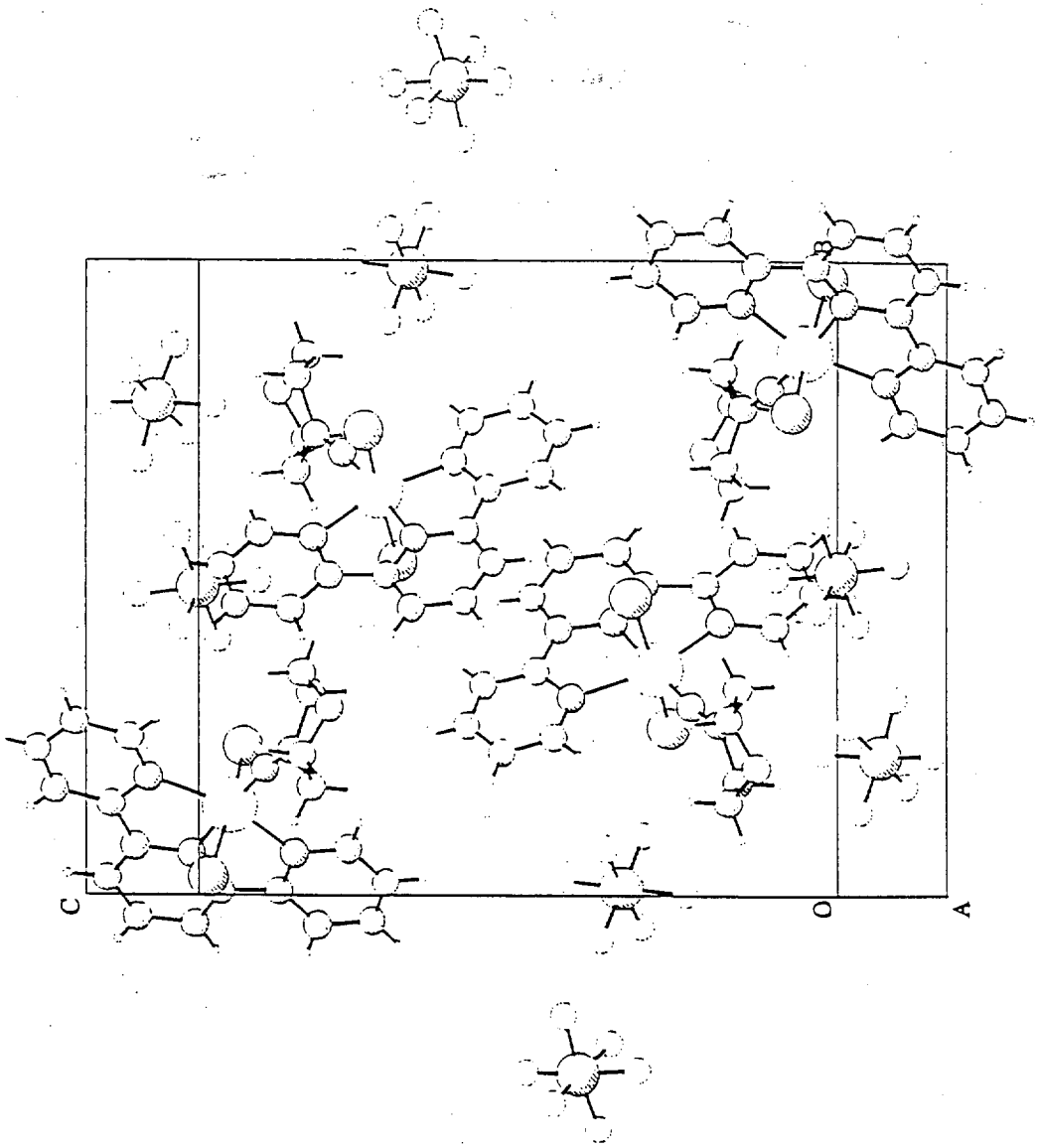
 

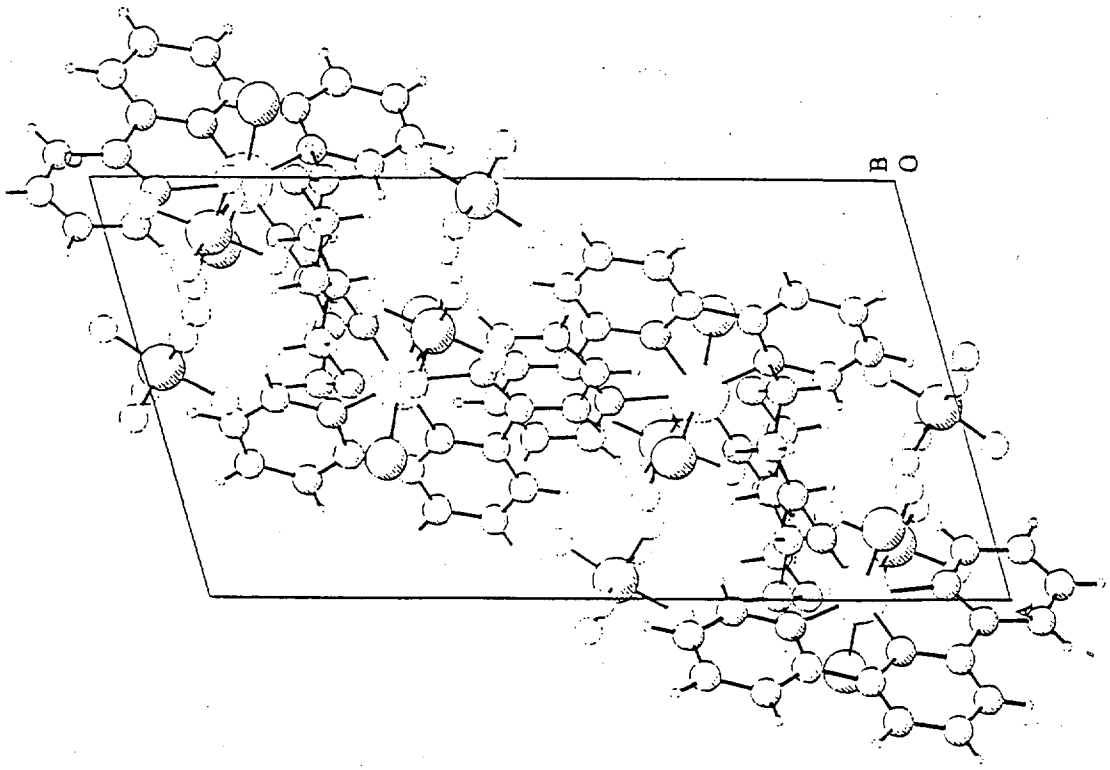
Space Group and Cell Dimensions  Monoclinic,  P 21/n
a  9.9697(5)  b  15.4863(7)  c  18.3680(8)
beta 105.642(1)
Volume  2730.88(22)A**3
Empirical formula : Os C19 H19 Cl2 F12 N5 O P2
Cell dimensions were obtained from 8192 reflections with 2Theta angle
in the range  3.00 -  50.00 degrees.
Crystal dimensions :  0.40  X  0.10  X  0.05  mm
FW =  884.42  Z =  4  F(000) =  1695.93
Dcalc  2.151Mg.m-3, mu  5.09mm-1, lambda 0.71073A, 2Theta(max)  50.0
The intensity data were collected on a Bruker SMART diffractometer,
using the omega scan mode.
The h,k,l ranges used during structure solution and refinement are :--
Hmin,max  -11  11;  Kmin,max  0  18;  Lmin,max  0  21
No. of reflections measured  13656
No. of unique reflections  4821
No. of reflections with Inet > 2.5sigma(Inet)  3624
Merging R-value on intensities  0.033
Correction was made for absorption using SADABS

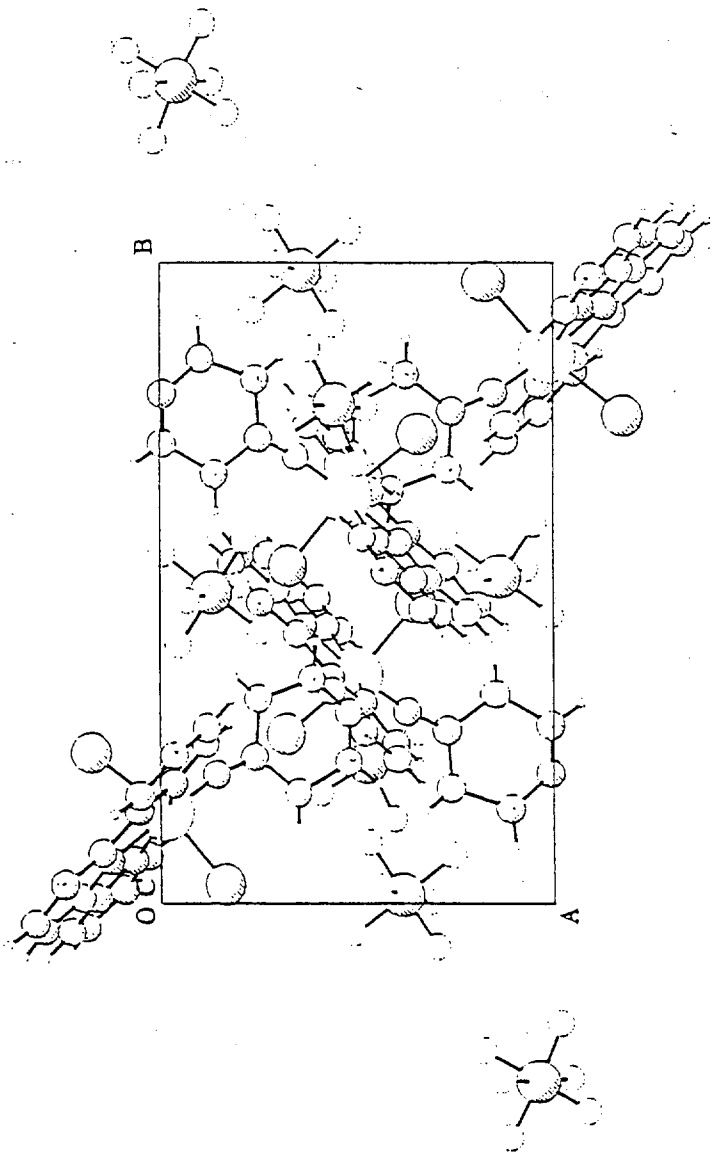
The last least squares cycle was calculated with
61 atoms, 379 parameters and 4790 out of 4821 reflections.
Weights based on counting-statistics were used.
The weight modifier K in KFo**2 is 0.000100
The residuals are as follows :--
For significant reflections,  RF 0.060, Rw 0.047 GoF  1.73
For all reflections,  RF 0.061, Rw 0.047.
where RF = Sum(Fo-Fc)/Sum(Fo),
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was  0.001.
In the last D-map, the deepest hole was  -1.950e/A**3,
and the highest peak  1.590e/A**3.

The following references are relevant to the NRCVAX System.

1. Full System Reference :
Gabe, E.J., Le Page, Y., Charland, J.-P., Lee, F.L. and White, P.S.
(1989) J. Appl. Cryst., 22, 384-387.
2. Scattering Factors from Int. Tab. Vol. 4 :
International Tables for X-ray Crystallography, Vol. IV, (1974)
Kynoch Press, Birmingham, England.
The following references may also be relevant.
3. ORTEP Plotting :
Johnson, C.K., (1976) ORTEP - A Fortran Thermal Ellipsoid Plot
Program, Technical Report ORNL-5138, Oak Ridge
4. Pluto Plotting :
S. Motherwell, University Chemical Laboratory, Cambridge, 1978
5. Missing Symmetry Treatment by MISSYM :
Le Page, Y., (1988) J. Appl. Cryst., 21, 983-984.
6. Grouping of Equivalent Reflections in DATRD2 :
Le Page, Y. and Gabe, E.J., (1979) J. Appl. Cryst., 12, 464-466.


C
O
A





21-Dec-1998

Table . Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

| | x | y | z | Biso |
|---|---|---|---|---|
| Os1 | 0.98620( 4) | 0.858238(21) | 0.186834(19) | 2.342(16) |
| Cl1 | 1.17177(25) | 0.76475 (14) | 0.23195 (13) | 3.18 (11) |
| Cl2 | 0.8331 ( 3) | 0.97109 (15) | 0.13490 (14) | 3.71 (12) |
| N1 | 0.8546 ( 8) | 0.7995 ( 4) | 0.2144 ( 4) | 2.8 ( 4) |
| N2 | 0.7554 ( 8) | 0.7709 ( 5) | 0.2352 ( 4) | 3.3 ( 4) |
| C3 | 0.6404 (16) | 0.8273 ( 8) | 0.2438 (10) | 8.6 (11) |
| C4 | 0.5063 (14) | 0.7787 (11) | 0.2118 (10) | 9.5 (10) |
| O5 | 0.5063 ( 8) | 0.7023 ( 5) | 0.2479 ( 4) | 5.2 ( 4) |
| C6 | 0.6036 (16) | 0.6478 ( 8) | 0.2258 (10) | 8.5 (10) |
| C7 | 0.7460 (15) | 0.6797 ( 8) | 0.2587 ( 7) | 6.1 ( 7) |
| N11 | 1.0650 ( 8) | 0.9329 ( 4) | 0.2834 ( 4) | 2.6 ( 3) |
| C12 | 1.0300 (10) | 0.9262 ( 6) | 0.3492 ( 5) | 3.2 ( 5) |
| C13 | 1.0894 (11) | 0.9789 ( 6) | 0.4095 ( 5) | 3.6 ( 5) |
| C14 | 1.1854 (12) | 1.0399 ( 7) | 0.4041 ( 5) | 4.1 ( 5) |
| C15 | 1.2234 (11) | 1.0464 ( 6) | 0.3365 ( 6) | 3.5 ( 5) |
| C16 | 1.1622 (10) | 0.9923 ( 6) | 0.2775 ( 5) | 2.8 ( 4) |
| N21 | 1.1244 ( 7) | 0.9337 ( 4) | 0.1557 ( 4) | 2.3 ( 3) |
| C22 | 1.1974 ( 9) | 0.9921 ( 5) | 0.2045 ( 5) | 2.5 ( 4) |
| C23 | 1.2926 (11) | 1.0448 ( 6) | 0.1839 ( 5) | 3.7 ( 5) |
| C24 | 1.3150 (12) | 1.0337 ( 7) | 0.1131 ( 6) | 4.1 ( 5) |
| C25 | 1.2400 (11) | 0.9719 ( 7) | 0.0634 ( 5) | 3.9 ( 5) |
| C26 | 1.1442 (10) | 0.9220 ( 6) | 0.0855 ( 5) | 2.8 ( 4) |
| N31 | 0.9668 ( 8) | 0.8130 ( 5) | 0.0768 ( 4) | 2.8 ( 3) |
| C32 | 1.0520 (10) | 0.8546 ( 6) | 0.0413 ( 5) | 3.0 ( 4) |
| C33 | 1.0503 (11) | 0.8323 ( 7) | -0.0323 ( 5) | 3.7 ( 5) |
| C34 | 0.9644 (13) | 0.7685 ( 8) | -0.0683 ( 6) | 5.4 ( 7) |
| C35 | 0.8806 (14) | 0.7255 ( 8) | -0.0312 ( 6) | 5.5 ( 7) |
| C36 | 0.8835 (11) | 0.7497 ( 7) | 0.0406 ( 6) | 4.1 ( 5) |
| P1 | 0.5424 ( 5) | 0.2194 ( 3) | 0.02204 (25) | 6.81 (24) |
| F11 | 0.4206 (10) | 0.1730 ( 8) | -0.0293 ( 7) | 15.9 ( 8) |
| F12 | 0.4620 (10) | 0.2252 ( 5) | 0.0870 ( 6) | 10.5 ( 6) |
| F13 | 0.4852 (11) | 0.3113 ( 6) | -0.0050 ( 6) | 11.2 ( 7) |
| F14 | 0.6731 (10) | 0.2682 ( 6) | 0.0835 ( 4) | 10.1 ( 6) |
| F15 | 0.6123 ( 8) | 0.1322 ( 5) | 0.0594 ( 4) | 7.2 ( 4) |
| F16 | 0.6331 ( 8) | 0.2212 ( 6) | -0.0349 ( 4) | 9.1 ( 6) |
| P2 | 0.8680 ( 4) | 0.5123 ( 3) | 0.12720 (21) | 6.94 (22) |
| F21 | 0.9529 ( 8) | 0.5949 ( 5) | 0.1665 ( 4) | 7.3 ( 4) |
| F22 | 0.9319 (11) | 0.5253 ( 7) | 0.0579 ( 5) | 11.5 ( 7) |
| F23 | 0.7827 (10) | 0.4307 ( 6) | 0.0875 ( 5) | 10.7 ( 6) |
| F24 | 0.8008 ( 9) | 0.5017 ( 5) | 0.1981 ( 4) | 8.0 ( 5) |
| F25 | 0.7403 ( 9) | 0.5745 ( 7) | 0.0883 ( 5) | 11.3 ( 6) |
| F26 | 0.9943 ( 7) | 0.4514 ( 5) | 0.1699 ( 4) | 7.0 ( 4) |
| H3a | 0.652 | 0.833 | 0.297 | 10.1 |
| H3b | 0.643 | 0.883 | 0.222 | 10.1 |
| H4a | 0.496 | 0.771 | 0.159 | 10.3 |
| H4b | 0.431 | 0.814 | 0.219 | 10.3 |
| H6a | 0.586 | 0.650 | 0.172 | 9.8 |
| H6b | 0.594 | 0.589 | 0.241 | 9.8 |
| H7a | 0.767 | 0.677 | 0.313 | 6.9 |
| H7b | 0.810 | 0.644 | 0.242 | 6.9 |
| H12 | 0.960 | 0.886 | 0.353 | 4.1 |

| | | | | |
|---|---|---|---|---|
| H13 | 1.067 | 0.972 | 0.457 | 4.4 |
| H14 | 1.226 | 1.078 | 0.445 | 4.8 |
| H15 | 1.291 | 1.088 | 0.331 | 4.2 |
| H23 | 1.345 | 1.086 | 0.219 | 4.5 |
| H24 | 1.383 | 1.069 | 0.098 | 5.0 |
| H25 | 1.253 | 0.965 | 0.014 | 4.8 |
| H33 | 1.113 | 0.861 | -0.056 | 4.6 |
| H34 | 0.961 | 0.754 | -0.120 | 6.3 |
| H35 | 0.817 | 0.682 | -0.057 | 6.3 |
| H36 | 0.825 | 0.720 | 0.066 | 5.0 |

