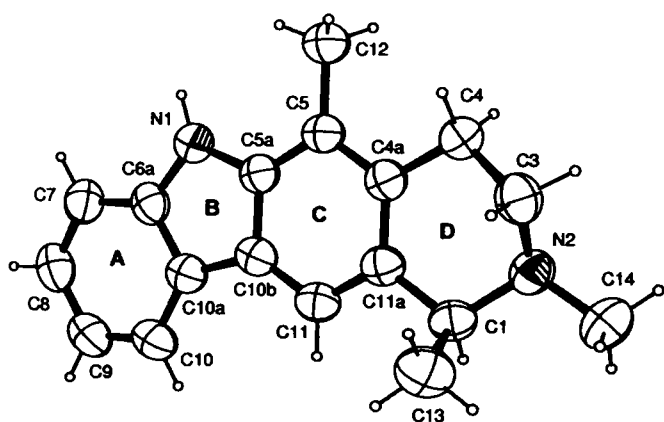


Crystal structure of 1,2,5-trimethyl-1,2,3,4-tetrahydropyrido[4,3-*b*]carbazole (guatambuine), C₁₈H₂₀N₂, from *Aspidosperma subincanum* Mart.

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Abstract

C₁₈H₂₀N₂, orthorhombic, *P*2₁2₁2₁ (no. 19), *a* = 11.587(5) Å, *b* = 8.130(5) Å, *c* = 15.239(5) Å, *V* = 1435.5 Å³, *Z* = 4, *R*_{gt}(*F*) = 0.055, *wR*_{ref}(*F*²) = 0.137, *T* = 293 K.

Source of material

The title compound, guatambuine, a pyrido[4,3-*b*]carbazole alkaloid, was isolated from the chloroform fraction of the ethanol extract from the stem of *Aspidosperma subincanum*, a tree of the *Apocynaceae* family. The crystals of the guatambuine were obtained by recrystallization from MeOH at room temperature.

Experimental details

H atoms attached to C atoms were located on stereochemical grounds and refined with fixed bond lengths and angles, each riding on a carrier atom, with an isotropic displacement parameter amounting to 1.5 (for methyl) or 1.2 (for the other H atoms) times the value of the equivalent isotropic displacement parameter of the atoms to which they are bonded. The H atom attached to the N atom was refined freely.

Discussion

The title compound, 1,2,5-trimethyl-1,2,3,4-tetrahydropyrido[4,3-*b*]carbazole, belongs to the class of indole alkaloids, a large group of biologically active compounds of naturally occurrence. The indole alkaloids have numerous biological activities such as anti-

tumor, anti-microbial, anti-hypertensive and stimulant for the central nervous system [1]. The occurrence of the indole alkaloids is described at the *Apocynaceae*, *Rubiaceae*, and *Loganiaceae* families [2]. Among the *Apocynaceae*, the genus *Aspidosperma* is especially rich in indole alkaloids [3]. *Aspidosperma subincanum* is a Brazilian medicinal plant used in the treatment of general debility, digestive tract disorders, dysentery and against fever [4]. Previous separate investigations of this plant revealed the presence of more than 15 indole alkaloids [5]. In our search for structurally unique and biologically interesting compounds from Brazilian medicinal plants we are working with the stem and stem bark of *A. subincanum*. From the ethanolic extract of stem of *A. subincanum* we isolated guatambuine or *N*-methyltetrahydro-olivacine, which has received considerable interest as result of this anti-tumor activity [6]. Guatambuine was isolated previously from others *Aspidosperma* species [7].

All the bond lengths and angles are within experimental error in good agreement with literature values. The atoms of three rings A, B and C of the molecule are nearly coplanar; the largest deviation (0.040(3) Å) from the least-squares plane is exhibited by atom C5. The heterocyclic ring D is in a half-chair conformation, as indicated by the Cremer & Pople puckering parameters [8]: *q*₂ = 6.221 Å, *q*₃ = −5.103 Å, *φ* = 263.59°, *Q* = 8.046 Å and *θ* = 129.35°. The C1 and C4 atoms of the heterocyclic ring D are located on the same plane of the rings A, B and C, while atoms C3 and N2 are located above and below respectively of that plane. Neighbored molecules are held together through one strong hydrogen interaction: N–H⋯N, where *d*(N1⋯N2ⁱ) = 3.015(4) Å, *d*(H1N⋯N2ⁱ) = 2.148(4) Å, *d*(N1–H1N) = 0.98(2) Å, ∠N1–H1N⋯N2ⁱ = 168(2)° (symmetry operation *i*: *x* − ½, *y* + ½, *z*).

Table 1. Data collection and handling.

Crystal:	colorless prism, size 0.09 × 0.12 × 0.18 mm
Wavelength:	Mo <i>K</i> _α radiation (0.71073 Å)
<i>μ</i> :	0.81 cm ^{−1}
Diffractionmeter, scan mode:	Nonius KappaCCD, <i>ω</i>
2 <i>θ</i> _{max} :	49.96°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	4743, 2497
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 <i>σ</i> (<i>I</i> _{obs}), 1830
<i>N</i> (<i>param</i>) _{refined} :	185
Programs:	SHELXS-97 [9], SHELXL-97 [10], ORTEP-3 [11], WinGX [12]

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

Atom	Site	x	y	z	U _{iso}
H(1N)	4a	0.758(4)	0.308(5)	−0.136(3)	0.10(1)
H(1)	4a	1.1958	−0.1424	0.0234	0.061
H(2)	4a	1.0625	−0.1496	−0.1027	0.062
H(3)	4a	0.9836	−0.1621	−0.2820	0.071
H(4)	4a	0.8872	−0.1235	−0.4120	0.077
H(5)	4a	0.7453	0.0755	−0.4241	0.076
H(6)	4a	0.6991	0.2426	−0.3066	0.070
H(8A)	4a	1.0477	0.2470	0.1500	0.063
H(8B)	4a	0.9307	0.1628	0.1754	0.063
H(9A)	4a	1.0954	0.0502	0.2496	0.070

Table 2. Continued.

