2i		0.7992(4)	0.4585(2)	1.0832(2)	0.086(2)	0.052(2)	0.046(2)	0.026(2)	0.014(2)	0.002(1)
C(6D)	2i		0.6455(4)	0.3927(2)	1.0206(2)	0.076(2)	0.046(2)	0.048(2)	0.019(2)	0.018(2)	-0.003(1)
C(7D)	2i	0.50	1.043(2)	0.630(2)	1.125(2)	0.06(1)	0.06(1)	0.06(1)	0.02(1)	-0.019(8)	-0.012(8)
C(8D)	2i	0.50	1.011(1)	0.663(1)	1.221(1)	0.073(6)	0.098(8)	0.089(8)	-0.002(5)	0.006(5)	-0.029(7)
N(9D)	2i	0.50	0.979(1)	0.696(1)	1.2874(9)	0.127(8)	0.24(2)	0.151(8)	-0.042(8)	0.048(7)	-0.13(1)
C(7D')	2i	0.50	1.039(3)	0.628(2)	1.133(2)	0.09(2)	0.08(2)	0.09(2)	0.00(1)	0.05(1)	-0.01(1)
C(8D')	2i	0.50	1.011(1)	0.720(1)	1.166(1)	0.089(6)	0.055(6)	0.126(9)	0.015(5)	-0.017(6)	-0.037(7)
N(9D')	2i	0.50	0.982(1)	0.7875(9)	1.194(1)	0.115(7)	0.132(8)	0.23(1)	0.035(6)	-0.045(8)	-0.12(1)
C(10D)	2i		0.5635(4)	0.2874(2)	1.0546(2)	0.095(2)	0.052(2)	0.052(2)	0.018(2)	0.029(2)	0.001(1)

References

- Gutsche, D. C.; Chun Nam, K.: Calixarenes. 22. Synthesis, Properties, and Metal Complexation of Aminocalixarenes. *J. Am. Chem. Soc.* **110** (1988) 6153-6162.
- Fourme, R.; Dhez, P.; Benoit, J. P.; Kahn, R.; Dubuisson, J. M.; Besson, P.; Frouin, J.: Bent crystal, bent multilayer optics on a multipole wiggler line for an X-Ray diffractometer with an imaging plate detector. *Rev. Sci. Instrum.* **63** (1992) 982-987.
- Ottwinowski, Z.; Minor, W.: Processing of X-Ray diffraction data collected in oscillation mode. *Methods in Enzymol.* **276** (1997) 307-326.
- Sheldrick, G. M.: SHELXL-97. A Program for Refining Crystal Structures. University of Göttingen, Germany 1997.
- Sheldrick, G. M.: SHELXS-86. Program for Solution of Crystal Structures. University of Göttingen, Germany 1985.
- Gutsche, D. C.; Bauer, L. J.: Calixarenes. 13. The Conformational Properties of Calix[4]arenes, Calix[6]arenes, Calix[8]arenes, and Oxacalixarenes. *J. Am. Chem. Soc.* **107** (1985) 6052-6059.
- Soi, A.; Bauer, W.; Mauser, H.; Moll, C.; Hampel, F.; Hirsch, A.: Investigations on the dynamic properties of 25,26,27,28-tetraalkoxy-calix[4]arenes: *para*-substituent- and solvent-dependent properties of paco conformers and determination of thermodynamic parameters of the pinched cone/pinched cone conversion. *J. Chem. Soc., Perkin Trans. II* (1998) 1471-1478.

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 135 (+ 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@verlag.olderbourg.de

Samples of CIF-files can be downloaded from:

<ftp://ftp.olderbourg.de/pub/zkrist>

For any question please ask the Technical Editor (e-mail: zkrist@verlag.olderbourg.de) or the Managing Editor (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 (<http://www.olderbourg.de/verlag/zkristallogr/mn-ncsc.htm>). 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.; Cockroft, 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 = 'ä', Å = 'a', ç = 'c', Ç = 'C'); 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. Substantial corrections exceeding the original typesetting costs by 5% 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 are available on
<http://www.olderbourg.de/verlag/zkristallogr/mn-ncsc.htm>.

