lel zu den mit Barium- und Sauerstoff-Ionen dichtest besetzten Ebenen.

Herrn Professor Dr O. W. Flörke danke ich vielmals für die Anregung zu dieser Arbeit, Dr K. Sahl, Dr K. Hanke und Dr V. Kupcik danke ich für viele klärende Diskussionen. Die Rechnungen wurden auf einer IBM 7040-Anlage in Göttingen und einer IBM 360/50-Anlage in Münster durchgeführt. Programme stellten Dr P. Süsse, Dr K. Sahl, Dr V. Kupcik, B. Neukäter und Frl H. v. Mertens zur Verfügung. Herrn Dr Schneider, Göttingen, danke ich für die Analyse mit der Mikrosonde.

### Literatur

ANDERSSON, S. & WADSLEY, A. D. (1961). *Acta Cryst*, **14**, 1245.
ANDERSSON, S. & WADSLEY, A. D. (1962). *Acta Cryst.* **15**, 194.
BERGHUIS, J., HAANAPPEL, IJ. M., POTTERS, M., LOOPSTRA, B. O., MACGILLAVRY, C. H. & VEENENDAAL, A. L. (1955) *Acta Cryst.* **8**, 478.
BERRY, K. L., AFTANDILIAN, V. D., GILBERT, W. W., MEIBOHM, E. P. H. & YOUNG, H. S. (1960). *J. Inorg. Nucl. Chem.* **14**, 231.
BURBANK, R. D. & EVANS, H. T. JR. (1948). *Acta Cryst.* **1**, 330.
CID-DRESDNER, H. & BUERGER, M. J. (1962). *Z. Kristallogr.* **117**, 411.
HAMILTON, W. C. (1955). *Acta Cryst.* **8**, 185.
HARRISON, F. W. (1956). *Acta Cryst.* **9**, 198.
HARRISON, F. W. (1956). *Acta Cryst.* **9**, 495.
LUKASZEWICZ, K. (1957). *Roczn. Chem.* **31**, 1111.
LUKASZEWICZ, K. & TRZEBIATOWSKI, W. (1955). *Roczn. Chem.* **29**, 942.
MEGAW, H. D. (1946). *Proc. Phys. Soc. (London)* **58**, 133.
PAULING, L. & SHERMAN, J. (1932). *Z. Kristallogr.* **81**, 1.
QURASHI, M. M. (1954). *Acta Cryst.* **7**, 310.

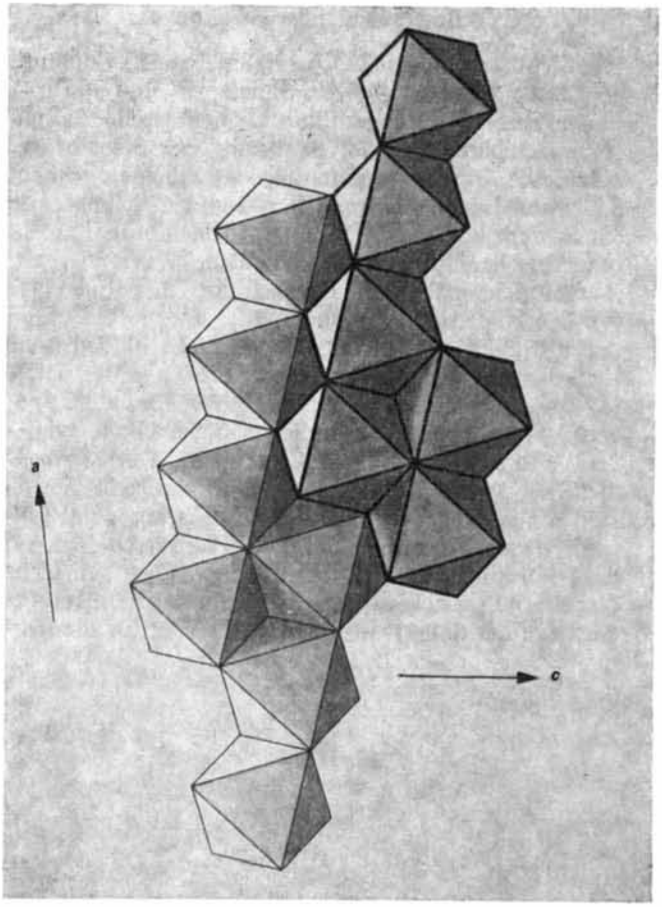

Fig. 4. Doppelkette aus zwei in *b*-Richtung übereinanderliegenden Einzelketten. Die Verknüpfung erfolgt über gemeinsame Ecken.

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*Acta Cryst.* (1969). B**25**, 1452

# The Crystal and Ionic Structures of Potassium Picrate and Ammonium Picrate

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(*Received* 12 *July* 1968)

Crystals of potassium picrate [2,4,6-trinitrophenoxide, $(NO_2)_3C_6H_2O)^-$] and ammonium picrate are orthorhombic, space group *Ibca* (No. 73), with cell dimensions 13·33, 19·09, 7·14 Å, and 13·45, 19·74, 7·12 Å. Both unit cells contain eight formula units. The phenoxide carbon–oxygen bond length is found to be 1·23 Å, and the carbon(1)–carbon(2) bond lengths 1·45 Å, while the other carbon–carbon bond lengths are 1·37 Å. The bond angle at carbon(1) in the benzene ring is 111°.

## Introduction

It is known from a number of crystal structure investigations of substituted benzenes and phenols that the bond angles, and to some extent also bond lengths, within the benzene ring are influenced by the substituents. The author thought it of interest to analyse derivatives of phenols in the form of phenoxides. These compounds seem to have been neglected by crystallographers and no earlier work in the field has been found in the literature.

## Experimental

Potassium picrate and ammonium picrate crystallize, in the form of long thin needles, from warm aqueous solutions of picric acid upon neutralization with potassium or ammonium hydroxide. Potassium picrate gives deep brown crystals, while the colour of the ammonium salt is orange-yellow.

The unit-cell dimensions and systematic absences were determined from oscillation and Weissenberg photographs of crystals mounted parallel to the shortest and next-shortest principal axes. The crystals were covered with finely ground sodium chloride before taking the Weissenberg photographs from which the unit-cell dimensions were determined, by use of the powder lines for calibration (NaCl, $d_{100} = 5{\cdot}640$ Å). Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å) was used for these as well as for all intensity photographs. All recordings were done at room temperature.

For the recording of the intensities, the crystals were cut to about cubical shape with the side-edge approximately 0·2 mm. The Weissenberg films were integrated and the multiple film technique was used. In the case of potassium picrate the following layers were recorded: $hk0$, $hk1$, $hk2$, $hk3$, $hk4$ and $0kl$, $1kl$, $2kl$. The relative intensities were measured with a densitometer. On these layers 758 independent reflexions are possible within $\sin\theta = 0{\cdot}97$, of these 199 were too weak to be measured. For ammonium picrate, only the $hk0$, $hk1$, $hk2$, $hk3$, and $hk4$ layers were recorded, and the relative intensities were estimated visually. Here, within $\sin\theta = 0{\cdot}97$, 703 reflexions are possible of which 79 were found below the observable intensity minimum.

*Crystal data*

Space group *Ibca* (No. 73).

| | Potassium picrate | Ammonium picrate |
|---|---|---|
| $a$ | $13{\cdot}32_5$ | $13{\cdot}45 \pm 0{\cdot}04$ Å |
| $b$ | 19·09 | $19{\cdot}74 \pm 0{\cdot}05$ |
| $c$ | 7·14 | $7{\cdot}12 \pm 0{\cdot}02$ |
| Density, experimental | 1·93 | 1·73 g.cm$^{-3}$ |
| Density, calculated | 1·96 | 1·71 |
| Formula units per unit cell | 8 | 8 |

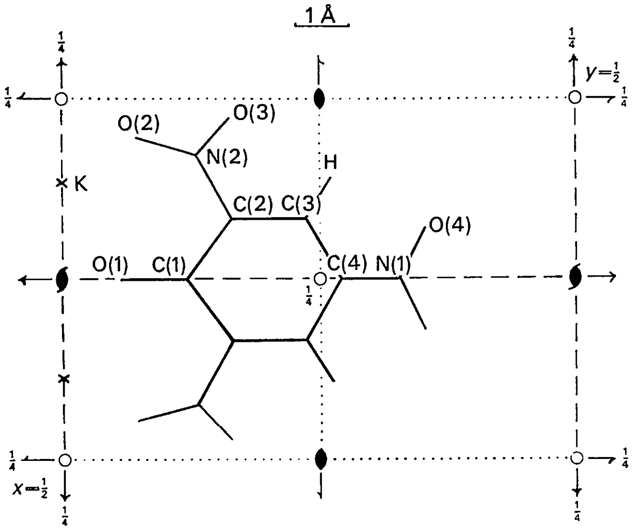

Fig. 1. The positions of the atoms of one formula unit of potassium picrate in the (001) projection.

## Structure analysis of potassium picrate

The measured intensities were corrected for spot extension, and the usual Lorentz and polarization factors applied. The relative structure amplitudes were put to the same scale by comparison of the values of common reflexions in the $hk0$–$hk4$ and the $0kl$–$2kl$ sets.

The space group *Ibca* has sixteenfold general positions, and with only 8 formula units per unit cell it is implied that O(1), C(1), C(4) and N(1) (Fig. 1) are situated on a twofold axis and most likely on one parallel to the $b$ axis. The potassium ion must lie on a twofold axis or on a centre of symmetry.

A three-dimensional Patterson synthesis yielded the necessary rough information on which a trial solution could be based. A model of the trinitrophenoxide ion was constructed assuming a regular benzene ring with carbon–carbon bonds of 1·38 Å, a carbon–oxygen bond of 1·35 Å, carbon–nitrogen bonds of 1·48 Å and nitrogen–oxygen bonds of 1·22 Å. All bond angles were assumed to be 120°. The nitro groups were, for the sake of simplicity, put coplanar with the benzene ring. On the basis of the vector density map this model of the trinitrophenoxide ion was placed as outlined above with the centre of the benzene ring at (0·25, 0·21, 0) and the normal to the plane of the molecule inclined 30° to the $c$ axis. The position of the potassium ion was fairly well indicated in the vector density map and was taken to be (0·125, 0, 0·25), which is on the twofold axis parallel to the $a$ axis. Calculated structure amplitudes based on these coordinates compared well enough with the experimental ones to allow progression directly to full-matrix least-squares refinement. The first iterations were carried out by use of isotropic temperature factors and fixed scale factors for the structure amplitudes belonging to the different layers. When an agreement residual of $R = \Sigma\,||F_{\text{exp}}| - |F_{\text{calc}}||/\,\Sigma\,|F_{\text{exp}}| = 0{\cdot}25$ was reached, the scale factors were allowed to vary. The hydrogen atom bonded to the benzene ring was included in the refinement at this stage, initially assuming a carbon–hydrogen bond length of 1·0 Å and the hydrogen atom to be coplanar with the benzene ring and equidistant from the *ortho* and *para* carbon atoms. At an agreement residual of 0·12, the least-squares refinement was interrupted and the experimental structure amplitudes corrected for secondary extinction (Zachariasen, 1963), neglecting absorption. Duplicate structure amplitudes were averaged and one common scale factor introduced. The last least-squares iterations were performed with anisotropic temperature factors for all atoms except hydrogen. The refinement converged with an agreement residual of 0·05.

The final atomic coordinates and temperature parameters are given in Table 1, and the experimental and calculated structure amplitudes in Table 3. The weights assigned the reflecting planes in the least-squares calculations are given by $(a + |F_{\text{exp}}| + c|F_{\text{exp}}|^2)^{-1}$, where $a = 20$ and $c = 0{\cdot}02$ (Rollet, 1965). The function minimized was $w(|F_{\text{exp}}| - |F_{\text{calc}}|)^2$. Unobserved reflexions were given zero weight where the calculated structure amplitudes were found less in value, but assigned the weight given by the weighting function if found greater in value than that corresponding to the observable intensity minimum. Atomic scattering factors used for the calculation of structure amplitudes were those given in *International Tables for X-ray Crystallography* (1962).

Table 1. *Positional and temperature parameters of potassium picrate*

The temperature parameters refer to the expressions:

$$\exp\left[-B(\sin\theta/\lambda)^2\right] \text{ and } \exp\left[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{23}kl+2\beta_{13}hl+2\beta_{12}hk)\right].$$

| | $x$ | $y$ | $z$ | $B$ | $\beta_{11}$ | $\beta_{22}$ | $\beta_{33}$ | $\beta_{23}$ | $\beta_{13}$ | $\beta_{12}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| K | 0·11697 | 0·0 | 0·25000 | | 0·00353 | 0·00149 | 0·01611 | −0·00001 | 0·0 | 0·0 |
| | 0·00009 | 0·0 | 0·0 | | 0·00006 | 0·00006 | 0·00032 | 0·00010 | 0·0 | 0·0 |
| O(1) | 0·25000 | 0·05656 | 0·0 | | 0·00372 | 0·00147 | 0·02744 | 0·0 | 0·00087 | 0·0 |
| | 0·0 | 0·00022 | 0·0 | | 0·00024 | 0·00012 | 0·00140 | 0·0 | 0·00051 | 0·0 |
| O(2) | 0·05469 | 0·07195 | −0·08275 | | 0·00458 | 0·00203 | 0·02744 | −0·00006 | −0·00176 | −0·00094 |
| | 0·00025 | 0·00018 | 0·00063 | | 0·00020 | 0·00009 | 0·00119 | 0·00026 | 0·00038 | 0·00012 |
| O(3) | 0·02622 | 0·16333 | −0·25266 | | 0·00490 | 0·00317 | 0·02220 | 0·00027 | −0·00343 | 0·00003 |
| | 0·00024 | 0·00020 | 0·00067 | | 0·00021 | 0·00011 | 0·00107 | 0·00030 | 0·00043 | 0·00013 |
| O(4) | 0·17847 | 0·37739 | −0·07122 | | 0·00629 | 0·00181 | 0·03035 | 0·00146 | −0·00175 | 0·00063 |
| | 0·00031 | 0·00018 | 0·00064 | | 0·00023 | 0·00009 | 0·00126 | 0·00027 | 0·00045 | 0·00012 |
| N(1) | 0·25000 | 0·34684 | 0·0 | | 0·00467 | 0·00168 | 0·01104 | 0·0 | 0·00039 | 0·0 |
| | 0·0 | 0·00027 | 0·0 | | 0·00033 | 0·00014 | 0·00133 | 0·0 | 0·00062 | 0·0 |
| N(2) | 0·07723 | 0·13099 | −0·13818 | | 0·00349 | 0·00177 | 0·01620 | −0·00063 | −0·00064 | −0·00004 |
| | 0·00028 | 0·00020 | 0·00064 | | 0·00019 | 0·00009 | 0·00110 | 0·00026 | 0·00040 | 0·00011 |
| C(1) | 0·25000 | 0·12167 | 0·0 | | 0·00322 | 0·00156 | 0·01539 | 0·0 | 0·00135 | 0·0 |
| | 0·0 | 0·00031 | 0·0 | | 0·00030 | 0·00016 | 0·00166 | 0·0 | 0·00064 | 0·0 |
| C(2) | 0·16651 | 0·16469 | −0·06227 | | 0·00286 | 0·00159 | 0·01231 | −0·00032 | 0·00064 | −0·00014 |
| | 0·00030 | 0·00022 | 0·00072 | | 0·00022 | 0·00010 | 0·00102 | 0·00026 | 0·00040 | 0·00011 |
| C(3) | 0·16657 | 0·23655 | −0·06642 | | 0·00368 | 0·00163 | 0·01155 | −0·00004 | 0·00062 | 0·00024 |
| | 0·00030 | 0·00021 | 0·00071 | | 0·00022 | 0·00012 | 0·00097 | 0·00025 | 0·00043 | 0·00013 |
| C(4) | 0·25000 | 0·27164 | 0·0 | | 0·00353 | 0·00132 | 0·01394 | 0·0 | 0·00045 | 0·0 |
| | 0·0 | 0·00030 | 0·0 | | 0·00029 | 0·00013 | 0·00170 | 0·0 | 0·00060 | 0·0 |
| H | 0·10833 | 0·26146 | −0·11837 | 0·60 | | | | | | |
| | 0·00400 | 0·00319 | 0·00875 | 0·90 | | | | | | |