Atom	Site	x	y	z	U _{iso}
H(9B)	4a	1.0189	−0.0828	0.2025	0.070
H(10A)	4a	1.3166	−0.1618	0.1537	0.105
H(10B)	4a	1.2182	−0.2302	0.2140	0.105
H(10C)	4a	1.2810	−0.0658	0.2387	0.105
H(11A)	4a	1.1349	−0.3653	0.1110	0.107
H(11B)	4a	1.0625	−0.3549	0.0243	0.107
H(11C)	4a	1.0097	−0.2926	0.1130	0.107
H(12A)	4a	0.7901	0.3938	−0.0010	0.091
H(12B)	4a	0.8964	0.4268	0.0602	0.091
H(12C)	4a	0.7964	0.3112	0.0918	0.091

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
N(1)	4a	0.8045(2)	0.2237(3)	−0.1432(2)	0.050(2)	0.055(1)	0.052(2)	0.005(1)	−0.004(1)	−0.005(1)
N(2)	4a	1.1678(2)	−0.0391(3)	0.1405(2)	0.053(2)	0.050(1)	0.057(2)	0.003(1)	−0.003(1)	0.006(1)
C(1)	4a	1.1282(3)	−0.1283(3)	0.0614(2)	0.054(2)	0.043(2)	0.056(2)	0.002(1)	0.005(1)	0.004(1)
C(1A)	4a	1.0417(3)	−0.0246(3)	0.0106(2)	0.047(2)	0.041(2)	0.054(2)	−0.002(1)	0.004(2)	0.002(1)
C(2)	4a	1.0220(3)	−0.0638(3)	−0.0765(2)	0.057(2)	0.042(1)	0.057(2)	0.001(1)	0.004(2)	−0.002(1)
C(2A)	4a	0.9414(3)	0.0258(3)	−0.1252(2)	0.047(2)	0.044(2)	0.049(2)	−0.006(1)	0.008(1)	−0.002(1)
C(2B)	4a	0.8998(3)	0.0172(3)	−0.2143(2)	0.048(2)	0.047(2)	0.051(2)	−0.005(1)	0.006(2)	−0.001(1)
C(3)	4a	0.9269(3)	−0.0815(4)	−0.2865(2)	0.064(2)	0.056(2)	0.059(2)	−0.007(2)	0.011(2)	−0.010(2)
C(4)	4a	0.8693(3)	−0.0582(4)	−0.3638(2)	0.070(2)	0.066(2)	0.057(2)	−0.012(2)	0.005(2)	−0.013(2)
C(5)	4a	0.7839(3)	0.0624(4)	−0.3711(2)	0.062(2)	0.078(2)	0.050(2)	−0.014(2)	−0.004(2)	−0.004(2)
C(6)	4a	0.7559(3)	0.1624(4)	−0.3013(2)	0.050(2)	0.068(2)	0.058(2)	−0.003(2)	−0.004(2)	−0.001(2)
C(6A)	4a	0.8146(3)	0.1401(3)	−0.2229(2)	0.047(2)	0.054(2)	0.048(2)	−0.010(1)	0.002(2)	−0.001(1)
C(6B)	4a	0.8817(2)	0.1553(3)	−0.0838(2)	0.042(2)	0.043(1)	0.050(2)	−0.003(1)	0.002(1)	0.001(1)
C(7)	4a	0.9022(2)	0.2005(3)	0.0027(2)	0.046(2)	0.043(1)	0.052(2)	−0.000(1)	0.004(1)	−0.002(1)
C(7A)	4a	0.9818(2)	0.1066(3)	0.0502(2)	0.046(2)	0.043(2)	0.050(2)	−0.004(1)	0.001(1)	0.001(1)
C(8)	4a	1.0040(3)	0.1455(4)	0.1460(2)	0.048(2)	0.056(2)	0.055(2)	0.003(1)	−0.001(2)	−0.005(1)
C(9)	4a	1.0693(3)	0.0108(4)	0.1929(2)	0.062(2)	0.061(2)	0.051(2)	−0.005(2)	−0.002(2)	0.002(1)
C(10)	4a	1.2533(3)	−0.1323(4)	0.1911(2)	0.068(2)	0.069(2)	0.073(2)	0.010(2)	−0.007(2)	0.015(2)
C(11)	4a	1.0792(3)	−0.3017(4)	0.0791(2)	0.091(3)	0.049(2)	0.074(2)	−0.004(2)	0.006(2)	0.009(2)
C(12)	4a	0.8407(3)	0.3463(4)	0.0420(2)	0.064(2)	0.056(2)	0.062(2)	0.010(2)	−0.002(2)	−0.006(2)

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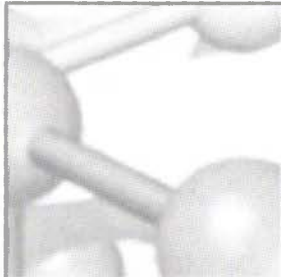
Author Index of Volume 221 Issues 1-2

