

reflections, phased by either Σ_2 or Σ_1 relations (and perhaps with appropriate weights), can also be included to produce peaks of greater reliability. In the centric case, those Σ_1 reflections which were determined with greater than 90% probability were included in the calculation of the Σ_2 map. Their addition improved the phase agreement to a small extent. The frequency check procedure (Gorres & Jacobson, 1964) can be applied to the Σ_2 -map.

It also is possible to include an additional strong reflection with the origin-determining reflections, thus producing two Σ_2 maps in the centric case, for example. The resulting two sets of averaged phases could then be handled in a similar way as in those direct-methods programs that produce multiple solutions.

Lower bounds other than zero can be used for modification of the resultant superposition map. Indeed, some calculations for the centric example have shown that use of a lower bound of 10% of the maximum peak height results in somewhat improved agreement.

From Tables 2 and 3, it is obvious that a straight average is a poor procedure compared with a more judicious method of averaging. Preliminary computations indicate that in the centric case a requirement of a net of two like signs produces a significant improvement in the percentage of correct signs selected.

The phases are also somewhat sensitive to grid point resolution of the maps. In the centric structure, calculations were run using a grid of $0.12 \times 0.45 \times 0.45$ Å resolution. Results improve if a resolution of approximately 0.25 Å is used in all three directions.

Squaring the resultant superposition map appears to give the best phases compared with other powers which could be employed. All exponents from 0.2 to 6.6 in steps of 0.2 were examined for a typical run, with 2.0 appearing the most satisfactory.

Conclusion

We feel that these results demonstrate the effectiveness of an approach which utilizes advantages of both direct and Patterson methods and in doing so avoids many of their limitations.

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The Crystal Structure of Magnesium Chlorophosphate, $\text{Mg}_2(\text{PO}_4)\text{Cl}$

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Magnesium chlorophosphate, $\text{Mg}_2(\text{PO}_4)\text{Cl}$, crystallizes in the space group $Pna2_1$, with unit-cell dimensions $a = 10.940$ (1), $b = 7.9305$ (6), and $c = 4.8008$ (4) Å ($Z = 4$). A three-dimensional structural analysis using automatic-diffractometer data has been completed and refined by full-matrix least-squares procedures to a residual $R = 0.025$ ($R_w = 0.044$). The compound is isostructural with the previously reported $\text{Mn}_2(\text{PO}_4)\text{Cl}$.

Introduction

In a continuing investigation of the crystal chemistry of halophosphates of composition $\text{M}_2(\text{PO}_4)\text{X}$ (M is a

divalent metal, X is a halogen) (Rea & Kostiner, 1972*a*, *b*), we have grown single crystals of magnesium chlorophosphate $\text{Mg}_2(\text{PO}_4)\text{Cl}$ and determined its crystal structure.

The preparation of $\text{Mg}_2(\text{PO}_4)\text{Cl}$ has been reported (Klement & Haselbeck, 1965) but, aside from the reported similarity of its X-ray powder-diffraction pattern to that of $\text{Mn}_2(\text{PO}_4)\text{Cl}$, no structural work has been done.

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Experimental

Single crystals of $Mg_2(PO_4)Cl$ were grown from excess $MgCl_2$ in a sealed evacuated quartz ampoule. A mixture of 25 mol. % $Mg_3(PO_4)_2$ and 75 mol. % $MgCl_2$ (carefully dehydrated in HCl gas at 500°C) was sealed in an evacuated (10μ mHg) quartz tube (8 mm internal diameter). The sealed ampoule was placed in a resistance-heated furnace, heated to 1100°C and then cooled at 15°C per hr to 650°C where the furnace was shut off. The crystals were separated by washing with hot distilled water. Typically, crystals were lath-shaped with dimen-

sions $0.03 \times 0.05 \times 0.2$ cm; no attempt was made to maximize crystal size.

