

intensities taken at 900°C correspond to the values given by Kreidler & Hummel. From geometrical considerations it seems obvious that $\beta\text{-CaZn}_2(\text{PO}_4)_2$ contains a double-sheet $[\text{Zn}_2\text{P}_2\text{O}_8]^{2-}$ with trigonal symmetry. The $[\text{Zn}_2\text{P}_2\text{O}_8]^{2-}$ -double sheet is built up from six-membered rings of tetrahedra. Each PO_4 tetrahedron is surrounded by four ZnO_4 tetrahedra and vice versa. The resulting symmetry of

Table 1. Coordinates of structure model for $\beta\text{-CaZn}_2\text{P}_2\text{O}_8$
Six oxygen atoms in general position xyz are not included.

	Equipoint of space group $P3$	x	y	z
Ca	1(a)	0	0	0
Zn(1)	1(c)	0.66	0.33	0.30
Zn(2)	1(b)	0.33	0.66	0.70
P(1)	1(c)	0.66	0.33	0.25
P(2)	1(b)	0.33	0.66	0.75
O(1)	1(c)	0.66	0.33	0.45
O(2)	1(b)	0.33	0.66	0.55

Table 2. Comparision of observed and calculated $F_{hkl,i}$'s corresponding to one formula unit (F_o , powder diffraction data at 900°C)

hkl	F_o	F_c
100	25.6	29.5
200	6.4	23.2
300	107.5	75.7
102	59.9	59.7
104	58.4	45.3
202	32.9	17.3
302	17.9	29.5
110	97.4	101.6
111	12.4	12.0
113	25.7	40.7
211	17.5	5.9
212	29.5	50.8

the double sheet is trigonal. With this assumption structure-factor calculations for a model with the coordinates of Table 1 were made. This led to an R value of 0.29. Table 2 gives the F_o and F_c values.

The crystal structure of scholzite (Taxer, 1970) shows some characteristics which make it possible to explain the topotactic reaction mechanism which leads to trigonal double-sheets $[\text{Zn}_2\text{P}_2\text{O}_8]^{2-}$ in the β -phase. Scholzite has layers of $[\text{Zn}_2(\text{PO}_4)_2]^{2-}$ parallel to (100) which alternate with Ca ions and water molecules. Ca has sixfold coordination with four oxygens from different isolated PO_4 groups and two water molecules. The ZnO_4 groups form chains parallel to c . Its bridging oxygens at the same time link the PO_4 groups to the chain. After dehydration the a axis, which is normal to the $[\text{Zn}_2(\text{PO}_4)_2]^{2-}$ layers shrinks from 17.19 to $2 \times 7.67 = 15.34$ Å and becomes the trigonal axis of the β -phase.
 P
 |

Within the $[\text{Zn}_2(\text{PO}_4)_2]^{2-}$ sheet the Zn–O–Zn arrangement is given up as all the oxygen atoms become bridging oxygen atoms. The resulting trigonal unit cell of $\beta\text{-CaZn}_2\text{P}_2\text{O}_8$ with $a_0 = 5.18$ and $c_0 = 7.67$ or 2×7.67 Å contains one or two molecules $\beta\text{-Ca}[\text{Zn}_2\text{P}_2\text{O}_8]$.

A determination of the structure of $\beta\text{-Ca}[\text{Zn}_2\text{P}_2\text{O}_8]$ on the basis of high-temperature single-crystal data is planned.

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The crystal structure of bis-(γ -picoline)zinc(II) dibromide. By L. FANFANI, A. NUNZI and P. F. ZANAZZI, *Istituto di Mineralogia dell'Università di Perugia, Perugia 06100, Italy*

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$\text{Zn}(\gamma\text{-pic})_2\text{Br}_2$ is monoclinic with $a = 14.42$, $b = 8.09$, $c = 13.89$ Å, $\beta = 101^\circ 10'$ and space group $P2_1/c$. The crystal structure has been solved by interpretation of the Patterson function employing three-dimensional photographic data and refined by the least-squares method to an R value of 0.082. The complex is tetrahedral; Zn–Br and Zn–N average distances are 2.35 and 2.05 Å respectively.