- Al-Harrasi, A., 12, 131
 Babizhetskyy, V., 1
 Balireddi, S., 20, 23
 Balliano, T. L., 49
 Bee, K., 15
 Bekaert, A., 45
 Blöß, S. P., 209
 Bolte, M., 219
 Brion, J. D., 45
 Brüdgam, I., 12, 131, 213
 Buchta, M., 97
 Burkhardt, U., 109
 Cai, T.-J., 231
 Cai, X.-Q., 37
 Caracelli, I., 159, 167
 Čejka, J., 97
 Cella, R., 167
 Cerqueira Jr., C. R., 165
 Chang, Y., 105
 Chen, F., 47
 Chen, X.-L., 171
 Cheng, H.-J., 197
 Cheng, X.-L., 105
 Chowdhury, M. A., 213
 Cioletti, A. G., 49
 Clemente, J., 15
 Costa, M. M. R., 157
 Criado, A., 157
 Cussigh, O., 159
 De Simone, C. A., 49, 233
 Decurtins, S., 135
 Deeken, S., 93
 Deiseroth, H.-J., 119
 Demchyna, R., 109
 Deng, Q., 231
 DiMuzio, S. J., 15
 Ding, J.-C., 57, 59, 83
 Dobosz, M., 151
 Domingues, N. L. C., 161, 163
 Dou, Y.-L., 25, 181, 183, 185
 Dunstan, P. O., 159
 Fan, R., 183
 Feng, Y.-L., 173
 Fettouhi, M., 221
 Frederick, J., 15
 Frey, W., 43, 87, 89, 215, 217
 Fu, F., 195
 Fucci, A., 15
 Fukuda, Y., 123, 126, 129
 Galanski, M., 226
 Giorgi, M., 75
 Gjikaj, M., 121
 Góger, S., 75
 Gordon, L., 15
 Goulart, M. O. F., 49
 Gu, S.-J., 200
 Gulla, M., 89, 215, 217
 Guo, J.-X., 195
 Guo, J.-Y., 229
 Guo, W.-F., 27
 Han, X.-Q., 73
 Harper, A., 15
 Hartl, H., 12, 131, 213
 Haug, E., 43
 Haukka, M., 226
 Haussühl, E., 35, 77
 He, D.-P., 25
 He, Y., 105
 He, Y.-H., 142
 Hinrichs, F., 121
 Holthouse, B., 91
 Horn, E., 123, 126, 129
 Hou, Y.-Q., 51
 Hu, M.-L., 37, 39, 47
 Hu, X.-J., 203
 Humberto, M. M. S., 233
 Hunter, A. D., 15
 Hušák, M., 97
 Irrgang, T., 20, 23, 93, 95
 Isab, A. A., 221
 Jäger, V., 87, 89, 215, 217
 Jansen, M., 206, 209
 Jegorov, A., 97
 Jégou, A., 87
 Jiang, W.-J., 231
 Jing, L.-H., 200
 Ju, Y.-L., 7, 9
 Kaizer, J., 75
 Kantlehner, W., 43
 Karthikeyan, S., 20, 23, 95
 Kasmar, A., 15
 Kasmar, C., 15
 Kelly, P. F., 226
 Kempe, R., 20, 23, 93, 95, 153
 Keppler, B. K., 226
 Khan, G. S., 153
 Koizumi, R., 123
 Koziol, A. E., 151
 Kratochvíl, B., 97
 Królikowska, M., 155
 Kuhn, P., 31
 Kukushkin, V. Yu., 226
 Kuzma, M., 97
 Labat, G., 135
 Lamenha, G. S., 233
 Lan, K., 171
 Laurent, M., 68, 71
 Laus, G., 103
 Lei, X.-X., 37
 Lemoine, P., 45
 Li, D.-S., 85, 195
 Li, J., 51, 85
 Li, M.-F., 41
 Li, P., 179
 Li, T.-B., 55
 Li, T.-H., 169
 Li, X., 5, 7, 9
 Li, Y., 203
 Li, Z.-F., 211
 Lima, F. S., 161, 163
 Lin, H., 173
 Liu, H.-Q., 185
 Liu, J.-K., 203
 Liu, L.-H., 229
 Liu, M.-C., 57, 59, 83
 Liu, S.-X., 135
 Liu, W.-L., 223
 Liu, X.-F., 223
 Liu, Z.-H., 179, 189
 Long, Y.-F., 231
 Loosli, C., 135
 Lorch, M., 219
 Louati, A., 31
 Lu, Y., 197
 Lü, Z.-X., 145
 Lukachuk, M., 3
 Ma, J.-Y., 53
 Ma, Z.-C., 65
 Maganhi, S., 165
 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
 Miyamoto, K., 123, 126, 129
 Mondino, M. G., 161, 163
 Nasiri, H. R., 219
 Neels, A., 135
 Noor, A., 153
 Nuss, H., 206
 Nuss, J., 209
 Olivato, P. R., 161, 163, 165
 Pan, X.-F., 53
 Peng, Z.-S., 231
 Pereira, M. A., 49
 Pitucha, M., 151
 Polomsky, S., 15
 Porto, K. R. A., 233
 Prots, Yu., 109, 112, 115
 Qadeer, G., 153
 Qin, D.-B., 200
 Rahmani, H., 133
 Rama, N. H., 153
 Réglier, M., 75
 Reis, A. K. C. A., 161, 163
 Reißig, H.-U., 12, 131, 213
 Ren, F.-J., 229
 Richter, K. W., 112, 115
 Rittner, R., 161, 163
 Rodrigues, V. H., 157
 Samareh Afsari, H., 133
 Sant'Ana, A. E. G., 233
 Scaffidi-Domianello, Yu. Yu., 226
 Schmalz, T., 95
 Schnelle, W., 109
 Schottenberger, H., 103
 Schreuer, J., 35, 77
 Schwalbe, H., 219
 Schwarz, U., 109
 Sedmera, P., 97
 Shan, Y.-K., 41
 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
 Simmons, A., 15
 Simon, A., 1, 3
 Skrzypczak, A., 155
 Smallsreed, D., 15
 Song, Q.-B., 169
 Speier, G., 75
 Stefani, H. A., 167
 Strasser, C. E., 103
 Su, H., 173
 Tang, L., 85, 195
 Tinant, B., 68, 71
 Toupet, L., 31
 Trindade, A. C., 159
 Underwood, T., 15
 Velasquez, N., 49
 Vinhato, E., 165
 Viossat, B., 45

Wang, C., 51
 Wang, G.-X., 101, 187, 211
 Wang, J.-J., 85
 Wang, J.-W., 85, 195
 Wang, P., 107, 211
 Wang, R.-J., 203
 Wang, X.-Q., 27, 55
 Wang, Y.-L., 27
 Wazeer, M. I. M., 221
 Wei, J.-F., 148
 Wen, Y.-H., 142
 Wheeler, K. A., 91
 Wiehl, L., 35, 77
 Wu, H.-Y., 57, 59, 83
 Wu, R.-F., 229
 Wu, T.-X., 53
 Wujec, M., 151
 Wurst, K., 103
 Xiong, J., 37, 39
 Xu, D., 27, 55
 Xu, W., 107
 Yang, H.-J., 203
 Yang, L., 229
 Yin, M.-H., 181
 Yin, P., 39
 Yu, W., 229
 Yu, W.-T., 27, 55
 Yu, Y.-Y., 63
 Yuan, J.-X., 37, 39
 Yue, G.-R., 73
 Zaiss, T., 119
 Zeller, M., 15
 Zhang, B.-S., 191
 Zhang, F.-X., 51
 Zhang, G.-F., 181, 183, 185
 Zhang, G.-H., 27, 55
 Zhang, G.-L., 223
 Zhang, H., 203
 Zhang, H.-X., 200
 Zhang, J.-G., 229
 Zhang, L.-J., 57, 83
 Zhang, M.-L., 195
 Zhang, Q.-W., 101, 187
 Zhang, T.-L., 229
 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
 Zhou, C.-H., 85
 Zhou, R., 197
 Zonouzi, A., 133
 Zukerman-Schpector, J., 159, 161, 163, 165, 167