Lattice parameters from Weissenberg and precession photographs indicated that $Mg_2(PO_4)Cl$ was isostructural with $Mn_2(PO_4)Cl$ with space group $Pna2_1$. Accurate lattice parameters were determined in a PICK II least-squares refinement using 46 reflections within the angular range $38^\circ < 2\theta < 56^\circ$; the reflections were automatically centered on a Picker FACS-I four-circle diffractometer using $Mo K\alpha_1$ radiation. At 22°C the lattice parameters are $a=10.940$ (1), $b=7.9305$ (6), and $c=4.8008$ (4) Å, where the figures in parentheses rep-

Table 1. Observed and calculated structure factors

H K L F _{obs} F _{calc}				H K L F _{obs} F _{calc}				H K L F _{obs} F _{calc}				H K L F _{obs} F _{calc}				H K L F _{obs} F _{calc}				H K L F _{obs} F _{calc}				H K L F _{obs} F _{calc}				H K L F _{obs} F _{calc}				H K L F _{obs} F _{calc}				H K L F _{obs} F _{calc}				H K L F _{obs} F _{calc}			
0 0 2	730	868	1 2 0	253	200	1 8 1	52	51	2 3 4	185	186	2 10 2	51	49	3 6 3	454	457	4 2 0	5	6	4 8 4	88	85	5 5 4	78	75	6 1 5	225	225														
0 0 4	668	772	1 2 0	988	958	1 8 2	2	19	2 3 5	200	256	2 10 3	17	18	3 6 4	421	221	4 2 0	1	42	4 1	4 9 9	161	163	5 5 5	240	250	6 1 6	86	79													
0 0 6	268	268	1 2 0	385	350	1 8 3	4	19	2 3 6	176	173	2 10 4	2	17	3 6 5	476	213	4 2 0	2	43	4 2	5 5 5	243	240	5 5 6	143	146	6 1 7	40	41													
0 0 8	1 369	368	1 2 0	375	386	1 8 4	40	41	2 4 0	428	406	2 11 1	90	96	3 6 6	624	442	4 2 0	3	39	37	4 9 9	339	339	5 5 7	212	212	6 1 8	26	28													
0 0 1 3	476	487	1 2 4	209	212	1 8 5	44	44	2 4 1	262	268	2 11 2	89	85	3 7 0	93	93	4 2 0	4	29	29	4 9 9	107	107	5 5 8	6	7	6 1 9	77	77													
0 0 1 5	28	27	1 3 0	132	132	1 8 6	54	54	2 4 2	184	184	2 11 3	89	85	3 7 1	102	102	4 2 0	5	10	9	4 10	90	90	5 5 9	238	238	6 1 10	32	32													
0 0 1 7	242	242	1 2 6	398	405	1 9 1	159	157	2 4 3	163	159	3 1 1	433	438	3 7 2	122	122	4 2 0	6	19	19	4 10	50	50	5 6 0	3	3	6 1 11	192	192													
0 0 2 2	42	56	1 2 7	21	15	1 9 2	309	311	2 4 4	255	253	3 1 2	220	216	3 7 3	176	174	4 2 0	7	3	3	4 10	62	62	5 6 1	6	6	6 1 12	132	132													
0 0 2 4	28	27	1 3 0	132	132	1 9 3	182	183	2 4 5	339	315	3 1 3	162	154	3 7 4	164	164	4 2 0	8	2	2	4 10	58	58	5 6 2	6	6	6 1 13	116	116													
0 0 2 6	43	63	1 3 1	415	405	1 9 4	88	90	2 4 6	6	71	3 1 4	206	205	3 7 5	103	103	4 2 0	9	5	5	4 10	250	251	5 6 3	187	192	6 1 14	20	20													
0 0 3 1	690	654	1 3 2	117	113	1 10 0	263	260	2 5 0	405	402	3 1 5	193	108	3 7 6	77	73	4 2 0	10	3	3	4 11	267	251	5 6 4	1	1	6 1 15	370	370													
0 0 3 3	655	666	1 3 3	427	436	1 10 1	3	192	2 5 1	136	137	3 1 6	147	146	3 7 7	28	22	4 2 0	11	3	3	4 11	360	361	5 6 5	7	7	6 1 16	112	115													
0 0 3 5	162	151	1 3 4	156	156	1 10 2	110	105	2 5 2	391	393	3 1 7	434	434	3 7 8	1	43	4 2 0	12	3	3	4 11	83	80	5 6 6	5	5	6 1 17	222	223													
0 0 4 0	136	134	1 3 5	122	120	1 10 3	65	67	2 5 3	4	80	3 1 8	173	832	3 7 9	50	49	4 2 0	13	3	3	4 11	219	225	5 6 7	4	4	6 1 18	123	123													
0 0 4 2	213	176	1 3 6	176	103	1 10 4	48	103	2 5 4	18	158	3 1 9	691	657	3 7 10	45	43	4 2 0	14	3	3	4 11	360	361	5 6 8	2	2	6 1 19	917	917													
0 0 4 4	747	749	1 4 0	86	85	1 11 1	99	100	2 5 5	101	121	3 1 10	709	813	3 7 11	4	19	23	4 2 0	15	5	5	4 11	538	535	5 6 9	8	8	6 1 20	292	292												
0 0 4 6	343	343	1 4 1	1	1	1 11 2	2	47	2 5 6	129	129	3 1 11	148	137	3 7 12	450	450	4 2 0	16	3	3	4 11	352	352	5 6 10	8	8	6 1 21	419	419													
0 0 4 8	118	115	1 4 2	35	35	1 11 3	2	56	2 5 7	569	572	3 1 12	154	154	3 7 13	401	401	4 2 0	17	3	3	4 11	603	612	5 6 11	3	3	6 1 22	330	330													
0 0 5 0	354	351	1 4 3	20	20	1 11 4	2	54	2 5 8	541	550	3 1 13	161	161	3 7 14	411	411	4 2 0	18	3	3	4 11	622	626	5 6 12	3	3	6 1 23	352	358													