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 217 Issues 1–3

- Abu-Surrah, A. S., 257
 Achary, S. N., 23
 Agostinho Moreira, J., 77, 79, 433
 Ahmed, I., 107
 Almeida, A., 77, 79, 433
 Alte da Veiga, L., 430
 Alvarez-Larena, A., 427
 Amarasekara, A. S., 213
 Andrade, L. C. R., 77, 79, 433
 Angelkort, J., 398
 Arendt, Y., 63
 Arif, A. M., 327, 329
 Arndt, P., 237
 Aycard, J. P., 389, 391, 289
 Bagieu-Beucher, M., 1
 Ballirano, P., 177
 Balogh-Hergovich, É., 61
 Barberan, O., 128
 Barbey, C., 137
 Barnes, C. L., 303
 Bauer, M., 421
 Baumann, W., 237
 Beck, W., 205
 Beckhaus, R., 47, 49
 Bekaert, A., 128
 Bente, K., 13
 Bentefrit, F., 263
 Bernstein J., 439
 Bhalla, V., 104
 Bibila Mayaya Bisseyou, Y., 289, 391
 Bildstein, B., 269
 Binnewies, M., 324, 325
 Bissky, G., 419
 Bodart, N., 109, 112
 Boeyens, J. C. A., 9
 Böhmer, V., 141, 144, 398
 Borrmann, H., 161, 167, 169, 171, 187, 305, 307, 324
 Brion, J. D., 128
 Bruhn, C., 63
 Bryan, J. C., 225
 Buchsbaum, N., 398
 Budnyk, S., 159
 Burgard, A., 139
 Burlakov, V. V., 237, 239, 241
 Capparelli, M. V., 427
 Carcelli, M., 203
 Cardoso Gil, R., 179, 181, 183
 Carrillo-Cabrera, W., 179, 181, 183
 Cendrowski-Guillaume, S., 35, 441
 Cetina, M., 273
 Chaban, N., 315
 Chan, S.-K., 413, 415
 Chaves, M. R., 77, 79, 433
 Chen, H.-H., 311
 Cheng, Y.-Q., 121
 Chiappe, C., 119
 Chiron, J., 287
 Chykhrij, S. I., 161
 Ci, X.-Y., 341
 Coindet-Benramdane, M., 154
 Cooper, M. A., 343, 345
 Costa, M. M. R., 77, 79, 433
 Courtney, S. C., 217
 Czado, W., 335, 337, 339
 Czaun, M., 379
 Dallmann, K., 239, 241
 Danan, A., 128
 Dave, C. G., 29, 32
 Deacon, G. B., 87
 de Almeida, E. T., 147, 366
 Declercq, J.-P., 385
 Dee, C. M., 85
 de Godoy Netto, A. V., 147, 366
 de la Encarnacion, E., 375
 Demchyna, R., 161
 Deng, J.-F., 169, 171, 305, 307, 309, 311
 Devillers, M., 109, 112, 385
 Dey, S., 369, 372
 Dieleman, C. B., 55
 Dinesh, C. U., 423, 425
 Djanhanl, J., 398
 Dorhout, P. K., 302
 Dridi, K., 275
 Dronskowski, R., 118
 Džolić, Z., 273
 Ebby, N., 289
 El Manouni, D., 154
 Elmes, P. S., 91
 Emirdag-Eanes, M., 17
 Ephritikhine, M., 35
 Ernst, R. D., 327, 329
 Fang, L.-P., 121
 Farran, J., 427
 Fleck, M., 15
 Fornasini, M. L., 173
 Frey, W., 123, 125, 279, 281, 401, 403, 405, 407, 409
 Friedrich, H. A., 24
 Fruziński, A., 259, 261, 437
 Gakh, A. A., 225
 Galy, J.-P., 233, 287
 Ganszky, I., 379
 Gerlach, U., 139
 Ghosez, L., 381, 383
 Giester, G., 69, 71
 Gillier, H., 154
 Giorgi, M., 61, 289
 Gouranlou, F., 74, 149, 228, 231, 395, 393
 Gream, G. E., 351, 353, 355
 Greatrex, B. W., 83
 Griesbeck, A. G., 235
 Grin, Yu., 159, 161, 179, 181, 183, 315
 Groy, T. L., 421
 Guillaume, B., 441
 Gültekin, Z., 125, 279, 281, 403, 405, 407
 Gumannl, N., 398
 Guo, H.-B., 413
 Gusing, H. J., 151
 Haase, D., 47, 49, 99, 101
 Hahn, D. U., 123, 409
 Hartenbach, I., 175
 Hartmann, Th., 186
 Haussühl, E., 69, 71
 Hay, B. P., 225
 Hegetschweiler, K., 133, 135
 Hernandez, O., 11
 Heuer, M., 13
 Ho, S. Y., 359
 Hofmann, A., 89
 Höhle, W., 314
 Horvath, M. J., 91
 Hu, M.-L., 121
 Huang, Y.-X., 3, 5, 7, 163, 165, 167, 169, 171, 305, 307
 Hundal, G., 104
 Ianelli, S., 203
 Ibers, J. A., 157
 Ichharam, V. V. H., 9
 Iijaali, I., 157
 Incarvito, C. D., 271
 Inoue, Y., 201
 Jackson, W. R., 91
 Jäger, V., 123, 125, 279, 281, 401, 403, 405, 407, 409
 Jalilian, A. R., 74, 149, 395
 Jamali, F., 74, 149, 228, 231, 395, 393
 Jansen, M., 19, 94, 95, 313
 Jäschke, T., 95
 Jeitschko, W., 25, 27
 Jeunesse, C., 51
 Jin, Q.-H., 292, 341
 Jin, Z.-M., 121, 435
 Joswig, W., 398
 Jotani, M. M., 29, 32
 Kabbani, R., 267
 Kaffashy, S., 231
 Kaisalo, L., 41
 Kaiser, J. W., 25
 Kakou-Yao, R., 289
 Kaloun, E. B., 128
 Karolak-Wojciechowska, J., 259, 261, 437
 Kastner, G., 107
 Kelling, A., 285
 Khodorkovsky, V., 439
 Kimber, M. C., 349
 Kirkbride, P. K., 351, 353, 355
 Klinga, M., 257
 Knip, R., 3, 5, 7, 163, 165, 167, 169, 171, 186, 187, 305, 307
 Koch, D., 186, 187
 Köhler, J., 23, 24
 Kolitsch, U., 15
 Kolomeitsev, A., 419
 Kong, Z.-P., 65, 195, 197, 333
 Kouvetakis, J., 421
 Krikava, A., 267
 Kristafor, V., 273
 Kumar, P., 369, 372
 Kumar, S., 104
 Kuz'ma, Yu. B., 159, 161, 315
 la Cour, A., 215
 Lang, H.-J., 139
 Lecouvey, M., 137, 445
 Le Gland, G., 35
 Leithe-Jasper, A., 319
 Lejeune, M., 51
 Lemoine, P., 128, 131, 263
 Lenoir, D., 119
 Lentz, D., 59
 Leroux, Y., 154
 Leskelä, M., 257
 Lex, J., 201, 235
 Li, M.-R., 3, 5, 165, 309, 311
 Li, S., 321
 Li, X., 292
 Liepa, A. J., 89