Formulae Index of Volume 221 Issues 1-2

- Ag₉AlS₆, 119
 Al₂₃Co_{10.14}Si_{8.72}, 112
 Al_{42.51}Co_{19.49}Si_{12.49}, 115
 Al_{43.14}Co_{18.86}Si_{11.86}, 115
 B₂C₅Pr₅, 1
 Ba_{0.73}Eu_{0.27}Ge₃Pt, 109
 BaGe₃Pt, 109
 Br₁₄K₂Mo₆, 107
 C₄H₇BF₃KS₂, 167
 C₅H₃N₃O₅, 183
 C₆H₅FN₂O₄, 57
 C₆H₈BrN₃O₂, 49
 C₆H₁₂Br₂N₄S₂Zn, 221
 C₆H₁₆Cl₄NOTa, 209
 C₇H₇CuNO₆, 35
 C₇H_{12.5}Br_{1.5}NO, 215
 C_{7.5}H_{12.5}B₅N_{1.5}O₁₀, 189
 C₈H₈FN₃O₅, 37
 C₈H₁₂N₆S₂, 151
 C₈H₂₅Br₂N₃NiO₃, 129
 C₉H₁₀N₄O₄, 59
 C₉H₁₁O_{4.5}, 187
 C₉H₁₄BrNO, 89
 C₉H₁₄CuN₆O₅S, 195
 C₁₀H₁₃NO₁₀, 229
 C₁₀H₁₆N₆NiO₁₆, 61
 C₁₁H₉ClN₂OS, 43
 C₁₁H₉FN₂O₂, 83
 C₁₁H₁₂BrNO, 217
 C₁₁H₁₄Cl₄CuN₂O, 53
 C₁₁H₁₄N₂O₅S, 161
 C₁₂H₁₄Cl₅FeN₈, 47
 C₁₂H₁₄O₇, 153
 C₁₂H₁₆K_{1.67}O₁₅Rb_{0.33}, 157
 C₁₄H₁₁N₅O₇, 29
 C₁₄H₂₁IN₂O₆, 87
 C₁₅H₃₃Cl₄CoMnN₃O₆, 77
 C₁₅H₃₃Cl₄MnN₃O₆Zn, 77
 C₁₆H₁₆BNO₆, 179
 C₁₆H₂₁NO₅S, 165
 C₁₇H₁₆N₈S₂, 185
 C₁₇H₁₉FN₄O₆, 39
 C₁₇H₂₃N₃O₇, 133
 C_{17.5}H₂₁Cl₂NOPtS₂, 226
 C₁₈H₁₅N₃O, 211
 C₁₈H₁₆ClNO₂S, 163
 C₁₈H₂₀N₂, 233
 C₁₈H₂₁NO₈S, 105
 C₁₈H₃₀Cu₃O₂₄, 101
 C₁₈H₄₉Cl₄IN₆Ni₃O, 123
 C₁₈H₄₉Cl₄N₆Ni₃O, 126
 C₁₉H₁₇O₂P, 171
 C₁₉H₂₅NO, 145
 C_{19.5}H₂₆N₂O_{1.5}, 219
 C₂₀H₁₈CuN₄O₆, 73
 C₂₀H₂₀HgN₂S₁₀, 27
 C₂₀H₂₂N₈S₂, 25
 C₂₀H₃₀F₂Ti, 206
 C₂₀H₃₉ClN₂O₂, 155
 C₂₂H₂₀CoF₆PRu, 103
 C₂₂H₄₉NO₅Si₂, 131
 C₂₃H₂₄O₁₁, 80
 C₂₃H₂₇NO₃, 68, 71
 C₂₃H₂₇NO₄, 213
 C₂₄H₃₂N₂O₂, 63
 C₂₅H₁₃N₇O₂, 91
 C₂₅H₂₂N₄NiO₇, 85
 C₂₅H₄₂AuNS₁₀, 55
 C₂₆H₂₃N₃O₃, 169
 C₂₆H₄₂N₄RuSi₂, 93
 C₂₇H₁₉CdClN₄O₂, 231
 C₂₈H₂₃MnN₂O₅, 51
 C₂₈H₂₈N₂NiO₄, 159
 C₂₈H₂₈N₄O₈S₂, 200
 C₂₈H₄₆Br₂Cu₂N₈O₄, 181
 C₂₈H₄₉NO₅Si₂, 12
 C₂₉H₂₀O₇, 176
 C₃₀H₃₆N₄O₁₄U₂, 45
 C₃₂H₂₆Fe₂O₄, 197
 C₃₃H₂₈N₂O₂, 65
 C₃₆H₃₀Cl₄O₂P₂Ti, 41
 C₃₆H₃₂N₄P₂Pt, 95
 C₃₆H₄₂N₈, 23
 C₃₉H₄₄O₁₂P₂W, 148
 C_{39.33}H₄₂Cl₄Cu₂N₆O_{8.67}, 75
 C₄₃H₄₂N₈O, 20
 C₄₈H₆₄Br₂N₂O₆, 203
 C₄₉H₄₀O₅, 31
 C₄₉H₆₂N₂O₁₄, 97
 C₅₄H₄₈Cl₄CuN₄O₈, 15
 C₅₄H₄₈Cl₄N₄NiO₈, 15
 C₅₄H₅₀Cl₄N₄O₈, 15
 C₆₀H₇₂Cl₄Cu₄N₁₂O₂₈, 223
 C₆₆H₄₀Cl₆La₂N₄O₁₂, 191
 C₆₆H₄₀Dy₂F₆N₄O₁₂, 7
 C₆₆H₄₀F₆N₄Nd₂O₁₂, 5
 C₇₂H₆₄Cu₆N₁₂O₃₅, 142
 C₇₈H₇₀N₄O₁₂Sm₂, 9
 C₈₁H₇₄DyN₁₇O₂, 135
 C₈₁H₇₅N₁₇O_{2.50}Tb, 135
 C₉₂H₁₄₀Cl₆Cu₂N₆O₃₈, 173
 EuGe₃Pt, 109
 Gd₄GeI₆, 3
 H₂₄MgN₂O₈P₂S₆, 121