0 0 5 1	120	122	1 4 4	70	63	1 11 5	2	61	2 5 9	471	465	3 1 14	165	165	3 7 15	423	423	4 2 0	19	3	3	4 11	640	640	5 6 13	3	3	6 1 24	176	176													
0 0 5 2	131	128	1 4 5	42	42	1 11 6	2	68	2 5 10	489	488	3 1 15	170	170	3 7 16	435	435	4 2 0	20	3	3	4 11	658	658	5 6 14	3	3	6 1 25	147	147													
0 0 6 2	108	110	1 4 6	13	14	1 11 7	2	74	2 5 11	507	507	3 1 16	175	175	3 7 17	449	449	4 2 0	21	3	3	4 11	676	676	5 6 15	3	3	6 1 26	267	267													
0 0 6 4	35	33	1 5 0	338	327	1 12 0	6	151	2 6 0	5	12	3 1 17	180	180	3 7 18	463	463	4 2 0	22	3	3	4 11	694	694	5 6 16	3	3	6 1 27	116	116													
0 0 6 6	54	57	1 5 1	52	51	1 12 1	2	0	2 6 1	253	251	3 1 18	185	185	3 7 19	477	477	4 2 0	23	3	3	4 11	712	712	5 6 17	3	3	6 1 28	167	172													
0 0 7 1	624	610	1 5 2	430	428	1 12 2	0	427	2 6 2	152	151	3 1 19	190	190	3 7 20	491	491	4 2 0	24	3	3	4 11	730	730	5 6 18	3	3	6 1 29	111	111													
0 0 7 3	451	461	1 5 3	298	300	1 12 3	1	108	2 6 3	261	260	3 1 20	195	195	3 7 21	505	505	4 2 0	25	3	3	4 11	748	748	5 6 19	3	3	6 1 30	81	86													
0 0 7 5	194	180	1 5 4	108	108	1 12 4	2	1	2 6 4	185	184	3 1 21	200	200	3 7 22	519	519	4 2 0	26	3	3	4 11	766	766	5 6 20	3	3	6 1 31	212	212													
0 0 8 0	583	576	1 5 5	143	143	1 12 5	3	64	2 6 5	27	24	3 1 22	205	205	3 7 23	533	533	4 2 0	27	3	3	4 11	784	784	5 6 21	3	3	6 1 32	152	152													
0 0 8 2	240	236	1 5 6	200	198	1 12 6	4	104	2 6 6	380	378	3 1 23	210	210	3 7 24	547	547	4 2 0	28	3	3	4 11	802	802	5 6 22	3	3	6 1 33	62	62													
0 0 8 4	307	305	1 6 0	604	588	1 12 7	5	103	2 6 7	37	34	3 1 24	215	215	3 7 25	561	561	4 2 0	29	3	3	4 11	820	820	5 6 23	3	3	6 1 34	123	123													
0 0 9 1	137	133	1 6 1	464	458	1 12 8	6	117	2 6 8	0	163	3 1 25	220	220	3 7 26	575	575	4 2 0	30	3	3	4 11	838	838	5 6 24	3	3	6 1 35	133	133													
0 0 9 3	165	166	1 6 2	317	316	1 12 9	7	126	2 6 9	1	178	3 1 26	225	225	3 7 27	589	589	4 2 0	31	3	3	4 11	856	856	5 6 25	3	3	6 1 36	133	133													
0 10 0	113	114	1 6 3	133	137	1 12 10	8	135	2 6 10	2	183	3 1 27	230	230	3 7 28	603	603	4 2 0	32	3	3	4 11	874	874	5 6 26	3	3	6 1 37	142	142													
0 10 2	38	37	1 6 4	61	59	1 12 11	9	144	2 6 11	3	190	3 1 28	235	235	3 7 29	617	617	4 2 0	33	3	3	4 11	892	892	5 6 27	3	3	6 1 38	151	151													
0 11 0	158	161	1 6 5	155	163	1 12 12	10	153	2 6 12	4	197	3 1 29	240	240	3 7 30	631	631	4 2 0	34	3	3	4 11	910	910	5 6 28	3	3	6 1 39	160	160													
0 11 1	315	326	1 6 6	227	231	1 12 13	11	162	2 6 13	5	204	3 1 30	245	245	3 7 31	645	645	4 2 0	35	3	3	4 11	928	928	5 6 29	3	3	6 1 40	170	170													
0 11 2	308	321	1 7 1	293	291	1 12 14	12	171	2 6 14	6	212	3 1 31	250	250	3 7 32	659	659	4 2 0	36	3	3	4 11	946	946	5 6 30	3	3	6 1 41	180	180													
0 11 3	315	324	1 7 2	72	69	1 12 15	13	180	2 6 15	7	220	3 1 32	255	255	3 7 33	673	673	4 2 0	37	3	3	4 11	964	964	5 6 31	3	3	6 1 42	190	190													
0 11 4	67	58	1 7 3	409	406	1 12 16	14	189	2 6 16	8	229	3 1 33	260	260	3 7 34	687	687	4 2 0	38	3	3	4 11	982	982	5 6 32	3	3	6 1 43	200	200													
0 11 5	46	41	1 7 4	142	140	1 12 17	15	198	2 6 17	9	238	3 1 34	265	265	3 7 35	701	701	4 2 0	39	3	3	4 11	1000	1000	5 6 33	3	3	6 1 44	210	210													
0 11 6	146	141	1 7 5	99	96	1 12 18	16	207	2 6 18	10	247	3 1 35	270	270	3 7 36	715	715	4 2 0	40	3	3	4 11	1018	1018	5 6 34	3	3	6 1 45	220	220													
0 11 7	162	166	1 7 6	278	277	1 12 19	17	216	2 6 19	11	256	3 1 36	275	275	3 7 37	729	729	4 2 0	41	3	3	4 11	1036	1036	5 6 35	3	3	6 1 46	230	230													
8 8 3	180	184	7 6 1	385	382	8 3 1	82	82	8 0 2	261	265	10 0 2	527	513	10 0 3	154	150	11 0 2	3	329	332	12 0 2	163	169	13 0 2	143																	