 Lin, J.-L., 65, 67, 189, 191, 193, 195, 197, 199, 299, 331, 333, 411
 Liu, W.-H., 199
 Liu, X., 118
 Lokshin, V., 57
 Lopes S. H., 430
 Lork, E., 419
 Lovel, C. G., 91
 Ludwig, R., 59
 Magull, J., 325
 Mahadevan, I. B., 207
 Mahjoub, A. R., 97, 443
 Mahuteau-Betzer, F., 381, 383

- Makker, J., 369, 372
 Malaun, M., 269
 Manfrinetti, P., 173
 Mao, S.-Y., 3, 5, 7, 165, 167, 307, 309, 311
 Maras, A., 177
 Martin, B. R., 302
 Matos Beja, A., 430
 Matt, D., 51, 55
 Mattausch, H., 321, 323
 Mauro, A. E., 147, 366
 Mayer, P., 205
 Mazor, R., 439
 Mi, J.-X., 3, 5, 7, 163, 165, 167, 169, 171, 305, 307, 309, 311
 Mintas, M., 273
 Miszta, S., 261
 Mitchell, K., 157
 Miyazaki, T., 43
 Mizuguchi, J., 43, 45, 244, 247, 249, 251, 253, 255
 Mochizuki, M., 244
 Mohammadi, B., 393
 Mokrosz, M., 259, 261, 437
 Momeni-Movahhed, A., 149
 Moody, K., 91
 Morgant, G., 131, 263
 Morsali, A., 74, 97, 149, 228, 231, 393, 395, 443
 Mosset, A., 1
 Mobaraki, B., 219, 223
 Mrvoš-Sermek, D., 273
 Mukherjee, S., 372
 Müller, U., 119, 335, 337, 339
 Murrmann, R. K., 303
 Murray, K. S., 215, 217, 219, 221, 223
 Mutikainen, I., 38, 41
 Neda, I., 55
 Nelson, K. T., 87
 Neuman, A., 154, 445
 Newbound, T. D., 329
 Nguyen-Huy, D., 131, 263
 Nierlich, M., 35, 441
 Niewa, R., 317
 Noshiranzadeh, N., 231, 393
 Nuss, J., 19, 21, 313, 314
 Oeckler, O., 323
 Oelgemöller, M., 201, 235
 Ostendorf, D., 99, 101
 O'Sullivan, P., 141, 144
 Paixão, J. A., 77, 79, 430, 433
 Palenzona, A., 173
 Palmer, C., 209
 Paluchowska, M., 259, 437
 Pan, Y.-J., 435
 Párkányi, L., 379
 Paschen, S., 183
 Patel, U. H., 29, 32
 Paulus, E. F., 139, 141, 144, 398
 Pèpe, G., 57
 Perrin, A., 11
 Peters, M., 398
 Pilet, G., 11
 Piniella, J. F., 427
 Pons, J., 375
 Poorheravi, M. R., 97
 Pothier, J., 401
 Prangé, T., 154, 445
 Prots, Yu., 159, 315
 Pu, S.-Z., 413, 415, 417
 Rabbi, C., 128
 Rademacher, O., 423, 425
 Rajeswaran, M., 151
 Ramazani, A., 74, 149, 228, 231, 395, 393
 Ramos Silva, M., 430
 Réglier, M., 61
 Reißig, H.-U., 423, 425
 Reuter, H., 107
 Rheingold, A. L., 271
 Robin, M., 233
 Rocha Gonsalves, A. M. d'A., 430
 Romba, J., 133, 135
 Ros, J., 375
 Röschenthaler, G.-V., 419
 Rosenthal, U., 237, 239, 241
 Rossollin, V., 57
 Rubin, J. M., 439
 Russell, R. A., 207, 209, 211, 213
 Rzaigui, M., 275, 277
 Saadioui, M., 398
 Saak, W., 47, 49, 99, 101
 Sachleben, R. A., 225
 Samat, A., 57
 Santana, A. M., 147, 366
 Santos, M. L., 77, 79, 433
 Santos, M. P., 366
 Santos, R. H. A., 147, 366
 Sasaki, T., 249
 Sato, A., 319
 Saylik, D., 91
 Schilde, U., 285
 Schleid, Th., 175
 Schlüter, M., 27
 Schmutzler, R., 55
 Schnering, H. G. von, 21, 314
 Schultz, A. C., 211
 Sefkow, M., 285
 Shah, H. C., 29, 32
 Shams, E., 97
 Shoja, M., 267
 Simon, A., 321, 323
 Singh, N., 104
 Singh, T. P., 369, 372
 Sireci, A., 271
 Smyth, D. R., 357, 361, 363
 So, W.-W., 302
 Sobral, A. J. F. N., 430
 Södervall, M., 38
 Soetebier, F., 22
 Souldozi, A., 393
 Souza Jr., J., 147
 Spannenberg, A., 237, 239, 241
 Speier, G., 61, 379
 Steinborn, D., 63
 Steinhauser, S., 133, 135
 Stroot, J., 47, 49
 Sun, F., 413, 415, 417
 Sun, H., 237
 Sun, J., 189, 193, 411
 Tanaka, T., 319
 Taylor, D. K., 83
 Tenon, J. A., 389, 391
 Tiekink, E. R. T., 81, 83, 85, 87, 89, 91, 207, 209, 211, 213, 215, 217, 219, 221, 223, 343, 345, 347, 349, 351, 353, 355, 357, 359, 361, 363
 Tillmanns, E., 69, 71
 Tinant, B., 109, 112, 381, 383, 385
 Toftlund, H., 215
 Tojo, K., 45, 247, 249, 253, 255
 Tomas, A., 131, 263
 Ton, Q. C., 398
 Torres, M. R., 375
 Torres-Castellanos, L., 427
 Trakarnpruk, W., 327
 Tran, V.-H., 181
 Tyagi, A. K., 23
 Uncuta, C., 289
 Urland, W., 22
 Van Langenberg, K. A., 221, 223
 Viossat, B., 128, 131, 263
 Walters, M. A., 271
 Wang, K.-W., 435
 Wang, P., 301
 Wang, R.-J., 413, 415, 417
 Ward, A. D., 343, 345, 347, 349
 Warrenner, R. N., 207, 209, 211, 213
 Wattenbach, C., 119
 Wei, D.-Y., 191
 Wei, Z.-B., 3, 5, 7, 165
 Weidenbruch, M., 99, 101
 Weisbarth, R., 94
 Williamson, N. M., 347
 Woisetschlager, O. E., 205
 Wolf, W. M., 115
 Wullens, H., 109, 112, 385
 Wurst, K., 269
 Xin, X.-L., 341
 Xu, W., 301
 Yap, Y. M., 389, 391
 Yu, K.-B., 292, 341
 Yuan, P., 415
 Zantour, H., 275, 277
 Zhang, F.-S., 413, 415, 417
 Zhang, H.-L., 67
 Zhao, J.-T., 3, 5, 7, 163, 165, 167, 169, 171, 305, 307, 309, 311
 Zheng, C., 321
 Zheng, H.-G., 341
 Zheng, Y.-Q., 65, 67, 189, 191, 193, 195, 197, 199, 299, 301, 331, 333, 411
 Zherebtsov, D. A., 317
 Zhou, X.-H., 413, 415
 Zhu, Y.-J., 299
 Zimmer, R., 423, 425
 Zou, Y.-Q., 292