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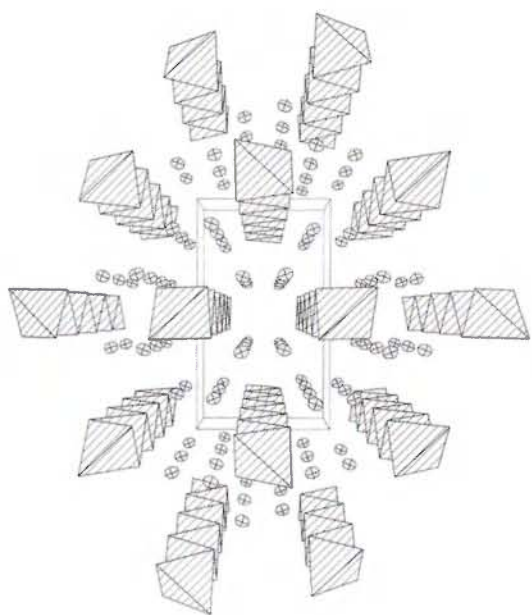
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Zeitschrift für Kristallographie

New Crystal Structures

Volume 221 · Issue 3 · 2006

Inorganic Crystal Structures

J.-P. Wang, P.-T. Ma and J.-Y. Niu
Re-investigation of the crystal structure of dodecasodium dodecaniobomanganate(IV) hydrate (1:52),
 $\text{Na}_{12}[\text{Mn}(\text{Nb}_6\text{O}_{19})_2] \cdot 52\text{H}_2\text{O}$ 235

S. Budnyk, Yu. Prots, Yu. B. Kuz'ma and Yu. Grin
Crystal structures of trigadolium tetraphosphidohepta-palladate, $\text{Gd}_3\text{Pd}_7\text{P}_4$, and triterbium tetraphosphidohepta-palladate, $\text{Tb}_3\text{Pd}_7\text{P}_4$ 238

A. Jiménez, J. D. Rodríguez, L. Torre-Fernández, M. Prieto and S. García-Granda
Crystal structure of dicalcium sodium monohydrogen diarsenate hexahydrate, $\text{Ca}_2\text{Na}[\text{HAsO}_4][\text{AsO}_4] \cdot 6\text{H}_2\text{O}$... 241

D. Phanon and I. Gautier-Luneau
Crystal structure of bismuth triiodate dihydrate,
 $\text{Bi}[\text{IO}_3]_3 \cdot 2\text{H}_2\text{O}$ 243

D. Phanon and I. Gautier-Luneau
Crystal structure of ytterbium triiodate dihydrate,
 $\text{Yb}[\text{IO}_3]_3 \cdot 2\text{H}_2\text{O}$ 245

D. Phanon and I. Gautier-Luneau
Crystal structure of indium triiodate dihydrate,
 $\text{In}[\text{IO}_3]_3 \cdot 2\text{H}_2\text{O}$ 247

D. Phanon and I. Gautier-Luneau
Crystal structure of indium triiodate trihydrate,
 $\text{In}[\text{IO}_3]_3 \cdot 3\text{H}_2\text{O}$ 249

P. W. Menezes, S. Hoffmann, Yu. Prots and R. Kniep
Crystal structure of potassium scandium (monophosphate-hydrogenmonoborate-monophosphate), $\text{KSc}[\text{BP}_2\text{O}_8(\text{OH})]$ 251

P. W. Menezes, S. Hoffmann, Yu. Prots and R. Kniep
Crystal structure of rubidium scandium (monophosphate-hydrogenmonoborate-monophosphate), $\text{RbSc}[\text{BP}_2\text{O}_8(\text{OH})]$ 253

A. Leithe-Jasper, R. Cardoso-Gil, R. Ramlau and U. Burkhardt
Crystal structure of tetraytterbium septarhodium hexaantimony, $\text{Yb}_4\text{Rh}_7\text{Sb}_6$ 255

F. Haarmann, Yu. Prots, S. Göbel and H. G. von Schnering
Crystal structure of tristrontium octagallide,
 $\text{Sr}_{3-x}\text{Ga}_{8+3x}$ ($x = 0.15$) 257

S. Stoyko, S. Oryshchyn, V. Babizhetskyy and R. Guérin
Crystal structure of yttrium nickel phosphide,
 $\text{Y}_{20}\text{Ni}_{42}\text{P}_{30.34}$ 259

O. Sichevych, R. Cardoso-Gil and Yu. Grin
Refinement of the crystal structure of europium digallide,
 EuGa_2 261

O. Sichevych, Yu. Prots, W. Schnelle, M. Schmidt and Yu. Grin
Crystal structure of dieuropium trigallium iridium,
 $\text{Eu}_2\text{Ga}_3\text{Ir}$ 263

O. Sichevych, Yu. Prots and Yu. Grin
Re-investigation of the crystal structure of trieuropium octagallide, $\text{Eu}_{3-x}\text{Ga}_{8+3x}$ ($x = 0.12$) 265

E. Dashjav, W. Schnelle, F. R. Wagner, G. Kreiner and R. Kniep
Crystal structure of praseodymium dimolybdenum disilicide carbide, $\text{PrMo}_2\text{Si}_2\text{C}$ 267

D. Grüner, A. Ormeci and G. Kreiner
Crystal structure of niobium chromium nickel,
 $\text{Nb}(\text{Cr}_{1-x}\text{Ni}_x)_2$ ($x = 0.49$) 269

O. Reckeweg and F. J. DiSalvo
Crystal structure of distrontium oxide diiodide, Sr_2OI_2 ... 271

Organic and Metalorganic Crystal Structures

D.-Y. Wei, S.-J. Huang, J. Sun and Y.-Q. Zheng
Crystal structure of diaquadysprosium triglutarate tetrahydrate, $\text{Dy}_2(\text{H}_2\text{O})_2[\text{O}_2\text{C}(\text{CH}_2)_3\text{CO}_2]_3 \cdot 4\text{H}_2\text{O}$ 273

I. Warad, S. Al-Resayes and K. Eichele
Crystal structure of *trans*-dichloro-1,3-propanediamine-bis[(2-methoxyethyl)diphenylphosphine]ruthenium(II),
 $\text{RuCl}_2(\text{C}_3\text{H}_{10}\text{N}_2)(\text{C}_{15}\text{H}_{17}\text{OP})_2$ 275