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

| | u11(U) | u22 | u33 | u12 | u13 | u23 |
|---|---|---|---|---|---|---|
| Os1 | 1.799(20) | 3.354(19) | 3.765(21) | 0.032(19) | 0.783(14) | -0.235(18) |
| C11 | 2.67 (14) | 3.92 (12) | 5.37 (15) | 0.90 (11) | 0.85 (11) | 0.40 (11) |
| C12 | 3.07 (15) | 5.00 (14) | 5.81 (16) | 1.19 (12) | 0.86 (12) | 0.54 (12) |
| N1 | 2.7 ( 5) | 3.6 ( 4) | 4.0 ( 5) | 0.5 ( 4) | 0.6 ( 4) | 0.2 ( 3) |
| N2 | 2.5 ( 5) | 4.5 ( 5) | 6.0 ( 6) | -1.2 ( 4) | 1.8 ( 4) | -1.2 ( 4) |
| C3 | 5.5 (10) | 6.6 ( 8) | 23.2 (18) | 1.4 ( 8) | 8.6 (11) | 1.6 (10) |
| C4 | 3.1 ( 9) | 15.2 (15) | 17.9 (16) | 1.4 ( 9) | 3.4 ( 9) | 9.7 (13) |
| O5 | 5.3 ( 6) | 6.7 ( 5) | 9.1 ( 6) | -0.8 ( 4) | 4.4 ( 4) | 0.9 ( 4) |
| C6 | 6.6 (11) | 5.7 ( 8) | 22.0 (18) | -0.6 ( 8) | 7.6 (11) | 1.6 (10) |
| C7 | 6.8 (10) | 8.0 ( 8) | 8.5 ( 9) | 1.7 ( 7) | 2.4 ( 7) | 4.7 ( 7) |
| N11 | 2.5 ( 5) | 3.7 ( 4) | 3.8 ( 5) | 0.7 ( 4) | 0.9 ( 4) | -0.1 ( 3) |
| C12 | 3.5 ( 6) | 5.0 ( 6) | 4.1 ( 6) | 0.3 ( 5) | 1.7 ( 5) | -0.2 ( 5) |
| C13 | 4.2 ( 7) | 5.6 ( 6) | 4.0 ( 6) | -0.1 ( 5) | 1.6 ( 5) | -1.0 ( 5) |
| C14 | 4.8 ( 8) | 5.9 ( 7) | 4.6 ( 7) | 0.0 ( 6) | 1.1 ( 5) | -1.8 ( 5) |
| C15 | 3.5 ( 7) | 4.3 ( 5) | 5.2 ( 7) | -1.1 ( 5) | 0.7 ( 5) | -0.7 ( 5) |
| C16 | 2.8 ( 6) | 3.5 ( 5) | 4.4 ( 6) | 0.4 ( 4) | 0.9 ( 4) | -0.3 ( 4) |
| N21 | 2.2 ( 4) | 3.0 ( 4) | 3.4 ( 4) | 0.3 ( 3) | 0.6 ( 3) | -0.2 ( 3) |
| C22 | 2.3 ( 6) | 3.0 ( 5) | 4.3 ( 6) | 0.0 ( 4) | 1.0 ( 4) | -0.3 ( 4) |
| C23 | 4.3 ( 7) | 5.2 ( 6) | 4.8 ( 6) | -1.6 ( 5) | 1.5 ( 5) | -0.9 ( 5) |
| C24 | 5.0 ( 8) | 5.9 ( 6) | 5.3 ( 7) | -2.7 ( 6) | 2.0 ( 5) | -1.1 ( 5) |
| C25 | 4.3 ( 7) | 6.7 ( 7) | 4.2 ( 6) | -0.6 ( 6) | 2.1 ( 5) | -0.3 ( 5) |
| C26 | 2.7 ( 6) | 4.1 ( 5) | 3.8 ( 6) | -0.3 ( 5) | 0.8 ( 4) | -0.4 ( 4) |
| N31 | 2.1 ( 5) | 4.5 ( 4) | 3.4 ( 5) | -0.8 ( 4) | -0.1 ( 3) | -0.6 ( 4) |
| C32 | 2.4 ( 6) | 4.9 ( 5) | 3.7 ( 5) | 0.2 ( 5) | -0.1 ( 4) | -0.6 ( 5) |
| C33 | 3.8 ( 7) | 7.5 ( 7) | 3.3 ( 6) | -1.3 ( 5) | 1.8 ( 5) | -1.9 ( 5) |
| C34 | 5.7 ( 9) | 11.0 (10) | 4.4 ( 7) | -2.8 ( 8) | 2.2 ( 6) | -3.8 ( 7) |
| C35 | 7.0 (10) | 9.1 ( 9) | 4.7 ( 7) | -3.7 ( 8) | 1.5 ( 6) | -3.7 ( 6) |
| C36 | 3.4 ( 7) | 6.1 ( 7) | 6.4 ( 7) | -1.4 ( 5) | 2.0 ( 5) | -1.0 ( 6) |
| P1 | 6.5 ( 3) | 9.2 ( 3) | 11.4 ( 3) | 1.70 (23) | 4.37 (24) | -0.62 (24) |
| F11 | 6.8 ( 7) | 27.7 (14) | 21.8 (12) | -1.9 ( 8) | -3.1 ( 8) | -14.5 (11) |
| F12 | 11.7 ( 9) | 11.8 ( 7) | 19.9 (10) | -0.8 ( 6) | 10.4 ( 7) | -4.1 ( 6) |
| F13 | 13.6 (10) | 13.3 ( 8) | 17.1 ( 9) | 4.9 ( 7) | 6.9 ( 7) | 1.5 ( 7) |
| F14 | 13.5 ( 9) | 14.4 ( 8) | 9.4 ( 6) | -6.1 ( 7) | 1.4 ( 6) | -1.2 ( 5) |
| F15 | 8.6 ( 6) | 9.4 ( 5) | 9.5 ( 5) | 1.8 ( 5) | 2.6 ( 4) | -2.8 ( 4) |
| F16 | 6.6 ( 6) | 22.2 (10) | 6.0 ( 5) | 5.1 ( 6) | 1.8 ( 4) | 0.0 ( 5) |
| P2 | 5.3 ( 3) | 13.1 ( 3) | 7.1 ( 3) | -1.4 ( 3) | 0.16 (20) | 1.23 (24) |
| F21 | 6.3 ( 6) | 10.2 ( 5) | 10.3 ( 6) | 1.0 ( 5) | 0.4 ( 4) | 1.8 ( 4) |
| F22 | 14.2 (10) | 21.0 (11) | 9.6 ( 7) | -5.3 ( 8) | 4.9 ( 6) | 0.2 ( 7) |
| F23 | 11.6 ( 8) | 16.4 ( 8) | 10.5 ( 7) | -6.5 ( 7) | -0.5 ( 6) | -0.9 ( 6) |
| F24 | 8.6 ( 7) | 11.5 ( 6) | 11.8 ( 6) | 1.4 ( 5) | 5.4 ( 5) | 2.2 ( 5) |
| F25 | 6.2 ( 6) | 19.0 ( 9) | 14.6 ( 8) | -1.0 ( 7) | -2.7 ( 6) | 6.2 ( 7) |
| F26 | 5.3 ( 5) | 9.9 ( 5) | 10.7 ( 6) | -0.8 ( 4) | 0.7 ( 4) | -0.9 ( 4) |
| H3a | 12.8 | | | | | |
| H3b | 12.8 | | | | | |
| H4a | 13.1 | | | | | |
| H4b | 13.1 | | | | | |
| H6a | 12.5 | | | | | |
| H6b | 12.5 | | | | | |
| H7a | 8.8 | | | | | |
| H7b | 8.8 | | | | | |
| H12 | 5.2 | | | | | |

| | |
|---|---|
| H13 | 5.6 |
| H14 | 6.1 |
| H15 | 5.4 |
| H23 | 5.8 |
| H24 | 6.4 |
| H25 | 6.1 |
| H33 | 5.9 |
| H34 | 8.0 |
| H35 | 8.0 |
| H36 | 6.3 |

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

DISANG -- The NRCVAX Distance and Angle Program
The Space Group is P 21/N Centrosymmetric
The Equivalent Positions are:
1) x y z 2) 1/2-x 1/2+y 1/2-z
The Lattice is Primitive. There are no Centering Vectors

| | | | |
|---|---|---|---|
| Os(1)-Cl(1) | 2.3193(22) | C(23)-C(24) | 1.389(14) |
| Os(1)-Cl(2) | 2.3472(23) | C(24)-C(25) | 1.393(14) |
| Os(1)-N(1) | 1.778(8) | C(25)-C(26) | 1.373(14) |
| Os(1)-N(11) | 2.086(7) | C(26)-C(32) | 1.480(12) |
| Os(1)-N(21) | 2.004(7) | N(31)-C(32) | 1.363(13) |
| Os(1)-N(31) | 2.099(7) | N(31)-C(36) | 1.340(12) |
| N(1)-N(2) | 1.234(12) | C(32)-C(33) | 1.392(12) |
| N(2)-C(3) | 1.483(16) | C(33)-C(34) | 1.358(14) |
| N(2)-C(7) | 1.487(14) | C(34)-C(35) | 1.383(18) |
| C(3)-C(4) | 1.508(22) | C(35)-C(36) | 1.364(15) |
| C(4)-O(5) | 1.357(16) | P(1)-F(11) | 1.504(9) |
| O(5)-C(6) | 1.424(18) | P(1)-F(12) | 1.610(10) |
| C(6)-C(7) | 1.470(21) | P(1)-F(13) | 1.563(10) |
| N(11)-C(12) | 1.349(12) | P(1)-F(14) | 1.658(9) |
| N(11)-C(16) | 1.361(12) | P(1)-F(15) | 1.589(8) |
| C(12)-C(13) | 1.374(13) | P(1)-F(16) | 1.556(9) |
| C(13)-C(14) | 1.369(16) | P(2)-F(21) | 1.595(9) |
| C(14)-C(15) | 1.394(15) | P(2)-F(22) | 1.582(10) |
| C(15)-C(16) | 1.376(12) | P(2)-F(23) | 1.587(9) |
| C(16)-C(22) | 1.474(13) | P(2)-F(24) | 1.626(9) |
| N(21)-C(22) | 1.342(10) | P(2)-F(25) | 1.603(9) |
| N(21)-C(26) | 1.368(11) | P(2)-F(26) | 1.599(8) |
| C(22)-C(23) | 1.379(14) | | |

| | | | |
|---|---|---|---|
| Cl(1)-Os(1)-Cl(2) | 168.16(9) | N(21)-C(26)-C(25) | 119.5(8) |
| Cl(1)-Os(1)-N(1) | 99.08(23) | N(21)-C(26)-C(32) | 112.6(8) |
| Cl(1)-Os(1)-N(11) | 87.77(20) | C(25)-C(26)-C(32) | 127.9(8) |
| Cl(1)-Os(1)-N(21) | 85.56(20) | Os(1)-N(31)-C(32) | 113.2(5) |
| Cl(1)-Os(1)-N(31) | 89.61(21) | Os(1)-N(31)-C(36) | 127.3(7) |
| Cl(2)-Os(1)-N(1) | 92.72(23) | C(32)-N(31)-C(36) | 119.5(8) |
| Cl(2)-Os(1)-N(11) | 89.27(19) | C(26)-C(32)-N(31) | 116.5(8) |
| Cl(2)-Os(1)-N(21) | 82.61(20) | C(26)-C(32)-C(33) | 123.4(9) |
| Cl(2)-Os(1)-N(31) | 88.64(21) | N(31)-C(32)-C(33) | 120.1(8) |
| N(1)-Os(1)-N(11) | 100.3(3) | C(32)-C(33)-C(34) | 119.6(10) |
| N(1)-Os(1)-N(21) | 175.0(3) | C(33)-C(34)-C(35) | 119.8(9) |
| N(1)-Os(1)-N(31) | 102.7(3) | C(34)-C(35)-C(36) | 119.1(9) |
| N(11)-Os(1)-N(21) | 77.8(3) | N(31)-C(36)-C(35) | 121.9(10) |
| N(11)-Os(1)-N(31) | 157.0(3) | F(11)-P(1)-F(12) | 90.7(7) |
| N(21)-Os(1)-N(31) | 79.2(3) | F(11)-P(1)-F(13) | 94.1(7) |
| Os(1)-N(1)-N(2) | 170.3(7) | F(11)-P(1)-F(14) | 176.1(7) |
| N(1)-N(2)-C(3) | 121.9(8) | F(11)-P(1)-F(15) | 92.9(6) |
| N(1)-N(2)-C(7) | 123.3(9) | F(11)-P(1)-F(16) | 96.0(7) |
| C(3)-N(2)-C(7) | 114.6(9) | F(12)-P(1)-F(13) | 88.4(5) |
| N(2)-C(3)-C(4) | 107.2(11) | F(12)-P(1)-F(14) | 85.8(5) |
| C(3)-C(4)-O(5) | 111.2(11) | F(12)-P(1)-F(15) | 88.6(5) |
| C(4)-O(5)-C(6) | 106.8(10) | F(12)-P(1)-F(16) | 173.2(6) |
| O(5)-C(6)-C(7) | 109.9(12) | F(13)-P(1)-F(14) | 87.4(6) |
| N(2)-C(7)-C(6) | 109.3(10) | F(13)-P(1)-F(15) | 172.4(6) |

| | | | |
|---|---|---|---|
| Os(1)-N(11)-C(12) | 126.2(6) | F(13)-P(1)-F(16) | 89.9(5) |
| Os(1)-N(11)-C(16) | 114.8(6) | F(14)-P(1)-F(15) | 85.5(5) |
| C(12)-N(11)-C(16) | 119.0(7) | F(14)-P(1)-F(16) | 87.5(5) |
| N(11)-C(12)-C(13) | 121.1(9) | F(15)-P(1)-F(16) | 92.3(5) |
| C(12)-C(13)-C(14) | 120.6(9) | F(21)-P(2)-F(22) | 89.0(5) |
| C(13)-C(14)-C(15) | 118.5(8) | F(21)-P(2)-F(23) | 179.5(5) |
| C(14)-C(15)-C(16) | 119.2(9) | F(21)-P(2)-F(24) | 90.0(5) |
| N(11)-C(16)-C(15) | 121.5(9) | F(21)-P(2)-F(25) | 88.9(5) |
| N(11)-C(16)-C(22) | 114.9(7) | F(21)-P(2)-F(26) | 90.0(4) |
| C(15)-C(16)-C(22) | 123.6(9) | F(22)-P(2)-F(23) | 90.8(5) |
| Os(1)-N(21)-C(22) | 119.5(6) | F(22)-P(2)-F(24) | 178.4(6) |
| Os(1)-N(21)-C(26) | 118.5(6) | F(22)-P(2)-F(25) | 90.5(6) |
| C(22)-N(21)-C(26) | 122.0(8) | F(22)-P(2)-F(26) | 92.0(6) |
| C(16)-C(22)-N(21) | 112.9(8) | F(23)-P(2)-F(24) | 90.1(5) |
| C(16)-C(22)-C(23) | 126.8(8) | F(23)-P(2)-F(25) | 90.6(5) |
| N(21)-C(22)-C(23) | 120.3(8) | F(23)-P(2)-F(26) | 90.6(5) |
| C(22)-C(23)-C(24) | 118.7(8) | F(24)-P(2)-F(25) | 88.2(5) |
| C(23)-C(24)-C(25) | 120.4(9) | F(24)-P(2)-F(26) | 89.3(4) |
| C(24)-C(25)-C(26) | 119.1(9) | F(25)-P(2)-F(26) | 177.2(6) |