Formulae Index of Volume 217 Issues 1–3

- $\text{Ag}_{2.16}\text{Ce}_2\text{P}_{3.80}$, 161
 $\text{AlBCsHO}_9\text{P}_2$, 169
 $\text{AlBHKO}_9\text{P}_2$, 186
 $\text{AlBHO}_9\text{P}_2\text{Rb}$, 171
 $\text{AlBH}_5\text{NO}_9\text{P}_2$, 305
 $\text{AlB}_2\text{H}_7\text{O}_{13}\text{P}_2$, 187
 As_2O_3 , 177
 $\text{As}_3\text{K}_6\text{NbO}$, 314
 As_5AuBa_8 , 313
 $\text{BGaH}_3\text{KO}_{10}\text{P}_2$, 167
 $\text{BGaH}_5\text{NO}_9\text{P}_2$, 165
 $\text{BHInKO}_9\text{P}_2$, 3
 $\text{BHInO}_9\text{P}_2\text{Rb}$, 163
 $\text{BH}_5\text{InNO}_9\text{P}_2$, 5
 B_4ErV , 315
 $\text{B}_4\text{H}_{12}\text{In}_4\text{Na}_4\text{O}_{40}\text{P}_8$, 7
 B_{12}Zr , 319
 $\text{Ba}_2\text{O}_7\text{Si}_2\text{Zn}$, 25
 $\text{Ba}_8\text{Ga}_{4.44}\text{Ge}_{39.14}$, 183
 $\text{Ba}_8\text{Ga}_{8.62}\text{Ge}_{36}$, 183
 $\text{Ba}_8\text{Ga}_{12.35}\text{Ge}_{33.27}$, 183
 $\text{Ba}_8\text{Ga}_{17.2}\text{Sn}_{28.8}$, 181
 BrIn_3La_5 , 321
 $\text{Br}_3\text{CsRe}_6\text{S}_8$, 11
 CClHgNS , 1
 $\text{C}_2\text{H}_{10}\text{CaO}_6\text{S}$, 441
 $\text{C}_4\text{H}_8\text{Br}_4\text{O}_2\text{Sn}$, 421
 $\text{C}_4\text{H}_8\text{Cl}_2\text{CuN}_8$, 118
 $\text{C}_4\text{H}_{12}\text{MnO}_8$, 411
 $\text{C}_4\text{H}_{12}\text{O}_3\text{P}_2$, 94
 $\text{C}_4\text{H}_{14}\text{ClN}_3\text{O}_5$, 433
 $\text{C}_5\text{H}_{19}\text{Ca}_{0.18}\text{Cl}_2\text{NO}_6\text{Sr}_{0.82}$, 79
 $\text{C}_7\text{H}_{13}\text{NO}_8\text{P}_2$, 137
 $\text{C}_7\text{H}_{21}\text{NO}_7\text{P}_2$, 154
 $\text{C}_8\text{H}_6\text{N}_3$, 203
 $\text{C}_9\text{H}_{13}\text{NO}_4$, 403
 $\text{C}_9\text{H}_{15}\text{NO}_4$, 279
 $\text{C}_{10}\text{H}_9\text{N}_5$, 273
 $\text{C}_{10}\text{H}_{10}\text{O}_8$, 63
 $\text{C}_{10}\text{H}_{12}\text{O}_3$, 59
 $\text{C}_{10}\text{H}_{17}\text{IO}_5$, 123
 $\text{C}_{10}\text{H}_{25}\text{Cl}_4\text{N}_7\text{O}_2\text{Pt}$, 131
 $\text{C}_{10}\text{H}_{27}\text{F}_2\text{N}_3\text{Si}$, 419
 $\text{C}_{11}\text{H}_{15}\text{NO}_5$, 405
 $\text{C}_{11}\text{H}_{17}\text{NO}_2$, 430
 $\text{C}_{11}\text{H}_{19}\text{NO}_9$, 77
 $\text{C}_{12}\text{H}_{12}\text{CuN}_4\text{O}_8$, 193
 $\text{C}_{12}\text{H}_{14}\text{MnN}_2\text{O}_7\text{S}$, 189
 $\text{C}_{12}\text{H}_{16}\text{N}_2\text{NiO}_8\text{S}$, 197
 $\text{C}_{12}\text{H}_{20}\text{ClNO}_4$, 289
 $\text{C}_{12}\text{H}_{37}\text{B}_2\text{N}_5\text{Si}_2$, 95
 $\text{C}_{12}\text{H}_{44}\text{Br}_2\text{CoN}_8\text{O}_{10}$, 121
 $\text{C}_{12}\text{H}_{44}\text{N}_2\text{O}_{18}\text{P}_4$, 154
 $\text{C}_{13}\text{H}_{16}\text{N}_4\text{OS}$, 275
 $\text{C}_{13}\text{H}_{18}\text{O}_4$, 201
 $\text{C}_{13}\text{H}_{22}\text{O}_6$, 409
 $\text{C}_{14}\text{H}_{18}\text{ClNO}_2$, 347
 $\text{C}_{14}\text{H}_{18}\text{CuN}_6\text{S}_2$, 215
 $\text{C}_{14}\text{H}_{24}\text{Cl}_3\text{N}_6\text{OPt}_{0.5}$, 263
 $\text{C}_{14}\text{H}_{24}\text{O}_3$, 41
 $\text{C}_{14}\text{H}_{26}\text{N}_2\text{NiO}_{12}$, 195
 $\text{C}_{14}\text{H}_{27}\text{N}_6\text{O}_{13.5}\text{Zr}$, 71
 $\text{C}_{15}\text{H}_{10}\text{O}_4$, 393
 $\text{C}_{15}\text{H}_{12}$, 99
 $\text{C}_{15}\text{H}_{12}\text{Br}_2\text{Cl}_3\text{N}$, 287
 $\text{C}_{15}\text{H}_{13}\text{ClN}_2\text{S}$, 233
 $\text{C}_{15}\text{H}_{17}\text{N}_5\text{S}_2$, 149
 $\text{C}_{15}\text{H}_{19}\text{N}_3\text{O}_4$, 91
 $\text{C}_{15}\text{H}_{20.68}\text{N}_2\text{O}_{4.34}\text{S}$, 139
 $\text{C}_{15}\text{H}_{31}\text{NO}_4\text{Si}$, 401
 $\text{C}_{16}\text{H}_{10}\text{BrClO}_2$, 267
 $\text{C}_{16}\text{H}_{14}\text{F}_8\text{N}_2\text{O}_2\text{Pt}$, 87
 $\text{C}_{16}\text{H}_{16}\text{CuN}_{10}\text{S}_2$, 221
 $\text{C}_{16}\text{H}_{16}\text{O}_2$, 425
 $\text{C}_{16}\text{H}_{18}\text{N}_2\text{O}_5\text{S}$, 235
 $\text{C}_{16}\text{H}_{18}\text{O}_4\text{Se}$, 345
 $\text{C}_{16}\text{H}_{20}\text{N}_2\text{Te}$, 427
 $\text{C}_{16}\text{H}_{20}\text{N}_5\text{O}_{0.5}\text{S}_2$, 74
 $\text{C}_{16}\text{H}_{21}\text{NO}_3\text{S}$, 381
 $\text{C}_{16}\text{H}_{21}\text{NO}_4$, 281, 283
 $\text{C}_{16}\text{H}_{26}\text{N}_2\text{O}_6$, 407
 $\text{C}_{17}\text{H}_{10}\text{F}_6\text{O}_2\text{S}_2$, 415
 $\text{C}_{17}\text{H}_{14}\text{O}_5$, 231
 $\text{C}_{17}\text{H}_{15}\text{ClCuN}_6\text{O}_2$, 223
 $\text{C}_{17}\text{H}_{17}\text{NO}_3\text{S}$, 379
 $\text{C}_{17}\text{H}_{18}\text{CoN}_2\text{O}_6$, 65
 $\text{C}_{17}\text{H}_{23}\text{NO}_3\text{S}$, 383
 $\text{C}_{18}\text{H}_{14}\text{N}_6$, 61
 $\text{C}_{18}\text{H}_{17}\text{FN}_4\text{O}$, 38
 $\text{C}_{18}\text{H}_{21}\text{NO}_3\text{SSe}$, 343
 $\text{C}_{18}\text{H}_{22}\text{F}_6\text{Ru}$, 327
 $\text{C}_{18}\text{H}_{22}\text{N}_2\text{O}_6$, 435
 $\text{C}_{18}\text{H}_{24}\text{O}_3$, 423
 $\text{C}_{18}\text{H}_{32}\text{BF}_4\text{OPRu}$, 329
 $\text{C}_{18}\text{H}_{36}\text{N}_4\text{O}_{14}\text{Zr}$, 69
 $\text{C}_{18}\text{H}_{42}\text{AlBr}_9\text{N}_6\text{O}_6$, 128
 $\text{C}_{19}\text{H}_{20}\text{O}_{10}$, 207
 $\text{C}_{19}\text{H}_{25}\text{N}_3\text{O}_4\text{S}_2$, 133
 $\text{C}_{20}\text{H}_{12}\text{N}_2\text{O}_2$, 249
 $\text{C}_{20}\text{H}_{15}\text{BrN}_2\text{O}_3\text{S}$, 115
 $\text{C}_{20}\text{H}_{15}\text{ClN}_2\text{O}_3\text{S}$, 115
 $\text{C}_{20}\text{H}_{22}\text{Cl}_{0.4}\text{N}_{9.6}\text{O}_{9.4}\text{Zn}$, 228
 $\text{C}_{20}\text{H}_{22}\text{Cu}_2\text{N}_4\text{O}_3$, 217
 $\text{C}_{20}\text{H}_{26}\text{CoN}_6\text{O}_{11}$, 331
 $\text{C}_{20}\text{H}_{26.67}\text{Cl}_2\text{N}_4\text{O}_{1.33}\text{Pt}$, 257
 $\text{C}_{20}\text{H}_{27}\text{BrO}$, 119
 $\text{C}_{20}\text{H}_{27}\text{NO}_4\text{S}$, 89
 $\text{C}_{20}\text{H}_{30}\text{Cl}_2\text{Ti}$, 49