Table 2. *Positional and temperature parameters of ammonium picrate*

*Cf.* legend of Table 1.

| | $x$ | $y$ | $z$ | $B$ | $\beta_{11}$ | $\beta_{22}$ | $\beta_{33}$ | $\beta_{23}$ | $\beta_{13}$ | $\beta_{12}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| N | 0·11652 | 0·0 | 0·0 | | 0·00264 | 0·00101 | 0·00485 | −0·00018 | 0·0 | 0·0 |
| | 0·00039 | 0·0 | 0·0 | | 0·0024 | 0·00010 | 0·00236 | 0·00033 | 0·0 | 0·0 |
| H(1) | 0·14916 | 0·01068 | 0·14639 | 2·55 | | | | | | |
| | 0·00495 | 0·00318 | 0·01153 | 1·46 | | | | | | |
| H(2) | 0·07665 | 0·03235 | 0·29644 | 2·18 | | | | | | |
| | 0·00494 | 0·00338 | 0·01088 | 1·46 | | | | | | |
| O(1) | 0·25000 | 0·06512 | 0·0 | | 0·00257 | 0·00092 | 0·01030 | 0·0 | 0·00217 | 0·0 |
| | 0·0 | 0·00018 | 0·0 | | 0·00019 | 0·00008 | 0·00167 | 0·0 | 0·00039 | 0·0 |
| O(2) | 0·05701 | 0·07928 | −0·08162 | | 0·00344 | 0·00167 | 0·02069 | 0·00010 | −0·00126 | −0·00080 |
| | 0·00022 | 0·00016 | 0·00066 | | 0·00017 | 0·00008 | 0·00154 | 0·00022 | 0·00035 | 0·00009 |
| O(3) | 0·02666 | 0·16857 | −0·24469 | | 0·00337 | 0·00233 | 0·01050 | −0·00023 | −0·00275 | 0·00024 |
| | 0·00021 | 0·00017 | 0·00062 | | 0·00016 | 0·00009 | 0·00141 | 0·00025 | 0·00031 | 0·00009 |
| O(4) | 0·17721 | 0·37504 | −0·06072 | | 0·00578 | 0·00125 | 0·02456 | 0·00104 | −0·00201 | 0·00086 |
| | 0·00026 | 0·00016 | 0·00065 | | 0·00022 | 0·00008 | 0·00168 | 0·00022 | 0·00043 | 0·00010 |
| N(1) | 0·25000 | 0·34622 | 0·0 | | 0·00418 | 0·00105 | 0·00480 | 0·0 | −0·00001 | 0·0 |
| | 0·0 | 0·00023 | 0·0 | | 0·00028 | 0·00011 | 0·00211 | 0·0 | 0·00053 | 0·0 |
| N(2) | 0·07776 | 0·13701 | −0·13650 | | 0·00212 | 0·00146 | 0·00419 | −0·00085 | −0·00041 | −0·00007 |
| | 0·00023 | 0·00016 | 0·00064 | | 0·00015 | 0·00008 | 0·00137 | 0·00023 | 0·00033 | 0·00008 |
| C(1) | 0·25000 | 0·12788 | 0·0 | | 0·00160 | 0·00111 | 0·00045 | 0·0 | 0·00030 | 0·0 |
| | 0·0 | 0·00024 | 0·0 | | 0·00023 | 0·00011 | 0·00222 | 0·0 | 0·00046 | 0·0 |
| C(2) | 0·16679 | 0·16925 | −0·06023 | | 0·00192 | 0·00128 | 0·00027 | −0·00014 | −0·00010 | −0·00002 |
| | 0·00024 | 0·00019 | 0·00069 | | 0·00018 | 0·00009 | 0·00177 | 0·00023 | 0·00036 | 0·00009 |
| C(3) | 0·16730 | 0·23877 | −0·06194 | | 0·00289 | 0·00119 | 0·00030 | 0·00061 | 0·00001 | 0·00025 |
| | 0·00026 | 0·00018 | 0·00068 | | 0·00019 | 0·00010 | 0·00164 | 0·00022 | 0·00038 | 0·00009 |
| C(4) | 0·25000 | 0·27243 | 0·0 | | 0·00325 | 0·00081 | 0·00446 | 0·0 | 0·00116 | 0·0 |
| | 0·0 | 0·00025 | 0·0 | | 0·00027 | 0·00010 | 0·00236 | 0·0 | 0·00057 | 0·0 |
| H | 0·10871 | 0·25951 | −0·12366 | 8·05 | | | | | | |
| | 0·00775 | 0·00575 | 0·01777 | 2·90 | | | | | | |

## Table 3. *Experimental and calculated structure amplitudes of potassium picrate*

Experimental structure amplitudes marked negative are unobserved; the value corresponds to the observable minimum. The values listed are $F_{\exp} \times 10$ and $F_{\mathrm{cal}} \times 10$.