Torsion angles

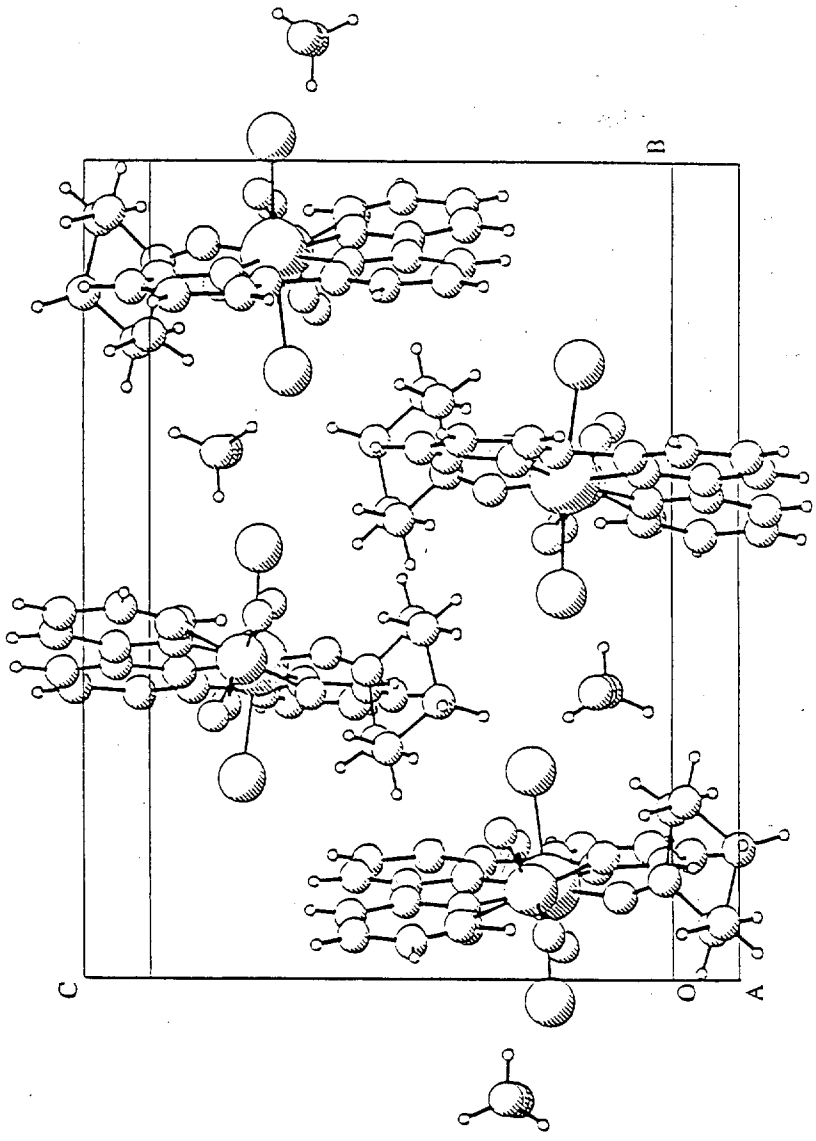
| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Cl1 | Os1 | N1 | N2 | 145.8(10) | Cl2 | Os1 | N1 | N2 | -33.3( 7) |
| N11 | Os1 | N1 | N2 | 56.5( 8) | N21 | Os1 | N1 | N2 | -11.4( 7) |
| N31 | Os1 | N1 | N2 | -122.5(10) | Cl1 | Os1 | N11 | C12 | -92.1( 9) |
| Cl1 | Os1 | N11 | C16 | 86.8( 8) | Cl2 | Os1 | N11 | C12 | 99.4( 9) |
| Cl2 | Os1 | N11 | C16 | -81.7( 8) | N1 | Os1 | N11 | C12 | 6.8( 8) |
| N1 | Os1 | N11 | C16 | -174.4(11) | N21 | Os1 | N11 | C12 | -178.0(11) |
| N21 | Os1 | N11 | C16 | 0.9( 7) | N31 | Os1 | N11 | C12 | -175.8(11) |
| N31 | Os1 | N11 | C16 | 3.1( 7) | Cl1 | Os1 | N21 | C22 | -88.9( 8) |
| Cl1 | Os1 | N21 | C26 | 89.2( 8) | Cl2 | Os1 | N21 | C22 | 90.6( 8) |
| Cl2 | Os1 | N21 | C26 | -91.3( 8) | N1 | Os1 | N21 | C22 | 68.6( 8) |
| N1 | Os1 | N21 | C26 | -113.3(10) | N11 | Os1 | N21 | C22 | -0.2( 7) |
| N11 | Os1 | N21 | C26 | 177.8(10) | N31 | Os1 | N21 | C22 | -179.3(10) |
| N31 | Os1 | N21 | C26 | -1.3( 7) | Cl1 | Os1 | N31 | C32 | -85.6( 8) |
| Cl1 | Os1 | N31 | C36 | 93.8( 9) | Cl2 | Os1 | N31 | C32 | 82.7( 8) |
| Cl2 | Os1 | N31 | C36 | -97.9( 9) | N1 | Os1 | N31 | C32 | 175.2(11) |
| N1 | Os1 | N31 | C36 | -5.4( 8) | N11 | Os1 | N31 | C32 | -2.2( 7) |
| N11 | Os1 | N31 | C36 | 177.2(11) | N21 | Os1 | N31 | C32 | 0.0( 7) |
| N21 | Os1 | N31 | C36 | 179.3(11) | Os1 | N1 | N2 | C3 | 11.2(10) |
| Os1 | N1 | N2 | C7 | -164.5(14) | N1 | N2 | C3 | C4 | 137.9(25) |
| C7 | N2 | C3 | C4 | -46.1(15) | N1 | N2 | C7 | C6 | -137.1(22) |
| C3 | N2 | C7 | C6 | 47.0(16) | N2 | C3 | C4 | O5 | 58.5(16) |
| C3 | C4 | O5 | C6 | -70.5(19) | C4 | O5 | C6 | C7 | 69.3(19) |
| O5 | C6 | C7 | N2 | -56.3(14) | Os1 | N11 | C12 | C13 | 179.7(15) |
| C16 | N11 | C12 | C13 | 0.8( 9) | Os1 | N11 | C16 | C15 | 179.8(14) |
| Os1 | N11 | C16 | C22 | -1.3( 6) | C12 | N11 | C16 | C15 | -1.2( 9) |
| C12 | N11 | C16 | C22 | 177.6(17) | N11 | C12 | C13 | C14 | 0.4( 9) |
| C12 | C13 | C14 | C15 | -1.2( 9) | C13 | C14 | C15 | C16 | 0.9( 9) |
| C14 | C15 | C16 | N11 | 0.4( 8) | C14 | C15 | C16 | C22 | -178.4(19) |
| N11 | C16 | C22 | N21 | 1.1( 7) | N11 | C16 | C22 | C23 | -179.5(18) |
| C15 | C16 | C22 | N21 | 180.0(18) | C15 | C16 | C22 | C23 | -0.7( 9) |
| Os1 | N21 | C22 | C16 | -0.4( 6) | Os1 | N21 | C22 | C23 | -179.8(14) |
| C26 | N21 | C22 | C16 | -178.4(16) | C26 | N21 | C22 | C23 | 2.2( 9) |
| Os1 | N21 | C26 | C25 | -178.8(14) | Os1 | N21 | C26 | C32 | 2.2( 6) |
| C22 | N21 | C26 | C25 | -0.8( 9) | C22 | N21 | C26 | C32 | -179.8(17) |
| C16 | C22 | C23 | C24 | 178.2(19) | N21 | C22 | C23 | C24 | -2.5( 8) |
| C22 | C23 | C24 | C25 | 1.4( 9) | C23 | C24 | C25 | C26 | -0.1( 9) |
| C24 | C25 | C26 | N21 | -0.2( 8) | C24 | C25 | C26 | C32 | 178.5(19) |
| N21 | C26 | C32 | N31 | -2.2( 7) | N21 | C26 | C32 | C33 | 178.5(19) |
| C25 | C26 | C32 | N31 | 179.0(19) | C25 | C26 | C32 | C33 | -0.3( 9) |
| Os1 | N31 | C32 | C26 | 1.2( 6) | Os1 | N31 | C32 | C33 | -179.5(14) |
| C36 | N31 | C32 | C26 | -178.2(18) | C36 | N31 | C32 | C33 | 1.1(10) |
| Os1 | N31 | C36 | C35 | -179.6(16) | C32 | N31 | C36 | C35 | -0.3(10) |
| C26 | C32 | C33 | C34 | 178.7(20) | N31 | C32 | C33 | C34 | -0.6( 9) |
| C32 | C33 | C34 | C35 | -0.8(10) | C33 | C34 | C35 | C36 | 1.6(10) |
| C34 | C35 | C36 | N31 | -1.1( 9) | | | | | |

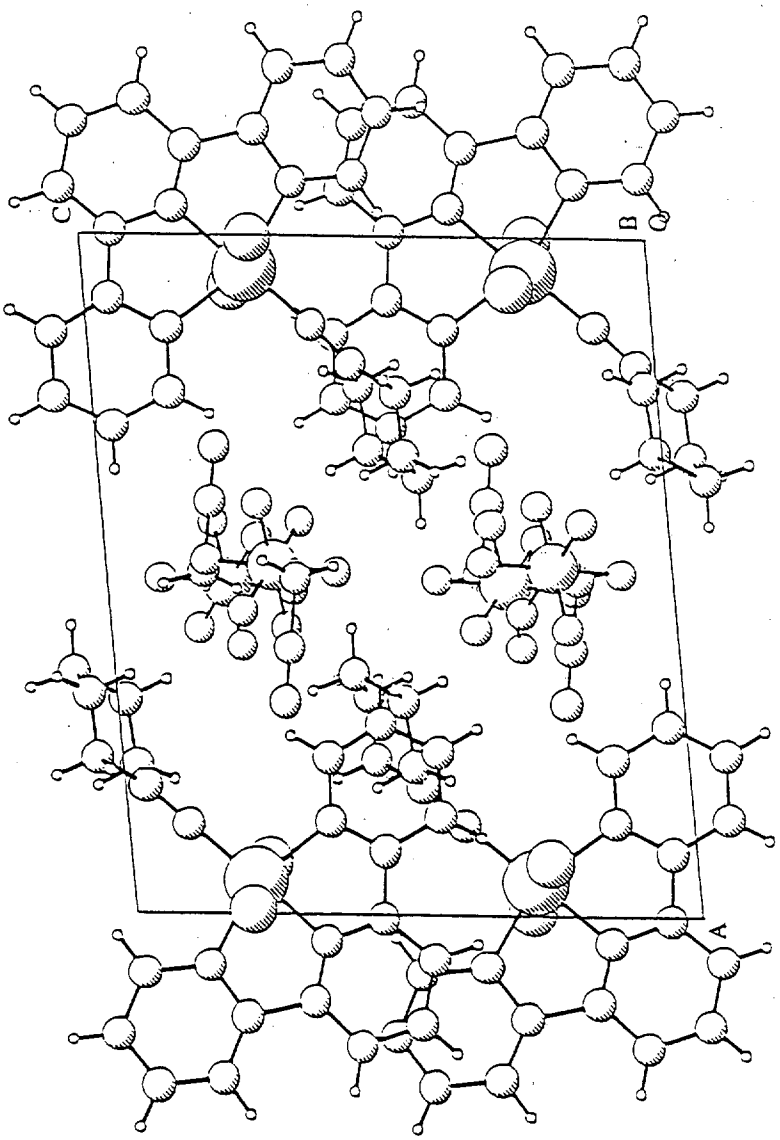
Space Group and Cell Dimensions  Monoclinic,  P 21/c
a 14.1724(17)  b 16.3483(20)  c 11.8853(14)
beta 95.436(2)
Volume 2741.4(6)A**3
Empirical formula : Os Cl2 P C22 H24 N6 F6
Cell dimensions were obtained from 5685 reflections with 2Theta angle in the range 3.00 - 50.00 degrees.
Crystal dimensions : 0.20 X 0.20 X 0.05 mm
FW = 778.53  Z = 4  F(000) = 1507.13
Dcalc 1.886Mg.m-3, mu 4.97mm-1, lambda 0.71073A, 2Theta(max) 50.0
The intensity data were collected on a Bruker SMART diffractometer, using the omega scan mode.
The h,k,l ranges used during structure solution and refinement are :--
Hmin,max -16 16; Kmin,max 0 19; Lmin,max 0 14
No. of reflections measured 15665
No. of unique reflections 4844
No. of reflections with Inet > 2.5sigma(Inet) 3570
Merging R-value on intensities 0.048
Correction was made for absorption using SADABS

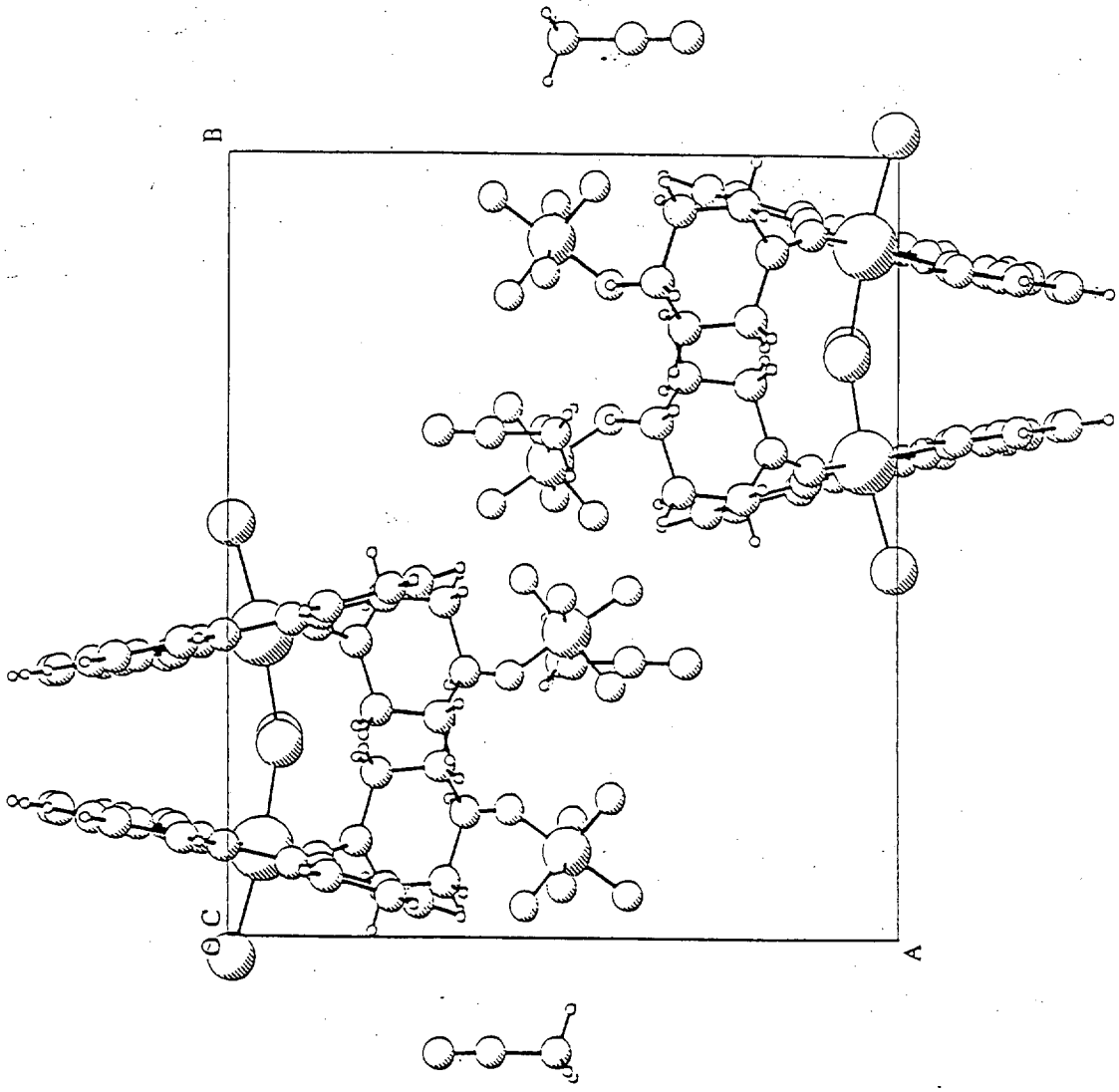
The last least squares cycle was calculated with
62 atoms, 344 parameters and 3570 out of 4844 reflections.
Weights based on counting-statistics were used.
The weight modifier K in KFo**2 is 0.000250
The residuals are as follows :--
For significant reflections, RF 0.048, Rw 0.059 GoF 2.09
For all reflections, RF 0.060, Rw 0.060.
where RF = Sum(Fo-Fc)/Sum(Fo),
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was 0.001.
In the last D-map, the deepest hole was -3.080e/A**3,
and the highest peak 3.100e/A**3.
Secondary ext. coeff. 0.0112microns sigma 0.0270

The following references are relevant to the NRCVAX System.

1. Full System Reference :
Gabe, E.J., Le Page, Y., Charland, J.-P., Lee, F.L. and White, P.S. (1989) J. Appl. Cryst., 22, 384-387.
2. Scattering Factors from Int. Tab. Vol. 4 :
International Tables for X-ray Crystallography, Vol. IV, (1974) Kynoch Press, Birmingham, England.
The following references may also be relevant.
3. ORTEP Plotting :
Johnson, C.K., (1976) ORTEP - A Fortran Thermal Ellipsoid Plot Program, Technical Report ORNL-5138, Oak Ridge
4. Pluto Plotting :
S. Motherwell, University Chemical Laboratory, Cambridge, 1978
5. Missing Symmetry Treatment by MISSYM :
Le Page, Y., (1988) J. Appl. Cryst., 21, 983-984.
6. Grouping of Equivalent Reflections in DATRD2 :
Le Page, Y. and Gabe, E.J., (1979) J. Appl. Cryst., 12, 464-466.
7. Extinction Treatment :
Larson, A.C., (1970) p.293, Crystallographic Computing, Munksgaard, Copenhagen.