 $\text{C}_{20}\text{H}_{31}\text{ClOTi}$, 47
 $\text{C}_{20}\text{H}_{34}\text{O}_{10}$, 125
 $\text{C}_{20}\text{H}_{35}\text{ClN}_2\text{O}_3$, 261
 $\text{C}_{20}\text{H}_{40}\text{Cd}_2\text{N}_4\text{S}_8$, 85
 $\text{C}_{20}\text{H}_{43.50}\text{N}_{10}\text{O}_{15.50}\text{Pr}$, 109
 $\text{C}_{20}\text{H}_{46.40}\text{N}_{12}\text{O}_{15.70}\text{Pr}$, 112
 $\text{C}_{21}\text{H}_{14}\text{N}_4$, 353, 355
 $\text{C}_{21}\text{H}_{18}\text{F}_6\text{O}_4\text{S}_2$, 413
 $\text{C}_{21}\text{H}_{24}\text{O}_4$, 211
 $\text{C}_{21}\text{H}_{24}\text{O}_4\text{S}_2$, 209
 $\text{C}_{21}\text{H}_{29}\text{N}_5\text{O}_5\text{S}_3$, 135
 $\text{C}_{21}\text{H}_{30}\text{O}_2$, 81
 $\text{C}_{22}\text{H}_{26}\text{O}_3$, 83
 $\text{C}_{22}\text{H}_{33}\text{ClN}_2\text{O}_2$, 259
 $\text{C}_{23}\text{H}_{18}\text{F}_6\text{OS}_2$, 417
 $\text{C}_{23}\text{H}_{19}\text{N}_3\text{O}_2$, 351
 $\text{C}_{23}\text{H}_{23}\text{N}_2\text{PS}$, 389
 $\text{C}_{23}\text{H}_{23}\text{N}_3\text{O}_3\text{S}$, 349
 $\text{C}_{23}\text{H}_{41}\text{AuNPS}_2$, 359
 $\text{C}_{24}\text{H}_8\text{O}_6$, 253, 255
 $\text{C}_{24}\text{H}_{10}\text{N}_2\text{O}_4$, 45
 $\text{C}_{24}\text{H}_{16}\text{BiN}_7\text{O}_9$, 443
 $\text{C}_{24}\text{H}_{18}\text{O}$, 213
 $\text{C}_{24}\text{H}_{20}\text{Br}_6\text{PSb}$, 337
 $\text{C}_{24}\text{H}_{20}\text{Cl}_6\text{PSb}$, 335
 $\text{C}_{24}\text{H}_{20}\text{Mo}_2\text{N}_2\text{O}_6\text{S}_2$, 271
 $\text{C}_{24}\text{H}_{22}\text{CuN}_6\text{O}_5$, 219
 $\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}_3$, 32
 $\text{C}_{24}\text{H}_{24}\text{CoN}_6\text{O}_{10}$, 67
 $\text{C}_{25}\text{H}_{20}\text{O}_2$, 57
 $\text{C}_{25}\text{H}_{25}\text{N}_3\text{O}_4\text{S}_2$, 104
 $\text{C}_{25}\text{H}_{29}\text{Cl}_4\text{O}_3\text{P}$, 339
 $\text{C}_{25}\text{H}_{30}\text{CuN}_4\text{O}_{10}$, 333
 $\text{C}_{25}\text{H}_{30}\text{N}_4\text{O}_{10}\text{Zn}$, 191
 $\text{C}_{25}\text{H}_{32}\text{ClN}_3\text{O}_4$, 437
 $\text{C}_{26}\text{H}_{12}\text{N}_8\text{O}_{16}$, 439
 $\text{C}_{26}\text{H}_{22}\text{Fe}_2\text{O}_4$, 205
 $\text{C}_{26}\text{H}_{30}\text{N}_2\text{O}_8\text{Zn}$, 199
 $\text{C}_{27}\text{H}_{33}\text{NO}_4\text{Si}$, 285
 $\text{C}_{28}\text{H}_{20}\text{N}_4\text{Pd}_2\text{S}_2$, 147
 $\text{C}_{28}\text{H}_{24}\text{NPS}$, 391
 $\text{C}_{28}\text{H}_{27}\text{AuNOPS}$, 357
 $\text{C}_{28}\text{H}_{46}\text{Cl}_8\text{N}_{12}\text{O}_2\text{Pt}$, 263
 $\text{C}_{30}\text{H}_{20}\text{N}_2\text{O}_2$, 43
 $\text{C}_{30}\text{H}_{20}\text{N}_2\text{S}_2$, 97
 $\text{C}_{30}\text{H}_{29}\text{Cl}_2\text{PRu}$, 375
 $\text{C}_{30}\text{H}_{62}\text{N}_6\text{O}_{24}\text{P}_6$, 277
 $\text{C}_{31}\text{H}_{39}\text{Co}_2\text{O}_5\text{Ti}$, 241
 $\text{C}_{32}\text{H}_{18}\text{MgN}_8\text{O}$, 251
 $\text{C}_{32}\text{H}_{26}\text{N}_2\text{O}$, 29
 $\text{C}_{33}\text{H}_{39}\text{Co}_2\text{O}_8\text{Ti}$, 239
 $\text{C}_{34}\text{H}_{40}\text{O}_7$, 225
 $\text{C}_{36}\text{H}_{28}\text{N}_4\text{O}_4$, 445
 $\text{C}_{36}\text{H}_{38}\text{N}_4\text{P}_2\text{Pd}$, 366
 $\text{C}_{36}\text{H}_{48}\text{N}_4\text{O}_7$, 372
 $\text{C}_{36}\text{H}_{72}\text{B}_2\text{KNdO}_8\text{P}_2$, 35
 $\text{C}_{38}\text{H}_{24}\text{N}_4\text{O}_4$, 247
 $\text{C}_{38}\text{H}_{26}\text{Fe}_2\text{N}_4\text{S}_6$, 269
 $\text{C}_{38}\text{H}_{29}\text{N}_9\text{S}_4$, 395
 $\text{C}_{40}\text{H}_{35}\text{Ag}_2\text{Br}_2\text{N}_3\text{P}_2$, 341
 $\text{C}_{40}\text{H}_{36}\text{Au}_2\text{N}_2\text{O}_2\text{P}_2\text{S}_2$, 361
 $\text{C}_{40}\text{H}_{76}\text{Si}_4$, 101
 $\text{C}_{41}\text{H}_{46.58}\text{O}_{5.29}$, 141
 $\text{C}_{42}\text{H}_{59}\text{N}_5\text{O}_8$, 369
 $\text{C}_{43}\text{H}_{46}\text{Au}_2\text{N}_2\text{O}_4\text{P}_2\text{S}_2$, 363
 $\text{C}_{45}\text{H}_{47}\text{Cl}_2\text{NO}_7$, 144
 $\text{C}_{48}\text{H}_{40}\text{Cl}_2\text{F}_2\text{O}_2\text{Sn}_4$, 107
 $\text{C}_{48}\text{H}_{58}\text{N}_6\text{O}_{12}\text{P}_2\text{S}_2$, 55
 $\text{C}_{56}\text{H}_{64}\text{Cl}_4\text{O}_8\text{S}_6$, 398
 $\text{C}_{56}\text{H}_{80}\text{O}_8\text{Si}_4\text{Zr}_2$, 237
 $\text{C}_{60}\text{H}_{52}\text{N}_6\text{Nd}_2\text{O}_{22}$, 291
 $\text{C}_{64}\text{H}_{80}\text{O}_{16}$, 295
 $\text{C}_{72}\text{H}_{88}\text{Cl}_4\text{Pd}_2\text{Te}_4$, 151
 $\text{C}_{74}\text{H}_{66}\text{BiCl}_5\text{N}_2\text{OP}_4$, 385
 $\text{C}_{79}\text{H}_{51}\text{Mg}_2\text{N}_9\text{O}_2$, 244
 $\text{C}_{89}\text{H}_{86}\text{Cl}_2\text{O}_4\text{P}_4$, 51
 $\text{CaH}_4\text{O}_6\text{S}$, 9
 $\text{Ce}_2\text{Ni}_7\text{P}_4$, 159
 Ce_2Sb , 21
 $\text{Ce}_4\text{O}_7\text{S}_3\text{Si}_2$, 175
 $\text{Cl}_6\text{Rb}_2\text{W}$, 301
 $\text{Cl}_8\text{O}_2\text{Si}_3$, 324
 $\text{Cl}_{10}\text{O}_7\text{Si}_6$, 325
 $\text{Cs}_3\text{S}_4\text{Sb}$, 302
 $\text{CuH}_{12}\text{O}_{14}\text{Rb}_2\text{Se}_2$, 15
 $\text{Cu}_{1.02}\text{In}_{0.87}\text{S}_2\text{Zn}_{0.11}$, 13
 $\text{F}_{34}\text{Pb}_8\text{Y}_6$, 23
 Fe_2ILa_2 , 323
 $\text{Ga}_9\text{Ru}_5\text{Sm}_2$, 27
 $\text{Ga}_{11.95}\text{Si}_{34.05}\text{Sr}_8$, 179
 $\text{Ga}_{13.82}\text{Si}_{32.18}\text{Sr}_8$, 179
 $\text{Ge}_2\text{H}_2\text{NaO}_{10}\text{Sm}_3$, 17
 Ge_6PdYb_2 , 173
 $\text{HInLi}_2\text{O}_8\text{P}_2$, 307
 HLi_4N , 317
 $\text{H}_4\text{K}_2\text{O}_6\text{Os}$, 303
 $\text{H}_6\text{InNO}_8\text{P}_2$, 311
 $\text{H}_9\text{InN}_2\text{O}_8\text{P}_2$, 309
 $\text{H}_{12}\text{NiO}_{14}\text{Rb}_2\text{Se}_2$, 15
 $\text{H}_{16}\text{O}_{20}\text{Pr}_2\text{S}_3$, 299
 In_7Pt_3 , 24
 $\text{Lu}_2\text{O}_7\text{Si}_2$, 22
 $\text{O}_4\text{SeSiTb}_2$, 157
 SbSc_2 , 19

