characteristic for the system water-active charcoal[1]. The steep rise of the adsorption isotherm is observed in the region of relative pressures 0·4–0·5 and the isotherm reveals a typical hysteresis.

From the point of view of adsorption selectivity the carbon molecular sieves are comparable to the classical 'Zeolite' sieves. In some cases the selectivity is even better. The carbon molecular sieve prepared by thermal processing of 'Saran' charcoal at 1,750° C selectively adsorbs benzene from the benzene-cyclohexane mixture[3]. These hydrocarbons, according to Barrer[4], belong to the same group of compounds separated by zeolites. Additional activation (by carbon dioxide) of the carbon molecular sieve prepared from the 'Saran' charcoal to a low burn-off (11 per cent) renders its microporous structure accessible for cyclohexane molecules[1]. It can therefore be concluded that the molecular sieve properties of carbon adsorbents on the basis of 'Saran' charcoal are caused by narrowing of the openings of micropores.

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Structures of Oxodiperoxo-1 : 10-phenanthrolinechromium(VI) and Diperoxoaquoethylenediaminechromium(VI)hydrate

As a part of an investigation of the structures of peroxochromates[1-4], peroxochromium complexes with ethylenediamine and 1 : 10-phenanthroline have been studied, and that of α,α'-bipyridyl is under investigation.

The structures of $[CrO(O_2)_2(C_{12}H_8N_2)]$ and $[Cr(O_2)_2(H_2O)(C_2H_6N_2)](H_2O)$ have been solved by three-dimensional Pattersson and Fourier methods, and refined some least-squares cycles. The R-factor has dropped to 0·13 and 0·18 respectively.

The unit cell dimensions of $[CrO(O_2)_2(C_{12}H_8N_2)]$ were determined from rotation and Weissenberg photographs, and were refined from Guinier photographs using CuK_a radiation. The unit cell is orthorhombic with 4 molecules in the cell and with $a = 10\cdot554$ Å, $b = 6\cdot857$ Å and $c = 16\cdot239$ Å. The systematically absent reflexions were $0kl$ with $k + l = 2n + 1$ and $hk0$ with $h = 2n + 1$. This is characteristic for the space groups $Pnma$ and $Pna2_1$. During the structure investigation it became obvious that a plausible structure could be obtained based on space group $Pnma$.

The investigation has revealed that chromium is coordinated to two peroxo groups, one oxide oxygen atom and to the two nitrogen atoms of the 1 : 10-phenanthroline molecule, the geometrical configuration of the co-ordinated atoms being a pentagonal bipyramid with the oxide oxygen and one nitrogen atom at the apices. The O—O distance is $1\cdot42 \pm 0\cdot02$ Å and the Cr—O_{oxo} distance is $1\cdot58 \pm 0\cdot03$ Å, values which are close to those obtained for similar compounds (1-4). Table 1 gives the atomic positions at the present stage of the refinement.

The unit cell dimensions of $[Cr(O_2)_2(H_2O)(C_2H_6N_2)](H_2O)$ were determined from rotation and Weissenberg photographs and were refined from Guinier photographs using CuK_a radiation. The orthorhombic unit cell contains 4 molecules and has the dimensions: $a = 7\cdot594$ Å, $b = 12\cdot258$ Å, and $c = 8\cdot168$ Å. The systematically absent

Table 1. PARAMETER VALUES FOR $[CrO(O_2)_2(C_{12}H_8N_2)]$
Space group $Pnma$

Atom	Equivalent position	x	y	z
Cr	4c	0·246	0·250	0·173
O₁	8d	0·239	0·519	0·156
O₂	8d	0·130	0·434	0·193
O₃	4c	0·327	0·250	0·255
N₁	4c	0·412	0·250	0·100
N₂	4c	0·175	0·250	0·042
C₁	4c	0·531	0·250	0·133
C₂	4c	0·631	0·250	0·079
C₃	4c	0·624	0·250	0·993
C₄	4c	0·499	0·250	0·962
C₅	4c	0·393	0·250	0·013
C₆	4c	0·473	0·250	0·875
C₇	4c	0·351	0·250	0·847
C₈	4c	0·242	0·250	0·901
C₉	4c	0·268	0·250	0·986
C₁₀	4c	0·110	0·250	0·877
C₁₁	4c	0·027	0·250	0·936
C₁₂	4c	0·046	0·250	0·017