21-Sep-1998

Table . Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

| | x | y | z | Biso |
|---|---|---|---|---|
| Os1 | 0.05021( 3) | 0.38753( 3) | 0.71446( 4) | 2.108(20) |
| Cl1 | 0.00531(23) | 0.52736(17) | 0.70451(23) | 2.68 (12) |
| Cl2 | 0.07681(22) | 0.24507(16) | 0.74195(25) | 2.83 (13) |
| N1 | 0.1316 ( 8) | 0.3994 ( 6) | 0.6021 ( 8) | 3.2 ( 5) |
| N2 | 0.1884 (10) | 0.3778 ( 7) | 0.5342 (10) | 4.9 ( 6) |
| C3 | 0.2187 (17) | 0.2903 (10) | 0.5229 (19) | 8.8 (13) |
| C4 | 0.3146 (14) | 0.2817 (11) | 0.5134 (20) | 8.5 (12) |
| C5 | 0.3539 (13) | 0.3398 (11) | 0.4269 (17) | 7.6 (11) |
| C6 | 0.3222 (18) | 0.4294 (13) | 0.4506 (22) | 11.2 (16) |
| C7 | 0.2286 (13) | 0.4368 (10) | 0.4554 (16) | 7.0 (10) |
| N11 | -0.0774 ( 7) | 0.3626 ( 5) | 0.6178 ( 7) | 2.1 ( 4) |
| C12 | -0.1532 ( 9) | 0.3517 ( 7) | 0.6774 (10) | 2.9 ( 6) |
| C13 | -0.2439 ( 9) | 0.3395 ( 8) | 0.6236 (11) | 3.2 ( 6) |
| C14 | -0.2545 (10) | 0.3379 ( 8) | 0.5081 (12) | 3.6 ( 7) |
| C15 | -0.1802 (12) | 0.3476 ( 8) | 0.4479 (11) | 3.9 ( 7) |
| C16 | -0.0885 (10) | 0.3584 ( 7) | 0.5032 (10) | 3.0 ( 6) |
| N21 | -0.0402 ( 7) | 0.3759 ( 5) | 0.8343 ( 8) | 2.5 ( 4) |
| C22 | -0.1298 ( 9) | 0.3577 ( 6) | 0.8029 (11) | 2.5 ( 5) |
| C23 | -0.1958 ( 9) | 0.3499 ( 7) | 0.8825 (11) | 2.9 ( 6) |
| C24 | -0.1626 ( 9) | 0.3564 ( 7) | 0.9958 (10) | 2.8 ( 6) |
| C25 | -0.0663 ( 9) | 0.3752 ( 6) | 1.0277 ( 9) | 2.4 ( 5) |
| C26 | -0.0061 ( 8) | 0.3853 ( 6) | 0.9435 ( 8) | 1.9 ( 4) |
| N31 | 0.1372 ( 7) | 0.4138 ( 5) | 0.8606 ( 8) | 2.6 ( 4) |
| C32 | 0.2316 ( 8) | 0.4367 ( 7) | 0.8663 (10) | 2.6 ( 6) |
| C33 | 0.2819 ( 8) | 0.4546 ( 7) | 0.9681 (11) | 3.0 ( 6) |
| C34 | 0.2399 ( 9) | 0.4470 ( 7) | 1.0666 (11) | 3.1 ( 6) |
| C35 | 0.1451 ( 9) | 0.4229 ( 7) | 1.0618 (10) | 2.7 ( 5) |
| C36 | 0.0944 ( 8) | 0.4064 ( 6) | 0.9572 ( 9) | 2.2 ( 5) |
| P1 | 0.51269(24) | 0.39096(23) | 0.7915 ( 3) | 3.46 (16) |
| F11 | 0.4464 ( 6) | 0.4592 ( 5) | 0.7323 ( 9) | 6.6 ( 5) |
| F12 | 0.5054 ( 6) | 0.4350 ( 7) | 0.9085 ( 7) | 6.9 ( 5) |
| F13 | 0.5217 ( 6) | 0.3500 ( 6) | 0.6729 ( 7) | 6.0 ( 5) |
| F14 | 0.5789 ( 6) | 0.3214 ( 5) | 0.8480 ( 9) | 6.5 ( 5) |
| F15 | 0.4230 ( 5) | 0.3359 ( 5) | 0.8085 ( 8) | 5.7 ( 5) |
| F16 | 0.6046 ( 6) | 0.4453 ( 5) | 0.7734 ( 7) | 5.0 ( 4) |
| C42 | 0.3924 (11) | 0.6463 ( 8) | 0.8110 (11) | 3.7 ( 7) |
| N43 | 0.3124 (10) | 0.6482 ( 9) | 0.7950 (10) | 5.3 ( 7) |
| C41 | 0.4955 (11) | 0.6463 ( 9) | 0.8325 (15) | 5.5 ( 9) |
| H3a | 0.188 | 0.270 | 0.453 | 10.2 |
| H3b | 0.199 | 0.259 | 0.584 | 10.2 |
| H4a | 0.344 | 0.298 | 0.585 | 9.6 |
| H4b | 0.331 | 0.226 | 0.498 | 9.6 |
| H5a | 0.423 | 0.335 | 0.428 | 11.8 |
| H5b | 0.329 | 0.323 | 0.348 | 11.8 |
| H6a | 0.345 | 0.466 | 0.395 | 12.5 |
| H6b | 0.351 | 0.443 | 0.524 | 12.5 |
| H7a | 0.211 | 0.491 | 0.475 | 8.1 |
| H7b | 0.201 | 0.424 | 0.380 | 8.1 |
| H13 | -0.297 | 0.332 | 0.667 | 4.0 |
| H14 | -0.317 | 0.330 | 0.470 | 4.3 |
| H15 | -0.189 | 0.347 | 0.367 | 4.6 |

| | | | | |
|---|---|---|---|---|
| H16 | -0.034 | 0.362 | 0.461 | 3.7 |
| H23 | -0.261 | 0.338 | 0.861 | 3.7 |
| H24 | -0.206 | 0.349 | 1.052 | 3.7 |
| H25 | -0.043 | 0.381 | 1.106 | 3.2 |
| H32 | 0.263 | 0.439 | 0.798 | 3.4 |
| H33 | 0.346 | 0.473 | 0.970 | 3.8 |
| H34 | 0.275 | 0.458 | 1.138 | 3.8 |
| H35 | 0.114 | 0.417 | 1.129 | 3.5 |
| H41a | 0.519 | 0.591 | 0.832 | 6.3 |
| H41b | 0.522 | 0.677 | 0.775 | 6.3 |
| H41c | 0.514 | 0.670 | 0.905 | 6.3 |

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

| | u11(U) | u22 | u33 | u12 | u13 | u23 |
|---|---|---|---|---|---|---|
| Os1 | 1.82( 3) | 2.595(24) | 3.67( 3) | -0.023(24) | 0.671(17) | 0.013(24) |
| Cl1 | 3.33(19) | 2.73 (15) | 4.23(16) | 0.32 (13) | 0.89 (14) | 0.24 (12) |
| Cl2 | 3.07(20) | 2.63 (14) | 5.07(18) | 0.33 (13) | 0.36 (14) | -0.03 (13) |
| N1 | 5.0 ( 8) | 4.0 ( 6) | 3.5 ( 5) | 0.4 ( 5) | 2.5 ( 5) | -0.7 ( 5) |
| N2 | 7.3 (10) | 4.6 ( 7) | 7.2 ( 8) | 2.1 ( 7) | 3.7 ( 7) | 1.2 ( 6) |
| C3 | 14.4 (21) | 5.1 (10) | 15.9 (19) | 4.0 (12) | 10.6 (17) | 3.7 (12) |
| C4 | 7.5 (15) | 6.2 (11) | 19.6 (23) | 4.4 (11) | 6.7 (15) | 3.3 (13) |
| C5 | 8.6 (16) | 7.2 (11) | 14.5 (17) | 4.0 (11) | 8.4 (13) | 3.8 (12) |
| C6 | 14.5 (23) | 9.9 (15) | 20. ( 3) | 5.4 (16) | 12.8 (20) | 8.5 (17) |
| C7 | 8.0 (15) | 6.2 (11) | 13.6 (16) | 3.2 (10) | 8.2 (13) | 5.3 (11) |
| N11 | 1.6 ( 6) | 3.4 ( 6) | 3.0 ( 5) | -0.4 ( 4) | -0.8 ( 4) | 0.6 ( 4) |
| C12 | 3.0 ( 8) | 3.4 ( 7) | 4.7 ( 7) | -0.4 ( 6) | 0.6 ( 6) | 0.2 ( 6) |
| C13 | 2.5 ( 8) | 3.7 ( 7) | 6.0 ( 9) | -0.5 ( 6) | 0.0 ( 6) | -0.7 ( 6) |
| C14 | 2.9 ( 9) | 3.9 ( 7) | 6.8 (10) | -0.2 ( 7) | -1.2 ( 7) | -0.1 ( 7) |
| C15 | 5.9 (11) | 3.1 ( 7) | 5.4 ( 8) | -0.3 ( 7) | -1.6 ( 8) | 0.4 ( 6) |
| C16 | 3.2 ( 9) | 3.1 ( 7) | 4.9 ( 8) | -0.2 ( 6) | 0.1 ( 6) | 0.4 ( 5) |
| N21 | 3.5 ( 7) | 2.3 ( 5) | 3.9 ( 5) | -0.4 ( 5) | 0.7 ( 5) | 1.2 ( 4) |
| C22 | 1.2 ( 7) | 2.1 ( 6) | 6.2 ( 8) | -0.8 ( 5) | -0.4 ( 6) | 0.5 ( 5) |
| C23 | 1.2 ( 7) | 4.0 ( 7) | 5.7 ( 8) | -0.4 ( 6) | 0.6 ( 6) | 0.1 ( 6) |
| C24 | 3.0 ( 8) | 3.6 ( 7) | 4.4 ( 7) | -0.2 ( 6) | 1.9 ( 6) | 0.2 ( 5) |
| C25 | 3.2 ( 8) | 2.9 ( 6) | 3.2 ( 6) | 0.4 ( 6) | 0.5 ( 5) | 0.7 ( 5) |
| C26 | 2.0 ( 6) | 1.9 ( 5) | 3.4 ( 6) | 0.2 ( 5) | 0.3 ( 5) | 0.3 ( 5) |
| N31 | 3.9 ( 7) | 2.7 ( 5) | 3.2 ( 5) | -0.6 ( 5) | 0.0 ( 5) | -0.2 ( 4) |
| C32 | 1.1 ( 7) | 3.0 ( 6) | 5.8 ( 8) | 0.2 ( 5) | 0.6 ( 6) | -0.5 ( 6) |
| C33 | 1.2 ( 7) | 4.0 ( 7) | 6.3 ( 9) | -0.9 ( 6) | 0.2 ( 6) | -0.2 ( 6) |
| C34 | 2.2 ( 8) | 3.8 ( 7) | 5.3 ( 8) | 0.3 ( 6) | -1.3 ( 6) | 0.0 ( 6) |
| C35 | 3.0 ( 8) | 3.2 ( 6) | 4.0 ( 7) | 0.6 ( 6) | 0.8 ( 6) | 0.6 ( 5) |
| C36 | 2.8 ( 8) | 2.4 ( 6) | 3.1 ( 6) | 0.1 ( 5) | 0.4 ( 5) | 0.1 ( 4) |
| P1 | 2.24(20) | 4.55 (20) | 6.44(22) | -0.52 (18) | 0.89 (16) | -1.12 (18) |
| F11 | 4.6 ( 7) | 6.7 ( 6) | 13.1 ( 8) | 0.7 ( 5) | -1.8 ( 6) | 0.0 ( 5) |
| F12 | 4.7 ( 6) | 13.3 ( 8) | 8.5 ( 7) | -0.8 ( 6) | 1.9 ( 5) | -4.8 ( 6) |
| F13 | 5.4 ( 6) | 9.0 ( 7) | 8.7 ( 6) | -1.5 ( 5) | 1.9 ( 5) | -3.8 ( 5) |
| F14 | 2.7 ( 6) | 6.7 ( 6) | 15.0 ( 9) | 0.7 ( 4) | 0.2 ( 5) | 3.2 ( 6) |
| F15 | 2.1 ( 5) | 7.3 ( 6) | 12.4 ( 8) | -1.9 ( 4) | 1.6 ( 5) | -0.3 ( 5) |
| F16 | 3.8 ( 6) | 5.9 ( 5) | 9.6 ( 6) | -2.2 ( 4) | 2.1 ( 5) | -1.2 ( 4) |
| C42 | 3.6 (10) | 5.0 ( 8) | 5.5 ( 9) | -0.1 ( 7) | 0.3 ( 7) | 0.8 ( 7) |
| N43 | 2.8 ( 8) | 10.8 (11) | 6.5 ( 8) | 0.0 ( 8) | 0.5 ( 6) | 0.0 ( 7) |
| C41 | 3.5 (11) | 5.9 (10) | 11.2 (13) | -0.3 ( 8) | 0.0 ( 9) | 0.8 ( 9) |
| H3a | 12.9 | | | | | |
| H3b | 12.9 | | | | | |
| H4a | 12.1 | | | | | |
| H4b | 12.1 | | | | | |
| H5a | 14.9 | | | | | |
| H5b | 14.9 | | | | | |
| H6a | 15.9 | | | | | |
| H6b | 15.9 | | | | | |
| H7a | 10.3 | | | | | |
| H7b | 10.3 | | | | | |
| H13 | 5.1 | | | | | |
| H14 | 5.5 | | | | | |
| H15 | 5.8 | | | | | |

| | |
|---|---|
| H16 | 4.7 |
| H23 | 4.6 |
| H24 | 4.7 |
| H25 | 4.1 |
| H32 | 4.3 |
| H33 | 4.8 |
| H34 | 4.8 |
| H35 | 4.4 |
| H41a | 7.9 |
| H41b | 7.9 |
| H41c | 7.9 |

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

DISANG -- The NRCVAX Distance and Angle Program
The Space Group is P 21/C Centrosymmetric
The Equivalent Positions are:
1) x y z 2) -x 1/2+y 1/2-z
The Lattice is Primitive. There are no Centering Vectors

| | | | |
|---|---|---|---|
| Os(1)-Cl(1) | 2.373(3) | N(21)-C(26) | 1.350(14) |
| Os(1)-Cl(2) | 2.377(3) | C(22)-C(23) | 1.398(18) |
| Os(1)-N(1) | 1.855(9) | C(23)-C(24) | 1.388(17) |
| Os(1)-N(11) | 2.089(9) | C(24)-C(25) | 1.415(18) |
| Os(1)-N(21) | 2.014(10) | C(25)-C(26) | 1.385(15) |
| Os(1)-N(31) | 2.078(9) | C(26)-C(36) | 1.459(16) |
| N(1)-N(2) | 1.243(15) | N(31)-C(32) | 1.385(16) |
| N(2)-C(3) | 1.504(20) | N(31)-C(36) | 1.353(15) |
| N(2)-C(7) | 1.495(18) | C(32)-C(33) | 1.376(17) |
| C(3)-C(4) | 1.38(3) | C(33)-C(34) | 1.367(19) |
| C(4)-C(5) | 1.54(3) | C(34)-C(35) | 1.395(18) |
| C(5)-C(6) | 1.57(3) | C(35)-C(36) | 1.402(16) |
| C(6)-C(7) | 1.34(3) | P(1)-F(11) | 1.580(9) |
| N(11)-C(12) | 1.354(16) | P(1)-F(12) | 1.579(9) |
| N(11)-C(16) | 1.357(15) | P(1)-F(13) | 1.576(9) |
| C(12)-C(13) | 1.395(18) | P(1)-F(14) | 1.583(9) |
| C(12)-C(22) | 1.499(17) | P(1)-F(15) | 1.585(8) |
| C(13)-C(14) | 1.367(19) | P(1)-F(16) | 1.607(8) |
| C(14)-C(15) | 1.337(23) | C(42)-N(43) | 1.132(21) |
| C(15)-C(16) | 1.411(20) | C(42)-C(41) | 1.459(23) |
| N(21)-C(22) | 1.322(16) | | |

| | | | |
|---|---|---|---|
| Cl(1)-Os(1)-Cl(2) | 171.54(11) | C(22)-N(21)-C(26) | 123.0(10) |
| Cl(1)-Os(1)-N(1) | 92.6(3) | C(12)-C(22)-N(21) | 114.3(11) |
| Cl(1)-Os(1)-N(11) | 86.92(25) | C(12)-C(22)-C(23) | 124.5(11) |
| Cl(1)-Os(1)-N(21) | 86.6(3) | N(21)-C(22)-C(23) | 121.0(11) |
| Cl(1)-Os(1)-N(31) | 88.7(3) | C(22)-C(23)-C(24) | 117.5(11) |
| Cl(2)-Os(1)-N(1) | 95.7(3) | C(23)-C(24)-C(25) | 120.4(11) |
| Cl(2)-Os(1)-N(11) | 90.14(24) | C(24)-C(25)-C(26) | 118.5(10) |
| Cl(2)-Os(1)-N(21) | 85.0(3) | N(21)-C(26)-C(25) | 119.4(10) |
| Cl(2)-Os(1)-N(31) | 90.8(3) | N(21)-C(26)-C(36) | 113.0(9) |
| N(1)-Os(1)-N(11) | 100.9(4) | C(25)-C(26)-C(36) | 127.6(10) |
| N(1)-Os(1)-N(21) | 178.8(4) | Os(1)-N(31)-C(32) | 126.2(8) |
| N(1)-Os(1)-N(31) | 102.7(4) | Os(1)-N(31)-C(36) | 114.4(8) |
| N(11)-Os(1)-N(21) | 78.2(4) | C(32)-N(31)-C(36) | 119.4(9) |
| N(11)-Os(1)-N(31) | 156.1(4) | N(31)-C(32)-C(33) | 121.2(11) |
| N(21)-Os(1)-N(31) | 78.2(4) | C(32)-C(33)-C(34) | 120.1(11) |
| Os(1)-N(1)-N(2) | 157.2(9) | C(33)-C(34)-C(35) | 119.1(11) |
| N(1)-N(2)-C(3) | 122.4(12) | C(34)-C(35)-C(36) | 120.1(11) |
| N(1)-N(2)-C(7) | 122.2(11) | C(26)-C(36)-N(31) | 116.0(9) |
| C(3)-N(2)-C(7) | 115.4(12) | C(26)-C(36)-C(35) | 123.8(10) |
| N(2)-C(3)-C(4) | 113.3(17) | N(31)-C(36)-C(35) | 120.1(11) |
| C(3)-C(4)-C(5) | 114.3(16) | F(11)-P(1)-F(12) | 89.1(6) |
| C(4)-C(5)-C(6) | 109.2(14) | F(11)-P(1)-F(13) | 89.9(6) |
| C(5)-C(6)-C(7) | 113.2(21) | F(11)-P(1)-F(14) | 178.7(6) |
| N(2)-C(7)-C(6) | 114.0(15) | F(11)-P(1)-F(15) | 90.4(5) |
| Os(1)-N(11)-C(12) | 115.2(7) | F(11)-P(1)-F(16) | 90.3(5) |

| | | | |
|---|---|---|---|
| Os(1)-N(11)-C(16) | 125.0(8) | F(12)-P(1)-F(13) | 177.9(6) |
| C(12)-N(11)-C(16) | 119.8(10) | F(12)-P(1)-F(14) | 92.3(6) |
| N(11)-C(12)-C(13) | 121.4(11) | F(12)-P(1)-F(15) | 91.5(5) |
| N(11)-C(12)-C(22) | 113.6(11) | F(12)-P(1)-F(16) | 89.3(5) |
| C(13)-C(12)-C(22) | 125.0(12) | F(13)-P(1)-F(14) | 88.8(6) |
| C(12)-C(13)-C(14) | 118.2(12) | F(13)-P(1)-F(15) | 90.4(5) |
| C(13)-C(14)-C(15) | 121.2(12) | F(13)-P(1)-F(16) | 88.9(5) |
| C(14)-C(15)-C(16) | 120.1(12) | F(14)-P(1)-F(15) | 89.3(5) |
| N(11)-C(16)-C(15) | 119.2(12) | F(14)-P(1)-F(16) | 89.9(5) |
| Os(1)-N(21)-C(22) | 118.6(8) | F(15)-P(1)-F(16) | 178.9(5) |
| Os(1)-N(21)-C(26) | 118.4(8) | N(43)-C(42)-C(41) | 178.5(16) |

