bond lengths and angles were computed by the function and error program (*ORFFE*) of Busing, Martin & Levy (1964).

Table 3. *Bond distances, polyhedral edge lengths, and bond angles for the phosphate tetrahedron*

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

P——O(1)	1·529 (4) Å	O(1)–O(2)	2·528 (6) Å
P——O(2)	1·537 (4)	O(1)–O(3)	2·511 (5)
P——O(3)	1·533 (4)	O(1)–O(4)	2·475 (5)
P——O(4)	1·548 (4)	O(2)–O(3)	2·503 (5)
		O(2)–O(4)	2·526 (5)
		O(3)–O(4)	2·511 (5)
O(1)–P–O(2)	111·1 (2)°	O(2)–P–O(3)	109·3 (2)°
O(1)–P–O(3)	110·2 (2)	O(2)–P–O(4)	110·0 (2)
O(1)–P–O(4)	107·1 (2)	O(3)–P–O(4)	109·2 (2)

As we predicted (Rea & Kostiner, 1972), $Cd_2(PO_4)F$ is isostructural with $Mn_2(PO_4)F$; the fluorine atom occupies a single position as opposed to the situation in both wagnerite $[Mg_2(PO_4)F]$ and tripoidite $[Mn_{1.5}Fe_{0.5}(PO_4)OH]$, in which the fluorine atom (or hydroxyl ion) half-occupies two sites in a doubled unit cell. Furthermore, it is undoubtedly the larger cadmium ion that causes a reduction in the unusually long

Table 4. *Bond distances and angles for the fluorine environment*

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

F–Cd(1)	2·468 (3) Å	Cd(1)–F–Cd(1')	109·0 (1)°
F–Cd(1')	2·270 (3)	Cd(1)–F–Cd(2)	95·4 (1)
F–Cd(2)	2·281 (3)	Cd(1)–F–Cd(2')	109·9 (1)
F–Cd(2')	2·414 (4)	Cd(1')–F–Cd(2)	139·1 (1)
		Cd(1')–F–Cd(2')	95·5 (1)
		Cd(2)–F–Cd(2')	106·6 (1)

metal–fluorine distances for one of the two fluorines in each of the two octahedra in $Mn_2(PO_4)F$. Table 4 presents the relevant bond angles and lengths about the fluorine atom.

The cadmium ion, with a six-coordinated ionic radius of 0·95 Å (Shannon & Prewitt, 1969), most probably represents the largest divalent metal cation which forms a fluorophosphate with the wagnerite structure type. Calcium ($r = 1·00$ Å) does not form a fluorophosphate with the 2:1:1 stoichiometry, and the compound chlorospodiosite $[Ca_2(PO_4)Cl]$ adopts an entirely different structure (Greenblatt, Banks & Post, 1967).

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Cyanomethyl 2-Picolyl Sulfone

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Abstract. $(C_5H_4N)CH_2SO_2CH_2CN$, $(C_8H_8N_2O_2S)$, $M = 196·32$, monoclinic, $P2_1/c$, $a = 10·609$ (1), $b = 9·964$ (1), $c = 9·124$ (1) Å, $\beta = 106·10$ (1)°, $V = 926·60$ Å³, $Z = 4$, $D_x = 1·406$, $D_m = 1·403$ g cm⁻³. Full-matrix least-squares refinement of 1686 reflections $[I > 3\sigma(I)]$ collected with θ–2θ scans on a Syntex $P2_1$ diffractometer yielded a conventional R of 0·036. Expected C–H$\cdots$O and/or C–H$\cdots$N interactions were not found.