| | | | | |
|---|---|---|---|---|
| 0 | 2 | 0 | 85 | -69 |
| 0 | 4 | 0 | 1350 | -1543 |
| 0 | 6 | 0 | 1038 | 1096 |
| 0 | 8 | 0 | 1678 | 1701 |
| 0 | 10 | 0 | 867 | -810 |
| 0 | 12 | 0 | 907 | 874 |
| 0 | 14 | 0 | 978 | 899 |
| 0 | 16 | 0 | 563 | 522 |
| 0 | 18 | 0 | 843 | 800 |
| 0 | 20 | 0 | 148 | -144 |
| 0 | 22 | 0 | 148 | 111 |
| 0 | 24 | 0 | 354 | 395 |
| 2 | 0 | 0 | 730 | -771 |
| 2 | 2 | 0 | 791 | 792 |
| 2 | 4 | 0 | 290 | -288 |
| 2 | 6 | 0 | 525 | 535 |
| 2 | 8 | 0 | 821 | -851 |
| 2 | 10 | 0 | 267 | 262 |
| 2 | 12 | 0 | 667 | 679 |
| 2 | 14 | 0 | 322 | 337 |
| 2 | 16 | 0 | -118 | -49 |
| 2 | 18 | 0 | 275 | -293 |
| 2 | 20 | 0 | -110 | -29 |
| 2 | 22 | 0 | -90 | 6 |
| 2 | 24 | 0 | 70 | 78 |
| 4 | 0 | 0 | 126 | 98 |
| 4 | 2 | 0 | 790 | -831 |
| 4 | 4 | 0 | 1395 | -1452 |
| 4 | 6 | 0 | 714 | -691 |
| 4 | 8 | 0 | 1417 | -1453 |
| 4 | 10 | 0 | 1078 | -1068 |
| 4 | 12 | 0 | 432 | -423 |
| 4 | 14 | 0 | 329 | -324 |
| 4 | 16 | 0 | 578 | -561 |
| 4 | 18 | 0 | 136 | -128 |
| 4 | 20 | 0 | 262 | -242 |
| 4 | 22 | 0 | 310 | -320 |
| 6 | 0 | 0 | 358 | -420 |
| 6 | 2 | 0 | 1133 | -1182 |
| 6 | 4 | 0 | 133 | -127 |
| 6 | 6 | 0 | 368 | 339 |
| 6 | 8 | 0 | -105 | 43 |
| 6 | 10 | 0 | -118 | -49 |
| 6 | 12 | 0 | 339 | 339 |
| 6 | 14 | 0 | 653 | -669 |
| 6 | 16 | 0 | 367 | -348 |
| 6 | 18 | 0 | -123 | 18 |
| 6 | 20 | 0 | 129 | -110 |
| 6 | 22 | 0 | 172 | -186 |
| 8 | 0 | 0 | 106 | 89 |
| 8 | 2 | 0 | 505 | 455 |
| 8 | 4 | 0 | 1110 | 1113 |
| 8 | 6 | 0 | 876 | 846 |
| 8 | 8 | 0 | 281 | 270 |
| 8 | 10 | 0 | 380 | 371 |
| 8 | 12 | 0 | 448 | 414 |
| 8 | 14 | 0 | -125 | 28 |
| 8 | 18 | 0 | 457 | 435 |
| 8 | 20 | 0 | 450 | 459 |
| 10 | 0 | 0 | 765 | -743 |
| 10 | 2 | 0 | 268 | 251 |
| 10 | 4 | 0 | 328 | 302 |
| 10 | 6 | 0 | 437 | 472 |
| 10 | 8 | 0 | 501 | 465 |
| 10 | 10 | 0 | 553 | 545 |
| 10 | 12 | 0 | -130 | -38 |
| 10 | 14 | 0 | -123 | -34 |
| 10 | 16 | 0 | 105 | 116 |
| 10 | 18 | 0 | -88 | -23 |
| 12 | 0 | 0 | 512 | 495 |
| 12 | 2 | 0 | 655 | -639 |
| 12 | 4 | 0 | 544 | -519 |
| 12 | 6 | 0 | 274 | -241 |
| 12 | 8 | 0 | -129 | 112 |
| 12 | 10 | 0 | 631 | -614 |
| 12 | 12 | 0 | 446 | -404 |
| 12 | 14 | 0 | 257 | -242 |
| 12 | 16 | 0 | -79 | -73 |
| 14 | 0 | 0 | 652 | -673 |
| 14 | 2 | 0 | -122 | -34 |
| 14 | 4 | 0 | 164 | -140 |
| 14 | 6 | 0 | 214 | -192 |
| 14 | 8 | 0 | 186 | -204 |
| 14 | 10 | 0 | -57 | -14 |
| 14 | 12 | 0 | 235 | -254 |
| 14 | 14 | 0 | 55 | -61 |
| 16 | 0 | 0 | 285 | 292 |
| 16 | 2 | 0 | 319 | 303 |
| 16 | 4 | 0 | -83 | 96 |
| 16 | 6 | 0 | -114 | -29 |
| 16 | 8 | 0 | 171 | 160 |
| 1 | 2 | 1 | 904 | -904 |
| 1 | 4 | 1 | 549 | -558 |
| 1 | 6 | 1 | 812 | -823 |
| 1 | 8 | 1 | 181 | -148 |
| 1 | 10 | 1 | 618 | 592 |
| 1 | 12 | 1 | 331 | 309 |
| 1 | 14 | 1 | -111 | -9 |
| 1 | 16 | 1 | 159 | 170 |
| 1 | 18 | 1 | 152 | -154 |
| 1 | 20 | 1 | -110 | -50 |
| 1 | 22 | 1 | -51 | -50 |
| 2 | 1 | 1 | 503 | -475 |
| 2 | 3 | 1 | 1873 | -1943 |
| 2 | 5 | 1 | 988 | -1053 |
| 2 | 7 | 1 | 836 | -868 |
| 2 | 9 | 1 | 1145 | -1201 |
| 2 | 11 | 1 | 748 | -783 |
| 2 | 13 | 1 | 261 | -249 |
| 2 | 15 | 1 | 520 | -518 |
| 2 | 17 | 1 | 379 | -363 |
| 2 | 19 | 1 | 420 | -429 |
| 2 | 21 | 1 | 304 | -322 |
| 2 | 23 | 1 | 222 | -244 |
| 3 | 2 | 1 | 1004 | -1077 |
| 3 | 4 | 1 | 237 | 246 |
| 3 | 6 | 1 | 353 | 367 |
| 3 | 8 | 1 | 152 | 127 |
| 3 | 10 | 1 | -108 | -42 |
| 3 | 12 | 1 | 411 | 394 |
| 3 | 14 | 1 | 251 | -265 |
| 3 | 16 | 1 | 268 | -257 |
| 3 | 18 | 1 | 143 | -133 |
| 3 | 20 | 1 | -124 | 89 |
| 3 | 22 | 1 | -59 | 81 |
| 4 | 1 | 1 | 539 | 556 |
| 4 | 3 | 1 | 981 | -1022 |
| 4 | 5 | 1 | 852 | -867 |
| 4 | 7 | 1 | 258 | 257 |
| 4 | 9 | 1 | 281 | -266 |
| 4 | 11 | 1 | 324 | -307 |
| 4 | 13 | 1 | -129 | -131 |
| 4 | 15 | 1 | 264 | 256 |
| 4 | 17 | 1 | -139 | -34 |
| 4 | 19 | 1 | 156 | -152 |
| 4 | 21 | 1 | 201 | -202 |
| 5 | 2 | 1 | 848 | -857 |
| 5 | 4 | 1 | 1667 | -1650 |
| 5 | 6 | 1 | 431 | 411 |
| 5 | 8 | 1 | 288 | 281 |
| 5 | 10 | 1 | -117 | 11 |
| 5 | 12 | 1 | -128 | -42 |
| 5 | 14 | 1 | 983 | 965 |
| 5 | 16 | 1 | 368 | -361 |
| 5 | 18 | 1 | 329 | -309 |
| 5 | 20 | 1 | 116 | -99 |
| 5 | 22 | 1 | 170 | 178 |
| 6 | 1 | 1 | 1347 | 1349 |
| 6 | 3 | 1 | 347 | 350 |
| 6 | 5 | 1 | 787 | 813 |
| 6 | 7 | 1 | 708 | 701 |
| 6 | 9 | 1 | 174 | 160 |
| 6 | 11 | 1 | 631 | 621 |
| 6 | 13 | 1 | 761 | 740 |
| 6 | 15 | 1 | 379 | 351 |
| 6 | 17 | 1 | 352 | 330 |
| 6 | 19 | 1 | 291 | 285 |
| 6 | 21 | 1 | 164 | 177 |
| 7 | 2 | 1 | -104 | 82 |
| 7 | 4 | 1 | 550 | 539 |
| 7 | 6 | 1 | 633 | -600 |
| 7 | 8 | 1 | -121 | 52 |
| 7 | 10 | 1 | 469 | 469 |
| 7 | 12 | 1 | 421 | 389 |
| 7 | 14 | 1 | 859 | -871 |
| 7 | 16 | 1 | -135 | 39 |
| 7 | 18 | 1 | -122 | 73 |
| 7 | 20 | 1 | 110 | 99 |
| 8 | 1 | 1 | 443 | 423 |
| 8 | 3 | 1 | -114 | -83 |
| 8 | 5 | 1 | 554 | 575 |
| 8 | 7 | 1 | 192 | 173 |
| 8 | 9 | 1 | 188 | -181 |
| 8 | 11 | 1 | 401 | 386 |
| 8 | 13 | 1 | 481 | 466 |
| 8 | 15 | 1 | 184 | -182 |
| 8 | 17 | 1 | 163 | 163 |
| 8 | 19 | 1 | 181 | 156 |
| 9 | 2 | 1 | -122 | -87 |
| 9 | 4 | 1 | 427 | -416 |
| 9 | 6 | 1 | -129 | -20 |
| 9 | 8 | 1 | -134 | 119 |
| 9 | 10 | 1 | -138 | 61 |
| 9 | 12 | 1 | 191 | -176 |
| 9 | 14 | 1 | 269 | 258 |
| 9 | 16 | 1 | -123 | 52 |
| 9 | 18 | 1 | 109 | -77 |
| 9 | 20 | 1 | 103 | -110 |
| 10 | 1 | 1 | 480 | -481 |
| 10 | 3 | 1 | 558 | -565 |
| 10 | 5 | 1 | 328 | -320 |
| 10 | 7 | 1 | 306 | -299 |
| 10 | 9 | 1 | 542 | -505 |
| 10 | 11 | 1 | 175 | -166 |
| 10 | 13 | 1 | 311 | -309 |
| 10 | 15 | 1 | 373 | -363 |
| 10 | 17 | 1 | 247 | -259 |
| 10 | 19 | 1 | 78 | -88 |
| 11 | 2 | 1 | 444 | 416 |
| 11 | 4 | 1 | 185 | 173 |
| 11 | 6 | 1 | -139 | 55 |
| 11 | 8 | 1 | -135 | 46 |
| 11 | 10 | 1 | -136 | -68 |
| 11 | 12 | 1 | 158 | -149 |
| 11 | 14 | 1 | 123 | -106 |
| 11 | 16 | 1 | 135 | -127 |
| 11 | 18 | 1 | 178 | 189 |
| 12 | 1 | 1 | 322 | -303 |
| 12 | 3 | 1 | 337 | -322 |
| 12 | 5 | 1 | -138 | -29 |
| 12 | 7 | 1 | -137 | -109 |
| 12 | 9 | 1 | 350 | -322 |
| 12 | 11 | 1 | 124 | -79 |
| 12 | 13 | 1 | 112 | -100 |
| 12 | 15 | 1 | 269 | -289 |
| 12 | 17 | 1 | 127 | -161 |
| 13 | 2 | 1 | -135 | 19 |
| 13 | 4 | 1 | -134 | 100 |
| 13 | 6 | 1 | -131 | -57 |
| 13 | 8 | 1 | -125 | -116 |
| 13 | 10 | 1 | -116 | 14 |
| 13 | 12 | 1 | -103 | -35 |
| 13 | 14 | 1 | -64 | -25 |
| 14 | 1 | 1 | 291 | 251 |
| 14 | 3 | 1 | -125 | 11 |
| 14 | 5 | 1 | 317 | 295 |
| 14 | 7 | 1 | 349 | 357 |
| 14 | 9 | 1 | 160 | 166 |
| 14 | 11 | 1 | 119 | 128 |
| 14 | 13 | 1 | 162 | 189 |
| 15 | 2 | 1 | -111 | -20 |
| 15 | 4 | 1 | 212 | 227 |
| 15 | 6 | 1 | 106 | 120 |
| 15 | 8 | 1 | -75 | -34 |
| 15 | 10 | 1 | 167 | -178 |
| 15 | 12 | 1 | 41 | 5 |
| 16 | 1 | 1 | 188 | 204 |
| 16 | 3 | 1 | -87 | 82 |
| 16 | 5 | 1 | 108 | 113 |
| 16 | 7 | 1 | 240 | 267 |
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| 0 | 4 | 2 | 1184 | -1188 |
| 0 | 6 | 2 | 2099 | -2153 |
| 0 | 8 | 2 | 483 | -476 |
| 0 | 10 | 2 | 1117 | -1100 |
| 0 | 12 | 2 | 884 | -847 |
| 0 | 14 | 2 | 358 | -370 |
| 0 | 16 | 2 | 152 | -137 |
| 0 | 18 | 2 | 158 | -133 |
| 0 | 20 | 2 | 468 | -471 |
| 0 | 22 | 2 | 329 | -343 |
| 1 | 1 | 2 | 1811 | 1574 |
| 1 | 3 | 2 | 1037 | 1024 |
| 1 | 5 | 2 | 73 | -81 |
| 1 | 7 | 2 | 470 | -481 |
| 1 | 9 | 2 | 255 | 256 |
| 1 | 11 | 2 | 299 | -270 |
| 1 | 13 | 2 | 312 | -304 |
| 1 | 15 | 2 | -118 | -39 |
| 1 | 17 | 2 | 311 | 322 |
| 1 | 19 | 2 | 191 | 185 |
| 1 | 21 | 2 | 121 | -142 |
| 1 | 23 | 2 | 89 | -103 |
| 2 | 0 | 2 | 2978 | -2926 |
| 2 | 2 | 2 | 817 | 858 |
| 2 | 4 | 2 | 770 | 774 |
| 2 | 6 | 2 | 812 | -859 |
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| 2 | 10 | 2 | 722 | 704 |
| 2 | 12 | 2 | -106 | -95 |
| 2 | 14 | 2 | -115 | 62 |
| 2 | 16 | 2 | -119 | 29 |
| 2 | 18 | 2 | 410 | -430 |
| 2 | 20 | 2 | -104 | -2 |
| 2 | 22 | 2 | -82 | 21 |
| 3 | 1 | 2 | 1059 | -1019 |
| 3 | 3 | 2 | 367 | 354 |
| 3 | 5 | 2 | 480 | 466 |
| 3 | 7 | 2 | 310 | 309 |
| 3 | 9 | 2 | 621 | -552 |
| 3 | 11 | 2 | -108 | -63 |
| 3 | 13 | 2 | 138 | -129 |
| 3 | 15 | 2 | 237 | 230 |
| 3 | 17 | 2 | -129 | 107 |
| 3 | 19 | 2 | 132 | -131 |
| 3 | 21 | 2 | -57 | 20 |
| 4 | 0 | 2 | 1227 | 1218 |
| 4 | 2 | 2 | 1451 | 1430 |
| 4 | 4 | 2 | 981 | 949 |
| 4 | 6 | 2 | 166 | 163 |
| 4 | 8 | 2 | 727 | 718 |
| 4 | 10 | 2 | 561 | 546 |
| 4 | 12 | 2 | 163 | 149 |
| 4 | 14 | 2 | 709 | 699 |
| 4 | 16 | 2 | 547 | 524 |
| 4 | 18 | 2 | 362 | 359 |
| 4 | 22 | 2 | 277 | 289 |
| 5 | 1 | 2 | 211 | 181 |
| 5 | 3 | 2 | 141 | -141 |
| 5 | 5 | 2 | -90 | -43 |
| 5 | 7 | 2 | -98 | -57 |
| 5 | 9 | 2 | -106 | 9 |
| 5 | 11 | 2 | -115 | 13 |
| 5 | 13 | 2 | 212 | 201 |
| 5 | 15 | 2 | -126 | -78 |
| 5 | 17 | 2 | -122 | -128 |
| 5 | 19 | 2 | -109 | 73 |
| 5 | 21 | 2 | -86 | 39 |
| 6 | 0 | 2 | 183 | -191 |
| 6 | 2 | 2 | -90 | -37 |
| 6 | 4 | 2 | 284 | 274 |
| 6 | 6 | 2 | 177 | 162 |
| 6 | 8 | 2 | 633 | 627 |
| 6 | 10 | 2 | 414 | 403 |
| 6 | 12 | 2 | 134 | 144 |
| 6 | 14 | 2 | -126 | -54 |
| 6 | 16 | 2 | 163 | 159 |
| 6 | 18 | 2 | -112 | -31 |
| 6 | 20 | 2 | -92 | 5 |
| 6 | 22 | 2 | 60 | 69 |
| 7 | 1 | 2 | 184 | -119 |
| 7 | 3 | 2 | 680 | -653 |
| 7 | 5 | 2 | -104 | 38 |
| 7 | 7 | 2 | 212 | 181 |
| 7 | 9 | 2 | -117 | -10 |
| 7 | 11 | 2 | -123 | -55 |
| 7 | 13 | 2 | 354 | 339 |
| 7 | 15 | 2 | -124 | 10 |
| 7 | 17 | 2 | 262 | -260 |
| 7 | 19 | 2 | -96 | -45 |
| 7 | 21 | 2 | -67 | 67 |
| 8 | 0 | 2 | 545 | -540 |
| 8 | 2 | 2 | 539 | -521 |
| 8 | 4 | 2 | 485 | -442 |
| 8 | 6 | 2 | 407 | -458 |
| 8 | 8 | 2 | 472 | -431 |
| 8 | 10 | 2 | 569 | -533 |
| 8 | 12 | 2 | 591 | -579 |
| 8 | 14 | 2 | 226 | -231 |
| 8 | 16 | 2 | 314 | -312 |
| 8 | 18 | 2 | 188 | -190 |
| 8 | 20 | 2 | 120 | -140 |
| 9 | 1 | 2 | 584 | -576 |
| 9 | 3 | 2 | 292 | -292 |
| 9 | 5 | 2 | -119 | -27 |
| 9 | 7 | 2 | 158 | 147 |
| 9 | 9 | 2 | -125 | -82 |
| 9 | 11 | 2 | 221 | 229 |
| 9 | 13 | 2 | -122 | 49 |
| 9 | 15 | 2 | -113 | 13 |
| 9 | 17 | 2 | 116 | -122 |
| 9 | 19 | 2 | 146 | -148 |
| 10 | 0 | 2 | 533 | -558 |
| 10 | 2 | 2 | 200 | -192 |
| 10 | 4 | 2 | 149 | -145 |
| 10 | 6 | 2 | -125 | -65 |
| 10 | 8 | 2 | -126 | -142 |
| 10 | 10 | 2 | -125 | 90 |
| 10 | 12 | 2 | 213 | -199 |
| 10 | 14 | 2 | 258 | -267 |
| 10 | 16 | 2 | 158 | -165 |
| 10 | 18 | 2 | 209 | -230 |
| 11 | 1 | 2 | 254 | 263 |
| 11 | 3 | 2 | -126 | -35 |
| 11 | 5 | 2 | 312 | -300 |
| 11 | 7 | 2 | -126 | -109 |
| 11 | 9 | 2 | 293 | 303 |
| 11 | 11 | 2 | -117 | 100 |
| 11 | 13 | 2 | -107 | -78 |
| 11 | 15 | 2 | 132 | -124 |
| 11 | 17 | 2 | -69 | -7 |
| 12 | 0 | 2 | 969 | 922 |
| 12 | 2 | 2 | -125 | 52 |
| 12 | 4 | 2 | 227 | 213 |
| 12 | 6 | 2 | 376 | 364 |
| 12 | 8 | 2 | 372 | 367 |
| 12 | 10 | 2 | -112 | -24 |
| 12 | 12 | 2 | 251 | 259 |
| 12 | 14 | 2 | 120 | 136 |