Torsion angles

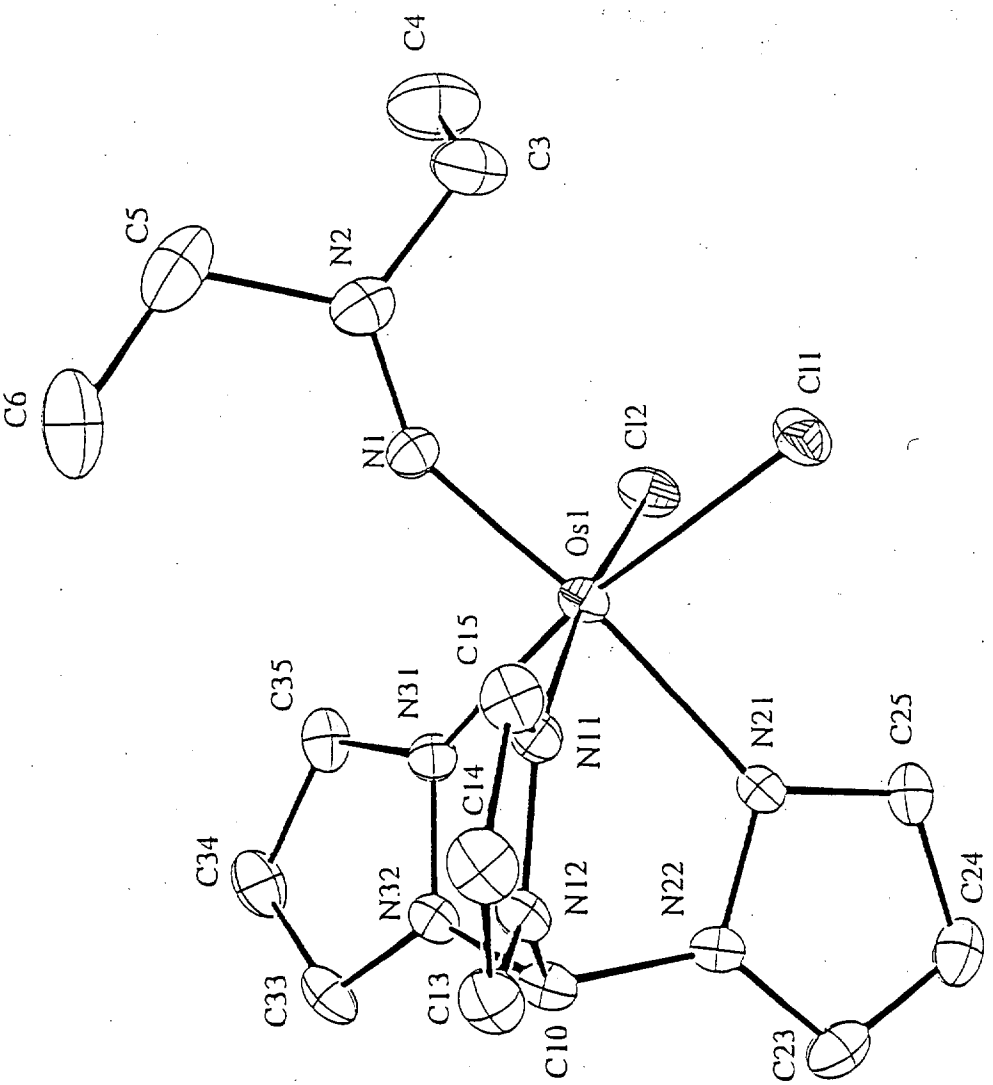
| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Cl1 | Os1 | N1 | N2 | -176.4(15) | Cl2 | Os1 | N1 | N2 | 2.2(10) |
| N11 | Os1 | N1 | N2 | -89.1(14) | N21 | Os1 | N1 | N2 | -127.2(15) |
| N31 | Os1 | N1 | N2 | 94.3(14) | Cl1 | Os1 | N11 | C12 | -87.1(11) |
| Cl1 | Os1 | N11 | C16 | 91.7(11) | Cl2 | Os1 | N11 | C12 | 85.0(11) |
| Cl2 | Os1 | N11 | C16 | -96.2(12) | N1 | Os1 | N11 | C12 | -179.1(15) |
| N1 | Os1 | N11 | C16 | -0.3(10) | N21 | Os1 | N11 | C12 | 0.1(10) |
| N21 | Os1 | N11 | C16 | 178.9(14) | N31 | Os1 | N11 | C12 | -7.3(10) |
| N31 | Os1 | N11 | C16 | 171.5(14) | Cl1 | Os1 | N21 | C22 | 89.0(12) |
| Cl1 | Os1 | N21 | C26 | -92.4(11) | Cl2 | Os1 | N21 | C22 | -89.7(12) |
| Cl2 | Os1 | N21 | C26 | 88.9(11) | N1 | Os1 | N21 | C22 | 39.8(11) |
| N1 | Os1 | N21 | C26 | -141.6(14) | N11 | Os1 | N21 | C22 | 1.5(10) |
| N11 | Os1 | N21 | C26 | -179.9(14) | N31 | Os1 | N21 | C22 | 178.4(15) |
| N31 | Os1 | N21 | C26 | -3.0( 9) | Cl1 | Os1 | N31 | C32 | -90.7(11) |
| Cl1 | Os1 | N31 | C36 | 89.9(11) | Cl2 | Os1 | N31 | C32 | 97.8(11) |
| Cl2 | Os1 | N31 | C36 | -81.6(11) | N1 | Os1 | N31 | C32 | 1.7(10) |
| N1 | Os1 | N31 | C36 | -177.7(15) | N11 | Os1 | N31 | C32 | -170.0(14) |
| N11 | Os1 | N31 | C36 | 10.5( 9) | N21 | Os1 | N31 | C32 | -177.5(14) |
| N21 | Os1 | N31 | C36 | 3.1( 9) | Os1 | N1 | N2 | C3 | 0.7(14) |
| Os1 | N1 | N2 | C7 | 178.5(22) | N1 | N2 | C3 | C4 | -138. ( 4) |
| C7 | N2 | C3 | C4 | 44.4(22) | N1 | N2 | C7 | C6 | 134. ( 4) |
| C3 | N2 | C7 | C6 | -48. ( 3) | N2 | C3 | C4 | C5 | -47.5(21) |
| C3 | C4 | C5 | C6 | 51. ( 3) | C4 | C5 | C6 | C7 | -53. ( 3) |
| C5 | C6 | C7 | N2 | 51.8(22) | Os1 | N11 | C12 | C13 | 176.1(20) |
| Os1 | N11 | C12 | C22 | -1.4( 8) | C16 | N11 | C12 | C13 | -2.8(12) |
| C16 | N11 | C12 | C22 | 179.7(24) | Os1 | N11 | C16 | C15 | -174.9(20) |
| C12 | N11 | C16 | C15 | 3.9(13) | N11 | C12 | C13 | C14 | 0.8(12) |
| C22 | C12 | C13 | C14 | 178. ( 3) | N11 | C12 | C22 | N21 | 2.6( 9) |
| N11 | C12 | C22 | C23 | 179. ( 3) | C13 | C12 | C22 | N21 | -175. ( 3) |
| C13 | C12 | C22 | C23 | 1.6(12) | C12 | C13 | C14 | C15 | 0.1(13) |
| C13 | C14 | C15 | C16 | 1.1(12) | C14 | C15 | C16 | N11 | -3.0(12) |
| Os1 | N21 | C22 | C12 | -2.6( 8) | Os1 | N21 | C22 | C23 | -179.2(19) |
| C26 | N21 | C22 | C12 | 178.9(23) | C26 | N21 | C22 | C23 | 2.3(11) |
| Os1 | N21 | C26 | C25 | -178.1(18) | Os1 | N21 | C26 | C36 | 2.3( 8) |
| C22 | N21 | C26 | C25 | 0.4(12) | C22 | N21 | C26 | C36 | -179.1(22) |
| C12 | C22 | C23 | C24 | 180. ( 3) | N21 | C22 | C23 | C24 | -4.2(11) |
| C22 | C23 | C24 | C25 | 3.7(11) | C23 | C24 | C25 | C26 | -1.2(11) |
| C24 | C25 | C26 | N21 | -0.9(11) | C24 | C25 | C26 | C36 | 178.5(23) |
| N21 | C26 | C36 | N31 | 0.5( 9) | N21 | C26 | C36 | C35 | 177.0(23) |
| C25 | C26 | C36 | N31 | -179.0(23) | C25 | C26 | C36 | C35 | -2.4(11) |
| Os1 | N31 | C32 | C33 | 178.4(19) | C36 | N31 | C32 | C33 | -2.2(12) |
| Os1 | N31 | C36 | C26 | -2.9( 7) | Os1 | N31 | C36 | C35 | -179.6(18) |
| C32 | N31 | C36 | C26 | 177.6(22) | C32 | N31 | C36 | C35 | 0.9(11) |
| N31 | C32 | C33 | C34 | 2.6(11) | C32 | C33 | C34 | C35 | -1.6(12) |
| C33 | C34 | C35 | C36 | 0.4(11) | C34 | C35 | C36 | C26 | -176.5(24) |
| C34 | C35 | C36 | N31 | -0.1(11) | | | | | |

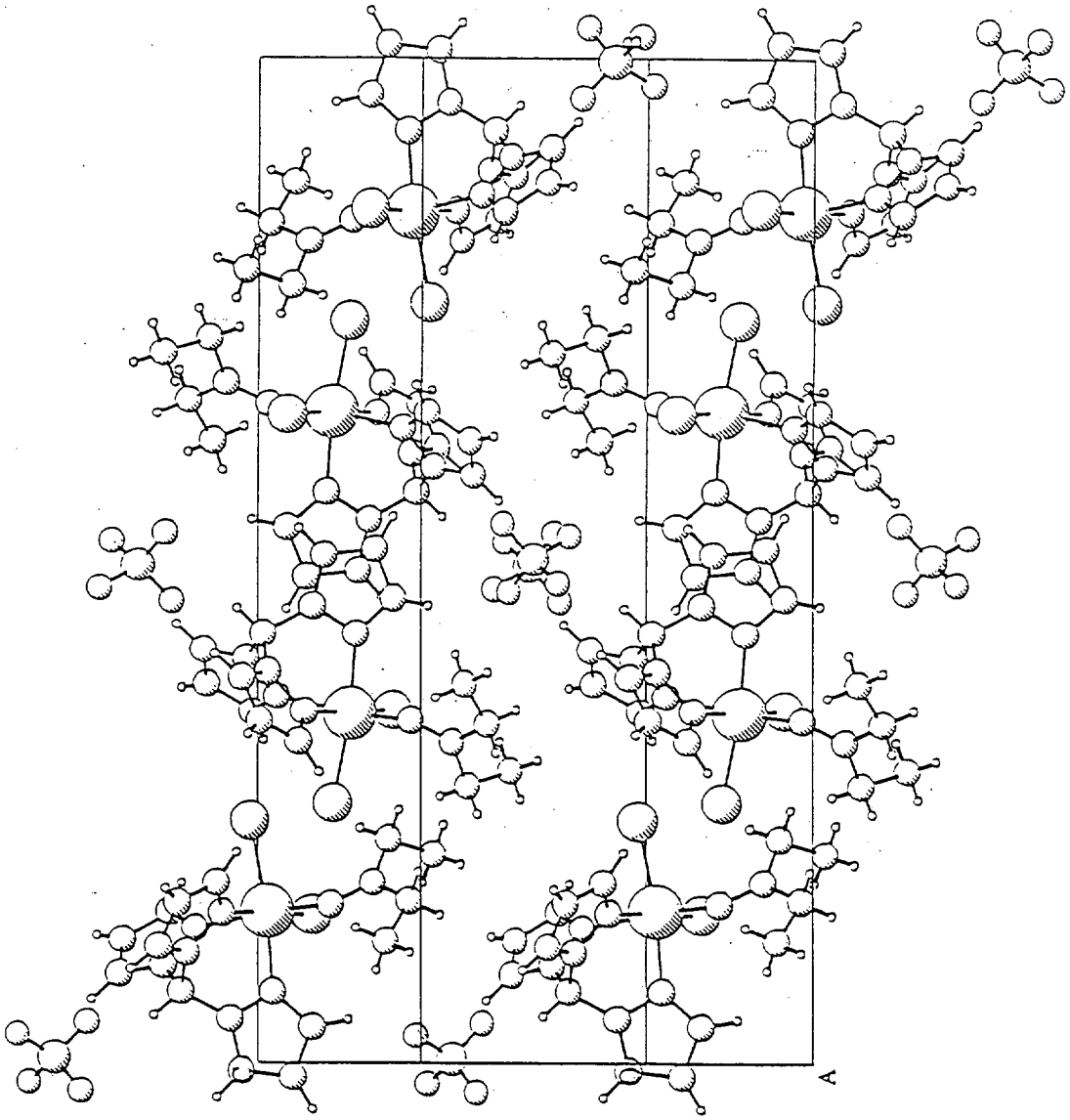
Space Group and Cell Dimensions  Monoclinic,  P 21/a
a  9.3411(5)  b  25.5779(14)  c  10.0974(6)
beta 116.554 (1)
Volume  2158.04(21)A**3
Empirical formula : Os Cl2 C14 H20 N8 B F4
Cell dimensions were obtained from 6126 reflections with 2Theta angle in the range  3.00 -  60.00 degrees.
Crystal dimensions :  0.20  X  0.20  X  0.35  mm
FW =  648.27  Z =  4  F(000) =  1242.53
Dcalc  1.995Mg.m-3, mu  6.21mm-1, lambda 0.71073A, 2Theta(max)  60.0
The intensity data were collected on a Bruker SMART diffractometer, using the omega scan mode.
The h,k,l ranges used during structure solution and refinement are :--
Hmin,max  -13  11;  Kmin,max  0  34;  Lmin,max  0  14
No. of reflections measured  10907
No. of unique reflections  5838
No. of reflections with Inet > 2.5sigma(Inet)  4562
Merging R-value on intensities  0.029
Correction was made for absorption using psi scams

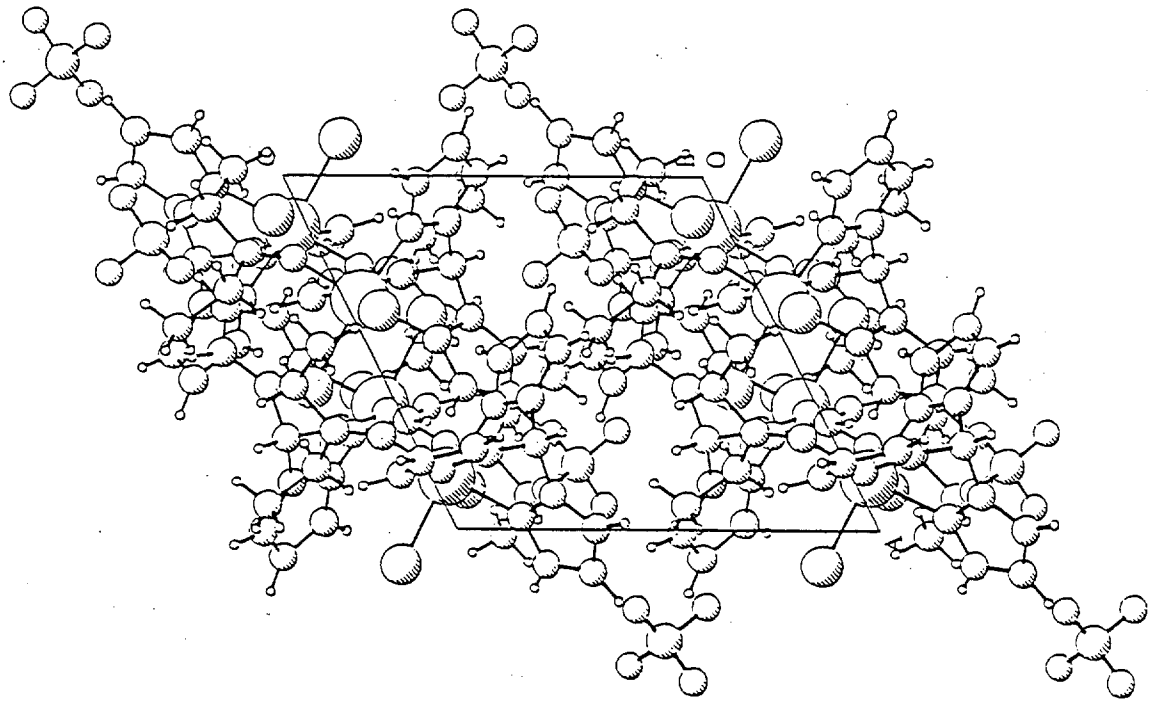
The last least squares cycle was calculated with
50 atoms, 272 parameters and 4561 out of 5838 reflections.
Weights based on counting-statistics were used.
The residuals are as follows :--
For significant reflections,  RF 0.031, Rw 0.033 GoF  2.03
For all reflections,  RF 0.045, Rw 0.048.
where RF = Sum(Fo-Fc)/Sum(Fo),
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was  0.000.
In the last D-map, the deepest hole was  -1.250e/A**3,
and the highest peak  1.620e/A**3.
Secondary ext. coeff.  0.2735microns  sigma  0.0166

The following references are relevant to the NRCVAX System.

1. Full System Reference :
Gabe, E.J., Le Page, Y., Charland, J.-P., Lee, F.L. and White, P.S. (1989) J. Appl. Cryst., 22, 384-387.
2. Scattering Factors from Int. Tab. Vol. 4 :
International Tables for X-ray Crystallography, Vol. IV, (1974) Kynoch Press, Birmingham, England.
The following references may also be relevant.
3. ORTEP Plotting :
Johnson, C.K., (1976) ORTEP - A Fortran Thermal Ellipsoid Plot Program, Technical Report ORNL-5138, Oak Ridge
4. Pluto Plotting :
S. Motherwell, University Chemical Laboratory, Cambridge, 1978
5. Missing Symmetry Treatment by MISSYM :
Le Page, Y., (1988) J. Appl. Cryst., 21, 983-984.
6. Grouping of Equivalent Reflections in DATRD2 :
Le Page, Y. and Gabe, E.J., (1979) J. Appl. Cryst., 12, 464-466.
7. Extinction Treatment :
Larson, A.C., (1970) p.293, Crystallographic Computing, Munksgaard, Copenhagen.