The crystal structure of $\text{ZnBr}_2(\gamma\text{-pic})_2$ has been determined in order to collect new information on tetrahedral Zn(II) complexes. The product was obtained in an unsuccessful attempt to synthesize the tetramethylammonium salt of $\text{ZnBr}_3(\gamma\text{-pic})_2^-$ according to a recent preparation (Guru & Ramana Rao, 1968). The crystals of $\text{ZnBr}_2(\gamma\text{-pic})_2$ were kindly supplied by Dr A. A. G. Tomlinson (Institute of Inorganic Chemistry of Perugia University). They are colourless, short and prismatic in habit with a density of 1.71

g.cm⁻³. The crystal data of the complex, determined by oscillation and Weissenberg photographs, are as follows: space group $P2_1/c$; $a = 14.42 \pm 0.01$, $b = 8.09 \pm 0.01$, $c = 13.89 \pm 0.01$ Å, $\beta = 101^\circ 10' \pm 5'$; $Z = 4$; $d_x = 1.72$ g.cm⁻³.

The intensity data for the structural determination were collected employing a Weissenberg equi-inclination technique using $\text{Cu K}\alpha$ radiation. Diffraction effects of the reciprocal lattice layers from $h0l$ to $h6l$ were recorded and measured with a microdensitometer. Absorption correction

($\mu = 86.7 \text{ cm}^{-1}$ for Cu $K\alpha$; crystal dimensions: $0.07 \times 0.08 \times 0.11 \text{ mm}$) was applied using the program of De Meulenaer & Tompa (1965). After the geometrical corrections the squared amplitudes were put on approximately the same relative scale by means of the common data on the $0k\ell$ layer.

About 2000 independent reflexions were obtained, of which 735 were in the measurable range.

From a three-dimensional Patterson function the Zn, Br(1) and Br(2) atoms were easily located. The coordinates of the atoms of the two picoline rings were determined by a Fourier synthesis computed with the signs given by the heavier atoms. The refinement of the structure was performed by the least-squares method, employing a block-diagonal program written by Shiono for the IBM 1130 computer. After four cycles with isotropic individual thermal factors, a last cycle was computed varying the temperature factors of Zn and Br atoms, anisotropically; the *R* index

reached the final value 0.082. The data were weighted using Hughes's (1941) scheme. Observed and calculated structure factors are compared in Table 1. The atomic coordinates and temperature factors are given in Table 2. The scattering factors used in the calculations for Br, Zn, N, and C were obtained from *International Tables for X-ray Crystallography* (1962).

Bond lengths and angles around the Zn^{2+} ion are listed with their estimated standard deviations in Table 3. The structure projected along the b axis is represented in Fig. 1. The complex is distorted tetrahedral; $Zn-Br$ distances, 2.35 Å, are in agreement with those reported by MacGillavry & Bijvoet (1936) for $Zn(NH_3)_2Br_2$, 2.38 Å. The $Zn-N$ distances (2.07 and 2.03 Å) are comparable with those found in bis(imidazole)zinc(II) dichloride (Lundberg, 1966) and in bis(pyridine)zinc(II) dichloride (Sokolova, Atovmyan & Poray-Koshits, 1966), (2.01 Å on average). The tetrahedral distortion may be caused by steric hindrance between the

Table 1. Observed and calculated structure factors ($\times 10$) of reflexions with intensities in the measurable range