| 12 | 16 | 2 | 176 | 157 |
| 13 | 1 | 2 | 217 | 158 |
| 13 | 3 | 2 | -120 | 2 |
| 13 | 5 | 2 | 143 | -138 |
| 13 | 7 | 2 | -112 | 10 |
| 13 | 9 | 2 | 159 | 163 |
| 13 | 11 | 2 | -94 | -50 |
| 13 | 13 | 2 | -78 | -57 |
| 14 | 0 | 2 | 165 | -163 |
| 14 | 2 | 2 | 208 | 227 |
| 14 | 4 | 2 | 228 | 240 |
| 14 | 6 | 2 | 270 | 275 |
| 14 | 8 | 2 | -95 | 34 |
| 14 | 10 | 2 | 215 | 248 |
| 14 | 12 | 2 | 169 | 208 |
| 15 | 1 | 2 | -96 | -100 |
| 15 | 3 | 2 | -135 | 137 |
| 15 | 5 | 2 | -88 | -5 |
| 15 | 7 | 2 | -80 | 0 |
| 16 | 0 | 2 | 88 | 90 |
| 16 | 2 | 2 | 110 | -129 |
| 16 | 4 | 2 | 207 | -237 |
| 16 | 6 | 2 | 112 | -143 |
| 1 | 2 | 3 | 70 | 84 |
| 1 | 4 | 3 | 439 | -444 |
| 1 | 6 | 3 | 342 | -361 |
| 1 | 8 | 3 | -78 | -18 |
| 1 | 10 | 3 | 258 | 252 |
| 1 | 12 | 3 | -96 | -53 |
| 1 | 14 | 3 | 192 | 169 |
| 1 | 16 | 3 | 151 | 147 |
| 1 | 18 | 3 | -99 | -61 |
| 1 | 20 | 3 | 104 | -95 |
| 1 | 22 | 3 | -63 | -12 |
| 2 | 1 | 3 | 1119 | 1185 |
| 2 | 3 | 3 | 790 | 835 |
| 2 | 5 | 3 | 854 | 536 |
| 2 | 7 | 3 | 295 | 249 |
| 2 | 9 | 3 | 355 | 349 |
| 2 | 11 | 3 | 510 | 526 |
| 2 | 13 | 3 | 886 | 930 |
| 2 | 15 | 3 | 298 | 291 |
| 2 | 17 | 3 | 430 | 434 |
| 2 | 19 | 3 | 200 | 197 |
| 2 | 21 | 3 | 236 | 266 |
| 3 | 2 | 3 | 452 | 486 |
| 3 | 4 | 3 | 554 | 527 |
| 3 | 6 | 3 | 338 | -319 |
| 3 | 8 | 3 | 63 | 70 |
| 3 | 10 | 3 | 209 | 194 |
| 3 | 12 | 3 | -98 | 19 |
| 3 | 14 | 3 | 578 | -553 |
| 3 | 16 | 3 | -104 | 64 |
| 3 | 18 | 3 | 203 | 152 |
| 3 | 20 | 3 | -82 | -4 |
| 3 | 22 | 3 | 76 | -89 |
| 4 | 1 | 3 | 749 | 771 |
| 4 | 3 | 3 | 499 | 471 |
| 4 | 5 | 3 | 547 | -538 |
| 4 | 7 | 3 | -82 | -33 |
| 4 | 9 | 3 | 513 | 486 |
| 4 | 11 | 3 | -97 | -63 |
| 4 | 13 | 3 | 280 | -244 |
| 4 | 15 | 3 | 756 | 763 |
| 4 | 17 | 3 | -99 | 66 |
| 4 | 19 | 3 | 142 | -139 |
| 4 | 21 | 3 | 101 | -101 |
| 5 | 2 | 3 | 150 | 139 |
| 5 | 4 | 3 | 600 | -593 |
| 5 | 6 | 3 | 94 | -113 |
| 5 | 8 | 3 | -90 | 83 |
| 5 | 10 | 3 | 148 | 140 |
| 5 | 12 | 3 | 246 | -224 |
| 5 | 14 | 3 | 405 | 374 |
| 5 | 16 | 3 | -101 | 38 |
| 5 | 18 | 3 | -91 | -33 |
| 5 | 20 | 3 | 122 | -130 |
| 6 | 1 | 3 | 573 | -557 |
| 6 | 3 | 3 | 154 | -123 |
| 6 | 5 | 3 | 836 | -831 |
| 6 | 7 | 3 | 1050 | -1022 |
| 6 | 9 | 3 | 454 | -474 |
| 6 | 11 | 3 | 419 | -403 |
| 6 | 13 | 3 | 281 | -244 |
| 6 | 15 | 3 | 119 | -106 |
| 6 | 17 | 3 | 342 | -336 |
| 6 | 19 | 3 | 331 | -365 |
| 6 | 21 | 3 | 170 | -202 |
| 7 | 2 | 3 | -86 | -80 |
| 7 | 4 | 3 | 456 | 491 |
| 7 | 6 | 3 | -99 | -8 |
| 7 | 8 | 3 | 119 | -104 |
| 7 | 10 | 3 | -103 | 12 |
| 7 | 12 | 3 | 199 | 198 |
| 7 | 14 | 3 | 412 | -393 |
| 7 | 16 | 3 | -94 | -10 |
| 7 | 18 | 3 | -80 | 59 |
| 7 | 20 | 3 | 77 | 79 |
| 8 | 1 | 3 | 310 | -299 |
| 8 | 3 | 3 | -99 | 3 |
| 8 | 5 | 3 | -97 | -94 |
| 8 | 7 | 3 | 568 | -557 |
| 8 | 9 | 3 | 133 | -126 |
| 8 | 11 | 3 | 109 | -97 |
| 8 | 13 | 3 | 106 | 98 |
| 8 | 15 | 3 | 290 | -299 |
| 8 | 17 | 3 | -81 | -47 |
| 8 | 19 | 3 | 126 | -139 |
| 9 | 2 | 3 | 324 | -302 |
| 9 | 4 | 3 | 273 | -260 |
| 9 | 6 | 3 | 204 | 186 |
| 9 | 8 | 3 | -104 | -41 |
| 9 | 10 | 3 | 118 | -93 |
| 9 | 12 | 3 | -101 | -20 |
| 9 | 14 | 3 | 350 | 349 |
| 9 | 16 | 3 | -81 | -30 |
| 9 | 18 | 3 | 131 | -131 |
| 10 | 1 | 3 | 166 | 153 |
| 10 | 3 | 3 | 737 | 710 |
| 10 | 5 | 3 | 112 | 100 |
| 10 | 7 | 3 | 257 | 276 |
| 10 | 9 | 3 | 599 | 597 |
| 10 | 11 | 3 | 308 | 294 |
| 10 | 13 | 3 | -91 | -64 |
| 10 | 15 | 3 | 408 | 432 |
| 10 | 17 | 3 | 86 | 103 |
| 11 | 2 | 3 | -104 | -57 |
| 11 | 4 | 3 | 147 | 144 |
| 11 | 6 | 3 | 140 | 128 |
| 11 | 8 | 3 | -100 | 5 |
| 11 | 10 | 3 | 138 | -127 |
| 11 | 12 | 3 | -87 | 78 |
| 11 | 14 | 3 | -75 | -69 |
| 11 | 16 | 3 | 102 | -108 |
| 12 | 1 | 3 | 119 | -110 |
| 12 | 3 | 3 | 379 | 368 |
| 12 | 5 | 3 | 289 | 279 |
| 12 | 7 | 3 | 159 | 136 |
| 12 | 9 | 3 | 257 | 243 |
| 12 | 11 | 3 | 159 | 178 |
| 12 | 13 | 3 | -70 | 76 |
| 12 | 15 | 3 | 65 | 69 |
| 13 | 2 | 3 | -99 | -93 |
| 13 | 4 | 3 | 110 | -101 |
| 13 | 6 | 3 | -89 | -39 |
| 13 | 8 | 3 | -84 | -22 |
| 13 | 10 | 3 | -74 | 40 |
| 13 | 12 | 3 | -62 | -11 |
| 13 | 14 | 3 | -32 | 86 |
| 14 | 1 | 3 | 229 | -239 |
| 14 | 3 | 3 | 258 | -278 |
| 14 | 5 | 3 | 80 | -53 |
| 14 | 7 | 3 | 106 | -109 |
| 14 | 9 | 3 | -64 | -72 |
| 14 | 11 | 3 | 189 | -226 |
| 15 | 2 | 3 | 126 | 129 |
| 15 | 4 | 3 | 82 | 79 |
| 15 | 6 | 3 | 79 | -80 |
| 16 | 1 | 3 | 163 | -200 |
| 0 | 2 | 4 | 400 | 356 |
| 0 | 4 | 4 | 719 | 655 |
| 0 | 6 | 4 | 1109 | 1070 |
| 0 | 8 | 4 | 284 | 238 |
| 0 | 10 | 4 | 221 | 204 |
| 0 | 12 | 4 | 713 | 652 |
| 0 | 14 | 4 | 298 | 269 |
| 0 | 16 | 4 | -86 | 46 |
| 0 | 18 | 4 | 609 | 617 |
| 0 | 20 | 4 | 340 | 377 |
| 0 | 22 | 4 | 94 | 120 |
| 1 | 1 | 4 | 583 | 550 |
| 1 | 3 | 4 | 237 | 246 |
| 1 | 5 | 4 | 220 | 219 |
| 1 | 7 | 4 | 83 | -68 |
| 1 | 9 | 4 | 87 | -82 |
| 1 | 11 | 4 | 299 | -298 |
| 1 | 13 | 4 | -88 | 62 |
| 1 | 15 | 4 | -88 | 1 |
| 1 | 17 | 4 | -83 | 28 |
| 1 | 19 | 4 | 136 | 154 |
| 1 | 21 | 4 | -52 | 10 |
| 2 | 0 | 4 | 566 | -567 |
| 2 | 2 | 4 | 181 | -159 |
| 2 | 4 | 4 | 151 | 163 |
| 2 | 6 | 4 | 560 | 532 |
| 2 | 8 | 4 | 101 | -93 |
| 2 | 10 | 4 | 209 | 208 |
| 2 | 12 | 4 | 330 | 323 |
| 2 | 14 | 4 | 201 | -188 |
| 2 | 16 | 4 | 137 | -124 |
| 2 | 18 | 4 | -77 | 2 |
| 2 | 20 | 4 | 70 | 76 |
| 3 | 1 | 4 | 814 | -769 |
| 3 | 3 | 4 | 211 | 158 |
| 3 | 5 | 4 | 327 | 318 |
| 3 | 7 | 4 | 236 | 218 |
| 3 | 9 | 4 | 471 | -444 |
| 3 | 11 | 4 | -89 | 31 |
| 3 | 13 | 4 | 140 | -139 |
| 3 | 15 | 4 | 182 | 166 |
| 3 | 17 | 4 | 104 | 102 |
| 3 | 19 | 4 | 131 | -144 |
| 3 | 21 | 4 | -47 | 22 |
| 4 | 0 | 4 | 558 | 541 |
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| 4 | 4 | 4 | 940 | -914 |
| 4 | 6 | 4 | 337 | -317 |
| 4 | 8 | 4 | 408 | -403 |
| 4 | 10 | 4 | 886 | -855 |
| 4 | 12 | 4 | 410 | -388 |
| 4 | 14 | 4 | 278 | -267 |
| 4 | 16 | 4 | 307 | -259 |
| 4 | 18 | 4 | 89 | -88 |
| 4 | 20 | 4 | 208 | -256 |
| 5 | 1 | 4 | 480 | 450 |
| 5 | 3 | 4 | 84 | 79 |
| 5 | 5 | 4 | 212 | -207 |
| 5 | 7 | 4 | 221 | -208 |
| 5 | 9 | 4 | 250 | 244 |
| 5 | 11 | 4 | -88 | 21 |
| 5 | 13 | 4 | -88 | 9 |
| 5 | 15 | 4 | 109 | -93 |
| 5 | 17 | 4 | -76 | 12 |
| 5 | 19 | 4 | 66 | 77 |
| 6 | 0 | 4 | 239 | -222 |
| 6 | 2 | 4 | 144 | -144 |
| 6 | 4 | 4 | 400 | -377 |
| 6 | 6 | 4 | -81 | 30 |
| 6 | 8 | 4 | 114 | -119 |
| 6 | 10 | 4 | -88 | -50 |
| 6 | 12 | 4 | -88 | -47 |
| 6 | 14 | 4 | 97 | -83 |
| 6 | 16 | 4 | -77 | -38 |
| 6 | 18 | 4 | 167 | -204 |
| 7 | 1 | 4 | 181 | 159 |
| 7 | 3 | 4 | 242 | -217 |
| 7 | 5 | 4 | 171 | -162 |
| 7 | 7 | 4 | -86 | -49 |
| 7 | 9 | 4 | 206 | 212 |
| 7 | 11 | 4 | -88 | 6 |
| 7 | 13 | 4 | -85 | 69 |
| 7 | 15 | 4 | -78 | -17 |
| 7 | 17 | 4 | -78 | -46 |
| 8 | 0 | 4 | 1182 | 1206 |
| 8 | 2 | 4 | 419 | 399 |
| 8 | 4 | 4 | -86 | 49 |
| 8 | 6 | 4 | 333 | 328 |
| 8 | 8 | 4 | 460 | 447 |
| 8 | 10 | 4 | 121 | 63 |
| 8 | 12 | 4 | 158 | 157 |
| 8 | 14 | 4 | 391 | 415 |
| 8 | 16 | 4 | 304 | 341 |
| 8 | 18 | 4 | 228 | 254 |
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| 9 | 7 | 4 | -88 | 35 |
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| 9 | 11 | 4 | 284 | 278 |
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| 9 | 15 | 4 | -65 | 15 |
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| 10 | 0 | 4 | 146 | -139 |
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| 10 | 4 | 4 | 271 | 256 |
| 10 | 6 | 4 | 125 | 126 |
| 10 | 8 | 4 | -85 | 28 |
| 10 | 10 | 4 | 246 | 261 |
| 10 | 12 | 4 | 236 | 246 |
| 10 | 14 | 4 | 96 | 98 |
| 10 | 16 | 4 | 62 | 78 |
| 11 | 1 | 4 | 51 | 82 |
| 11 | 3 | 4 | 133 | -124 |
| 11 | 5 | 4 | 76 | -66 |
| 11 | 7 | 4 | 72 | -73 |
| 11 | 9 | 4 | 129 | 132 |
| 11 | 11 | 4 | 78 | 55 |
| 11 | 13 | 4 | 68 | 67 |
| 11 | 15 | 4 | 80 | -91 |
| 12 | 0 | 4 | 126 | -128 |
| 12 | 2 | 4 | 182 | -206 |
| 12 | 4 | 4 | 147 | -184 |
| 12 | 6 | 4 | 300 | -322 |
| 12 | 8 | 4 | 238 | -265 |
| 12 | 10 | 4 | 182 | -217 |
| 12 | 12 | 4 | 137 | -159 |
| 13 | 1 | 4 | -74 | 31 |
| 13 | 3 | 4 | 107 | -119 |
| 13 | 5 | 4 | -69 | 49 |
| 13 | 7 | 4 | -64 | 39 |
| 13 | 9 | 4 | -56 | 29 |
| 13 | 11 | 4 | 55 | -57 |
| 14 | 0 | 4 | 419 | -499 |
| 14 | 2 | 4 | 53 | -101 |
| 14 | 4 | 4 | -59 | 8 |
| 14 | 6 | 4 | 134 | -170 |
| 14 | 8 | 4 | 147 | -179 |
| 15 | 1 | 4 | 175 | -222 |
| 15 | 3 | 4 | 54 | 67 |
| 0 | 0 | 2 | 1300 | 1333 |
| 0 | 0 | 4 | 1230 | 1208 |
| 0 | 0 | 6 | 787 | -711 |
| 0 | 2 | 6 | 267 | -241 |
| 0 | 4 | 6 | 380 | -354 |
| 0 | 6 | 6 | 430 | -369 |
| 0 | 8 | 6 | 227 | -206 |
| 0 | 10 | 6 | 263 | -249 |
| 0 | 12 | 6 | 648 | -606 |
| 0 | 14 | 6 | 159 | -137 |
| 0 | 16 | 6 | 199 | -221 |
| 0 | 18 | 6 | 193 | -226 |
| 0 | 0 | 8 | 310 | 272 |
| 0 | 2 | 8 | 268 | 269 |
| 0 | 4 | 8 | -114 | 41 |
| 0 | 6 | 8 | 276 | 291 |
| 0 | 8 | 8 | 225 | 224 |
| 0 | 10 | 8 | 141 | 151 |
| 1 | 2 | 5 | -107 | 40 |
| 1 | 4 | 5 | 361 | -341 |
| 1 | 6 | 5 | 182 | 154 |
| 1 | 8 | 5 | -117 | 16 |
| 1 | 10 | 5 | -119 | -56 |
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| 1 | 14 | 5 | 422 | 416 |
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| 1 | 5 | 6 | -115 | 103 |
| 1 | 7 | 6 | -120 | 51 |
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| 1 | 11 | 6 | -115 | -61 |
| 1 | 13 | 6 | 119 | 124 |
| 1 | 15 | 6 | -93 | 2 |
| 1 | 17 | 6 | 87 | -52 |
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| 1 | 4 | 7 | 233 | -250 |
| 1 | 6 | 7 | 209 | 211 |
| 1 | 8 | 7 | -109 | 14 |
| 1 | 10 | 7 | 117 | -108 |
| 1 | 12 | 7 | 166 | -176 |
| 1 | 14 | 7 | 234 | 386 |
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| 1 | 3 | 8 | -97 | 0 |
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| 1 | 7 | 8 | -86 | -1 |
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| 2 | 3 | 5 | 519 | -546 |
| 2 | 5 | 5 | 115 | -111 |
| 2 | 7 | 5 | 648 | -685 |
| 2 | 9 | 5 | 664 | -704 |
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| 2 | 13 | 5 | -117 | 27 |
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| 2 | 17 | 5 | 172 | -181 |
| 2 | 19 | 5 | 123 | -146 |
| 2 | 0 | 6 | 453 | -460 |
| 2 | 2 | 6 | -118 | -83 |
| 2 | 4 | 6 | -119 | 79 |
| 2 | 6 | 6 | -119 | -69 |
| 2 | 8 | 6 | 172 | 181 |
| 2 | 10 | 6 | 127 | 124 |
| 2 | 12 | 6 | 113 | -127 |
| 2 | 14 | 6 | 132 | -149 |
| 2 | 16 | 6 | -82 | 42 |
| 2 | 18 | 6 | 99 | -119 |
| 2 | 1 | 7 | 222 | 243 |
| 2 | 3 | 7 | 258 | 264 |
| 2 | 5 | 7 | 299 | 321 |
| 2 | 7 | 7 | 241 | 261 |
| 2 | 9 | 7 | 219 | 236 |
| 2 | 11 | 7 | 175 | 198 |
| 2 | 13 | 7 | 179 | 229 |
| 2 | 15 | 7 | 98 | 126 |
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| 2 | 2 | 8 | -96 | -69 |
| 2 | 4 | 8 | -93 | -8 |
| 2 | 6 | 8 | -87 | 109 |
| 2 | 8 | 8 | 99 | 52 |