S. Sörgel, I. Brüdgam, H. Hartl and H.-U. Reißig
Crystal structure of 2-bromo-1,4,5,7,8-pentamethoxy-naphthalene, $\text{C}_{10}\text{H}_2\text{Br}(\text{OCH}_3)_5$ 278

L. Yang, W. Yu, T. Wu, T.-L. Zhang, J.-G. Zhang, J.-Y. Guo, R.-F. Wu and F.-J. Ren
Crystal structure of carbohydrazidium(1+) *p*-toluene-sulfonate, $(\text{NH}_2\text{NHCONHNH}_3)[\text{CH}_3\text{C}_6\text{H}_4\text{SO}_3]$ 281

A. Noor, T. Irrgang and R. Kempe
Crystal structure of (2,6-diisopropyl-phenyl)[*N*-tris(pentafluorophenyl)-boronyl-pyridin-2-yl]amine,
 $(\text{C}_6\text{F}_5)_3\text{B}(\text{C}_5\text{H}_4\text{N})(\text{C}_{12}\text{H}_{18}\text{N})$ 283

- Q.-B. Song and J. Zhang*
Crystal structure of (1,8-diethyl-1,3,4,9-tetrahydropyrano[3,4-*b*]indol-1-yl)acetic acid (2-hydroxy-benzylidene)hydrazide, $C_{24}H_{27}N_3O_3$ 285
- Q. Deng, W.-J. Jiang, Z.-S. Peng, Y.-F. Long and T.-J. Cai*
Crystal structure of aquabis(acrylate-*O,O'*)-(1,10-phenanthroline-*N,N'*)zinc(II) hydrate, $Zn(C_3H_3O_2)_2(H_2O)(C_{12}H_{10}N_2) \cdot H_2O$ 287
- R. D. Ernst, R. Basta and A. M. Arif*
Crystal structure of bis(6,6-dimethyl-cyclohexadienyl)vanadium, $V(C_8H_{11})_2$ 289
- R. D. Ernst, B. G. Harvey and A. M. Arif*
Crystal structure of (hydrido)(η^3 -butenyl)-bis(η^5 -pentamethylcyclopentadienyl)zirconium, $Zr(C_4H_7)[C_5(CH_3)_5]_2(H)$ 291
- R. D. Ernst, V. Kulsomphob and A. M. Arif*
Crystal structure of (η^5 -2,4-dimethylpentadienyl)[η^2 -*rel*-(*aR*)-a-[[[(1*R*,5*E*)-5-[(1,1-dimethylethyl)imino]-1,3-dimethyl-2-cyclopenten-1-yl]methyl]-*N*-(1-methylethyl)-benzenemethanaminato- κN][2-(isocyano- κC)-2-methylpropane]zirconium, $Zr(C_7H_{11})(C_{22}H_{33}N_2)(C_4H_9NC)$ 293
- X. Feng, X. Han and L.-Y. Wang*
Crystal structure of bis(*N*-(2-aminoethyl)salicylaldiminato)iron(III) isothiocyanide, $[Fe(C_9H_{11}N_2O)_2][NCS]$ 296
- M.-Q. Cheng, L.-F. Ma and L.-Y. Wang*
Crystal structure of *catena*-[(1,10-phenanthroline-*N,N'*)-bis(μ -acetato-*O,O'*)lead(II)], $Pb(C_{12}H_8N_2)(CH_3COO)_2$... 299
- G. Steiner, K. Wurst, B. Bildstein and H. Kopacka*
Crystal structure of dichlorobis[*N*-(2,6-diisopropylphenyl)benzimidimidazolid]palladium(II), $PdCl_2(C_{22}H_{25}N_3)_2$ 301
- G. Steiner, K. Wurst, B. Bildstein and H. Kopacka*
Crystal structure of dichloro(3-cyclopentadienyl-3-methyl-1-phenyl-butyliden-2,6-dimethylphenyl-amino)chromium(III), $CrCl_2(C_{24}H_{26}N)$ 303
- M. Zareef, R. Iqbal, G. Qadeer, W.-Y. Wong, H. Akhtar and M. Arfan*
Crystal structure of 2-bromobenzoic acid hydrazide, $C_7H_7BrN_2O$ 305
- M. Zareef, R. Iqbal, J. H. Zaidi, G. Qadeer, W.-Y. Wong and H. Akhtar*
Crystal structure of picolinic acid hydrazide, $C_6H_7N_3O$... 307
- P. Lemoine, A. Bekaert, J. D. Brion and B. Viosat*
Crystal structure of hexakis(μ_2 -acetato)tris(acetonitrile- κN)- μ_3 -oxo-trialuminum(III) tetrachloroaluminate, $[Al_3(C_2H_3O_2)_6(C_2H_3N)_3O][AlCl_4]$ 309
- J. Zukerman-Schpector, R. Oliveira da Silva, P. R. Olivato, E. Vinhato, A. Rodrigues and C. R. Cerqueira Jr.*
Crystal structure of 2-phenylsulfinyl-cyclohexanone, $C_{12}H_{14}O_2S$ 311
- Z.-X. Du, M.-L. Han and X. Feng*
Crystal structure of tetrakis(melaminium) 1,2,4,5-benzenetetracarboxylate octahydrate, $(C_3H_7N_6)_4[C_6H_2(COO)_4] \cdot 8H_2O$ 313
- Y.-H. Deng, Y.-L. Yang and X.-J. Yang*
Crystal structure of diiodo-bis[(4*R*,5*R*)-*trans*-4,5-bis[(diphenylphosphinomethyl)-2,2-dimethyl-1,3-dioxalane]dicopper(I)], $Cu_2I_2(C_{31}H_{32}O_2P_2)_2$ 316
- L. Yu, P.-T. Ma, J. Li and J.-P. Wang*
Refinement of the crystal structure of bis(2-hydroxy-1,10-phenanthroline)dicopper(I), $Cu_2(C_{12}H_7N_2O)_2$ 319
- A.-Q. Wang, Y. Wu and H. Guo*
Crystal structure of 8-bromo-6-chloro-1',3',3'-trimethylspiro[2*H*-1-benzopyran-2,2'-indoline], $C_{19}H_{17}BrClNO$ 321
- M.-H. Wu, X.-H. Yang, W.-D. Zou, W.-J. Liu and C. Li*
Refinement of the crystal structure of (*E*)-1,3-diphenyl-2-propen-1-one, $C_{15}H_{12}O$ 323
- Y.-J. Wei and F.-W. Wang*
Crystal structure of bis(cyclopropyl-4-bromosalicylaldiminato)cobalt(II), $Co(C_{20}H_{18}BrNO)_2$ 325
- Y.-H. Luo, X.-J. Hu, J.-K. Liu, H. Zhang, Y. Li, H.-J. Yang and R.-J. Wang*
Crystal structure of 5,11,17,23-tetrabromo-25,27-dihydroxy-26,28-dimethoxycalix[4]arene, $C_{30}H_{24}Br_4O_4$ 327
- X.-J. Hu, H.-J. Yang, J.-K. Liu, H. Zhang, Y. Li, Y.-H. Luo, Y.-H. Luo and R.-J. Wang*
Crystal structure of 5,17-bis(*N-tert*-butylhydroxyamine)-25,26,27,28-tetrapropoxycalix[4]arene, $C_{48}H_{66}N_2O_6$ 329
- Q.-H. Jin, J.-C. Dong, H.-W. Gao, X.-L. Xin, L. Yang and P.-Z. Li*
Crystal structure of *catena*-poly[(μ -2-aminopyrimidine-*N,N'*)bis(μ -chloro)bis(triphenylphosphine)dicopper(I)], $Cu_2Cl_2[P(C_6H_5)_3]_2(C_4H_5N_3)$ 332
- Z.-S. Peng, W.-J. Jiang, Q. Deng, Y.-F. Long and T.-J. Cai*
Refinement of the crystal structure of *catena*-[(1,10-phenanthroline-*N,N'*)-(μ^3 -molybdate(VI))copper(II)] monohydrate, $Cu(C_2H_{10}N_2)(MoO_4) \cdot H_2O$ 335
- D. B. Werz, S. Balalaie, F. Rominger and Z. Oloumi*
Crystal structure of 2-(2-propynyloxy)benzaldehyde, $C_{10}H_8O_2$ 337
- D. B. Werz, S. Balalaie, F. Rominger and Z. Oloumi*
Crystal structure of 2-[6-(2-formylphenoxy)-2,4-hexadiynyloxy]benzaldehyde, $C_{20}H_{14}O_4$ 339
- X.-S. Tai and F.-Y. Kong*
Crystal structure of 2'-hydroxyacetophenone nicotinoyl-hydrazone monohydrate, $C_{14}H_{15}N_3O_3 \cdot H_2O$ 341