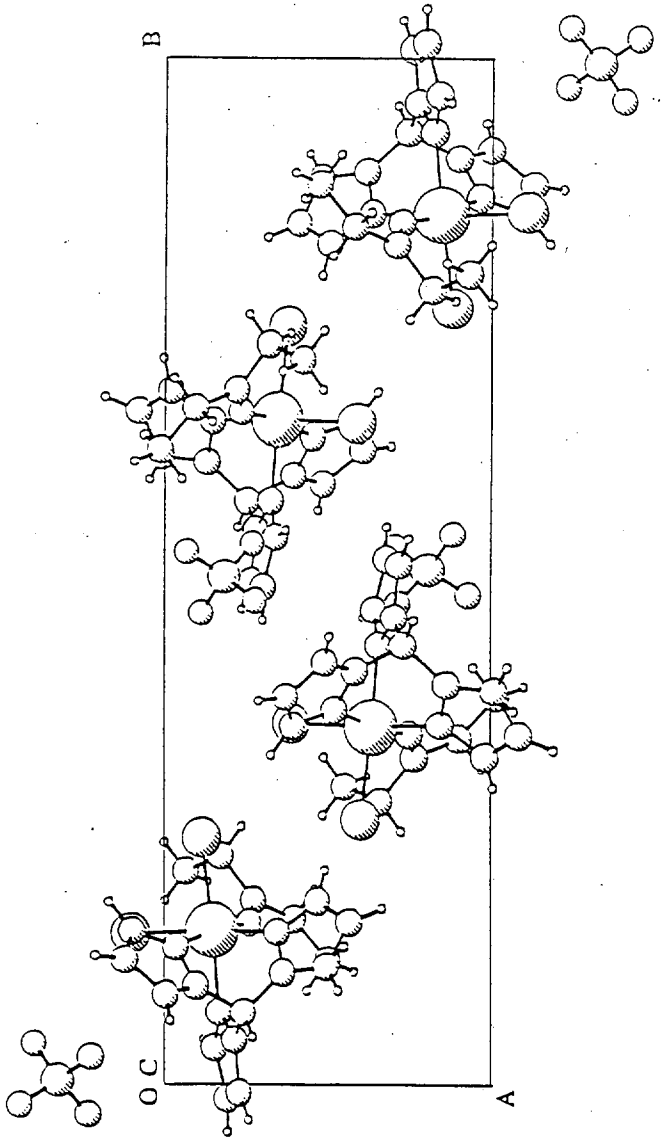


Table . Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

| | x | y | z | Biso |
|---|---|---|---|---|
| Os1 | 0.648156(21) | 0.349051( 7) | 0.037459(21) | 1.938( 9) |
| Cl1 | 0.61526 (15) | 0.25884 ( 5) | 0.06791 (15) | 2.90 ( 7) |
| Cl2 | 0.39776 (15) | 0.35234 ( 5) | -0.17641 (14) | 2.91 ( 6) |
| N1 | 0.7627 ( 5) | 0.34162 (16) | -0.0714 ( 4) | 2.32 (19) |
| N2 | 0.7774 ( 5) | 0.32007 (19) | -0.1737 ( 5) | 3.23 (24) |
| C3 | 0.6732 ( 8) | 0.2764 ( 3) | -0.2584 ( 7) | 4.5 ( 4) |
| C4 | 0.5666 (10) | 0.2914 ( 3) | -0.4176 ( 8) | 6.4 ( 5) |
| C5 | 0.9047 ( 9) | 0.3382 ( 3) | -0.2155 ( 8) | 5.2 ( 4) |
| C6 | 1.0139 ( 7) | 0.3786 ( 3) | -0.1093 ( 9) | 5.9 ( 4) |
| C10 | 0.7441 ( 6) | 0.42914 (20) | 0.2951 ( 6) | 2.52 (24) |
| N11 | 0.8518 ( 4) | 0.35062 (16) | 0.2370 ( 4) | 2.10 (18) |
| N12 | 0.8696 ( 4) | 0.39047 (16) | 0.3339 ( 4) | 2.24 (19) |
| C13 | 1.0086 ( 6) | 0.38492 (23) | 0.4589 ( 6) | 3.0 ( 3) |
| C14 | 1.0805 ( 6) | 0.34135 (22) | 0.4420 ( 6) | 3.1 ( 3) |
| C15 | 0.9816 ( 6) | 0.32104 (21) | 0.3044 ( 6) | 2.66 (24) |
| N21 | 0.5349 ( 5) | 0.36593 (16) | 0.1731 ( 5) | 2.13 (19) |
| N22 | 0.5973 ( 5) | 0.40388 (16) | 0.2776 ( 4) | 2.37 (19) |
| C23 | 0.5036 ( 7) | 0.41223 (22) | 0.3460 ( 6) | 3.1 ( 3) |
| C24 | 0.3788 ( 7) | 0.37833 (24) | 0.2860 ( 7) | 3.4 ( 3) |
| C25 | 0.4014 ( 6) | 0.34983 (21) | 0.1802 ( 6) | 2.70 (25) |
| N31 | 0.6688 ( 4) | 0.42907 (16) | 0.0325 ( 4) | 2.21 (19) |
| N32 | 0.7165 ( 4) | 0.45661 (17) | 0.1605 ( 4) | 2.26 (19) |
| C33 | 0.7305 ( 6) | 0.50817 (20) | 0.1380 ( 7) | 3.0 ( 3) |
| C34 | 0.6933 ( 6) | 0.51383 (22) | -0.0073 ( 7) | 3.3 ( 3) |
| C35 | 0.6545 ( 6) | 0.46434 (21) | -0.0709 ( 6) | 2.8 ( 3) |
| B1 | 0.1840 ( 8) | 0.4964 ( 3) | 0.3751 ( 8) | 3.4 ( 4) |
| F1 | 0.2726 ( 7) | 0.5294 ( 3) | 0.3462 ( 6) | 12.4 ( 4) |
| F2 | 0.0681 ( 5) | 0.52078 (25) | 0.3921 ( 5) | 11.0 ( 4) |
| F3 | 0.2807 ( 5) | 0.47328 (16) | 0.5097 ( 4) | 6.27 (24) |
| F4 | 0.1123 ( 5) | 0.46092 (18) | 0.2637 ( 4) | 6.81 (24) |
| H3a | 0.739 | 0.248 | -0.259 | 5.2 |
| H3b | 0.608 | 0.266 | -0.212 | 5.2 |
| H4a | 0.499 | 0.263 | -0.472 | 6.9 |
| H4b | 0.502 | 0.320 | -0.416 | 6.9 |
| H4c | 0.632 | 0.302 | -0.464 | 6.9 |
| H5a | 0.854 | 0.352 | -0.314 | 6.6 |
| H5b | 0.972 | 0.309 | -0.212 | 6.6 |
| H6a | 1.094 | 0.390 | -0.138 | 6.6 |
| H6b | 0.947 | 0.408 | -0.113 | 6.6 |
| H6c | 1.065 | 0.365 | -0.010 | 6.6 |
| H10 | 0.775 | 0.454 | 0.374 | 3.2 |
| H13 | 1.047 | 0.408 | 0.543 | 3.4 |
| H14 | 1.181 | 0.328 | 0.514 | 3.6 |
| H15 | 1.005 | 0.290 | 0.263 | 3.3 |
| H23 | 0.518 | 0.438 | 0.421 | 4.0 |
| H24 | 0.293 | 0.374 | 0.313 | 4.4 |
| H25 | 0.333 | 0.322 | 0.123 | 3.5 |
| H33 | 0.761 | 0.535 | 0.213 | 3.6 |
| H34 | 0.694 | 0.546 | -0.054 | 3.9 |
| H35 | 0.622 | 0.457 | -0.174 | 3.5 |

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

| | u11(U) | u22 | u33 | u12 | u13 | u23 |
|---|---|---|---|---|---|---|
| Os1 | 2.468(10) | 2.106(11) | 2.507(10) | 0.037( 9) | 0.860( 8) | -0.084( 9) |
| Cl1 | 4.18 ( 7) | 2.26 ( 7) | 4.59 ( 8) | -0.10 ( 6) | 1.97 ( 7) | -0.03 ( 6) |
| Cl2 | 3.12 ( 6) | 3.53 ( 8) | 3.24 ( 6) | 0.13 ( 6) | 0.39 ( 5) | -0.49 ( 6) |
| N1 | 3.21 (22) | 2.8 ( 3) | 2.90 (22) | 0.66 (19) | 1.47 (19) | 0.28 (18) |
| N2 | 5.0 ( 3) | 3.7 ( 3) | 3.8 ( 3) | 1.22 (24) | 2.21 (24) | 0.64 (22) |
| C3 | 8.0 ( 5) | 4.0 ( 4) | 5.0 ( 4) | 0.3 ( 4) | 2.8 ( 4) | -0.7 ( 3) |
| C4 | 10.2 ( 6) | 8.1 ( 6) | 4.8 ( 5) | 1.2 ( 5) | 2.3 ( 5) | -1.4 ( 4) |
| C5 | 7.2 ( 5) | 7.7 ( 6) | 7.1 ( 5) | 2.2 ( 4) | 5.2 ( 4) | 2.4 ( 4) |
| C6 | 3.9 ( 4) | 9.2 ( 6) | 9.1 ( 6) | -0.8 ( 4) | 2.6 ( 4) | 2.7 ( 5) |
| C10 | 3.4 ( 3) | 2.7 ( 3) | 3.2 ( 3) | -0.13 (23) | 1.26 (24) | -0.63 (22) |
| N11 | 2.77 (20) | 2.22 (23) | 2.83 (21) | 0.10 (19) | 1.12 (18) | 0.08 (18) |
| N12 | 2.65 (21) | 2.5 ( 3) | 2.75 (22) | -0.15 (18) | 0.70 (19) | -0.12 (18) |
| C13 | 3.3 ( 3) | 4.3 ( 4) | 2.5 ( 3) | -0.2 ( 3) | 0.24 (24) | 0.24 (24) |
| C14 | 3.0 ( 3) | 4.3 ( 4) | 3.4 ( 3) | 0.5 ( 3) | 0.29 (24) | 0.7 ( 3) |
| C15 | 2.8 ( 3) | 3.3 ( 3) | 3.5 ( 3) | 0.62 (23) | 0.94 (24) | 0.62 (24) |
| N21 | 2.58 (20) | 2.32 (24) | 2.98 (22) | -0.22 (17) | 1.06 (19) | -0.18 (17) |
| N22 | 3.20 (22) | 2.9 ( 3) | 2.81 (23) | -0.04 (19) | 1.21 (19) | -0.43 (18) |
| C23 | 4.7 ( 3) | 4.2 ( 4) | 3.4 ( 3) | 1.4 ( 3) | 2.3 ( 3) | 0.48 (25) |
| C24 | 4.0 ( 3) | 4.4 ( 4) | 5.2 ( 4) | 0.7 ( 3) | 2.9 ( 3) | 1.1 ( 3) |
| C25 | 3.0 ( 3) | 3.3 ( 3) | 4.2 ( 3) | 0.17 (24) | 1.81 (24) | 1.0 ( 3) |
| N31 | 2.85 (22) | 2.72 (25) | 2.72 (21) | 0.23 (18) | 1.15 (19) | -0.02 (18) |
| N32 | 2.63 (20) | 2.44 (24) | 3.05 (23) | 0.17 (19) | 0.86 (19) | -0.04 (19) |
| C33 | 3.4 ( 3) | 2.0 ( 3) | 5.2 ( 4) | -0.32 (23) | 1.2 ( 3) | -0.39 (25) |
| C34 | 3.6 ( 3) | 2.9 ( 3) | 5.3 ( 4) | -0.1 ( 3) | 1.3 ( 3) | 1.2 ( 3) |
| C35 | 3.1 ( 3) | 3.1 ( 3) | 4.3 ( 3) | 0.54 (23) | 1.5 ( 3) | 1.21 (24) |
| B1 | 3.6 ( 4) | 5.6 ( 5) | 4.0 ( 4) | -0.3 ( 3) | 1.9 ( 3) | -0.9 ( 3) |
| F1 | 13.1 ( 4) | 23.5 ( 7) | 6.9 ( 3) | -11.9 ( 5) | 1.4 ( 3) | 3.1 ( 4) |
| F2 | 7.1 ( 3) | 23.9 ( 7) | 7.5 ( 3) | 6.9 ( 4) | 0.4 ( 3) | -7.9 ( 4) |
| F3 | 7.9 ( 3) | 6.7 ( 3) | 5.6 ( 3) | 0.32 (23) | -0.19 (23) | 0.66 (21) |
| F4 | 8.8 ( 3) | 8.2 ( 3) | 5.9 ( 3) | 1.6 ( 3) | 0.66 (23) | -2.91 (23) |
| H3a | 6.6 | | | | | |
| H3b | 6.6 | | | | | |
| H4a | 8.7 | | | | | |
| H4b | 8.7 | | | | | |
| H4c | 8.7 | | | | | |
| H5a | 8.3 | | | | | |
| H5b | 8.3 | | | | | |
| H6a | 8.4 | | | | | |
| H6b | 8.4 | | | | | |
| H6c | 8.4 | | | | | |
| H10 | 4.1 | | | | | |
| H13 | 4.4 | | | | | |
| H14 | 4.6 | | | | | |
| H15 | 4.2 | | | | | |
| H23 | 5.1 | | | | | |
| H24 | 5.6 | | | | | |
| H25 | 4.5 | | | | | |
| H33 | 4.5 | | | | | |
| H34 | 4.9 | | | | | |
| H35 | 4.5 | | | | | |

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+----+2*h*k*u12*astar*bstar+---)

DISANG -- The NRCVAX Distance and Angle Program
The Space Group is P 21/A Centrosymmetric
The Equivalent Positions are:
1) x y z 2) 1/2-x 1/2+y -z
The Lattice is Primitive. There are no Centering Vectors

| | | | |
|---|---|---|---|
| Os(1)-Cl(1) | 2.3661(13) | N(21)-N(22) | 1.358(6) |
| Os(1)-Cl(2) | 2.3718(12) | N(21)-C(25) | 1.346(6) |
| Os(1)-N(1) | 1.855(4) | N(22)-C(23) | 1.353(6) |
| Os(1)-N(11) | 2.062(4) | C(23)-C(24) | 1.359(9) |
| Os(1)-N(21) | 2.116(4) | C(24)-C(25) | 1.385(8) |
| Os(1)-N(31) | 2.059(4) | N(31)-N(32) | 1.361(6) |
| N(1)-N(2) | 1.231(6) | N(31)-C(35) | 1.340(6) |
| N(2)-C(3) | 1.476(8) | N(32)-C(33) | 1.354(7) |
| N(2)-C(5) | 1.502(8) | C(33)-C(34) | 1.356(9) |
| C(3)-C(4) | 1.513(10) | C(34)-C(35) | 1.392(8) |
| C(5)-C(6) | 1.510(12) | B(1)-F(1) | 1.304(8) |
| C(10)-N(12) | 1.448(6) | B(1)-F(2) | 1.326(8) |
| C(10)-N(22) | 1.453(6) | B(1)-F(3) | 1.384(8) |
| C(10)-N(32) | 1.447(7) | B(1)-F(4) | 1.366(8) |
| N(11)-N(12) | 1.371(6) | F(1)-F(2) | 2.170(8) |
| N(11)-C(15) | 1.330(6) | F(1)-F(3) | 2.164(6) |
| N(12)-C(13) | 1.354(6) | F(2)-F(3) | 2.173(6) |
| C(13)-C(14) | 1.351(8) | F(2)-F(4) | 2.162(5) |
| C(14)-C(15) | 1.381(8) | | |

| | | | |
|---|---|---|---|
| Cl(1)-Os(1)-Cl(2) | 91.17(5) | N(22)-N(21)-C(25) | 105.2(4) |
| Cl(1)-Os(1)-N(1) | 96.89(13) | C(10)-N(22)-N(21) | 117.8(4) |
| Cl(1)-Os(1)-N(11) | 90.50(12) | C(10)-N(22)-C(23) | 131.2(4) |
| Cl(1)-Os(1)-N(21) | 89.05(11) | N(21)-N(22)-C(23) | 111.0(4) |
| Cl(1)-Os(1)-N(31) | 172.70(11) | N(22)-C(23)-C(24) | 107.1(5) |
| Cl(2)-Os(1)-N(1) | 93.41(13) | C(23)-C(24)-C(25) | 106.5(5) |
| Cl(2)-Os(1)-N(11) | 172.92(11) | N(21)-C(25)-C(24) | 110.2(5) |
| Cl(2)-Os(1)-N(21) | 90.42(11) | Os(1)-N(31)-N(32) | 119.1(3) |
| Cl(2)-Os(1)-N(31) | 90.43(11) | Os(1)-N(31)-C(35) | 135.3(4) |
| N(1)-Os(1)-N(11) | 93.22(16) | N(32)-N(31)-C(35) | 105.5(4) |
| N(1)-Os(1)-N(21) | 172.87(17) | C(10)-N(32)-N(31) | 119.1(4) |
| N(1)-Os(1)-N(31) | 90.13(16) | C(10)-N(32)-C(33) | 129.8(4) |
| N(11)-Os(1)-N(21) | 82.73(15) | N(31)-N(32)-C(33) | 111.1(4) |
| N(11)-Os(1)-N(31) | 87.08(16) | N(32)-C(33)-C(34) | 106.7(5) |
| N(21)-Os(1)-N(31) | 83.82(15) | C(33)-C(34)-C(35) | 106.9(5) |
| Os(1)-N(1)-N(2) | 148.5(4) | N(31)-C(35)-C(34) | 109.8(5) |
| N(1)-N(2)-C(3) | 122.2(5) | F(1)-B(1)-F(2) | 111.2(7) |
| N(1)-N(2)-C(5) | 119.8(5) | F(1)-B(1)-F(3) | 107.2(6) |
| C(3)-N(2)-C(5) | 118.0(5) | F(1)-B(1)-F(4) | 111.9(6) |
| N(2)-C(3)-C(4) | 112.0(6) | F(2)-B(1)-F(3) | 106.6(6) |
| N(2)-C(5)-C(6) | 112.3(5) | F(2)-B(1)-F(4) | 106.9(5) |
| N(12)-C(10)-N(22) | 109.6(4) | F(3)-B(1)-F(4) | 112.9(6) |
| N(12)-C(10)-N(32) | 111.6(4) | B(1)-F(1)-F(2) | 34.7(4) |
| N(22)-C(10)-N(32) | 109.9(4) | B(1)-F(1)-F(3) | 37.7(4) |
| Os(1)-N(11)-N(12) | 118.5(3) | F(2)-F(1)-F(3) | 60.19(23) |
| Os(1)-N(11)-C(15) | 136.1(4) | B(1)-F(2)-F(1) | 34.1(4) |
| N(12)-N(11)-C(15) | 105.4(4) | B(1)-F(2)-F(3) | 37.6(4) |