### Structure analysis of ammonium picrate

The visually estimated intensities were corrected in the same way as those of the potassium picrate. No Patterson synthesis was computed, as the initial coordinates used in the least-squares refinement were derived from the results obtained in the analysis of the potassium salt. The scale factors of the five parallel layers and the isotropic temperature parameters were first adjusted by allowing them to vary while the positional parameters were kept constant. Subsequently the coordinates, isotropic temperature parameters and the scale factors were allowed to vary. When the parameters had converged, the experimental structure amplitudes were corrected for secondary extinction (Zachariasen, 1963), neglecting absorption. The least-squares refinement was then continued with the scale factors kept constant and with anisotropic temperature factors on all atoms except the hydrogen atoms. The hydrogen atoms of the ammonium ion were included in the refinement under the assumption that the nitrogen–hydrogen bond length is approximately 0·9 Å and that the ammonium hydrogen atoms form a tetrahedron. One of the two crystallographically independent hydrogen atoms of the ammonium ion was assumed to be situated on the line between the phenoxide oxygen and the ammonium nitrogen; the position of the second hydrogen atom is then implicit. The final agreement residual was 0·07.

The final coordinates and temperature parameters are given in Table 2 and the experimental and calculated structure amplitudes in Table 4. The weights assigned to the reflecting planes in the least-squares calculations were computed according to the same scheme and with the same constants as for the potassium salt. Atomic scattering factors were identical in the two analyses.

### Discussion

Tables 5 and 6 give interatomic distances and angles together with the standard deviations, as calculated from the positional data obtained in the two analyses. The content of Table 5 is illustrated in Fig. 2. The standard deviations listed are probably too small since no account has been taken of the uncertainty in the cell dimensions.

The two analyses of the picrate ion are in good agreement, considering bond lengths and angles. The anisotropic temperature parameters do, on the other hand, deviate more than would be expected in the two isomorphous salts. The extreme anisotropy assigned to the carbon atoms in the ammonium salt is probably not real, but a consequence of inaccurate scaling of the five parallel layers on which the analysis of the ammonium salt is based. It should be mentioned that the separate scale factors of the layers have *not* been refined with anisotropic temperature factors (Lingafelter & Donohue, 1966).

In order to consider the planarity of the picrate ion and groups therein, planes were fitted by least-squares with equal weights assigned to carbon, nitrogen and oxygen atoms; hydrogen atoms were assigned zero weight. Relative to the least-squares plane of the carbon atoms of the ion, the deviations are:

| O(2) | O(3) | O(4) | N(2) | C(2) | C(3) | H |
|---|---|---|---|---|---|---|
| 0·448 | −0·529 | −0·106 | −0·033 | 0·014 | −0·014 | −0·060 Å |
| 0·401 | −0·532 | −0·047 | −0·064 | 0·007 | −0·007 | −0·107 |

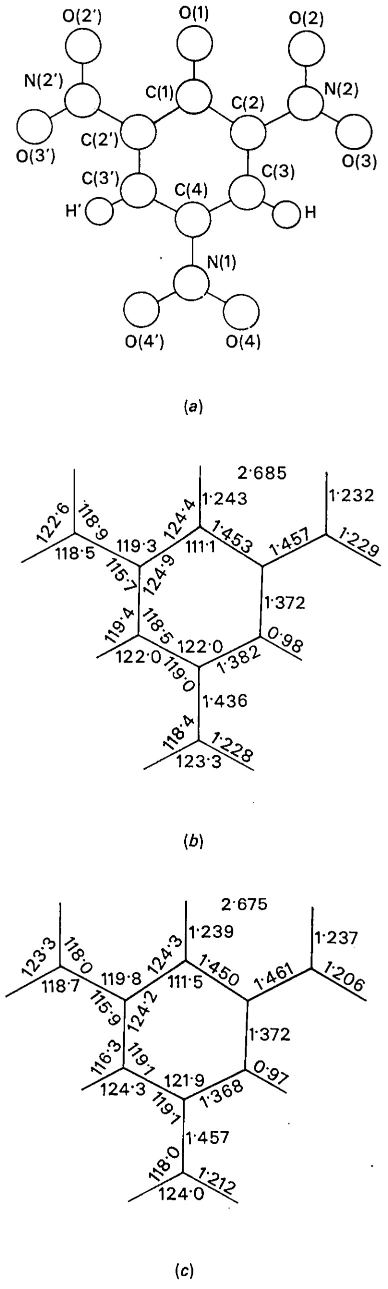

Fig. 2. Atomic numbering, bond lengths and angles in the picrate ion. (*b*) and (*c*) refer to potassium picrate and ammonium picrate, respectively.

Table 4. *Experimental and calculated structure amplitudes of ammonium picrate*

*Cf.* the legend of Table 3.