Zeitschrift für Kristallographie

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

New Crystal Structures

4/2002

Volume 217

Since 1877 Zeitschrift für
Kristallographie und Mineralogie
125
YEARS

Oldenbourg

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 electronically submitted to the publisher:

Oldenbourg Wissenschaftsverlag

Lektorat MINT
K. Berber-Nerlinger
Postfach 80 13 60
D-81613 München
Tel.: 49/89/4 50 51-3 24
Telefax: 49/89/4 50 51-2 92
e-mail: zkrist@verlag.oldenbourg.de
www: <http://www.zkristallogr.de>

Editor in chief:

Prof. W. Steurer

Managing Editor:

Dr. Yuri Grin.
Fax: +49-3 51-46 46-33 40
e-mail: grin@cpfs.mpg.de

(Addresses are printed on the inside cover page.)

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

© Copyright 2002 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 217 (2002)

ISSN 1433-7266

Oldenbourg Wissenschaftsverlag, München

Subscription information

Volume **217**: 4 issues will appear in **2002**

Annual subscription prices: EUR 236.– + postage: EUR 38.– (Germany), EUR 54.– (elsewhere).

Single issue: EUR 71.– + 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

Zeitschrift für Kristallographie

New Crystal Structures

Volume 217 • Issue 4 • 2002

Inorganic Crystal Structures

S.-Y. Yu, J.-X. Lu., Y.-K. Shan, M.-Y. He and L.-Y. Dai
Crystal structure of tetrapotassium dihydrogen tetratungsteno heptamolybdeno mononickel monoquasilicate hydrate, $K_4H_2[SiW_4Mo_7Ni(H_2O)O_{39}] \cdot 13H_2O$ 449

S.-R. Ye, Y.-K. Shan, M.-Y. He and L.-Y. Dai
Crystal structure of tetrapotassium dihydrogen heptatungsteno tetramolybdeno monomanganese monoquasilicate hydrate, $K_4H_2[SiW_7Mo_4Mn(H_2O)O_{39}] \cdot 13H_2O$ 451

L. Spina, M. Tillard and C. Belin
Crystal structure of the intermetallic compound lithium aluminum germanium, $Li_{16}Al_4Ge_7$ 453

J.-P. Jemietio Feudjio, Th. Doert and P. Böttcher
Refinement of the crystal structure of five ternary arsenides, $YCuAs_2$, $TbCuAs_2$, $DyCuAs_2$, $ErCuAs_2$ and $TmCuAs_2$ 455

Hj. Mattausch, O. Oeckler and A. Simon
Crystal structure of pentaterbium nonabromide monoethanide, $Tb_5Br_9C_2$ 458

Hj. Mattausch, O. Oeckler and A. Simon
Crystal structure of triterbium tribromide monosilicide, Tb_3Br_3Si 459

A. Grzechnik, J. Nuss, K. Friese, J.-Y. Gesland and M. Jansen
Refinement of the crystal structure of potassium triyttrium decafluoride, KY_3F_{10} 460

K. R. Dey, Th. M. Gesing, C. H. Rüschler and A. Hussain
Crystal structure of caesium niobium tungsten bronzes, $Cs_{0.23}(Nb_{0.09}W_{0.91})O_3$ and $Cs_{0.29}(Nb_{0.10}W_{0.90})O_3$ 461

P. Held, J. Liebertz and L. Bohatý
Crystal structure of dibarium pentaborate chloride, $Ba_2B_5O_9Cl$ 463

M. Heuer, A. Huber and G. Bromiley
Crystal structure of calcium iron zinc catena-disilicate, $Ca(Fe_{0.52}Zn_{0.48})Si_2O_6$ 465

M. Heuer, A. Huber and G. J. Redhammer
Crystal structure of calcium iron zinc catena-disilicate, $Ca(Fe_{0.19}Zn_{0.81})Si_2O_6$ 467

D. A. Zhrebtssov, L. G. Akselrud and R. Niewa
Crystal structure of dicalcium trinitrido monovanadate(V), $Ca_2[VN_3]$ 469

U. Schwarz
Crystal structure of indium monosulfide, InS , at 7.9 GPa 470

M. Fleck and U. Kolitsch
Crystal structure of ammonium hexaaquacobalt(II) selenate, $(NH_4)_2Co(SeO_4)_2 \cdot 6H_2O$, and of ammonium hexaaquazinc selenate, $(NH_4)_2Zn(SeO_4)_2 \cdot 6H_2O$, hydrogen bonds in two ammonium selenate Tutton's salts 471

K. O. Klepp and M. Sing
Crystal structure of rubidium dithiotricuprate, $RbCu_3S_2$... 474

K. O. Klepp and F. Fabian
Crystal structure of tetrarubidium tetrathioantimonate(IV), Rb_4SnS_4 475

L.-R. Zhang, H. Zhang, H. Borrmann and R. Kniep
Crystal structure of sodium vanadium(III) (monohydrogenmonophosphate-dihydrogenmonoborate-monophosphate), $NaV[BP_2O_7(OH)_3]$ 477

J.-X. Mi, H. Zhang, J.-F. Deng, S.-Y. Mao and J.-T. Zhao
Crystal structure of rubidium tetrachlorogallate, $RbGaCl_4$... 479

M. L. Mrad, A. Ben Slimane and M. Rzaigui
Crystal structure of hydrated tetrazinc cyclo-octaphosphate, $Zn_4[P_8O_{24}] \cdot 18H_2O$ 481

W. Hönle, J. Buresch, K. Peters, J. H. Chang and H. G. von Schnering
Crystal structure of the catena-pentelides KAs and $Na(As_{0.5}Sb_{0.5})$ 483

W. Hönle, J. Buresch, K. Peters, J. H. Chang and H. G. von Schnering
Crystal structure of the low-temperature modification of trilithium heptaarsenide, $LT-Li_3As_7$ 485

W. Hönle, J. Buresch, K. Peters, J. H. Chang and H. G. von Schnering
Crystal structure of the low-temperature modification of trisodium heptaarsenide, $LT-Na_3As_7$ 487

W. Hönle, J. Buresch, J. Wolf, K. Peters, J.-H. Chang and H. G. von Schnering
Crystal structure of the low-temperature modification of trirubidium heptaarsenide, $LT-Rb_3As_7$ 489

W. Hönle, J. Buresch, K. Peters, J. H. Chang and H. G. von Schnering
Crystal structure of tripotassium heptapentelides $K_3[As_xSb_{1-x}]_7$ with $x = 5/14$ and $x = 13/14$ 491