M	O	O	-3 779 800	1 807 756	M	2 3	M	2 10	-3 283 283	M	4 3	M	4 10	-10 266 198	-1 193 471				
2	2122-2610	-5 786 -565	-2 582 529	1 224 251	-5 389 362	-10 1130-1119	-5 389 362	-1 257 -240	M	5 >	M	5 >	M	5 >	M	5 >			
3	1366-1247	M	O 14	3 709 700	1 -1 314 -843	0 450 -623	0 450 -623	0 297 -331	-6	257 -240	M	4 11	M	4 11	0 280 -333	1 477 -444			
4	1657 1812	-	-8 812 812	2 542 -534	-2 318 242	4 682 -607	8 680 -686	1 1617 1715	-6	1470 -1504	M	4 11	M	4 11	0 222 336	1 477 -366			
5	1465-1466	-1	371 319	-5 782 -813	3 266 -229	-5 367 -342	M	3 6	-2 412 381	-6	1470 -1504	M	4 11	M	4 11	-1 467 -366	-2 339 227		
6	1374-1745	-6 485 -488	-7 709 -225	3 -777 343	0 593 204	3 1149-1187	-2 490 456	0 243 231	1 246 -268	M	4 11	M	4 11	3 222 233	3 497 -553				
7	356 333	-5 484 509	-7 424 -410	4 -10 393	7 595 654	1 635 588	1 642 -700	3 1183 1226	1 246 -268	M	4 11	M	4 11	3 222 233	3 497 -553				
8	731 739	-7 485 -461	-9 450 -438	-7 432 -621	-9 387 -317	-1 682 -700	-2 339 231	2 239 -256	M	4 11	M	4 11	3 222 233	3 497 -553					
M	O 2	M	1 > 0	M	1 > 7	M	2 > *	M	2 > 12	M	3 > 7	M	3 > 8	M	3 > 9				
0	1156-1250	2 615 355	M	1 > 7	M	2 > *	M	2 > 12	-3 310 318	5 825 89	-5 740 -834	3 256 258	-5 424 -588	0 243 231	1 477 -366				
1	666 572	3 1209-1466	0 968 -960	0 968 -914	0 468 393	M	3 > 7	-6 290 259	-3 426 -588	3 256 258	7 346 -500	7 346 -500	M	4 11	0 280 -333	1 477 -366			
-1	897 -919	4 454 -413	2 1003 938	1 813 773	0 468 393	1 481 -676	7 649 -687	-6 333 416	1 246 -268	M	4 11	M	4 11	3 222 233	3 497 -553				
2	1257 1349	5 836 907	-9 988 -1234	1 817 -500	2 178 1106	-2 468 -442	-1 723 713	0 454 -487	3 115 -332	M	4 11	M	4 11	3 222 233	3 497 -553				
3	550 -692	9 479 -479	-5 562 -333	-2 297 193	M	3 > 0	-3 586 -593	-7 241 -238	M	4 11	M	4 11	3 222 233	3 497 -553					
-4	956 800	M	1 > 1	6 758 730	3 1081-1111	M	3 > 0	6 611 636	M	4 11	M	4 11	3 222 233	3 497 -553					
-5	503 -655	M	1 > 1	7 567 -574	-3 433 371	-5 420 406	M	4 11	3 222 233	M	5 > 0	M	5 > 0	M	5 > 0				
-6	2959-3556	M	1 > 1	-7 763 738	4 330 -29	-6 369 -363	0 245 -217	M	5 > 0	M	5 > 0	M	5 > 0	M	5 > 0				
-7	1288-1353	-2 1303 1710	-6 559 -559	4 330 -29	2 343 -29	2 444 -579	1 311 -311	M	5 > 0	M	5 > 0	M	5 > 0	M	5 > 0				
-8	2241 2055	-2 398 380	-11 1179 734	-5 761 -702	3 614 -602	M	3 > 8	-1 546 -698	1 988 997	1 348 421	M	4 11	M	4 11	3 222 233	3 497 -553			
-9	421 2	3 598 -556	M	1 > 8	6 826 667	M	3 > 1	2 585 611	2 213 -127	M	4 11	M	4 11	3 222 233	3 497 -553				
-10	493 -693	-3 930 831	M	1 > 8	6 833 -612	M	3 > 1	3 365 658	3 657 -552	M	4 11	M	4 11	3 222 233	3 497 -553				
-11	426 516	3 1394-1722	-10 553 -553	7 765 -532	M	3 > 1	3 629 -691	5 403 309	5 511 -353	M	4 11	M	4 11	3 222 233	3 497 -553				
-12	466 -442	5 553 -553	1 680 -596	0 1213-1342	M	3 > 0	5 305 502	6 335 -504	M	4 11	M	4 11	3 222 233	3 497 -553					
M	O 4	M	1032 1111	-3 630 -651	8 466 -446	-1 1010 1142	5 316 320	M	5 > 1	M	5 > 1	M	5 > 1	M	5 > 1				
0	1239-1289	7 973-1034	-7 706 -757	-10 456 -407	-2 583 484	-6 294 -297	2 209 227	M	5 > 1	M	5 > 1	M	5 > 1	M	5 > 1				
1	1233-1333	-7 592 565	M	1 > 9	11 507 -332	3 350 -424	0 621 613	-2 339 -404	4 259 337	M	5 > 1	M	5 > 1	M	5 > 1				
2	1011 961	-8 729 837	M	1 > 9	-11 740 824	-1 541 -504	1 377 385	M	4 5	M	4 5	M	4 5	M	4 5				
-3	810 593	9 802 889	0 929 883	-6 493 280	2 664 -700	1 858 -822	-6 520 500	7 292 -292	M	4 5	M	4 5	M	4 5	M	4 5			
-4	532 476	-7 792 -761	2 812 -706	M	2 > 5	-5 508 526	-2 477 -461	-1 1031 1059	5 516 -394	M	4 5	M	4 5	M	4 5				
-5	1037 -927	-10 543 -553	-2 850 -832	0 600 847	3 366 -607	3 561 -545	-6 526 -504	6 203 -333	M	4 5	M	4 5	M	4 5	M	4 5			
-6	812 790	-11 621 513	6 699 654	0 371 -324	8 527 -561	-2 342 564	-3 224 -1010	6 678 -677	7 217 -289	M	4 5	M	4 5	11 206 -256	11 206 -256				
-7	1013 1037	-13 719 -546	M	2 > 0	-2 596 -582	M	3 > 2	-6 429 409	-5 935 988	-8 424 416	M	4 5	M	4 5	-11 409 431	-11 409 431			
-8	485 -607	M	1 > 2	1 562 -545	-6 454 -443	0 796 607	-7 497 536	-7 709 -699	-9 291 337	M	5 > 2	M	5 > 2	M	5 > 2	M	5 > 2		
-9	371 -346	0 1213-1452	3 567 -567	-7 715 -738	-1 535 -486	M	3 > 10	-9 368 239	M	5 > 2	M	5 > 2	M	5 > 2	M	5 > 2			
M	O 6	M	1 > 6	M	1 > 6	M	2 > 7	M	2 > 10	M	3 > 11	M	3 > 11	M	3 > 11	M	3 > 11		
-1	645 581	5 593 -614	M	1 > 6	-8 570 622	-2 361 -546	1 419 -336	M	4 6	M	4 6	M	4 6	M	4 6	M	4 6		