| | | | | |
|---|---|---|---|---|
| 0 | 2 | 0 | 954 | -1075 |
| 0 | 4 | 0 | 1981 | -2261 |
| 0 | 6 | 0 | 866 | 666 |
| 0 | 8 | 0 | 931 | 966 |
| 0 | 10 | 0 | 1263 | -1167 |
| 0 | 12 | 0 | 971 | 915 |
| 0 | 14 | 0 | 630 | 587 |
| 0 | 16 | 0 | 575 | 548 |
| 0 | 18 | 0 | 188 | 180 |
| 0 | 20 | 0 | 652 | -613 |
| 0 | 22 | 0 | 113 | 122 |
| 0 | 24 | 0 | 350 | 338 |
| 2 | 0 | 0 | 776 | -850 |
| 2 | 2 | 0 | 680 | 681 |
| 2 | 4 | 0 | 343 | -314 |
| 2 | 6 | 0 | 578 | 566 |
| 2 | 8 | 0 | 1009 | -989 |
| 2 | 10 | 0 | 566 | 452 |
| 2 | 12 | 0 | 720 | 651 |
| 2 | 14 | 0 | -54 | -22 |
| 2 | 16 | 0 | 382 | -355 |
| 2 | 18 | 0 | 323 | -306 |
| 2 | 20 | 0 | 56 | 93 |
| 2 | 22 | 0 | 150 | 133 |
| 2 | 24 | 0 | 153 | 174 |
| 4 | 0 | 0 | 701 | 655 |
| 4 | 2 | 0 | 334 | -343 |
| 4 | 4 | 0 | 886 | -904 |
| 4 | 6 | 0 | 154 | -193 |
| 4 | 8 | 0 | 1006 | -1025 |
| 4 | 10 | 0 | 468 | -444 |
| 4 | 12 | 0 | 152 | 128 |
| 4 | 14 | 0 | 118 | 77 |
| 4 | 16 | 0 | 302 | -275 |
| 4 | 18 | 0 | 170 | 154 |
| 4 | 20 | 0 | 183 | -183 |
| 4 | 22 | 0 | 173 | -193 |
| 4 | 24 | 0 | 183 | -174 |
| 6 | 0 | 0 | 341 | -321 |
| 6 | 2 | 0 | 1067 | -1054 |
| 6 | 4 | 0 | 298 | 293 |
| 6 | 6 | 0 | 650 | 566 |
| 6 | 8 | 0 | 206 | 190 |
| 6 | 10 | 0 | 134 | 119 |
| 6 | 12 | 0 | 251 | 255 |
| 6 | 14 | 0 | 971 | -1012 |
| 6 | 16 | 0 | -60 | 32 |
| 6 | 18 | 0 | 251 | 285 |
| 6 | 20 | 0 | 113 | -96 |
| 6 | 22 | 0 | 108 | -111 |
| 8 | 0 | 0 | 472 | -439 |
| 8 | 2 | 0 | 127 | 104 |
| 8 | 4 | 0 | 756 | 731 |
| 8 | 6 | 0 | 480 | 452 |
| 8 | 8 | 0 | 201 | -151 |
| 8 | 10 | 0 | -56 | 12 |
| 8 | 12 | 0 | 88 | 57 |
| 8 | 14 | 0 | 161 | 163 |
| 8 | 16 | 0 | 85 | -80 |
| 8 | 18 | 0 | 357 | 402 |
| 8 | 20 | 0 | 197 | 228 |
| 10 | 0 | 0 | 1037 | -1045 |
| 10 | 2 | 0 | 159 | 123 |
| 10 | 4 | 0 | 248 | 228 |
| 10 | 6 | 0 | 357 | 369 |
| 10 | 8 | 0 | 339 | 299 |
| 10 | 10 | 0 | 272 | 297 |
| 10 | 12 | 0 | 318 | -325 |
| 10 | 14 | 0 | 171 | -184 |
| 10 | 16 | 0 | 61 | 41 |
| 10 | 18 | 0 | -44 | 21 |
| 10 | 20 | 0 | 235 | 249 |
| 12 | 0 | 0 | 934 | 918 |
| 12 | 2 | 0 | 444 | -433 |
| 12 | 4 | 0 | 361 | -348 |
| 12 | 6 | 0 | -59 | -6 |
| 12 | 8 | 0 | 302 | 324 |
| 12 | 10 | 0 | 554 | -559 |
| 12 | 12 | 0 | 182 | -182 |
| 12 | 14 | 0 | 74 | 85 |
| 12 | 16 | 0 | 165 | 177 |
| 14 | 0 | 0 | 555 | -585 |
| 14 | 2 | 0 | 178 | 176 |
| 14 | 4 | 0 | -55 | 0 |
| 14 | 6 | 0 | 104 | -95 |
| 14 | 8 | 0 | -50 | -61 |
| 14 | 10 | 0 | 65 | 62 |
| 14 | 12 | 0 | 162 | -171 |
| 14 | 14 | 0 | 109 | 107 |
| 16 | 0 | 0 | 177 | 215 |
| 16 | 2 | 0 | 210 | 244 |
| 16 | 4 | 0 | 81 | -75 |
| 16 | 6 | 0 | 274 | -241 |
| 1 | 2 | 1 | 566 | -555 |
| 1 | 4 | 1 | 556 | -524 |
| 1 | 6 | 1 | 756 | -768 |
| 1 | 8 | 1 | 58 | 30 |
| 1 | 10 | 1 | 901 | 891 |
| 1 | 12 | 1 | 265 | 241 |
| 1 | 14 | 1 | 175 | -171 |
| 1 | 16 | 1 | -46 | 12 |
| 1 | 18 | 1 | 254 | -304 |
| 1 | 20 | 1 | -45 | 51 |
| 1 | 22 | 1 | -39 | -26 |
| 1 | 24 | 1 | -29 | 0 |
| 2 | 1 | 1 | 203 | 141 |
| 2 | 3 | 1 | 1437 | -1467 |
| 2 | 5 | 1 | 392 | -409 |
| 2 | 7 | 1 | 338 | -304 |
| 2 | 9 | 1 | 744 | -716 |
| 2 | 11 | 1 | 170 | -165 |
| 2 | 13 | 1 | 229 | 218 |
| 2 | 15 | 1 | 241 | -245 |
| 2 | 17 | 1 | 135 | -128 |
| 2 | 19 | 1 | 227 | -237 |
| 2 | 21 | 1 | 63 | -52 |
| 2 | 23 | 1 | 43 | -47 |
| 3 | 2 | 1 | 1052 | -1121 |
| 3 | 4 | 1 | 355 | 388 |
| 3 | 6 | 1 | 428 | 415 |
| 3 | 8 | 1 | 146 | 105 |
| 3 | 10 | 1 | 56 | -53 |
| 3 | 12 | 1 | 290 | 301 |
| 3 | 14 | 1 | 473 | -483 |
| 3 | 16 | 1 | 226 | -205 |
| 3 | 18 | 1 | 115 | 110 |
| 3 | 20 | 1 | 213 | 212 |
| 3 | 22 | 1 | 53 | 47 |
| 3 | 24 | 1 | 43 | 34 |
| 4 | 1 | 1 | 1005 | 1015 |
| 4 | 3 | 1 | 1009 | -1027 |
| 4 | 5 | 1 | 680 | -633 |
| 4 | 7 | 1 | 351 | 353 |
| 4 | 9 | 1 | 239 | -211 |
| 4 | 11 | 1 | 93 | -80 |
| 4 | 13 | 1 | 111 | 88 |
| 4 | 15 | 1 | 287 | 269 |
| 4 | 17 | 1 | 136 | -113 |
| 4 | 19 | 1 | 209 | -153 |
| 4 | 21 | 1 | 59 | -52 |
| 4 | 23 | 1 | 154 | 146 |
| 5 | 2 | 1 | 1028 | -1078 |
| 5 | 4 | 1 | 1652 | -1600 |
| 5 | 6 | 1 | 783 | 738 |
| 5 | 8 | 1 | 400 | 395 |
| 5 | 10 | 1 | 92 | 78 |
| 5 | 12 | 1 | 52 | 50 |
| 5 | 14 | 1 | 784 | 804 |
| 5 | 16 | 1 | 719 | -730 |
| 5 | 18 | 1 | 364 | -292 |
| 5 | 20 | 1 | 71 | 56 |
| 5 | 22 | 1 | 281 | 280 |
| 6 | 1 | 1 | 814 | 828 |
| 6 | 3 | 1 | 288 | -275 |
| 6 | 5 | 1 | 410 | 385 |
| 6 | 7 | 1 | 213 | 221 |
| 6 | 9 | 1 | 249 | -257 |
| 6 | 11 | 1 | 454 | 452 |
| 6 | 13 | 1 | 420 | 406 |
| 6 | 15 | 1 | -47 | -18 |
| 6 | 17 | 1 | 109 | 102 |
| 6 | 19 | 1 | 47 | 47 |
| 6 | 21 | 1 | -36 | 15 |
| 6 | 23 | 1 | 133 | 135 |
| 7 | 2 | 1 | 159 | 142 |
| 7 | 4 | 1 | 655 | 554 |
| 7 | 6 | 1 | 714 | -670 |
| 7 | 8 | 1 | 127 | 90 |
| 7 | 10 | 1 | 455 | 475 |
| 7 | 12 | 1 | 121 | 112 |
| 7 | 14 | 1 | 948 | -956 |
| 7 | 16 | 1 | 306 | 299 |
| 7 | 18 | 1 | 187 | 216 |
| 7 | 20 | 1 | 110 | 128 |
| 7 | 22 | 1 | 123 | -129 |
| 8 | 1 | 1 | 238 | 238 |
| 8 | 3 | 1 | 319 | -288 |
| 8 | 5 | 1 | 477 | 483 |
| 8 | 7 | 1 | 72 | -51 |
| 8 | 9 | 1 | 302 | -325 |
| 8 | 11 | 1 | 419 | 427 |
| 8 | 13 | 1 | 221 | 202 |
| 8 | 15 | 1 | 383 | -353 |
| 8 | 17 | 1 | 219 | 220 |
| 8 | 19 | 1 | 86 | 99 |
| 8 | 21 | 1 | 77 | -86 |
| 9 | 2 | 1 | 73 | -79 |
| 9 | 4 | 1 | 448 | -420 |
| 9 | 6 | 1 | 64 | 29 |
| 9 | 8 | 1 | 167 | 153 |
| 9 | 10 | 1 | 72 | 62 |
| 9 | 12 | 1 | 201 | -199 |
| 9 | 14 | 1 | 298 | 320 |
| 9 | 16 | 1 | 55 | 48 |
| 9 | 18 | 1 | 174 | -202 |
| 9 | 20 | 1 | 122 | -137 |
| 10 | 1 | 1 | 163 | -140 |
| 10 | 3 | 1 | 249 | -241 |
| 10 | 5 | 1 | 84 | 56 |
| 10 | 7 | 1 | 46 | -54 |
| 10 | 9 | 1 | 286 | -273 |
| 10 | 11 | 1 | 134 | 116 |
| 10 | 13 | 1 | 199 | -208 |
| 10 | 15 | 1 | 209 | -230 |
| 10 | 17 | 1 | -37 | 17 |
| 10 | 19 | 1 | 69 | 63 |
| 11 | 2 | 1 | 488 | 515 |
| 11 | 4 | 1 | 211 | 207 |
| 11 | 6 | 1 | 51 | 23 |
| 11 | 8 | 1 | 56 | -26 |
| 11 | 10 | 1 | 188 | -215 |
| 11 | 12 | 1 | 167 | -165 |
| 11 | 14 | 1 | -41 | -34 |
| 11 | 16 | 1 | -36 | 14 |
| 11 | 18 | 1 | 319 | 313 |
| 12 | 1 | 1 | 148 | -140 |
| 12 | 3 | 1 | 192 | -158 |
| 12 | 5 | 1 | 109 | 204 |
| 12 | 7 | 1 | -47 | 33 |
| 12 | 9 | 1 | 216 | -229 |
| 12 | 11 | 1 | 79 | 63 |
| 12 | 13 | 1 | 74 | -55 |
| 12 | 15 | 1 | 158 | -242 |
| 12 | 17 | 1 | 42 | 34 |
| 13 | 2 | 1 | -46 | 1 |
| 13 | 4 | 1 | 147 | 143 |
| 13 | 6 | 1 | 113 | -97 |
| 13 | 8 | 1 | 163 | -169 |
| 13 | 10 | 1 | 78 | 66 |
| 13 | 12 | 1 | -37 | 6 |
| 13 | 14 | 1 | 34 | 40 |
| 13 | 16 | 1 | 189 | 212 |
| 14 | 1 | 1 | 139 | 143 |
| 14 | 3 | 1 | 201 | -199 |
| 14 | 5 | 1 | 192 | 193 |
| 14 | 7 | 1 | 196 | 234 |
| 14 | 9 | 1 | -37 | -45 |
| 14 | 11 | 1 | -33 | 1 |
| 14 | 13 | 1 | 77 | 76 |
| 15 | 2 | 1 | -39 | 2 |
| 15 | 4 | 1 | 258 | 273 |
| 15 | 6 | 1 | 78 | 100 |
| 15 | 8 | 1 | 59 | -116 |
| 15 | 10 | 1 | 216 | -217 |
| 16 | 1 | 1 | 112 | 110 |
| 16 | 3 | 1 | 63 | -67 |
| 16 | 5 | 1 | -29 | 7 |
| 16 | 7 | 1 | 201 | 216 |
| 17 | 2 | 1 | 38 | -41 |
| 0 | 2 | 2 | 574 | -630 |
| 0 | 4 | 2 | 909 | -891 |
| 0 | 6 | 2 | 1761 | -1739 |
| 0 | 8 | 2 | 402 | 354 |
| 0 | 10 | 2 | 661 | -648 |
| 0 | 12 | 2 | 338 | -316 |
| 0 | 14 | 2 | 276 | 241 |
| 0 | 16 | 2 | 246 | 239 |
| 0 | 18 | 2 | 130 | -121 |
| 0 | 20 | 2 | 344 | -408 |
| 0 | 22 | 2 | 151 | -154 |
| 0 | 24 | 2 | 50 | -38 |
| 1 | 1 | 2 | 1576 | 1720 |
| 1 | 3 | 2 | 920 | 998 |
| 1 | 5 | 2 | 273 | -316 |
| 1 | 7 | 2 | 413 | -438 |
| 1 | 9 | 2 | 237 | 230 |
| 1 | 11 | 2 | 436 | -354 |
| 1 | 13 | 2 | 158 | -181 |
| 1 | 15 | 2 | 198 | 174 |
| 1 | 17 | 2 | 337 | 342 |
| 1 | 19 | 2 | -46 | -11 |
| 1 | 21 | 2 | 237 | -258 |
| 1 | 23 | 2 | 62 | -51 |
| 2 | 0 | 2 | 3260 | -3093 |
| 2 | 2 | 2 | 971 | 1061 |
| 2 | 4 | 2 | 758 | 814 |
| 2 | 6 | 2 | 859 | -885 |
| 2 | 8 | 2 | 229 | -185 |
| 2 | 10 | 2 | 844 | 829 |
| 2 | 12 | 2 | 238 | -187 |
| 2 | 14 | 2 | -44 | 39 |
| 2 | 16 | 2 | 178 | -156 |
| 2 | 18 | 2 | 388 | -412 |
| 2 | 20 | 2 | 226 | 244 |
| 2 | 22 | 2 | 80 | 75 |
| 3 | 1 | 2 | 880 | -928 |
| 3 | 3 | 2 | 472 | 437 |
| 3 | 5 | 2 | 379 | 343 |
| 3 | 7 | 2 | 264 | 239 |
| 3 | 9 | 2 | 610 | -577 |
| 3 | 11 | 2 | 55 | -1 |
| 3 | 13 | 2 | -43 | -44 |
| 3 | 15 | 2 | 359 | 370 |
| 3 | 17 | 2 | -47 | -4 |
| 3 | 19 | 2 | 177 | -191 |
| 3 | 21 | 2 | 47 | 56 |
| 3 | 23 | 2 | 85 | 68 |
| 4 | 0 | 2 | 588 | 598 |
| 4 | 2 | 2 | 890 | 892 |
| 4 | 4 | 2 | 325 | 276 |
| 4 | 6 | 2 | 452 | -424 |
| 4 | 8 | 2 | 355 | 342 |
| 4 | 10 | 2 | 135 | 88 |
| 4 | 12 | 2 | 175 | -172 |
| 4 | 14 | 2 | 653 | 691 |
| 4 | 16 | 2 | 181 | 159 |
| 4 | 18 | 2 | 59 | 41 |
| 4 | 20 | 2 | 118 | 104 |
| 4 | 22 | 2 | 73 | 73 |
| 5 | 1 | 2 | 194 | 167 |
| 5 | 3 | 2 | 277 | -260 |
| 5 | 5 | 2 | 73 | 14 |
| 5 | 7 | 2 | -35 | -42 |
| 5 | 9 | 2 | -38 | -8 |
| 5 | 11 | 2 | 50 | 48 |
| 5 | 13 | 2 | 261 | 247 |
| 5 | 15 | 2 | 242 | -250 |
| 5 | 17 | 2 | 148 | -124 |
| 5 | 19 | 2 | 174 | 184 |
| 5 | 21 | 2 | -36 | 26 |
| 5 | 23 | 2 | 128 | -119 |
| 6 | 0 | 2 | 325 | -317 |
| 6 | 2 | 2 | 271 | -203 |
| 6 | 4 | 2 | 246 | 244 |
| 6 | 6 | 2 | 161 | 119 |
| 6 | 8 | 2 | 579 | 625 |
| 6 | 10 | 2 | 210 | 181 |
| 6 | 12 | 2 | 129 | -101 |
| 6 | 14 | 2 | 365 | -386 |
| 6 | 16 | 2 | 162 | 164 |
| 6 | 18 | 2 | 83 | -75 |
| 6 | 20 | 2 | 48 | 57 |
| 6 | 22 | 2 | 68 | 73 |
| 7 | 1 | 2 | 237 | -246 |
| 7 | 3 | 2 | 759 | -723 |
| 7 | 5 | 2 | 93 | 76 |
| 7 | 7 | 2 | 231 | 212 |
| 7 | 9 | 2 | -43 | -16 |
| 7 | 11 | 2 | -45 | 18 |
| 7 | 13 | 2 | 322 | 315 |
| 7 | 15 | 2 | 295 | -223 |
| 7 | 17 | 2 | 274 | -283 |
| 7 | 19 | 2 | 97 | 100 |
| 7 | 21 | 2 | 129 | 109 |
| 8 | 0 | 2 | 201 | -171 |
| 8 | 2 | 2 | 134 | -113 |
| 8 | 4 | 2 | 140 | -83 |
| 8 | 6 | 2 | 162 | -130 |
| 8 | 8 | 2 | 192 | -162 |
| 8 | 10 | 2 | 335 | -334 |