Introduction. Produced by sublimation, the colorless crystal used in this study measured $0.28 \times 0.27 \times 0.45 \times 0.38$ mm perpendicular to (010), (100), (011), (01$\bar{1}$) respectively. The unit-cell parameters were refined with the Cu $K\alpha_1$ Bragg angles for 28 high-angle reflections ($136 < 2\theta < 150°$) measured on a G. E. XRD-5 diffractometer (Cu $K\alpha_1 = 1.54050$ Å). Intensity data for 2134 independent reflections were collected on a Syntex $P2_1$ diffractometer with Mo $K\alpha$ radiation monochromatized by a graphite crystal. The θ–2θ scan technique was employed with the scan rate, S, varying from 1.5 to $5.0°$ min^{-1}. The reflections were scanned from $1.1°$ in 2θ below the $K\alpha_1$ peak to $1.1°$ above the $K\alpha_2$ peak accumulating P counts. Background measurements, B_1 and B_2, were taken at both ends of the scan range, each for a time equal to one-half of the scan time. The intensities of four standard reflections were measured after every 96 reflections; the average intensity fluctuated by 2% and a correction as a function of exposure time was applied. Lorentz and polarization corrections were applied; no absorption corrections were made ($\mu = 3.12$ cm^{-1}, Mo $K\alpha$). Standard deviations in the intensities, $\sigma(I)$, and in the structure amplitudes, $\sigma(F_o)$, were derived from counting statistics: $\sigma(I) = S(P + B_1 + B_2)^{1/2}$. The 1686 reflections for which $I > 3\sigma(I)$ were the only reflections used in the solution and refinement of the structure; weights for these reflections were assigned as $1/\sigma^2(F_o)$.

The structure was solved by the heavy-atom method and all non-hydrogen atoms were located in subsequent Fourier syntheses. A difference Fourier was used to locate the hydrogen atoms. Full-matrix least-squares refinement (*NUCLS*: J. A. Ibers's modification of *ORFLS*) of all positional and thermal (anisotropic for non-hydrogen atoms; isotropic for hydrogen atoms) parameters converged at a conventional $R = (\sum ||F_o| - |F_c||/\sum|F_o|)$ of 0.036 and a weighted $R_w = (\sum w(|F_o| - |F_c|)^2/\sum w|F_o|^2)^{1/2}$ of 0.027. When all 2134 reflections were included, the conventional R was found to be 0.049. The largest shift of any parameter in the final cycle of refinement was 0.14. The largest peak in the final difference map had a magnitude of 0.16 e Å^{-3} and

was located near atom O(2). Extinction did not prove to be a serious problem. For S, O, N, and C, the atomic scattering factors of Cromer & Waber (1965) were used; those of Stewart, Davidson & Simpson (1965) were used for the hydrogen atoms. The final positional and thermal parameters are given in Tables 1 and 2.*

Table 2. *Positional and thermal parameters for the hydrogen atoms*

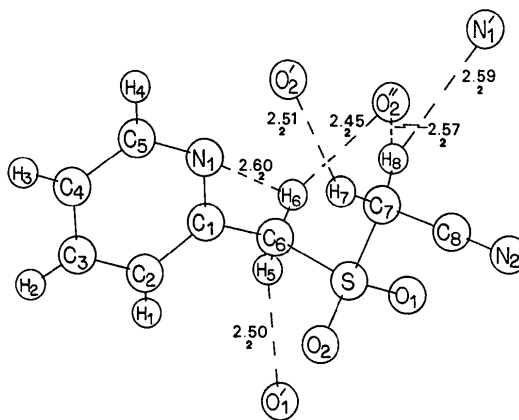|				
H(1)	−0.320 (2)	0.102 (3)	0.052 (3)	6.4 (8)
H(2)	−0.476 (3)	0.210 (3)	0.154 (3)	9.0 (10)
H(3)	−0.461 (3)	0.440 (3)	0.193 (3)	7.4 (9)
H(4)	−0.299 (2)	0.557 (3)	0.114 (3)	5.8 (7)
H(5)	−0.148 (2)	0.125 (2)	−0.081 (2)	4.1 (6)
H(6)	−0.113 (2)	0.256 (2)	−0.121 (2)	3.4 (5)
H(7)	0.047 (2)	0.409 (2)	0.188 (3)	5.5 (7)
H(8)	0.092 (2)	0.395 (2)	0.025 (2)	4.7 (6)

Fig. 1. Atom numbering scheme with H···O and H···N interactions.