0	1917 1948	3 831 791	8 580 -603	M	2 > 6	-3 538 -475	5 427 -422	0 693 698	-13 437 -49	M	4 6	M	4 6	M	4 6	M	4 6		
1	1037 1037	-5 1027 997	10 335 317	M	2 > 6	-4 562 -450	-8 381 388	5 432 -467	5 512 527	M	4 6	M	4 6	M	4 6	M	4 6		
2	1786-1818	-6 548 475	M	2 > 6	1 -394 305	0 805 626	-5 363 526	-2 502 -467	1 241 -218	M	4 6	M	4 6	M	4 6	M	4 6		
-3	1675-1723	7 533 465	M	2 > 6	-2 769 -795	-6 468 -487	4 369 -416	-2 367 -411	-11 287 271	M	4 6	M	4 6	M	4 6	M	4 6		
-4	512 -664	-7 890 -817	M	2 > 6	-3 545 582	8 359 595	-2 491 473	5 229 -262	4 371 313	M	4 6	M	4 6	M	4 6	M	4 6		
-5	1116 1059	M	1 > 3	1 961 -888	-3 545 582	8 359 595	-2 491 473	5 229 -262	5 609 528	M	4 6	M	4 6	M	4 6	M	4 6		
-6	1452 1499	-2 373 422	-8 658 -652	-8 688 -601	-8 612 842	-3 361 -391	-5 337 -322	-7 389 413	6 323 -330	M	4 6	M	4 6	M	4 6	M	4 6		
-7	373 401	0 1379 1703	-7 781 652	-8 533 -524	9 607 421	-4 481 -523	-5 337 -339	-7 389 413	-9 222 -211	M	4 6	M	4 6	M	4 6	M	4 6		
-8	1179-1238	1 611 -563	3 343 277	5 629 -671	-5 325 -346	M	3 > 3	-6 325 346	-9 596 -527	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6		
-9	576 566	-1 451 -368	-2 451 -368	-2 360 -302	M	3 > 3	-7 260 -302	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6		
-10	1037 1037	-2 168 -172	-2 168 -172	-2 361 -305	M	3 > 3	-7 261 -305	-10 266 -260	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6			
-11	621 626	-2 1839-1793	-6 966 -908	-8 341 -279	0 1627 1718	M	4 6	0 271 220	8 337 -324	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6		
-12	841 645	-3 1037 1119	5 475 -505	M	2 > 7	-1 574 -478	2 386 -695	-2 308 -406	-10 314 332	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6		
-13	689 667	4 1115 1180	775 803	M	2 > 7	-1 590 -525	2 395 -695	-2 308 -406	12 188 167	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6		
-14	384 -337	-4 479 -453	-6 801 832	0 200 -336	-2 477 -451	4 771 -511	-2 477 -451	-2 477 -451	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6			
-15	326 -344	-3 326 -338	8 659 -697	1 -195 -593	-3 477 -494	5 337 -339	-7 221 -272	9 939 -322	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6			
M	O 8	6 489 -451	-8 397 -385	-1 275 233	4 124 1394	6 257 -266	-5 206 -260	-9 229 -242	M	6 > 6	M	6 > 6	M	6 > 6	M	6 > 6			
-7	636 636	10 512 549	-2 467 499	-4 1552 1160	7 602 617	6 257 -266	-5 206 -260	-9 229 -242	1 360 -323	M	6 > 6	M	6 > 6	M	6 > 6	M	6 > 6		
0	1514-1533	-10 529 568	-2 408 328	5 381 -333	M	4 6	0 426 -333	3 488 656	M	6 > 6	M	6 > 6	M	6 > 6	M	6 > 6			
1	466 -466	M	1 > 4	-12 358 -356	-2 466 -349	5 381 -333	-1 426 -333	-12 267 -275	-1 391 -339	M	6 > 6	M	6 > 6	M	6 > 6	M	6 > 6		
2	867 781	0 680 688	M	2 > 2	+ 4 39 -412	-6 761 -702	1 1092 -962	0 404 -398	-6 253 203	M	6 > 6	M	6 > 6	M	6 > 6	M	6 > 6		
-3	1259 1190	1 699 -627	-6 811 -851	4 360 259	5 330 -322	1 378 822	2 374 -377	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6		
-4	863 -802	2 733 -770	0 837 -684	-5 309 -554	-2 476 -442	2 489 -435	3 229 -273	7 373 373	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6			
-5	753 -693	-2 567 -564	1 781 -740	-2 370 320	M	3 > 4	-6 265 -490	2 486 -490	-2 461 -482	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6		
-6	1271 -1272	-2 568 -564	-7 733 -733	-5 355 -537	-2 476 -442	2 489 -435	-6 265 -490	-2 461 -482	-3 395 382	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6		
-7	844 -820	-5 367 533	2 682 -659	-5 309 -528	0 493 -660	-3 471 -529	-5 337 -339	-8 562 -636	-3 395 -337	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6		
-8	983 1011	-9 645 -607	-2 949 901	-8 318 -570	1 474 -248	5 478 -689	-3 477 -529	-7 221 -272	9 939 -322	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6		
-9	588 -582	-7 415 -412	3 305 -321	-10 455 435	-1 646 -647	7 602 617	7 602 617	-9 229 -242	1 426 -321	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6		
-10	753 -756	-3 946 -946	M	2 > 8	-4 266 846	9 275 -299	M	4 6	0 143 -399	-12 210 -234	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6	
-11	583 625	M	1 > 5	-6 475 642	-3 325 -308	1 122 1141	M	4 6	-1 646 -666	-12 267 -275	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6	
M	O 10	-1 709 736	-10 1091 1091	-3 598 -615	-6 456 -624	0 786 -684	-1 509 -539	-6 253 203	5 322 -348	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6	M	5 > 6
-12																			