| 8 | 12 | 2 | 312 | -318 |
| 8 | 14 | 2 | 154 | 156 |
| 8 | 16 | 2 | 121 | -127 |
| 8 | 18 | 2 | 67 | -16 |
| 8 | 20 | 2 | 35 | -11 |
| 9 | 1 | 2 | 555 | -651 |
| 9 | 3 | 2 | 285 | -279 |
| 9 | 5 | 2 | 68 | 17 |
| 9 | 7 | 2 | 227 | 206 |
| 9 | 9 | 2 | -47 | -51 |
| 9 | 11 | 2 | 252 | 258 |
| 9 | 13 | 2 | 92 | -76 |
| 9 | 15 | 2 | 40 | -38 |
| 9 | 17 | 2 | 166 | -174 |
| 9 | 19 | 2 | 45 | -50 |
| 10 | 0 | 2 | 930 | -913 |
| 10 | 2 | 2 | -45 | -11 |
| 10 | 4 | 2 | 57 | 39 |
| 10 | 6 | 2 | 169 | 137 |
| 10 | 8 | 2 | 60 | -31 |
| 10 | 10 | 2 | 158 | 215 |
| 10 | 12 | 2 | 155 | -190 |
| 10 | 14 | 2 | 244 | -279 |
| 10 | 16 | 2 | 77 | -76 |
| 10 | 18 | 2 | 74 | -56 |
| 11 | 1 | 2 | 311 | 307 |
| 11 | 3 | 2 | 74 | -59 |
| 11 | 5 | 2 | 305 | -324 |
| 11 | 7 | 2 | -47 | -31 |
| 11 | 9 | 2 | 333 | 379 |
| 11 | 11 | 2 | -45 | 32 |
| 11 | 13 | 2 | 91 | -85 |
| 11 | 15 | 2 | 133 | -152 |
| 11 | 17 | 2 | 46 | 56 |
| 12 | 0 | 2 | 830 | 887 |
| 12 | 2 | 2 | 259 | -235 |
| 12 | 4 | 2 | 56 | -38 |
| 12 | 6 | 2 | 178 | 176 |
| 12 | 8 | 2 | 145 | 144 |
| 12 | 10 | 2 | 233 | -249 |
| 12 | 12 | 2 | 149 | 181 |
| 12 | 14 | 2 | -35 | 28 |
| 12 | 16 | 2 | 184 | 190 |
| 13 | 1 | 2 | 275 | 261 |
| 13 | 3 | 2 | -46 | 34 |
| 13 | 5 | 2 | 161 | -153 |
| 13 | 7 | 2 | -43 | 33 |
| 13 | 9 | 2 | 183 | 186 |
| 13 | 11 | 2 | 135 | -135 |
| 13 | 13 | 2 | 102 | -99 |
| 13 | 15 | 2 | 77 | 37 |
| 14 | 0 | 2 | 330 | -350 |
| 14 | 2 | 2 | 122 | 115 |
| 14 | 4 | 2 | 146 | 152 |
| 14 | 6 | 2 | 179 | 183 |
| 14 | 8 | 2 | 107 | -145 |
| 14 | 10 | 2 | 198 | 204 |
| 14 | 12 | 2 | 125 | 139 |
| 15 | 1 | 2 | 110 | -112 |
| 15 | 3 | 2 | 179 | 191 |
| 15 | 5 | 2 | -35 | -12 |
| 15 | 7 | 2 | -32 | -33 |
| 15 | 9 | 2 | 67 | -55 |
| 16 | 0 | 2 | 442 | 303 |
| 16 | 2 | 2 | 35 | -24 |
| 16 | 4 | 2 | 265 | -211 |
| 16 | 6 | 2 | 64 | -52 |
| 1 | 2 | 3 | 151 | 141 |
| 1 | 4 | 3 | 480 | -529 |
| 1 | 6 | 3 | 389 | -427 |
| 1 | 8 | 3 | 114 | 120 |
| 1 | 10 | 3 | 436 | 459 |
| 1 | 12 | 3 | 76 | -72 |
| 1 | 14 | 3 | 151 | 166 |
| 1 | 16 | 3 | -73 | 76 |
| 1 | 18 | 3 | 219 | -230 |
| 1 | 20 | 3 | 71 | -80 |
| 1 | 22 | 3 | 62 | 47 |
| 2 | 1 | 3 | 688 | 694 |
| 2 | 3 | 3 | 219 | 214 |
| 2 | 5 | 3 | 316 | 334 |
| 2 | 7 | 3 | 232 | -248 |
| 2 | 9 | 3 | 55 | -16 |
| 2 | 11 | 3 | 312 | 280 |
| 2 | 13 | 3 | 663 | 678 |
| 2 | 15 | 3 | 51 | -81 |
| 2 | 17 | 3 | 139 | 120 |
| 2 | 19 | 3 | 66 | -91 |
| 2 | 21 | 3 | 152 | 181 |
| 3 | 2 | 3 | 543 | 557 |
| 3 | 4 | 3 | 459 | 427 |
| 3 | 6 | 3 | 393 | -413 |
| 3 | 8 | 3 | 165 | 154 |
| 3 | 10 | 3 | -60 | 47 |
| 3 | 12 | 3 | 211 | -179 |
| 3 | 14 | 3 | 518 | -509 |
| 3 | 16 | 3 | 317 | 305 |
| 3 | 18 | 3 | 287 | 255 |
| 3 | 20 | 3 | 74 | -71 |
| 3 | 22 | 3 | 52 | -53 |
| 4 | 1 | 3 | 663 | 723 |
| 4 | 3 | 3 | 358 | 363 |
| 4 | 5 | 3 | 1239 | -1208 |
| 4 | 7 | 3 | -54 | 18 |
| 4 | 9 | 3 | 553 | 572 |
| 4 | 11 | 3 | 239 | -224 |
| 4 | 13 | 3 | 158 | -132 |
| 4 | 15 | 3 | 680 | 782 |
| 4 | 17 | 3 | 292 | -313 |
| 4 | 19 | 3 | 221 | -223 |
| 4 | 21 | 3 | -54 | -39 |
| 4 | 23 | 3 | 154 | 144 |
| 5 | 2 | 3 | 59 | 52 |
| 5 | 4 | 3 | 729 | -782 |
| 5 | 6 | 3 | 78 | -4 |
| 5 | 8 | 3 | 157 | 213 |
| 5 | 10 | 3 | 88 | 92 |
| 5 | 12 | 3 | 250 | -214 |
| 5 | 14 | 3 | 482 | 504 |
| 5 | 16 | 3 | 154 | -140 |
| 5 | 18 | 3 | 188 | -200 |
| 5 | 20 | 3 | 126 | -139 |
| 5 | 22 | 3 | 126 | 128 |
| 6 | 1 | 3 | 143 | -124 |
| 6 | 3 | 3 | 308 | 305 |
| 6 | 5 | 3 | 570 | -559 |
| 6 | 7 | 3 | 635 | -640 |
| 6 | 9 | 3 | -66 | -21 |
| 6 | 11 | 3 | 104 | -50 |
| 6 | 13 | 3 | 103 | 51 |
| 6 | 15 | 3 | 92 | 54 |
| 6 | 17 | 3 | 308 | -330 |
| 6 | 19 | 3 | 154 | -210 |
| 6 | 21 | 3 | -46 | 17 |
| 7 | 2 | 3 | -55 | 63 |
| 7 | 4 | 3 | 574 | 522 |
| 7 | 6 | 3 | 157 | -130 |
| 7 | 8 | 3 | 126 | -58 |
| 7 | 10 | 3 | -70 | 2 |
| 7 | 12 | 3 | 166 | 129 |
| 7 | 14 | 3 | 450 | -488 |
| 7 | 16 | 3 | 138 | 133 |
| 7 | 18 | 3 | 180 | 179 |
| 7 | 20 | 3 | 119 | 110 |
| 8 | 1 | 3 | 272 | -293 |
| 8 | 3 | 3 | 218 | 193 |
| 8 | 5 | 3 | -66 | -13 |
| 8 | 7 | 3 | 458 | -486 |
| 8 | 9 | 3 | 120 | 100 |
| 8 | 11 | 3 | -73 | 32 |
| 8 | 13 | 3 | 159 | 128 |
| 8 | 15 | 3 | 312 | -256 |
| 8 | 17 | 3 | -61 | 34 |
| 8 | 19 | 3 | 70 | -73 |
| 9 | 2 | 3 | 354 | -382 |
| 9 | 4 | 3 | 338 | -272 |
| 9 | 6 | 3 | 317 | 250 |
| 9 | 8 | 3 | -72 | -39 |
| 9 | 10 | 3 | 92 | -79 |
| 9 | 12 | 3 | 111 | 104 |
| 9 | 14 | 3 | 363 | 384 |
| 9 | 16 | 3 | 151 | -207 |
| 9 | 18 | 3 | 226 | -205 |
| 10 | 1 | 3 | 242 | -156 |
| 10 | 3 | 3 | 602 | 554 |
| 10 | 5 | 3 | 225 | -201 |
| 10 | 7 | 3 | 103 | 85 |
| 10 | 9 | 3 | 454 | 473 |
| 10 | 11 | 3 | -71 | -40 |
| 10 | 13 | 3 | 249 | -271 |
| 10 | 15 | 3 | 321 | 385 |
| 10 | 17 | 3 | 123 | -62 |
| 11 | 2 | 3 | -73 | 4 |
| 11 | 4 | 3 | 160 | 165 |
| 11 | 6 | 3 | 166 | 181 |
| 11 | 8 | 3 | -71 | -35 |
| 11 | 10 | 3 | 218 | -218 |
| 11 | 12 | 3 | 91 | 55 |
| 11 | 14 | 3 | 85 | -83 |
| 11 | 16 | 3 | 133 | -118 |
| 12 | 1 | 3 | 285 | -307 |
| 12 | 3 | 3 | 321 | 327 |
| 12 | 5 | 3 | 187 | 190 |
| 12 | 7 | 3 | 75 | 48 |
| 12 | 9 | 3 | 167 | 168 |
| 12 | 11 | 3 | -61 | -20 |
| 12 | 13 | 3 | 67 | -61 |
| 12 | 15 | 3 | -42 | 0 |
| 13 | 2 | 3 | -68 | -59 |
| 13 | 4 | 3 | 153 | -135 |
| 13 | 6 | 3 | -65 | -25 |
| 13 | 8 | 3 | -61 | -2 |
| 13 | 10 | 3 | 75 | 83 |
| 13 | 12 | 3 | -48 | 7 |
| 13 | 14 | 3 | 105 | 111 |
| 14 | 1 | 3 | 124 | -109 |
| 14 | 3 | 3 | 145 | -140 |
| 14 | 5 | 3 | 50 | 69 |
| 14 | 7 | 3 | -54 | 28 |
| 14 | 9 | 3 | -49 | -1 |
| 14 | 11 | 3 | 158 | -188 |
| 15 | 2 | 3 | 240 | 219 |
| 15 | 4 | 3 | 107 | 76 |
| 15 | 6 | 3 | 137 | -133 |
| 15 | 8 | 3 | 54 | 88 |
| 16 | 1 | 3 | 114 | -114 |
| 16 | 3 | 3 | 46 | 37 |
| 0 | 2 | 4 | 180 | -185 |
| 0 | 4 | 4 | 232 | 219 |
| 0 | 6 | 4 | 612 | 557 |
| 0 | 8 | 4 | 237 | -217 |
| 0 | 10 | 4 | 131 | -120 |
| 0 | 12 | 4 | 440 | 456 |
| 0 | 14 | 4 | 95 | -65 |
| 0 | 16 | 4 | 54 | 45 |
| 0 | 18 | 4 | 552 | 577 |
| 0 | 20 | 4 | 43 | -30 |
| 0 | 22 | 4 | 116 | -126 |
| 1 | 1 | 4 | 459 | 565 |
| 1 | 3 | 4 | 258 | 252 |
| 1 | 5 | 4 | 250 | 265 |
| 1 | 7 | 4 | 300 | -275 |
| 1 | 9 | 4 | 157 | -170 |
| 1 | 11 | 4 | 263 | -230 |
| 1 | 13 | 4 | 190 | 172 |
| 1 | 15 | 4 | -45 | -17 |
| 1 | 17 | 4 | 140 | 126 |
| 1 | 19 | 4 | 123 | 127 |
| 1 | 21 | 4 | 138 | -119 |
| 2 | 0 | 4 | 722 | -757 |
| 2 | 2 | 4 | 185 | -182 |
| 2 | 4 | 4 | 332 | 335 |
| 2 | 6 | 4 | 554 | 600 |
| 2 | 8 | 4 | 305 | -309 |
| 2 | 10 | 4 | 328 | 258 |
| 2 | 12 | 4 | 301 | 287 |
| 2 | 14 | 4 | 482 | -519 |
| 2 | 16 | 4 | 131 | -126 |
| 2 | 18 | 4 | 130 | 145 |
| 2 | 20 | 4 | 113 | 82 |
| 2 | 22 | 4 | 40 | -29 |
| 3 | 1 | 4 | 904 | -1003 |
| 3 | 3 | 4 | 299 | 277 |
| 3 | 5 | 4 | 366 | 366 |
| 3 | 7 | 4 | 93 | 97 |
| 3 | 9 | 4 | 552 | -542 |
| 3 | 11 | 4 | 197 | 169 |
| 3 | 13 | 4 | 215 | -152 |
| 3 | 15 | 4 | 354 | 348 |
| 3 | 17 | 4 | -47 | 3 |
| 3 | 19 | 4 | 223 | -240 |
| 3 | 21 | 4 | 74 | 70 |
| 4 | 0 | 4 | 1112 | 1121 |
| 4 | 2 | 4 | 509 | -494 |
| 4 | 4 | 4 | 560 | -638 |
| 4 | 6 | 4 | 122 | 109 |
| 4 | 8 | 4 | 207 | -157 |
| 4 | 10 | 4 | 632 | -601 |
| 4 | 12 | 4 | 43 | -23 |
| 4 | 14 | 4 | 136 | 121 |
| 4 | 16 | 4 | 97 | -76 |
| 4 | 18 | 4 | 62 | 56 |
| 4 | 20 | 4 | 229 | -236 |
| 4 | 22 | 4 | 55 | -59 |
| 5 | 1 | 4 | 465 | 494 |
| 5 | 3 | 4 | 49 | 14 |
| 5 | 5 | 4 | 182 | -174 |
| 5 | 7 | 4 | 222 | -201 |
| 5 | 9 | 4 | 333 | 332 |
| 5 | 11 | 4 | -48 | 0 |
| 5 | 13 | 4 | -49 | 0 |
| 5 | 15 | 4 | 164 | -166 |
| 5 | 17 | 4 | 69 | 61 |
| 5 | 19 | 4 | 72 | 69 |
| 5 | 21 | 4 | 69 | -61 |
| 6 | 0 | 4 | 60 | -45 |
| 6 | 2 | 4 | 139 | -133 |
| 6 | 4 | 4 | 402 | -361 |
| 6 | 6 | 4 | 223 | 231 |
| 6 | 8 | 4 | 46 | 22 |
| 6 | 10 | 4 | -48 | -6 |
| 6 | 12 | 4 | -49 | 32 |
| 6 | 14 | 4 | 154 | -140 |
| 6 | 16 | 4 | -45 | -16 |
| 6 | 18 | 4 | 185 | -210 |
| 6 | 20 | 4 | -30 | 7 |
| 7 | 1 | 4 | 162 | 162 |
| 7 | 3 | 4 | 345 | -298 |
| 7 | 5 | 4 | 131 | -176 |
| 7 | 7 | 4 | 47 | 29 |
| 7 | 9 | 4 | 332 | 332 |
| 7 | 11 | 4 | -49 | -9 |
| 7 | 13 | 4 | 65 | 45 |
| 7 | 15 | 4 | 118 | -92 |
| 7 | 17 | 4 | 57 | -45 |
| 7 | 19 | 4 | -31 | -28 |
| 8 | 0 | 4 | 1026 | 1080 |
| 8 | 2 | 4 | 121 | 87 |
| 8 | 4 | 4 | 331 | -302 |
| 8 | 6 | 4 | 104 | 87 |
| 8 | 8 | 4 | 203 | 158 |
| 8 | 10 | 4 | 221 | -222 |
| 8 | 12 | 4 | 73 | 67 |
| 8 | 14 | 4 | 401 | 452 |
| 8 | 16 | 4 | 159 | 148 |
| 8 | 18 | 4 | 38 | 22 |
| 9 | 1 | 4 | 678 | -672 |
| 9 | 3 | 4 | 74 | -46 |
| 9 | 5 | 4 | -49 | 33 |
| 9 | 7 | 4 | 98 | 84 |
| 9 | 9 | 4 | -49 | -48 |
| 9 | 11 | 4 | 309 | 320 |
| 9 | 13 | 4 | 286 | -265 |
| 9 | 15 | 4 | 90 | 75 |
| 9 | 17 | 4 | 61 | -64 |
| 10 | 0 | 4 | 434 | -411 |
| 10 | 2 | 4 | 207 | 178 |
| 10 | 4 | 4 | 231 | 217 |
| 10 | 6 | 4 | -49 | 3 |
| 10 | 8 | 4 | 57 | -52 |
| 10 | 10 | 4 | 259 | 274 |
| 10 | 12 | 4 | 170 | 144 |
| 10 | 14 | 4 | 123 | -89 |
| 10 | 16 | 4 | 57 | -55 |
| 11 | 1 | 4 | 127 | 131 |
| 11 | 3 | 4 | 216 | -172 |
| 11 | 5 | 4 | 81 | -84 |
| 11 | 7 | 4 | 59 | -89 |
| 11 | 9 | 4 | 184 | 190 |
| 11 | 11 | 4 | 49 | 33 |
| 11 | 13 | 4 | 68 | 66 |
| 11 | 15 | 4 | 215 | -201 |
| 12 | 0 | 4 | 89 | 67 |
| 12 | 2 | 4 | 70 | -35 |
| 12 | 4 | 4 | -46 | 0 |
| 12 | 6 | 4 | 251 | -279 |
| 12 | 8 | 4 | 105 | -98 |
| 12 | 10 | 4 | 73 | -81 |
| 12 | 12 | 4 | 78 | -52 |
| 13 | 1 | 4 | 94 | 74 |
| 13 | 3 | 4 | 138 | -123 |
| 13 | 5 | 4 | 82 | 91 |
| 13 | 7 | 4 | 42 | 47 |
| 13 | 9 | 4 | 38 | -10 |
| 13 | 11 | 4 | 111 | -116 |
| 14 | 0 | 4 | 459 | -620 |
| 14 | 2 | 4 | -37 | 31 |
| 14 | 4 | 4 | 230 | 215 |
| 14 | 6 | 4 | 125 | -123 |
| 14 | 8 | 4 | 116 | -111 |
| 15 | 1 | 4 | 250 | -295 |
| 15 | 3 | 4 | 139 | 137 |
| 15 | 5 | 4 | 77 | 72 |