Table 1. *Positional and thermal parameters* ($\times 10^4$) *for the non-hydrogen atoms*

Estimated standard deviations are in parentheses.
Thermal parameters are in the form: $\exp[-(h^2\beta_{11} + \ldots + 2kl\beta_{23})]$.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
S	0.0327 (1)	0.1886 (1)	0.0939 (1)	81 (1)	54 (1)	100 (1)	5 (1)	39 (1)	1 (1)
O(1)	0.1140 (2)	0.1196 (2)	0.0167 (2)	122 (2)	82 (2)	176 (3)	15 (2)	80 (2)	−11 (2)
O(2)	0.0197 (1)	0.1331 (1)	0.2344 (2)	100 (2)	79 (2)	112 (2)	2 (1)	37 (2)	19 (2)
N(1)	−0.2180 (2)	0.4053 (2)	0.0472 (2)	88 (2)	81 (2)	153 (3)	−2 (2)	41 (2)	−0 (2)
N(2)	0.3345 (2)	0.3437 (3)	0.3002 (3)	96 (3)	184 (4)	254 (5)	−5 (3)	40 (3)	1 (4)
C(1)	−0.2240 (2)	0.2726 (2)	0.0317 (2)	76 (3)	82 (3)	88 (3)	4 (2)	13 (2)	−7 (2)
C(2)	−0.3162 (3)	0.1951 (3)	0.0745 (3)	103 (3)	112 (4)	162 (4)	24 (3)	34 (3)	−13 (4)
C(3)	−0.4056 (3)	0.2588 (4)	0.1358 (4)	86 (3)	197 (5)	191 (5)	20 (4)	52 (4)	−32 (4)
C(4)	−0.4000 (3)	0.3948 (4)	0.1519 (3)	85 (3)	182 (5)	181 (5)	−23 (3)	40 (3)	5 (4)
C(5)	−0.3055 (3)	0.4632 (3)	0.1071 (3)	95 (3)	114 (4)	192 (5)	−17 (3)	37 (3)	12 (4)
C(6)	−0.1245 (2)	0.2102 (2)	−0.0363 (3)	110 (3)	80 (3)	89 (3)	4 (2)	30 (3)	5 (3)
C(7)	0.0966 (2)	0.3568 (2)	0.1324 (3)	87 (3)	61 (2)	138 (4)	−2 (2)	44 (3)	3 (3)
C(8)	0.2301 (3)	0.3500 (2)	0.2282 (3)	85 (3)	87 (3)	163 (4)	−6 (2)	48 (3)	−4 (3)

Discussion. This structure represents the second in a series to study C–H···O and C–H···N interactions in compounds where the C–H bond is polarized by adjacent electron-withdrawing groups. Such an interaction, with a short H···O distance of 2·22 Å, was found for the first compound in the series, 2,4-dinitrobenzyl p-tolyl sulfone, but the geometry of the molecule left doubt as to whether the interaction was a result of an H···O attraction or a result of packing forces (Harlow, Pfluger, Sammes & Simonsen, 1974). It was hoped that the study of the present molecule, where the geometry does not 'force' the methylene hydrogen to approach either an oxygen or a nitrogen atom, would yield additional information on the nature of this interaction.

The results of this study can be seen in Fig. 1; all H···O and H···N distances less than 2·6 Å, the classical if unrealistic van der Waals H···O distance, are given. For the methylene group of most interest, –SO₂–CH₂–CN, the shortest H···O distance is 2·51 Å. The second methylene group, pyridine–CH₂SO₂–, where the C–H bond should be less polarized than the first, shows in fact a shorter H···O distance of 2·45 Å. In short, no significant C–H···O or C–H···N interactions occur in this structure, even if a correction is applied to lengthen the C–H bonds to chemically reasonable distances and hence shorten the H···O and H···N distances.

The intramolecular bond distances and angles are given in Table 3. The sulfonyl S–O distances and the O–S–O angle are within 2σ of those found in the first compound of this series. The C–S distances are significantly different and may reflect the different inductive effects of the pyridine and cyano groups. The C≡N bond length, 1·122 (4) Å, is typically short because of the large thermal motion of this group and of the nitrogen atom in particular (Little, Pautler & Coppens, 1971; Matthews, Swanson, Mueller & Stucky, 1971). The C–C≡N angle of 178·6 (3)° is normal.