Organic and Metalorganic Crystal Structures

- L.-X. Zhang, M.-L. Hu, A.-J. Zhang and G.-Q. Xiang
Crystal structure of 2,6,6-trimethyl-2-hydroxybi-
cyclo[3.1.1]-3-heptanone oxime, $C_{10}H_{17}NO_2$ 494
- M.-D. Ye, M.-L. Hu, J.-X. Yuan and S. Wang
Crystal structure of 2,2'-bipyridine-1,1'-dioxide dihydrate,
 $C_{10}H_8N_2O_2 \cdot 2H_2O$ 497
- J.-C. Ding, M.-C. Liu, Y.-J. Zhao and M.-L. Hu
Crystal structure of 1-benzylthymine, $C_{12}H_{12}N_2O_2$ 499
- M.-D. Ye, M.-L. Hu and C.-P. Ye
Crystal structure of 2-aminopyrimidin-1-ium perchlorate,
($C_4H_6N_3$)ClO₄ 501
- S. Gupta, S. Henk, G. Kees, G.-Y. Yeap, I. Susanti,
W. A. K. Wan Mahmood and S. P. Sen Gupta
Crystal structure of E-1-(phenyl)-3-(4-hydroxyphenyl)-2-
propene-1-one, $C_{15}H_{12}O_2$ 503
- F. Bentefrit, A. Tomas, G. Morgant, D. Nguyen-Huy,
P. Lemoine and B. Viossat
Crystal structure of dichloro[1-(p-chlorophenyl)-5-isopropyl-
biguanide]-palladium(II), $C_{11}H_{16}Cl_3N_5Pd$ 505
- A. Bekaert, O. Barberan, E. B. Kaloun, C. Rabhi,
A. Danan, J. D. Brion, P. Lemoine and B. Viossat
Crystal structure of tetrakis(*N,N*-dimethylformamide-O)-
borane bis(tribromide) bromide,
{B[(CH₃)₂NCHO]₄}(Br₃)₂Br 507
- B. Tinant, J. P. Declercq, J. C. Mulatier and J. P. Dutasta
Crystal structure of ethyl-[3-thioxo-2-(3-thioxo-11,14,-
17,20-tetraoxa-2,4-diaza-3λ⁵-phospha-tricyclo[19.4.0.0^{5,10}]-
pentacosa-1(25),5(10),6,8,21,23-hexaene-3-yl)-11,14,17,20-
tetraoxa-2,4-diaza-3λ⁵-phospha-tricyclo[19.4.0.0^{5,10}]-
pentacosa-1(25),5(10),6,8,21,23-hexaene-3-yl]-amine
monohydrate, ($C_{38}H_{49}N_5O_8P_2S_2$) · H₂O 510
- A. R. Mahjoub and A. Morsali
Refinement of the crystal structure of
trans-bis(1,10-phenanthroline)bismuth(III) tribromide,
 $C_{24}H_{16}BiBr_3N_4$ 513
- J. Mizuguchi and H. Shikamori
Crystal structure of 3-[4-(1,1-dimethylethyl)phenyl]-2,5-
dihydro-6-phenylpyrrolo[3,4-*c*]pyrrole-1,4-dione,
 $C_{22}H_{20}N_2O_2$, at 93 K 515
- K. Tojo and J. Mizuguchi
Crystal structure of *N,N'*-bis(2-phenylpropyl)perylene-
3,4:9,10-bis(dicarboximide), $C_{42}H_{30}N_2O_4$ 517
- J. Mizuguchi, H. Takahashi and H. Yamakami
Crystal structure of 3,6-bis(4'-pyridyl)-pyrrolo[3,4-*c*]-
pyrrole-1,4-dione, $C_{16}H_{10}N_4O_2$, at 93 K 519
- K. Kobayashi, N. Tanifuji and J. Mizuguchi
Crystal structure of 11-(3'-oxodihydro[1]benzothiophen-2'-
ylidene)-cyclopenta[1,2-*b*:4,3-*b'*]di[1]benzothiophene,
 $C_{25}H_{12}OS_3$, at 93K 521
- J. Mizuguchi and T. Senju
Crystal structure of 5,12-dihydro-5-methylquino[2,3-*b*]-
acridine-7,14-dione, $C_{21}H_{14}N_2O_2$, at 93 K 523
- J. Mizuguchi, T. Senju and M. Sakai
Crystal structure of 5,12-dihydro-2,9-dimethylquino[2,3-*b*]-
acridine-7,14-dione, $C_{22}H_{16}N_2O_2$, at 123 K 525
- J. Zukerman-Schpector, P. R. Olivato and A. K. C. A. Reis
Crystal structure of 4'-methylphenyl-2-ethylsulfonyl
acetate, $C_{11}H_{14}O_4S$ 527
- F. Baysen, R. Yağbasan, S. Ide, E. Şahin, B. Çakır
and Y. Dünder
Crystal structure of ethyl 4-(2-oxobenzothiazolin-3-
yl)butanoate, $C_{13}H_{15}NO_3S$ 529
- E. Haussühl, S. Haussühl and E. Tillmanns
Crystal structure of bis(aminoguanidinium)
bis(nitrilotriacetato)zirconate,
[(NH₂)₂CNHNH₂]₂Zr[N(CH₂COO)₃]₂ 531
- E. Haussühl
Crystal structure of *N,N,N',N'*-tetramethylethylenedi-
ammonium bis(nitrilotriacetato)zirconate pentahydrate,
[(CH₃)₂NH(CH₂)₂NH(CH₃)₂]₂Zr[N(CH₂COO)₃]₂ · 5H₂O ... 533
- M. Ramos Silva, A. Matos Beja, J. A. Paixão,
A. J. F. N. Sobral, L. M. L. Cabral, S. H. Lopes
and A. M. d'A. Rocha Gonsalves
Crystal structure of iminodiacetic acid monomethyl ester
monohydrate, $C_5H_9NO_4 \cdot H_2O$ 535
- L. C. R. Andrade, M. M. R. Costa, J. A. Paixão, M. L. Santos,
J. Agostinho Moreira, M. R. Chaves and A. Almeida
Crystal structure of diammonium hydrogen-2-hydroxy-
1,2,3-propanetricarboxylate, (NH₄)₂(C₆H₆O₇) 537
- A. Kirfel, H. Euler, C. Valder, M. Neugebauer, M. Meier
and N. A. Braun
Crystal structure of (1*R*,2*S*,5*S*,6*R*,7*R*)-6-(4-bromo-
benzene-sulfonyloxy)-methyl-2,7-dimethyl-tri-
cyclo[5.2.2.0^{1,5}]undec-8-ene, $C_{20}H_{25}BrO_3S$ 539
- H. Euler, A. Kirfel, S. J. Freudenthal and C. E. Müller
Crystal structure of 4-bromobutyric acid 3-((4,4-difluoro-
1,3,5,7-tetramethyl-4-bora-3a,4a-diaza-*s*-indacen)-8-yl)-
propyl ester, $C_{20}H_{26}BBrF_2N_2O_2$ 541
- H. Euler, A. Kirfel, S. J. Freudenthal and C. E. Müller
Crystal structure of 8-(5-bromopentyl)-4,4-difluoro-
1,3,5,7-tetramethyl-4-bora-3a,4a-diaza-*s*-indacene,
 $C_{18}H_{24}BBrF_2N_2$ 543
- A. Spannenberg, V. V. Burlakov, P. Arndt, W. Baumann,
V. B. Shur and U. Rosenthal
Crystal structure of [1,2-ethylene-1,1'-bis(η⁵-tetra-
hydroindenyl)] [hydroxytris(pentafluorophenyl)-
borato]titanium(III), $C_{38}H_{24}BF_{15}OTi$ 546
- A. Spannenberg, N. Fdil, L. El Firdoussi and A. Karim
Crystal structure of [(1*R*)-(+)-3-benzoyl-camphoryl-*O,O'*]-
(cycloocta-1,5-diene)rhodium(I), $C_{25}H_{31}O_2Rh$ 549

H. Brunner, Th. Zwack and M. Zabel

Crystal structure of η^6 -benzene(chloro)(*N*-[(*S*)-(-)-1-phenylethyl]-thiobenzamido)ruthenium(II), (C₆H₆)Ru(C₁₅H₁₄NS)Cl

551

V. Huang and R. J. Staples

Crystal structure of 3-bromochromone, C₉H₅BrO₂ 554

J. C. Schlenker and R. J. Staples

Crystal structure of 6-methylnicotinamide, C₇H₈N₂O 555

M. Polamo and M. Hämäläinen

Crystal structure of bis(2,6-di(phenylamino)pyridinium) hexachlorotantalate(V) chloride—toluene (1/1), (C₁₇H₁₆N₃)₂(TaCl₆)Cl · C₇H₈ 557