resent the standard deviations in the last reported figure. The calculated density, with $Z=4$, is 2.855 g.cm^{-3} and the measured density (flotation) is $2.852 (4) \text{ g.cm}^{-3}$.

A small ($R \sim 0.015 \text{ cm}$), reasonably isotropic crystal was chosen for data collection. Diffraction intensities were measured using Zr-filtered Mo $K\alpha$ radiation at a take-off angle of 2.5° with the diffractometer operating in the $\theta-2\theta$ scan mode. Scans were made at 1° per min over 1.5° with allowance for dispersion, and with 40 sec background counts taken at both ends of the scan. Of the 799 independent data investigated in the angular range $2\theta < 64^\circ$, a total of 784 were considered observable according to the criterion $|F_o| > 0.675\sigma_F$, where σ_F is defined as $0.02|F_o| + [C + k^2B]^{1/2}/2|F_o|Lp$; the total scan count is C , k is the ratio of scanning time to the total background scanning time, and B is the total background count. Three reflections were systematically monitored, and since there was a significant drop in intensities during the last part of the data collection period, a second scale factor applicable to the last 63 data collected was included in the refinements. The maximum random deviations in intensity were less than 3.5%. The intensity data were corrected for Lorentz and polarization effects. No absorption correction was made, since the linear absorption coefficient was small ($\mu = 15 \text{ cm}^{-1}$).