Table 2. Fractional atomic coordinates ($\times 10^4$) and thermal parameters with relative standard deviations

	x/a	y/b	z/c	$B(\text{\AA})^2$
Zn	7535 (4)	1970 (7)	1894 (4)	*
Br(1)	7075 (4)	4757 (6)	1734 (4)	*
Br(2)	7572 (4)	541 (7)	3376 (4)	*
N(1)	8857 (21)	1864 (35)	1530 (21)	3.2 (0.6)
N(2)	6743 (22)	677 (35)	775 (22)	2.7 (0.6)
C(1)	9524 (27)	801 (43)	2027 (28)	3.5 (0.8)
C(2)	10420 (27)	627 (45)	1740 (27)	4.1 (0.8)
C(3)	10568 (29)	1525 (44)	898 (27)	3.5 (0.8)
C(4)	9907 (27)	2631 (44)	390 (27)	3.5 (0.8)
C(5)	9054 (27)	2698 (46)	803 (27)	3.6 (0.8)
C(6)	11473 (28)	1312 (46)	605 (27)	3.9 (0.8)
C(7)	6433 (29)	1457 (44)	-131 (27)	2.7 (0.8)
C(8)	5936 (27)	548 (46)	-940 (30)	3.6 (0.8)
C(9)	5820 (28)	-1006 (45)	-892 (28)	3.4 (0.8)
C(10)	6132 (29)	-1826 (44)	6 (27)	3.4 (0.8)
C(11)	6616 (27)	-947 (44)	832 (28)	2.9 (0.8)
C(12)	5362 (26)	-2166 (47)	-1787 (26)	3.3 (0.8)