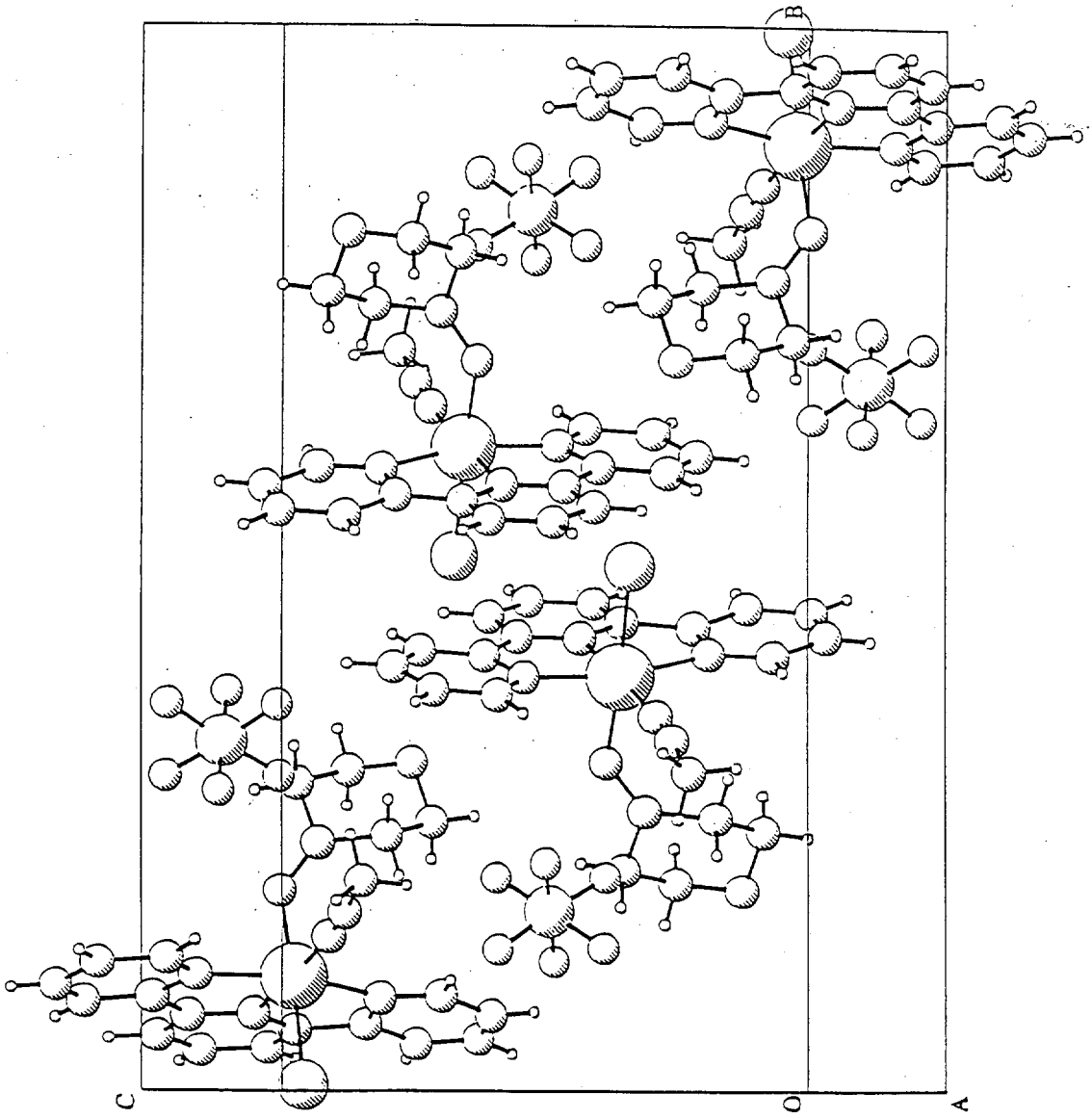
| | | | |
|---|---|---|---|
| C(10)-N(12)-N(11) | 119.3(4) | B(1)-F(2)-F(4) | 37.2(3) |
| C(10)-N(12)-C(13) | 130.3(4) | F(1)-F(2)-F(3) | 59.77(22) |
| N(11)-N(12)-C(13) | 110.3(4) | F(1)-F(2)-F(4) | 61.39(25) |
| N(12)-C(13)-C(14) | 107.0(5) | F(3)-F(2)-F(4) | 63.82(19) |
| C(13)-C(14)-C(15) | 106.9(5) | B(1)-F(3)-F(1) | 35.1(3) |
| N(11)-C(15)-C(14) | 110.4(5) | B(1)-F(3)-F(2) | 35.8(3) |
| Os(1)-N(21)-N(22) | 118.9(3) | F(1)-F(3)-F(2) | 60.0(3) |
| Os(1)-N(21)-C(25) | 135.7(4) | B(1)-F(4)-F(2) | 35.9(3) |

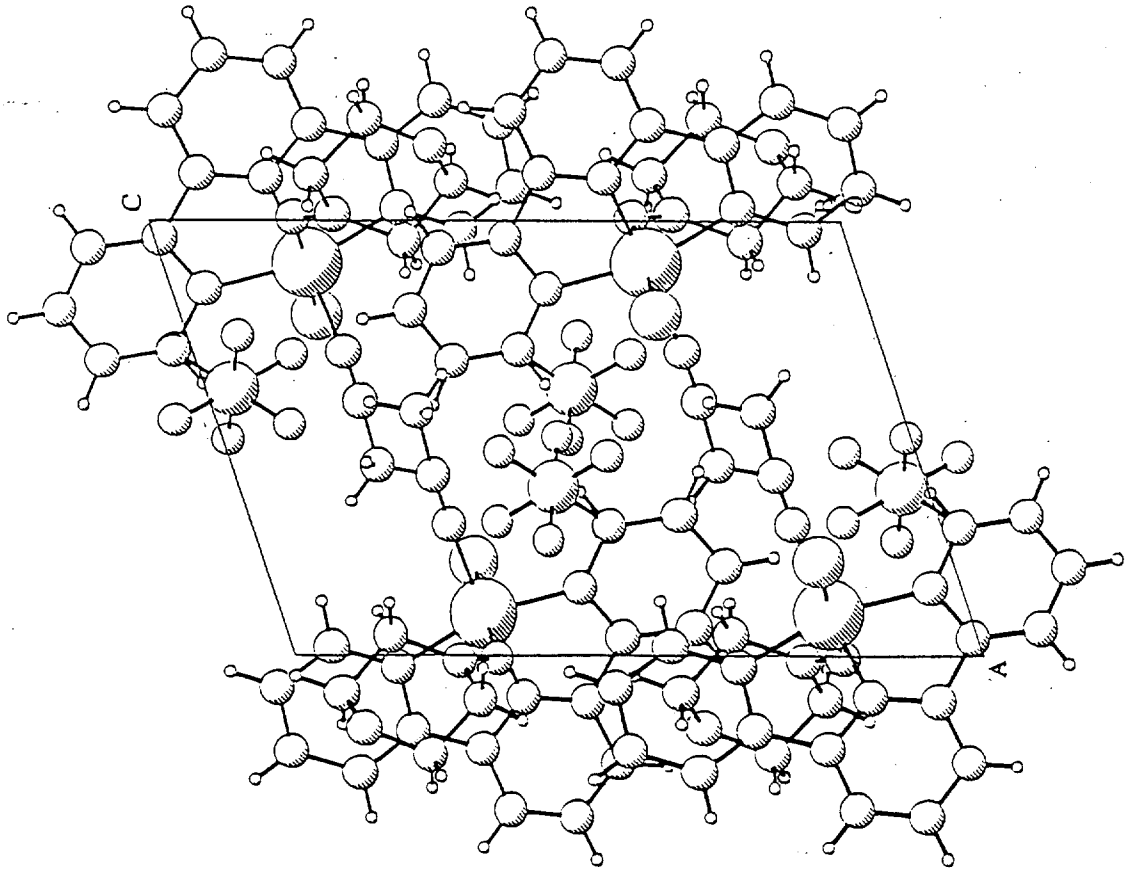
Torsion angles

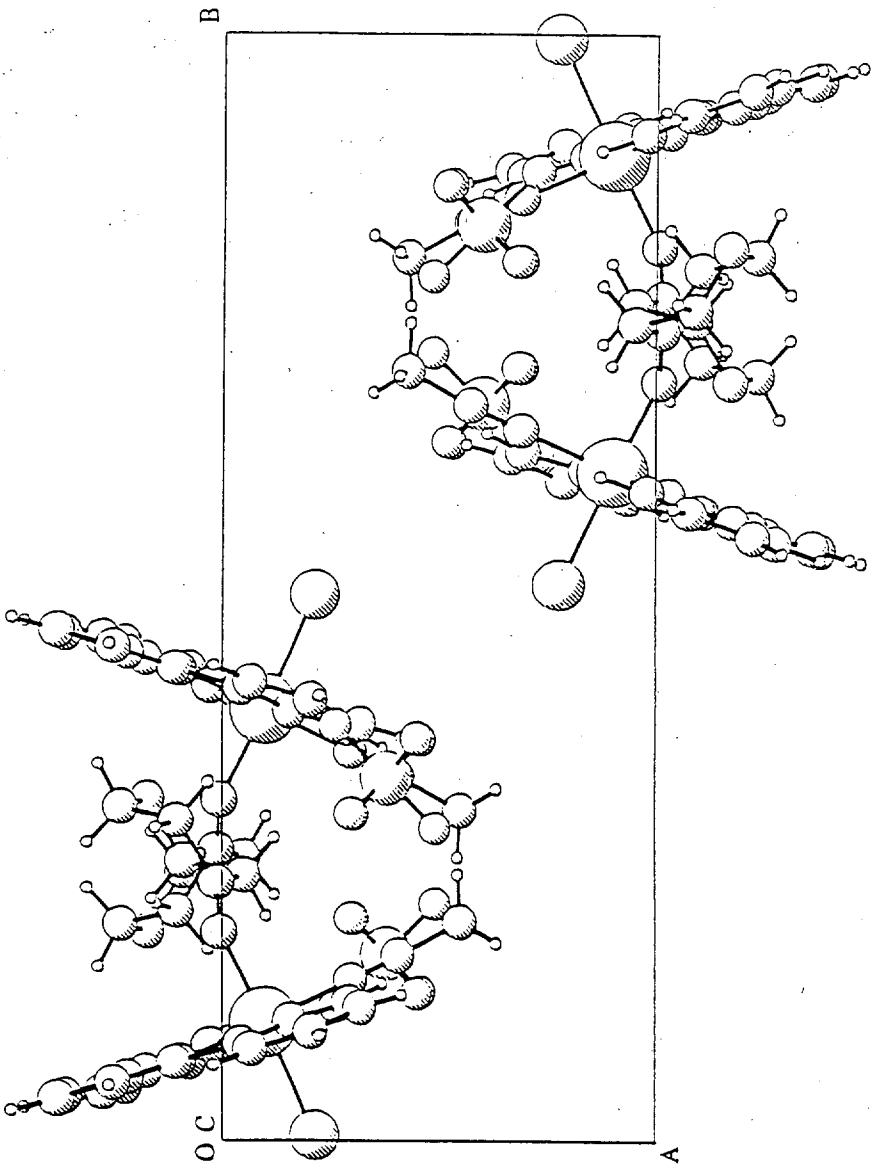
| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Cl1 | Os1 | N1 | N2 | 46.0( 4) | Cl2 | Os1 | N1 | N2 | -45.6( 4) |
| N11 | Os1 | N1 | N2 | 136.9( 6) | N21 | Os1 | N1 | N2 | -167.9( 6) |
| N31 | Os1 | N1 | N2 | -136.0( 6) | Cl1 | Os1 | N11 | N12 | -133.9( 5) |
| Cl1 | Os1 | N11 | C15 | 45.4( 4) | Cl2 | Os1 | N11 | N12 | -30.3( 3) |
| Cl2 | Os1 | N11 | C15 | 149.1( 5) | N1 | Os1 | N11 | N12 | 129.2( 5) |
| N1 | Os1 | N11 | C15 | -51.5( 4) | N21 | Os1 | N11 | N12 | -44.9( 4) |
| N21 | Os1 | N11 | C15 | 134.4( 5) | N31 | Os1 | N11 | N12 | 39.2( 3) |
| N31 | Os1 | N11 | C15 | -141.4( 6) | Cl1 | Os1 | N21 | N22 | 137.0( 5) |
| Cl1 | Os1 | N21 | C25 | -47.6( 4) | Cl2 | Os1 | N21 | N22 | -131.9( 5) |
| Cl2 | Os1 | N21 | C25 | 43.6( 4) | N1 | Os1 | N21 | N22 | -9.4( 3) |
| N1 | Os1 | N21 | C25 | 166.0( 6) | N11 | Os1 | N21 | N22 | 46.3( 4) |
| N11 | Os1 | N21 | C25 | -138.2( 6) | N31 | Os1 | N21 | N22 | -41.5( 4) |
| N31 | Os1 | N21 | C25 | 134.0( 6) | Cl1 | Os1 | N31 | N32 | 32.0( 3) |
| Cl1 | Os1 | N31 | C35 | -152.6( 5) | Cl2 | Os1 | N31 | N32 | 134.6( 5) |
| Cl2 | Os1 | N31 | C35 | -50.0( 4) | N1 | Os1 | N31 | N32 | -132.0( 5) |
| N1 | Os1 | N31 | C35 | 43.5( 4) | N11 | Os1 | N31 | N32 | -38.7( 4) |
| N11 | Os1 | N31 | C35 | 136.7( 6) | N21 | Os1 | N31 | N32 | 44.3( 4) |
| N21 | Os1 | N31 | C35 | -140.3( 6) | Os1 | N1 | N2 | C3 | -6.4( 4) |
| Os1 | N1 | N2 | C5 | 173.6( 8) | N1 | N2 | C3 | C4 | 113.3(10) |
| C5 | N2 | C3 | C4 | -66.7( 8) | N1 | N2 | C5 | C6 | 6.5( 6) |
| C3 | N2 | C5 | C6 | -173.4(12) | N22 | C10 | N12 | N11 | 61.8( 5) |
| N22 | C10 | N12 | C13 | -115.5( 8) | N32 | C10 | N12 | N11 | -60.1( 5) |
| N32 | C10 | N12 | C13 | 122.6( 8) | N12 | C10 | N22 | N21 | -59.7( 5) |
| N12 | C10 | N22 | C23 | 122.4( 8) | N32 | C10 | N22 | N21 | 63.2( 6) |
| N32 | C10 | N22 | C23 | -114.7( 8) | N12 | C10 | N32 | N31 | 61.0( 5) |
| N12 | C10 | N32 | C33 | -119.1( 8) | N22 | C10 | N32 | N31 | -60.7( 5) |
| N22 | C10 | N32 | C33 | 119.1( 8) | Os1 | N11 | N12 | C10 | 1.6( 3) |
| Os1 | N11 | N12 | C13 | 179.3( 7) | C15 | N11 | N12 | C10 | -178.0( 8) |
| C15 | N11 | N12 | C13 | -0.2( 5) | Os1 | N11 | C15 | C14 | -179.2( 8) |
| N12 | N11 | C15 | C14 | 0.2( 4) | C10 | N12 | C13 | C14 | 177.6(10) |
| N11 | N12 | C13 | C14 | 0.1( 4) | N12 | C13 | C14 | C15 | 0.0( 4) |
| C13 | C14 | C15 | N11 | -0.1( 4) | Os1 | N21 | N22 | C10 | -3.0( 3) |
| Os1 | N21 | N22 | C23 | 175.3( 7) | C25 | N21 | N22 | C10 | -179.7( 9) |
| C25 | N21 | N22 | C23 | -1.4( 5) | Os1 | N21 | C25 | C24 | -174.6( 8) |
| N22 | N21 | C25 | C24 | 1.3( 5) | C10 | N22 | C23 | C24 | 178.9(10) |
| N21 | N22 | C23 | C24 | 1.0( 5) | N22 | C23 | C24 | C25 | -0.1( 4) |
| C23 | C24 | C25 | N21 | -0.8( 4) | Os1 | N31 | N32 | C10 | -2.9( 3) |
| Os1 | N31 | N32 | C33 | 177.2( 7) | C35 | N31 | N32 | C10 | -179.5( 9) |
| C35 | N31 | N32 | C33 | 0.6( 5) | Os1 | N31 | C35 | C34 | -175.8( 8) |
| N32 | N31 | C35 | C34 | 0.0( 4) | C10 | N32 | C33 | C34 | 179.2(10) |
| N31 | N32 | C33 | C34 | -0.9( 5) | N32 | C33 | C34 | C35 | 0.9( 4) |
| C33 | C34 | C35 | N31 | -0.6( 4) | F2 | B1 | F1 | F2 | 0.0( 5) |
| F2 | B1 | F1 | F3 | 116.2(10) | F3 | B1 | F1 | F2 | -116.2( 9) |
| F3 | B1 | F1 | F3 | 0.0( 4) | F4 | B1 | F1 | F2 | 119.5( 9) |
| F4 | B1 | F1 | F3 | -124.3( 9) | F1 | B1 | F2 | F1 | 0.0( 5) |
| F1 | B1 | F2 | F3 | -116.6(10) | F1 | B1 | F2 | F4 | 122.4(10) |
| F3 | B1 | F2 | F1 | 116.6( 9) | F3 | B1 | F2 | F3 | 0.0( 4) |
| F3 | B1 | F2 | F4 | -121.1( 9) | F4 | B1 | F2 | F1 | -122.4( 9) |
| F4 | B1 | F2 | F3 | 121.1( 9) | F4 | B1 | F2 | F4 | 0.0( 4) |
| F1 | B1 | F3 | F1 | 0.0( 5) | F1 | B1 | F3 | F2 | 119.2( 9) |
| F2 | B1 | F3 | F1 | -119.2( 9) | F2 | B1 | F3 | F2 | 0.0( 5) |
| F4 | B1 | F3 | F1 | 123.7( 9) | F4 | B1 | F3 | F2 | -117.1( 8) |
| F1 | B1 | F4 | F2 | -122.0( 9) | F2 | B1 | F4 | F2 | 0.0( 5) |
| F3 | B1 | F4 | F2 | 117.0( 8) | B1 | F1 | F2 | B1 | 0.0( 7) |
| B1 | F1 | F2 | F3 | 39.2( 6) | B1 | F1 | F2 | F4 | -35.5( 6) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| F3 | F1 | F2 | B1 | -39.2( 6) | F3 | F1 | F2 | F3 | 0.00(23) |
| F3 | F1 | F2 | F4 | -74.7( 5) | B1 | F1 | F3 | B1 | 0.0( 7) |
| B1 | F1 | F3 | F2 | -36.1( 6) | F2 | F1 | F3 | B1 | 36.1( 6) |
| F2 | F1 | F3 | F2 | 0.0( 3) | B1 | F2 | F3 | B1 | 0.0( 7) |
| B1 | F2 | F3 | F1 | 35.4( 6) | F1 | F2 | F3 | B1 | -35.4( 6) |
| F1 | F2 | F3 | F1 | 0.0( 3) | F4 | F2 | F3 | B1 | 35.2( 6) |
| F4 | F2 | F3 | F1 | 70.7( 4) | B1 | F2 | F4 | B1 | 0.0( 7) |
| F1 | F2 | F4 | B1 | 32.6( 6) | F3 | F2 | F4 | B1 | -35.6( 6) |

```
  Space Group and Cell Dimensions    Monoclinic,    P 21/c
a   8.9615(5)    b  21.5547(12)    c  13.4873(8)
beta 108.280(1)
       Volume  2473.77(24)A**3
Empirical formula : Os C21 H22 N6 O P F6 Cl
Cell dimensions were obtained from 5262 reflections with 2Theta angle
in the range   3.00 -  50.00 degrees.
Crystal dimensions :  0.20  X  0.15  X  0.15  mm
FW =    745.05     Z =    4     F(000) =    1438.56
Dcalc  2.001Mg.m-3, mu   5.40mm-1, lambda 0.71073A, 2Theta(max)  50.0
The intensity data were collected on a Bruker SMART diffractometer,
using the omega scan mode.
The h,k,l ranges used during structure solution and refinement are :--
Hmin,max  -10  10;  Kmin,max    0  25;  Lmin,max   0  16
No. of reflections measured                    18276
No. of unique reflections                       4366
No. of reflections with Inet > 2.5sigma(Inet)  3057
Merging R-value on intensities  0.050
Correction was made for absorption using SADABS

The last least squares cycle was calculated with
 59 atoms, 334 parameters and 4098 out of 4366 reflections.
Weights based on counting-statistics were used.
The weight modifier K in KFo**2 is 0.000200
The residuals are as follows :--
For significant reflections,  RF 0.065, Rw 0.055 GoF  1.85
For all reflections,          RF 0.076, Rw 0.055.
where RF = Sum(Fo-Fc)/Sum(Fo),
      Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
     GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was  0.005.
In the last D-map, the deepest hole was  -1.720e/A**3,
and the highest peak   3.170e/A**3.

      The following references are relevant to the NRCVAX System.

1. Full System Reference :
   Gabe, E.J., Le Page, Y., Charland, J.-P., Lee, F.L. and White, P.S.
   (1989) J. Appl. Cryst., 22, 384-387.
2. Scattering Factors from Int. Tab. Vol. 4 :
   International Tables for X-ray Crystallography, Vol. IV, (1974)
   Kynoch Press, Birmingham, England.
      The following references may also be relevant.
3. ORTEP Plotting :
   Johnson, C.K., (1976) ORTEP - A Fortran Thermal Ellipsoid Plot
   Program, Technical Report ORNL-5138, Oak Ridge
4. Pluto Plotting :
   S. Motherwell, University Chemical Laboratory, Cambridge, 1978
5. Missing Symmetry Treatment by MISSYM :
   Le Page, Y., (1988) J. Appl. Cryst., 21, 983-984.
6. Grouping of Equivalent Reflections in DATRD2 :
   Le Page, Y. and Gabe, E.J., (1979) J. Appl. Cryst., 12, 464-466.
```