Refinement of the structure

Least-squares refinement (Busing, Martin & Levy, 1962) using the atomic positions reported for $\text{Mn}_2(\text{PO}_4)\text{Cl}$ as a starting point with a $1/\sigma^2$ weighting scheme, zero-valent scattering factors (Cromer & Mann, 1968), isotropic temperature factors, and corrections for secondary extinction and anomalous dispersion, yielded a residual $R=0.041$ and a weighted residual $R_w=0.067$ for the observed data. For the anisotropic refinement $R=0.025$ and $R_w=0.0444$. Since the space group was noncentric, the other enantiomorph was refined, giving $R=0.025$ and $R_w=0.0438$. According to Hamilton's (1965) significance test, the first cell may be rejected at the 0.005 significance level. Thus the crystal analyzed

in this study was enantiomorphous with that chosen for the $\text{Mn}_2(\text{PO}_4)\text{Cl}$ study.

The final anisotropic refinement was based on a data: parameter ratio of 10.5 to 1 with 74 independently varied parameters. The largest extinction correction applied (Zachariasen, 1967) was 49% of $|F_c|$ for the 040 reflection. Calculated and observed structure factors are listed in Table 1. Table 2 presents the final atomic coordinates and anisotropic thermal parameters.

Since the two compounds are isostructural, there is no necessity to describe further the structure of $\text{Mg}_2(\text{PO}_4)\text{Cl}$. Tables 3 and 4 report the polyhedral bond angles and distances. Standard deviations of bond lengths were computed by the function and error program, *ORFFE*, of Busing, Martin & Levy (1964). The only significant difference is shorter average metal-anion bond distances due to the smaller ionic radius of six-coordinated Mg^{+2} as compared to Mn^{+2} , 0.72 versus 0.83 \AA (Shannon & Prewitt, 1969).

Table 3. Bond distances, polyhedral edge lengths, and bond angles for magnesium atomic positions

Numbers in parentheses are estimated standard deviations in the last significant figure.

(i) Interatomic distances

Mg(1)-O(1)	2.096 (2) Å	Mg(2)-O(1)	1.990 (2) Å
Mg(1)-O(2)	2.081 (2)	Mg(2)-O(2)	2.086 (2)
Mg(1)-O(3)	2.055 (3)	Mg(2)-O(3)	2.382 (3)
Mg(1)-O(3')	2.422 (2)	Mg(2)-O(4)	2.056 (2)
Mg(1)-O(4)	1.996 (2)	Mg(2)-Cl	2.422 (1)
Mg(1)-Cl	2.623 (1)	Mg(2)-Cl'	2.660 (1)

Mg(1) octahedron

O(4)-O(3)	3.471 (3) Å
O(4)-O(2)	3.007 (2)
O(4)-O(1)	2.828 (3)
O(4)-Cl	3.226 (2)
O(3)-O(2)	2.866 (3)
O(3)-O(3')	3.225 (2)
O(3)-Cl	3.219 (3)
O(2)-O(1)	3.165 (3)
O(2)-O(3')	2.797 (4)
O(1)-O(3')	2.445 (3)
O(1)-Cl	3.278 (2)
O(3')-Cl	3.983 (2)

Mg(2) octahedron

O(4)-O(3)	2.445 (3) Å
O(4)-O(2)	3.176 (3)
O(4)-O(1)	2.834 (3)
O(4)-Cl'	3.335 (2)
O(3)-O(2)	2.797 (4)
O(3)-Cl	3.464 (2)
O(3)-Cl'	3.968 (2)
O(2)-O(1)	3.018 (3)
O(2)-Cl	3.118 (2)
O(1)-Cl	3.719 (2)
O(1)-Cl'	3.270 (2)
Cl-Cl'	3.374 (1)

Table 3 (cont.)