- J.-N. Feng, Y.-Z. Zhou, H.-J. Zhu and S.-J. Tu*
Crystal structure of ethanolammonium dioxo-(*N*-(2-ethanolato)-2-oxy-3-methoxybenzaldiminato-*O,N,O'*)-vanadate(V),
(NH₃CH₂CH₂OH)[VO₂{(C₆H₄(OCH₃)(O)CHNCCCH₂CH₂O)}] . . . 343
- G. N. Kaluderovic, G. A. Bogdanovic and T. J. Sabo*
Crystal structure of ethylenediammonium-*N,N'*-di-3-propionic acid tetrachloroplatinate(II),
(CH₂NH₂(CH₂)₂COOH)₂[PtCl₄] . . . 345
- W. Frey, S. Shiva and V. Jäger*
Crystal structure of *rel*-(3*aR*,4*S*,6*aS*)-4-chloromethyl-6-methyl-3,6*a*-diphenyl-3*a*,4,6,6*a*-tetrahydro-isoxazolo-[5,4-*c*]isoxazole, C₁₈H₁₇ClN₂O₂ . . . 347
- W. Frey, S. Shiva and V. Jäger*
Crystal structure of *rel*-(3*aR*,6*aS*)-6-methyl-3,6*a*-diphenyl-3*a*,4,6,6*a*-tetrahydro-isoxazolo[5,4-*c*]isoxazole, C₁₇H₁₆N₂O₂ . . . 349
- H.-M. Guo, B.-S. Zhang and Y.-H. Wang*
Crystal structure of bis(1,10-phenanthroline-*N,N'*)bis(2-chlorobenzoato)lead(II) hydrate (1:2.5),
[Pb(C₇H₄O₂Cl)₂(C₁₂H₈N₂)₂] · 2.5 H₂O . . . 352
- B.-S. Zhang*
Crystal structure of (2,2'-bipyridine-*N,N'*)bis(2-fluorobenzoato)lead(II), Pb(C₇H₄O₂F)₂(C₁₀H₈N₂) . . . 355
- C. A. De Simone, V. L. M. Guarda, S. L. Galdino and I. R. Pitta*
Crystal structure of 4-butyl-6-nitro-2*H*-1,4-benzothiazin-3-one, C₁₂H₁₄N₂O₃S . . . 357
- C. R. Doyle, M. D. Zimmerman, M. Chruszcz, M. Cymborowski, A. Gawlicka-Chruszcz and W. Minor*
Crystal structure of 6-(4-difluoromethoxy-3-methoxyphenyl)-3(2*H*)-pyridazinone, C₁₂H₁₀F₂N₂O₃ . . . 359
- X.-L. Wang*
Refinement of the crystal structure of sinoacutine, C₁₉H₂₁NO₄ . . . 361
- I.-C. Hwang and K. Ha*
Crystal structure of aquachloro[*N,N'*-bis(3-ethoxy-salicylidene)ethylenediiminato]manganese(III) dihydrate, [Mn(C₂₀H₂₂N₂O₄)Cl(H₂O)] · 2H₂O . . . 363
- I.-C. Hwang and K. Ha*
Crystal structure of aquachloro[*N,N'*-bis(3-ethoxy-salicylidene)propylenediiminato]manganese(III) dihydrate, [Mn(C₂₁H₂₄N₂O₄)Cl(H₂O)] · 2H₂O . . . 365
- Y. B. Lee, T. H. Kim, I.-C. Hwang and K. Ha*
Crystal structure of *N*-benzoyl-4,4-dimethyl-2-methyl-amino-2-thiazoline, C₁₃H₁₆N₂OS . . . 367
- M.-Q. Cheng, L.-F. Ma and L.-Y. Wang*
Crystal structure of (phenanthroline-*N,N'*)-*N*-carbamoyl-methyliminodiacetato-copper(II) dihydrate, [Cu(C₆H₈N₂)(C₁₂H₈N₂)] · 2H₂O . . . 369
- Z. An and R.-S. Wang*
Crystal structure of tetraqua-bis(norfloroxacin)barium(II) 1,4-benzenedicarboxylate hydrate, [Ba(H₂O)₄(C₁₆H₁₇FN₃O₃)₂][C₆H₄(COO)₂] · H₂O . . . 372
- W.-D. Wang, H. Wang, W.-J. Feng, Z.-M. Jin and M.-L. Hu*
Crystal structure of caffeineium perchlorate monohydrate, (C₈H₁₁N₄O₂)[ClO₄] · H₂O . . . 375
- H.-L. Keller and T. Oldag*
Crystal structure of (acetonitrile-*N*)copper(I) cyanide, [Cu(CH₃CN)][CN] . . . 377
- H.-L. Keller and T. Oldag*
Crystal structure of dicyano(*N*-(1-iminoethyl)-acetamidine)palladium(II), Pd(CN)₂(C₄H₉N₃) . . . 379
- G. Le Bras, A. Bekaert, B. Viossat, J.-F. Peyrat, M. Alami, J. D. Brion and P. Lemoine*
Crystal structure of cyclonovobiocin, C₄₄H₄₂N₂O₁₂ . . . 381
- Q.-H. Jin, L. Yang, X.-L. Xin, H.-W. Gao, J.-C. Dong and P.-Z. Li*
Crystal structure of aqua(phenanthroline-*N,N'*)-(glycinato-*N,O*)copper(II) bromide hydrate, [Cu(NH₂CH₂COO)(C₁₂H₈N₂)(H₂O)]Br · H₂O . . . 383
- C.-C. Wang*
Refinement of the crystal structure of aquabis(2,2'-bipyridine)bis(terephthalato)dycopper(II), Cu₂(H₂O)(C₁₀H₈N₂)₂(C₈H₄O₄)₂ . . . 385
- C.-C. Wang*
Crystal structure of bis[(1,3-bis(4-pyridinium)-propane)][β-hexacosaoxoctamolybdate(VI)], (C₁₃H₁₆N₂)₂[Mo₈O₂₆] . . . 388
- P.-G. Li, Q.-L. Wang, D.-S. Li, F. Fu and G.-C. Qi*
Crystal structure of bis(1,10-phenanthroline-*N,N'*)silver(I) mononitrate, [Ag(C₁₂H₈N₂)₂][NO₃] . . . 391
- S. Guo, R. Hauptmann, C. Beyer, T. Kollmann and J. J. Schneider*
Crystal structure of pentamethylpyrylium triiodide, [(CH₃)₅C₅O][I₃] . . . 393
- F.-Q. Cao, Y. Wang, N. Okabe and M. Odoko*
Crystal structure of aquabis(4-aminobenzoato)cadmium dihydrate, Cd(H₂O)(NH₂C₆H₄COO)₂ · 2H₂O . . . 395
- S. Florio, V. Capriati, R. Luisi, A. Salomone and C. Cuocci*
Crystal structure of (*N*-*tert*-butyl-3,4-diphenyl-1,2-oxazetidin-4-yl)methanol, C₁₉H₂₃NO₂ . . . 398
- S.-P. Xu, C.-H. Liu and Y. Zhu*
Crystal structure of tetra(2-aminopyrimidine)di-methanolato-dicobalt(II) diperchlorate, [Co₂(CH₃O)₂(C₄H₅N₃)₄][ClO₄]₂ . . . 401
- S.-P. Xu, C.-H. Liu and P. Cao*
Crystal structure of tetra(2-aminopyrimidine)di-methanolato-dinickel(II) di(tetrafluoroborate), [Ni₂(CH₃O)₂(C₄H₅N₃)₄][BF₄]₂ . . . 403