The usual pattern of angles within the pyridine ring is also found here; the C–N–C angle is less than 120°, 118·4 (3)°; the neighboring N–C–C angles are greater than 120°, 122·8 (2)° and 124·0 (3)°; the remaining angles are generally somewhat less than 120° and such is the case here (Kim, Jeffrey & Rosenstein, 1971; Campsteyn, Dupont & Dideberg, 1974; Kvick & Backéus, 1974). The C(6)–C(1)–N(1) and C(6)–C(1)–C(2) angles of 116·0 (2) and 121·2 (2)°, respectively, are also reasonable. The bond distances within the ring agree quite well with those previously noted; the C(3)–C(4) and C(4)–C(5) are shortened as a result of the large thermal motions of these atoms. The pyridine ring is planar to within one standard deviation, 0·003 Å; substituent atom C(6) deviates from the plane by only –0·008 (2) Å.

Table 3. *Bond distances and angles for cyanomethyl 2-picolyl sulfone*

Bond distances (Å)

S——O(1)	1·432 (2)	C(7)–C(8)	1·446 (4)
S——O(2)	1·438 (2)	C(8)–N(2)	1·122 (4)
S——C(6)	1·774 (3)		
S——C(7)	1·805 (2)	C(2)–H(1)	0·95 (3)
C(1)–N(1)	1·329 (3)	C(3)–H(2)	0·94 (3)
C(1)–C(2)	1·385 (4)	C(4)–H(3)	0·95 (3)
C(1)–C(6)	1·500 (3)	C(5)–H(4)	0·93 (3)
C(2)–C(3)	1·383 (4)	C(6)–H(5)	0·95 (2)
C(3)–C(4)	1·363 (5)	C(6)–H(6)	0·93 (2)
C(4)–C(5)	1·365 (4)	C(7)–H(7)	0·98 (2)
C(5)–N(1)	1·333 (4)	C(7)–H(8)	1·04 (2)

Bond angles (°)

O(1)–S——O(2)	118·3 (1)	C(1)–C(2)–H(1)	119 (2)
O(1)–S——C(6)	108·2 (1)	C(3)–C(2)–H(1)	123 (2)
O(1)–S——C(7)	107·3 (1)	C(2)–C(3)–H(2)	120 (2)
O(2)–S——C(6)	109·8 (1)	C(4)–C(3)–H(2)	121 (3)
O(2)–S——C(7)	107·9 (1)	C(3)–C(4)–H(3)	120 (2)
C(6)–S——C(7)	104·5 (1)	C(5)–C(4)–H(3)	122 (2)
C(2)–C(1)–N(1)	122·8 (2)	C(4)–C(5)–H(4)	121 (2)
C(2)–C(1)–C(6)	121·2 (2)	N(1)–C(5)–H(4)	115 (2)
N(1)–C(1)–C(6)	116·0 (2)	C(1)–C(6)–H(5)	115 (1)
C(1)–C(2)–C(3)	118·4 (3)	C(1)–C(6)–H(6)	114 (1)
C(2)–C(3)–C(4)	119·1 (3)	S——C(6)–H(5)	105 (1)
C(3)–C(4)–C(5)	118·6 (3)	S——C(6)–H(6)	107 (1)
C(4)–C(5)–N(1)	124·0 (3)	H(5)–C(6)–H(6)	100 (2)
C(1)–N(1)–C(5)	117·2 (2)	C(8)–C(7)–H(7)	107 (1)
C(1)–C(6)–S	114·4 (2)	C(8)–C(7)–H(8)	112 (1)
C(8)–C(7)–S	109·1 (2)	S——C(7)–H(7)	111 (1)
C(7)–C(8)–N(2)	178·6 (3)	S——C(7)–H(8)	104 (1)
		H(7)–C(7)–H(8)	114 (2)

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