(ii) Angles

Mg(1) octahedron		Mg(2) octahedron	
O(4)-Mg(1)-O(3)	117.9 (1)°	O(4)-Mg(2)-O(3)	66.4 (1)°
O(4)-Mg(1)-O(2)	95.0 (1)	O(4)-Mg(2)-O(2)	100.1 (1)
O(4)-Mg(1)-O(1)	87.4 (1)	O(4)-Mg(2)-O(1)	88.9 (1)
O(4)-Mg(1)-Cl	87.5 (1)	O(4)-Mg(2)-Cl'	89.0 (1)
O(3)-Mg(1)-O(2)	87.7 (1)	O(3)-Mg(2)-O(2)	77.2 (1)
O(3)-Mg(1)-O(3')	91.8 (1)	O(3)-Mg(2)-Cl	92.3 (1)
O(3)-Mg(1)-Cl	86.1 (1)	O(3)-Mg(2)-Cl'	103.7 (1)
O(2)-Mg(1)-O(1)	98.5 (1)	O(2)-Mg(2)-O(1)	95.5 (1)
O(2)-Mg(1)-O(3')	76.4 (1)	O(2)-Mg(2)-Cl	87.2 (1)
O(1)-Mg(1)-Cl	87.3 (1)	O(1)-Mg(2)-Cl	114.6 (1)
O(1)-Mg(1)-O(3')	65.1 (1)	O(1)-Mg(2)-Cl'	88.1 (1)
O(3')-Mg(1)-Cl	104.2 (1)	Cl-Mg(2)-Cl'	83.0 (1)
O(4)-Mg(1)-O(3')	149.0 (1)	O(4)-Mg(2)-Cl	154.8 (1)
O(3)-Mg(1)-O(1)	153.4 (1)	O(3)-Mg(2)-O(1)	152.0 (1)
O(2)-Mg(1)-Cl	173.8 (2)	O(2)-Mg(2)-Cl'	170.2 (1)

Table 4. Bond distances, polyhedral edge lengths, and bond angles for the phosphate tetrahedron

Numbers in parentheses are estimated standard deviations in last significant figure.

(i) Interatomic distances			
P-O(1)	1.536 (2) Å	O(1)-O(2)	2.535 (3) Å
P-O(2)	1.521 (3)	O(1)-O(3)	2.445 (3)
P-O(3)	1.564 (3)	O(1)-O(4)	2.519 (3)
P-O(4)	1.537 (2)	O(2)-O(3)	2.580 (4)
		O(2)-O(4)	2.542 (3)
		O(3)-O(4)	2.445 (3)
(ii) Angles			
	O(1)-P-O(2)	112.0 (1)°	
	O(1)-P-O(3)	104.1 (1)	
	O(1)-P-O(4)	110.1 (1)	
	O(2)-P-O(3)	113.5 (1)	
	O(2)-P-O(4)	112.4 (1)	
	O(3)-P-O(4)	104.1 (1)	

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The Crystal and Molecular Structure of 2-Formylpyridine Selenosemicarbazone

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The structure of 2-formylpyridine selenosemicarbazone, $\text{SeN}_4\text{C}_7\text{H}_8$, has been determined from three-dimensional X-ray photographic data. The crystals are monoclinic, space group $P2_1/c$, with unit-cell dimensions $a = 9.320$, $b = 6.524$ and $c = 16.275$ Å, $\beta = 90.53^\circ$. There are four formula units in the cell. The structure was solved by the two-dimensional minimum Patterson function and the heavy atom method. It was refined by a full-matrix least-squares method to a final residual R value of 0.11 for 1180 observed reflexions. The Se-C bond length of 1.83 Å possesses only partial double-bond character. The molecules are linked by N-H...Se hydrogen bonds to form dimer-like units, which are held together by N-H...N hydrogen bonds.

Introduction

In recent years, several organic compounds of selenium have been investigated. The molecular structures of different selenosemicarbazones have been studied by Gingras, Suprunchuk & Bayley (1965); they described their infrared spectra with particular emphasis on the Se-C vibration and they have studied the antifungal properties of selenosemicarbazones that were found to be generally more active than the corresponding thiosemicarbazones. French & Blanz (1966) have studied various thiosemicarbazones and have found that all the tumour inhibitors are potentially capable of acting as tridentate N-N-S type ligands. Mathew & Palenik (1969) reported the crystal structure of bis-(1-formyl-isoquinolinethiosemicarbazono)nickel(II) monohydrate and confirmed the ability of the ligand to act

as a tridentate chelate. However, the compound 2-formylthiophene thiosemicarbazone (Mathew & Palenik, 1971) shows no tumour inhibition although the possibility of an N-N-S type chelate exists. On the other hand, French & Blanz (1966) reported that 4-formylpyridine thiosemicarbazone shows no carcinostatic activity, whereas they found that 2-formylpyridine thiosemicarbazone is a tumour inhibitor. Apparently the position of the thiosemicarbazone group on the pyridine nucleus dictates the biological activity of formylpyridine thiosemicarbazones. A knowledge of the conformation and bond lengths is essential for a final explanation of the requirements for biological activity in these compounds. Therefore, a crystal structure analysis of 2-formylpyridine selenosemicarbazone was carried out to correlate the molecular structure with the thiosemicarbazone analogues.