* The anisotropic temperature factors of Zn, Br(1) and Br(2), given in the form $T = \exp \{ - (h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23}) \times 10^{-4} \}$ are as follows:

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Zn	66 (4)	166 (11)	79 (4)	12 (6)	12 (3)	3 (5)
Br(1)	89 (4)	240 (10)	60 (4)	14 (5)	16 (3)	10 (5)
Br(2)	54 (4)	186 (11)	59 (4)	8 (5)	7 (3)	3 (5)

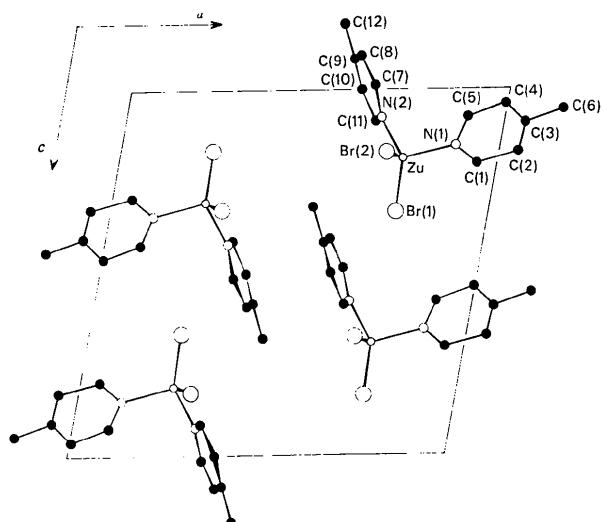


Fig. 1. Projection of the structure along the b axis.

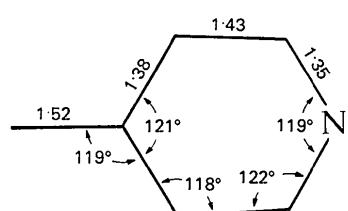


Fig. 2. Sketch of the ligand with averaged bond lengths and angles.

two bromine atoms: the angle Br(1)-Zn-Br(2) is 120.9° ; the Br-Br distance in the complex is 4.09 \AA .

Table 3. Distances and angles around Zn with their standard deviations

Zn-Br(1)	2.35	$\pm 0.01 \text{ \AA}$
Zn-Br(2)	2.35	0.01
Zn-N(1)	2.07	0.03
Zn-N(2)	2.03	0.03
Br(1)-Zn-Br(2)	120.9°	$\pm 0.3^\circ$
Br(1)-Zn-N(1)	105.9	0.9
Br(1)-Zn-N(2)	108.3	0.9
Br(2)-Zn-N(1)	109.1	0.9
Br(2)-Zn-N(2)	109.3	0.9
N(1)-Zn-N(2)	101.6	1.3

Individual bond lengths and angles in the picoline rings are not reported in detail because they have poor significance for the high standard deviations (σ_{C-C} and $\sigma_{C-N} = 0.05 \text{ \AA}$). However a sketch of the ligand with the averaged values of equivalent bond lengths and angles in the two molecules is reported in Fig. 2. The rings are planar within experimental error, the least-square plane equations computed for the six atoms of the heterocyclic ring being:

$0.682x + 1.038y + 1.311z = 1$ for the ring containing N(1) and

$1.581x - 0.166y - 0.728z = 1$ for that containing N(2).

The interplanar angle is 77.15° . The central Zn^{2+} ion is out of both the mean square planes with deviations of about 0.18 \AA . The carbon atoms of the methyl groups, C(6) and

Table 4. Shortest intermolecular contacts

(a)	$2-x, \frac{1}{2}+y, \frac{1}{2}-z$	(d)	$2-x, -\frac{1}{2}+y, \frac{1}{2}-z$
(b)	$x, \frac{1}{2}-y, \frac{1}{2}+z$	(e)	$2-x, -y, -z$
(c)	$x, 1+y, z$	(f)	$1-x, -y, -z$
Br(1)-C(2) (a)	3.86 \AA	Br(2)-C(5) (b)	3.90 \AA
Br(1)-C(8) (b)	3.92	Br(2)-C(7) (b)	3.77
Br(1)-C(10) (c)	3.75	Br(2)-C(6) (d)	3.85
Br(1)-C(11) (c)	3.72		
C(3)-C(3) (e)	3.67 \AA	C(7)-C(10) (f)	3.61 \AA
		C(7)-C(11) (f)	3.70

C(12), deviate by 0.01 \AA and 0.12 \AA respectively from the planes of relative rings.

The shortest intermolecular contacts are given in Table 4.

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