5-Jan-1999

Table . Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

| | x | y | z | Biso |
|---|---|---|---|---|
| Os1 | 0.90316( 5) | 0.891845(23) | 0.20485( 4) | 2.098(21) |
| Cl1 | 0.7841 ( 3) | 0.99522 (14) | 0.19452(25) | 2.46 (14) |
| N1 | 1.0062 (10) | 0.8102 ( 5) | 0.2061 ( 7) | 2.0 ( 4) |
| N2 | 1.0128 (11) | 0.7648 ( 5) | 0.2640 ( 8) | 2.5 ( 5) |
| C3 | 0.9531 (15) | 0.7582 ( 6) | 0.3545 (11) | 3.0 ( 7) |
| C4 | 1.0877 (16) | 0.7456 ( 6) | 0.4524 (11) | 3.4 ( 7) |
| O5 | 1.1683 (11) | 0.6898 ( 5) | 0.4379 ( 8) | 4.0 ( 5) |
| C6 | 1.2295 (15) | 0.6966 ( 6) | 0.3537 (12) | 3.4 ( 7) |
| C7 | 1.1020 (15) | 0.7088 ( 6) | 0.2520 (11) | 2.9 ( 6) |
| N8 | 0.6999 (10) | 0.8537 ( 4) | 0.2145 ( 8) | 2.1 ( 4) |
| C9 | 0.5852 (15) | 0.8312 ( 6) | 0.2143 (10) | 2.9 ( 6) |
| C10 | 0.4376 (14) | 0.8009 ( 6) | 0.2080 (12) | 3.5 ( 7) |
| N11 | 1.0277 (10) | 0.9125 ( 4) | 0.3592 ( 8) | 2.0 ( 5) |
| C12 | 0.9801 (15) | 0.9104 ( 5) | 0.4442 (11) | 2.9 ( 7) |
| C13 | 1.0755 (16) | 0.9291 ( 6) | 0.5427 (11) | 3.2 ( 7) |
| C14 | 1.2211 (15) | 0.9514 ( 7) | 0.5522 (11) | 3.5 ( 7) |
| C15 | 1.2703 (15) | 0.9560 ( 6) | 0.4654 (11) | 3.1 ( 6) |
| C16 | 1.1732 (13) | 0.9371 ( 5) | 0.3675 (10) | 2.3 ( 6) |
| N21 | 1.0959 (10) | 0.9274 ( 4) | 0.1850 ( 8) | 1.9 ( 5) |
| C22 | 1.2156 (14) | 0.9425 ( 5) | 0.2726 (11) | 2.5 ( 6) |
| C23 | 1.3559 (14) | 0.9600 ( 6) | 0.2596 (11) | 3.2 ( 6) |
| C24 | 1.3722 (14) | 0.9625 ( 6) | 0.1623 (12) | 3.1 ( 7) |
| C25 | 1.2475 (14) | 0.9479 ( 6) | 0.0744 (11) | 2.8 ( 6) |
| C26 | 1.1063 (13) | 0.9288 ( 5) | 0.0894 ( 9) | 1.9 ( 5) |
| N31 | 0.8437 (10) | 0.8903 ( 4) | 0.0458 ( 7) | 2.1 ( 4) |
| C32 | 0.9588 (13) | 0.9110 ( 5) | 0.0074 (10) | 2.0 ( 5) |
| C33 | 0.9365 (15) | 0.9159 ( 6) | -0.0980 (11) | 2.7 ( 6) |
| C34 | 0.7942 (16) | 0.9004 ( 6) | -0.1694 (10) | 3.0 ( 6) |
| C35 | 0.6775 (15) | 0.8786 ( 6) | -0.1317 (11) | 3.1 ( 6) |
| C36 | 0.7046 (15) | 0.8741 ( 6) | -0.0256 (11) | 2.9 ( 6) |
| P1 | 0.6135 ( 5) | 0.66995 (22) | 0.0374 ( 3) | 4.31 (22) |
| F11 | 0.7005 (19) | 0.7022 ( 6) | -0.0273 (12) | 11.8 (11) |
| F12 | 0.736 ( 3) | 0.6226 (10) | 0.0708 (16) | 23.2 (22) |
| F13 | 0.5318 (20) | 0.6353 (11) | 0.1034 (10) | 19.1 (15) |
| F14 | 0.496 ( 3) | 0.7157 (15) | 0.0075 (15) | 30. ( 3) |
| F15 | 0.541 ( 3) | 0.6340 (12) | -0.0579 (10) | 25.4 (21) |
| F16 | 0.6934 (20) | 0.7024 ( 5) | 0.1399 ( 9) | 11.7 (10) |
| H3a | 0.900 | 0.796 | 0.362 | 3.9 |
| H3b | 0.880 | 0.724 | 0.341 | 3.9 |
| H4a | 1.048 | 0.740 | 0.510 | 4.2 |
| H4b | 1.159 | 0.780 | 0.466 | 4.2 |
| H6a | 1.305 | 0.730 | 0.367 | 4.2 |
| H6b | 1.280 | 0.658 | 0.348 | 4.2 |
| H7a | 1.031 | 0.674 | 0.233 | 3.7 |
| H7b | 1.150 | 0.716 | 0.198 | 3.7 |
| H10a | 0.417 | 0.806 | 0.273 | 4.6 |
| H10b | 0.354 | 0.820 | 0.153 | 4.6 |
| H10c | 0.443 | 0.758 | 0.193 | 4.6 |
| H12 | 0.875 | 0.896 | 0.436 | 3.7 |
| H13 | 1.039 | 0.925 | 0.602 | 4.0 |
| H14 | 1.288 | 0.966 | 0.619 | 4.1 |

| | | | | |
|---|---|---|---|---|
| H15 | 1.374 | 0.971 | 0.472 | 3.8 |
| H23 | 1.444 | 0.970 | 0.320 | 3.8 |
| H24 | 1.471 | 0.973 | 0.153 | 3.9 |
| H25 | 1.256 | 0.951 | 0.005 | 3.7 |
| H33 | 1.019 | 0.931 | -0.123 | 3.6 |
| H34 | 0.774 | 0.904 | -0.243 | 3.7 |
| H35 | 0.576 | 0.867 | -0.179 | 3.8 |
| H36 | 0.623 | 0.857 | -0.001 | 3.7 |

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

| | u11(U) | u22 | u33 | u12 | u13 | u23 |
|---|---|---|---|---|---|---|
| Os1 | 3.000(23) | 2.154(25) | 3.06( 3) | -0.41( 3) | 1.298(18) | 0.06( 3) |
| Cl1 | 3.38 (15) | 2.59 (17) | 3.63(19) | -0.02(13) | 1.47 (14) | 0.15(15) |
| N1 | 2.1 ( 5) | 3.2 ( 6) | 2.1 ( 6) | -0.1 ( 4) | 0.7 ( 4) | 0.5 ( 5) |
| N2 | 3.5 ( 6) | 2.0 ( 6) | 3.5 ( 7) | -0.2 ( 5) | 0.6 ( 5) | -0.5 ( 5) |
| C3 | 4.8 ( 8) | 2.5 ( 8) | 4.4 ( 9) | -0.7 ( 6) | 1.7 ( 7) | 0.8 ( 7) |
| C4 | 5.7 ( 9) | 3.2 ( 8) | 3.9 ( 9) | -1.0 ( 7) | 1.3 ( 7) | 0.7 ( 7) |
| O5 | 5.1 ( 6) | 4.5 ( 7) | 5.2 ( 7) | -0.5 ( 5) | 1.0 ( 5) | 1.4 ( 6) |
| C6 | 3.8 ( 7) | 3.5 ( 9) | 5.6 (10) | -0.7 ( 6) | 1.2 ( 7) | -0.5 ( 8) |
| C7 | 4.6 ( 8) | 1.9 ( 7) | 4.4 ( 9) | 0.6 ( 6) | 1.6 ( 7) | 1.1 ( 6) |
| N8 | 2.5 ( 5) | 2.5 ( 6) | 2.9 ( 6) | -0.5 ( 4) | 0.7 ( 4) | -0.4 ( 5) |
| C9 | 5.0 ( 8) | 2.6 ( 8) | 3.9 ( 9) | 0.7 ( 6) | 2.1 ( 7) | 0.8 ( 7) |
| C10 | 3.9 ( 8) | 4.1 ( 9) | 6.3 (10) | -0.5 ( 6) | 2.9 ( 8) | -0.1 ( 8) |
| N11 | 2.9 ( 5) | 1.4 ( 5) | 3.5 ( 7) | 0.3 ( 4) | 1.1 ( 5) | 0.8 ( 5) |
| C12 | 4.8 ( 8) | 2.0 ( 8) | 4.3 ( 9) | 0.3 ( 6) | 1.4 ( 7) | 0.2 ( 6) |
| C13 | 5.5 ( 9) | 3.6 ( 9) | 3.2 ( 9) | 0.5 ( 7) | 1.8 ( 7) | -0.2 ( 7) |
| C14 | 4.2 ( 8) | 4.2 ( 9) | 4.1 ( 9) | 0.3 ( 7) | 0.3 ( 7) | -0.1 ( 7) |
| C15 | 4.0 ( 7) | 3.4 ( 8) | 4.0 ( 9) | -0.5 ( 6) | 0.5 ( 7) | -0.5 ( 7) |
| C16 | 2.9 ( 6) | 1.5 ( 6) | 4.1 ( 8) | 0.3 ( 5) | 0.5 ( 6) | -0.1 ( 6) |
| N21 | 2.4 ( 5) | 1.5 ( 5) | 3.2 ( 6) | 0.3 ( 4) | 0.9 ( 4) | 0.4 ( 5) |
| C22 | 3.4 ( 7) | 1.7 ( 7) | 4.5 ( 9) | -0.2 ( 5) | 1.5 ( 6) | -0.1 ( 6) |
| C23 | 3.7 ( 7) | 2.7 ( 8) | 5.0 (10) | 0.6 ( 6) | 0.4 ( 7) | 0.2 ( 7) |
| C24 | 3.0 ( 7) | 2.3 ( 7) | 6.6 (10) | -0.5 ( 5) | 1.8 ( 7) | 0.5 ( 7) |
| C25 | 3.8 ( 7) | 2.2 ( 7) | 5.0 ( 9) | 0.7 ( 6) | 2.1 ( 7) | 0.5 ( 7) |
| C26 | 3.1 ( 6) | 1.6 ( 7) | 2.7 ( 8) | 0.1 ( 5) | 1.4 ( 5) | 0.4 ( 6) |
| N31 | 3.5 ( 5) | 1.0 ( 5) | 3.9 ( 6) | 0.1 ( 5) | 1.6 ( 4) | 0.0 ( 5) |
| C32 | 3.5 ( 6) | 1.0 ( 6) | 3.2 ( 8) | 0.6 ( 5) | 1.4 ( 6) | -0.1 ( 5) |
| C33 | 4.6 ( 8) | 1.6 ( 6) | 4.5 ( 9) | 0.4 ( 5) | 1.9 ( 7) | -0.2 ( 6) |
| C34 | 5.8 ( 8) | 2.7 ( 8) | 2.6 ( 7) | 1.1 ( 6) | 0.8 ( 6) | -0.1 ( 6) |
| C35 | 4.0 ( 7) | 3.5 ( 9) | 4.0 ( 8) | -0.1 ( 6) | 0.6 ( 6) | -0.1 ( 7) |
| C36 | 4.0 ( 7) | 2.9 ( 8) | 4.3 ( 9) | -1.0 ( 6) | 1.8 ( 6) | -0.3 ( 7) |
| P1 | 5.34 (23) | 6.5 ( 3) | 4.6 ( 3) | -0.68(22) | 1.58 (20) | -0.49(25) |
| F11 | 21.4 (16) | 10.8 (11) | 17.0 (14) | -3.3 (10) | 12.1 (13) | 1.5 (10) |
| F12 | 54. ( 4) | 22.2 (20) | 21.8 (21) | 29. ( 3) | 26. ( 3) | 11.8 (17) |
| F13 | 19.8 (16) | 46. ( 3) | 5.9 ( 9) | -23.6 (19) | 2.3 ( 9) | 0.1 (14) |
| F14 | 32. ( 3) | 69. ( 5) | 16.6 (18) | 44. ( 3) | 14.2 (19) | 24. ( 3) |
| F15 | 51. ( 4) | 36. ( 3) | 3.8 ( 8) | -38. ( 3) | 1.9 (14) | -4.9 (13) |
| F16 | 24.4 (16) | 6.8 ( 9) | 8.3 (10) | -1.5 (10) | -2.0 (10) | 1.0 ( 7) |
| H3a | 4.9 | | | | | |
| H3b | 4.9 | | | | | |
| H4a | 5.3 | | | | | |
| H4b | 5.3 | | | | | |
| H6a | 5.3 | | | | | |
| H6b | 5.3 | | | | | |
| H7a | 4.7 | | | | | |
| H7b | 4.7 | | | | | |
| H10a | 5.8 | | | | | |
| H10b | 5.8 | | | | | |
| H10c | 5.8 | | | | | |
| H12 | 4.7 | | | | | |
| H13 | 5.1 | | | | | |
| H14 | 5.2 | | | | | |