reflexions were $0kl$ with $k = 2n + 1$ and $h0l$ with $l = 2n + 1$, which is characteristic for the space groups $Pbcm$ and $Pbc2_1$.

As there are only 4 molecules in the unit cell and as it was supposed from other evidence that the molecules did not contain a mirror plane, the correct space group was thought to be $Pbc2_1$. The fractional co-ordinates of the atoms, based on this assumption, are at the present stage of the refinement those given in Table 2 ($R = 0\cdot176$). During the structure investigation it soon became evident that all atoms except the two carbon atoms were situated at positions that fitted space group $Pbcm$ equally well (within the limits of error). With the carbon atoms assumed to occupying positions $8e$ of $Pbcm$ with only half the equivalent positions occupied (evidently this means that in half the unit cells C_1 is above and C_2 below the 'mirror' plane, while in the rest of the unit cells the reverse is true), refinement was undertaken and the R-value became 0·183 after six cycles, the parameters being those given in parenthesis in Table 2.

Table 2. PARAMETER VALUES FOR $[Cr(O_2)_2(H_2O)(C_2H_6N_2)](H_2O)$
Space group $Pbc2_1$ assumed. In parenthesis are given the values obtained by assuming $Pbcm$ to be the correct space group with O_1 and O_2 in $8d$, C_1 and C_2 in $8d$ (half-filled), O_6 in $4b$ and all the others in $4c$

Atom	x	y	z
Cr	0·241 (0·241)	0·013 (0·013)	0·251 (0·250)
O₁	0·237 (0·237)	0·018 (0·020)	0·014 (0·017)
O₂	0·282 (0·281)	0·913 (0·912)	0·082 (0·084)
O₃	0·238	0·021	0·480
O₄	0·278	0·913	0·412
O₅	0·977 (0·978)	0·984 (0·983)	0·246 (0·250)
O₆	0·955 (0·955)	0·241 (0·250)	0·000 (0·000)
N₁	0·501 (0·500)	0·059 (0·058)	0·247 (0·250)
N₂	0·204 (0·204)	0·183 (0·182)	0·259 (0·250)
C₁	0·520 (0·519)	0·172 (0·173)	0·220 (0·219)
C₂	0·369 (0·369)	0·234 (0·232)	0·302 (0·302)

This molecule can also be described as being co-ordinated to five ligands, namely, to two peroxo groups, one water molecule and the two nitrogen atoms of one ethylenediamine molecule as co-ordinating groups. The geometrical arrangement of the co-ordinated atoms is a pentagonal bipyramid. The water molecules are involved in hydrogen bonding, one with one peroxidic oxygen atom of each of two neighbouring $[Cr(O_2)_2(H_2O)en]$ molecules and the other with two peroxidic oxygen atoms of one neighbouring complex molecule, forming chains through the whole crystal. The O—O distances are $1\cdot44 \pm 0\cdot04$ Å and $1\cdot46 \pm 0\cdot04$ Å, the Cr—O_{water} distance is $2\cdot04 \pm 0\cdot02$ Å, and the hydrogen bonding distances $O_{peroxo} \cdots H \cdots O_{water}$ are $2\cdot69$ Å, $2\cdot86$ Å, $2\cdot72$ Å and $2\cdot72$ Å. $\angle$ $O_{peroxo} \cdots O_{water} \cdots O_{peroxo}$ are 102° and 107° respectively.

The refinement will be continued to convergence, and complete reports will be published elsewhere.

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