S.-P. Xu, C.-H. Liu and J. Shao
Crystal structure of bis(1,3-diaminepropane)carbonato-
manganese(III) chloride monohydrate,
[Mn(C₃H₁₀N₂)₂(CO₃)]Cl · H₂O 405

S.-P. Xu, C.-H. Liu and C.-H. Zhu
Crystal structure of μ -terephthalatobis[bis(1,3-diamino-
propane)manganese(II)] diperchlorate,
[Mn₂(C₃H₆(NH₂)₂)₄{C₆H₄(COO)₂}] [ClO₄]₂ 407

S.-P. Xu, C.-H. Liu and S.-F. Wang
Crystal structure of acetato- μ -N,N'-bis(salicylidene)-
3-methyl-3-aza-1,5-pentanediaminocobalt(III),
Co(C₂H₃O₂)(C₂₁H₂₅N₃O₂) 409

H. Maisel, G. Glatz, T. Irrgang and R. Kempe
Crystal structure of dicyclohexyl-2,2'-dipyridylamido-
phosphane, C₂₂H₃₀N₃P 411

T. Irrgang, A. Spannenberg and R. Kempe
Crystal structure of bis(1,3-bis[{4-methyl-pyridin-2-yl}-
amido]-1,1,3,3-tetramethyldisiloxane)dichromium
dichloride, [(C₁₆H₂₄N₄OSi₂)CrCl]₂ 413

A. Noor, T. Irrgang and R. Kempe
Crystal structure of tetrakis[(4-methyl-pyridin-2-yl)tri-
methylsilanyl-amido]zirconium(IV), Zr(C₉H₁₅N₂Si)₄ 415

Z. García-Hernández, B. Wrackmeyer, M. Herberhold,
T. Irrgang and R. Kempe
Crystal structure of 3,4,7,8-bis(1,2-dicarba-closo-
dodecaborano[1,2])-1,2,5,6-tetraselenacyclooctane
benzene solvate, [(C₂B₁₀H₁₀)Se₂]₂ · C₆D₆ 419

T.-J. Cai, W.-J. Jiang, Z.-S. Peng, Y.-F. Long and Q. Deng
Crystal structure of aquabis(acrylato-O,O')(1,10-
phenanthroline-N,N')cadmium(II),
Cd(H₂O)(C₃H₃O₂)₂(C₁₂H₁₀N₂) 421

H. Reuter and M. Izaaryene
Crystal structure of dichloro-bis(*n*-pentyl)tin(IV),
Sn(C₅H₁₁)₂Cl₂, tin-halide compounds – part VI 423

Instructions to Contributors

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-
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