M. Polamo, K. Lappalainen and M. Hämäläinen

Crystal structure of 2,6-di[(2-ethyl)phenylamino]pyridine, C₂₁H₂₃N₃ 559

M. Polamo and M. Hämäläinen

Crystal structure of 2-[2,6-bis(1-methylethyl)phenyl]-2,3-dihydro-1*H*-isoindol-1-one, C₂₀H₂₃NO, at 193K 561

M. Polamo and M. Hämäläinen

Crystal structure of 2-(2,6-dimethylphenylamino)pyridine, C₁₃H₁₄N₂ 563

J. Makker, S. Kumar, S. Dey and T. P. Singh

Crystal structure of Boc-Trp-ΔPhe-OH, C₂₅H₂₆N₃O₅ 565

K. O. Klepp and H. Schmidt

Crystal structure of 1,3,5-tri-2-propyl-2,4-dioxo-hexahydro-1,3,5-triazine, C₁₂H₂₃N₃O₂ 567

M. Fleck

Crystal structure of diaqualutetium(III) succinate dihydrate, Lu(H₂O)₂(C₄H₄O₄)_{1.5} · 2H₂O, the first succinate of a trivalent cation 569

J. A. Rusanova, S. Decurtins, E. B. Rusanov and H. Stoeckli-Evans

Crystal structure of bis(2,2'-bipyridine-*N,N'*)-[1,10-phenanthroline-5,6-dione]ruthenium(II) dihexafluorophosphate acetone solvate, [Ru(C₁₀H₈N₂)₂(C₁₂H₆N₂O₂)](PF₆)₂ · 1.75(CH₃)₂CO 571

K. Peters, M. Neumann and W. Tochtermann

Crystal structure of dimethyl (1*R**,2*R**,4*S**,6*S**,10*S**,13*S**,14*S**)-1-bromo-3,5-dioxapentacyclo[8.2.1.1^{6,13}.0^{4,6}.0^{2,14}]-tetradecane-13,14-dicarboxylate, C₁₂H₁₃BrO₂(COOCH₃)₂

575

K. Peters, A. Taugerbeck and W. Tochtermann

Crystal structure of (2'*R**,3'*R**,4'*R**,5'*R**,6'*R**)-1-(6'-hydroxy-5'-methoxy-2',3',4',5'-tetrahydro-2',4'-heptanofuran-3'-yl)-5-methyl-(1*H*,3*H*)-pyrimidine-2,4-dione, [C₄H₄O(OCH₃)(C₅H₅N₂O₂)](C₇H₁₃OH)

577

L.-G. Zhu and S. Kitagawa

Crystal structure of di(3-aminopyridine)disalicylato-copper(II), C₂₄H₂₂CuN₄O₆ 579

J. Karolak-Wojciechowska, R. Czyłkowski, K. Kieć-Kononowicz, E. Szymańska and A. Dzierżawska

Crystal structure of *Z*-5-(4-phenylbenzylidene)-2-methylthio-imidazoline-4-one, C₁₇H₁₄N₂OS 581

L. Liu, R. N. Warrener, R. A. Russell and E. R. T. Tiekink

Crystal structure of (13*S**,13*aR**)-2,3-dimethoxy-13-hydroxy-13*a*-methyl-8-oxo-5,6,13,13*a*-tetrahydro-8*H*-dibenzo[*a,g*]quinolizine, C₂₀H₂₁NO₄ 583

L. Liu, R. N. Warrener, R. A. Russell and E. R. T. Tiekink

Crystal structure of (3*S**,4*S**)-4-hydroxy-2-(2'-methoxyethyl)-3-phenyl-3,4-dihydroisoquinol-1(2*H*)-one, C₁₈H₁₉NO₃ 585

B. W. Greatrex, M. Jevric, M. C. Kimber, S. J. Krivickas, D. K. Taylor and E. R. T. Tiekink

Crystal structure of 1-(4-methoxyphenyl)-1,3*a*,4,11*c*-tetrahydro-3*H*-benzo[*f*]furo[3,4-*c*]chromen-3,4-dione, C₂₂H₁₆O₅ 587

S. Y. Ho and E. R. T. Tiekink

Refinement of the crystal structure of bis[(di-*n*-propyl-dithiocarbamato)gold(I)], C₇H₁₄AuNS₂ 589

S. Y. Ho and E. R. T. Tiekink

Crystal structure of chloro[tris(2-furyl)phosphine]gold(I), (C₄H₃O)₃PAuCl 591

C. S. Lai and E. R. T. Tiekink

Refinement of the crystal structure of bis[bis(*N,N*-diethylthiocarbamato)mercury(II)], [Hg(S₂CNEt₂)₂]₂ 593

A. Ramazani, A. Morsali, N. Noshiranzadeh,
B. Mohammadi, H. Arjmandfar, Z. Starikova,
A. Yanovsky and A. A. Korlyukov
Crystal structure of dimethyl 6-bromo-2*H*-1-benzopyran-
2,3-dicarboxylate, C₁₃H₁₁BrO₅ 595

A. Mahjoub, H. Zantour and S. Masson
Crystal structure of dithioacetic acid trimers,
(CH₃C(SH)S)₃ 597

H.-L. Zhu, S.-Y. Li, W.-M. He and K.-B. Yu
Crystal structure of aqua-*N*-(2-hydroxyphenylmethenyl-
imino)-1,5-diamine-3-azapentane-copper(II) chloride,
[(C₁₁H₁₆N₃O)Cu(H₂O)]Cl 599

H.-L. Zhu, Y.-J. Pan, X.-J. Wang and K.-B. Yu
Crystal structure of tetraaqua(*o*-phenanthroline)cobalt(II)
sulfate dihydrate, [C₁₂H₈N₂Co(H₂O)₄]SO₄ · 2H₂O 601

H. Punnapayak, J. Pechwang, N. Chaichit, N. Jaiboon,
S. Pornpakakul and A. Petsom
Crystal structure of ent-(7β,11α)-dihydroxy-1-oxo-kaur-
16-en-19-oic acid, C₂₀H₂₈O₅ 603

P. Laavanya, K. Panchanatheswaran, M. Muthukumar,
R. Jeyaraman and J. A. Krause Bauer
Crystal structure of *N*-nitroso-2,3,4,5-tetrahydro-2,2,4-tri-
methyl-1,5-benzothiazepine, C₁₂H₁₆N₂OS 605

A. Daut-Özdemir, O. Anaç, H. Borrmann and M. Somer
Crystal structure of 3*R*(*S*)-1'*S*(*R*)-2,2-dimethoxycarbonyl-
3-(2',6',6'-trimethyl-2'-cyclohexen-1'-yl)-2,3-dihydrofuran,
C₁₈H₂₆O₅ 607

A. Daut-Özdemir, O. Anaç, H. Borrmann and M. Somer
Crystal structure of *cis*-5-methoxy-2,2-dimethoxycarbonyl-
5-methyl-3-(2',6',6'-trimethyl-1'-cyclohexen-1'-yl)-tetra-
hydrofuran, C₁₉H₃₀O₆ 609

Q.-H. Jin, H.-G. Zheng and K.-B. Yu
Crystal structure of μ₃-bromo-2:3:4κ³*Br*-oxo-1κ*O*-tri-μ₃-
sulfido-1:2:3κ³*S*;1:2:4κ³*S*;1:3:4κ³*S*-tris(triphenyl-phos-
phine)-2κ*P*;3κ*P*;4κ*P*;tricopper molybdenum—quinoline
(2:1), {MoOS₃Cu₃Br[P(C₆H₅)₃]₃} · 0.5C₉H₇N 612

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).