where the first and second lines refer to the potassium and ammonium picrate, respectively. It is immediately apparent that the *ortho* nitro groups are twisted relative to the plane of the benzene ring, (between 25 and 27°), while the *para*-positioned nitro group is almost coplanar with the benzene ring. In the case of the potassium picrate the twist is about 6°, whilst in ammonium picrate it is about 2·5°. The planarity of the benzene ring itself is questionable since the deviations of C(2) and C(3) from the least-squares plane are to the same side of the plane in the two analyses, and in the case of potassium picrate, the deviations reach the level of significance.

The deviations from the least-squares plane defined by C(2),N(2),O(2) and O(3) are:

| C(2) | N(2) | O(2) | O(3) |
|---|---|---|---|
| 0·002 | −0·007 | 0·003 | 0·003 Å |
| 0·003 | −0·012 | 0·004 | 0·004 |

Similarly, the deviations from the least-squares plane defined by C(1),C(2),C(3) and N(2) are:

| C(1) | C(2) | C(3) | N(2) |
|---|---|---|---|
| −0·007 | 0·022 | −0·008 | −0·007 Å |
| −0·007 | 0·022 | −0·008 | −0·007 |

As above, the first and second lines refer to potassium and ammonium picrate, respectively. The two last-mentioned sets of planes are inclined to each other by 26·6 and 25·7°. Regarding the *para* position, the corresponding groups of atoms must, by crystal symmetry, be exactly planar. The inclinations of the planes in the two salts are 5·0 and 2·2°. The strong rotation of the bond C(2)–N(2) must be due to the interaction between O(1) and O(2), which are only 2·685 and 2·675 Å apart. The nonplanarity of the benzene ring may be a consequence of the tendency of a conjugated system to maintain planarity on rotation of the nitro groups.

The bond lengths in the nitro groups conform with the results obtained in earlier investigations of nitrobenzenes and nitropyridines (Eichhorn, 1956; Trotter, 1959; Trueblood, Goldish & Donohue, 1961; Hanson, 1964; Coppens & Schmidt, 1964; Mugnoli, Mariani & Simonetti, 1965). The length of the bond between C(1) and O(1), 1·24 Å, is the same as that found in many ketones, aldehydes and carboxylic acids and their salts (*Tables of Interatomic Distances and Configuration in Molecules and Ions*, 1958, 1965). The C(1)–C(2) bond length, 1·45 Å, corresponds to that found in conjugated unsaturated systems such as acraldehyde and acrylic acid, and one may assume that the density of delocalized $\pi$-electrons is reduced from the even distribution in benzene to a degree similar to that for 'single bonds' in short conjugated unsaturated systems. The C(2)–C(3) and C(3)–C(4) bonds of 1·37 Å do not deviate significantly from what is normally found in benzene and its derivatives, neither do the C–N bonds of 1·44 to 1·46 Å to the nitro groups.

The bond angle C(2′)–C(1)–C(2) of 111·0° to 111·5° is, to the knowledge of the author, the smallest observed in a benzene ring. One may ask, on the basis of the bond lengths and angles of the carbon system, whether the term 'benzene ring' is appropriate in cases like these.

In Table 6 the shortest cation–anion distances and related angles are listed. The coordination of oxygen atoms around the potassium cation is illustrated in Fig. 3(*a*). As may be seen, the coordination is roughly square-antiprismatic. The potassium–oxygen distances, ranging from 2·74 to 2·92 Å, are as usually found in potassium salts of organic acids (Manojlović & Speakman, 1968; Manojlović, 1968; Larson & Nahringbauer, 1968). The corresponding distances and

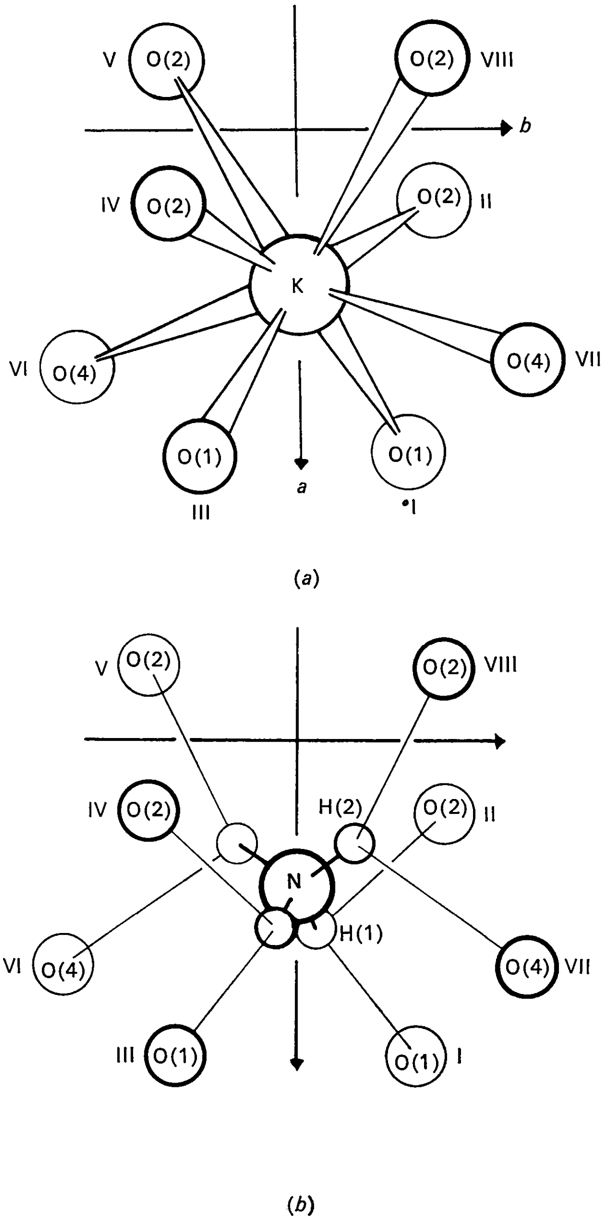

Fig. 3. The coordination of oxygen atoms around the potassium and ammonium ion. *Cf.* Table 6.

angles in ammonium picrate are also given in Table 6, together with the hydrogen–oxygen distances and angles relevant to the hydrogen bonding (*cf.* Donohue, 1952 and Fuller, 1959). It should be noted that each of the two crystallographically independent hydrogen atoms of the ammonium ion is shared by two acceptor oxygen atoms (*cf.* Albrecht & Corey, 1936 and Marsh, 1958); the bifurcations are indicated by thin, solid

Table 5. *Distances and angles within the picrate ion*

The standard deviations are in Å × $10^3$ and in degrees × 10.
Upper lines refer to potassium picrate, lower lines to ammonium picrate.

| | | | |
|---|---|---|---|
| C(1)–O(1) | 1·243 (7) Å | O(1)–C(1)–C(2) | 124·3 (3)° |
| | 1·239 (6) | | 124·3 (2) |
| C(1)–C(2) | 1·452 (5) | C(2)–C(1)–C(2′) | 111·1 (5) |
| | 1·450 (5) | | 111·5 (4) |
| C(2)–C(3) | 1·372 (6) | C(1)–C(2)–C(3) | 124·9 (4) |
| | 1·372 (5) | | 124·2 (3) |
| C(3)–C(4) | 1·382 (5) | C(1)–C(2)–N(2) | 119·3 (3) |
| | 1·368 (4) | | 119·8 (3) |
| C(3)–H | 0·983 (60) | C(3)–C(2)–N(2) | 115·7 (3) |
| | 0·966 (97) | | 115·9 (3) |
| N(1)–O(4) | 1·228 (5) | C(2)–C(3)–C(4) | 118·5 (4) |
| | 1·212 (4) | | 119·1 (3) |
| N(1)–C(4) | 1·436 (8) | C(2)–C(3)–H | 119·4 (50) |
| | 1·457 (7) | | 116·3 (60) |
| N(2)–O(2) | 1·232 (5) | C(4)–C(3)–H | 122·0 (40) |
| | 1·237 (5) | | 124·3 (60) |
| N(2)–O(3) | 1·229 (5) | C(3)–C(4)–C(3′) | 122·0 (5) |
| | 1·206 (5) | | 121·9 (3) |
| N(2)–C(2) | 1·457 (6) | C(3)–C(4)–N(1) | 119·0 (3) |
| | 1·461 (5) | | 119·1 (2) |
| O(1)–O(2) | 2·685 (3) | C(4)–N(1)–O(4) | 118·4 (3) |
| | 2·675 (3) | | 118·0 (2) |
| | | O(4)–N(1)–O(4′) | 123·3 (5) |
| | | | 124·0 (4) |
| | | C(2)–N(2)–O(2) | 118·9 (4) |
| | | | 118·0 (3) |
| | | C(2)–N(2)–O(3) | 118·5 (4) |
| | | | 118·7 (3) |
| | | O(2)–N(2)–O(3) | 122·6 (4) |
| | | | 123·3 (3) |

Table 6. *Distances and angles related to the coordination of oxygen atoms around the potassium and ammonium cations*

| | | | K/N | I | II | III | IV | V | VI | VII |
|---|---|---|---|---|---|---|---|---|---|---|
| I | O(1) | $(x, y, z)$ | 2·738 (2) Å | | | | | | | |
| | | | 2·836 (4) | | | | | | | |
| II | O(2) | $(x, y, z)$ | 2·867 (4) | 57·2° | | | | | | |
| | | | 2·944 (5) | 55·1 | | | | | | |
| III | O(1) | $(x, \bar{y}, \frac{1}{2}+z)$ | 2·738 | 99·3 | 156·5 | | | | | |
| | | | 2·836 | 101·5 | 156·5 | | | | | |
| IV | O(2) | $(x, \bar{y}, \frac{1}{2}-z)$ | 2·867 | 156·5 | 146·3 | 57·2 | | | | |
| | | | 2·944 | 156·5 | 148·4 | 55·1 | | | | |
| V | O(2) | $(x, \bar{y}, \bar{z})$ | 2·923 (4) | 115·2 | 70·2 | 126·0 | 83·5 | | | |
| | | | 3·056 (5) | 118·0 | 75·5 | 119·8 | 80·5 | | | |
| VI | O(4) | $(x, -\frac{1}{2}+y, \bar{z})$ | 2·789 (4) | 80·9 | 96·2 | 77·1 | 93·6 | 69·4 | | |
| | | | 2·927 (4) | 85·2 | 98·9 | 74·4 | 89·8 | 66·5 | | |
| VII | O(4) | $(x, \frac{1}{2}-y, \frac{1}{2}+z)$ | 2·789 | 77·1 | 93·6 | 80·9 | 96·2 | 144·2 | 145·8 | |
| | | | 2·927 | 74·4 | 89·8 | 85·2 | 98·9 | 145·6 | 147·7 | |
| VIII | O(2) | $(\bar{x}, y, \frac{1}{2}+z)$ | 2·923 | 126·0 | 83·5 | 115·2 | 70·1 | 77·0 | 144·2 | 69·4 |
| | | | 3·056 | 119·8 | 80·5 | 118·0 | 75·5 | 80·3 | 145·6 | 66·5 |

Column under 'K/N' gives the potassium–oxygen and nitrogen–oxygen distances. The angles following are the O–K–O and O–N–O angles, respectively.

| | | | | | |
|---|---|---|---|---|---|
| N––H(1) | 0·90 (90) Å | C(1)–O(1)–H(1) | 122° | O(1)–H(1) | 2·00 (80) Å |
| N––H(2) | 0·85 (60) | C(1)–O(1)–N | 117·0 | O(1)–N | 2·836 (4) |
| H(1)–N–H(1′) | 121° | N(2)–O(2)–H(1) | 127 | O(2)–H(1) | 2·44 (80) |
| H(2)–N–H(2′) | 110 | N(2)–O(2)–N | 133·0 | O(2)–N | 2·944 (5) |
| H(1)–N–H(2) | 114 | N(2)–O(2)–H(2″) | 116 | O(2)–H(2″) | 2·25 (60) |
| H(1)–N–H(2′) | 99 | N(2)–O(2)–N″ | 121·4 | O(2)–N″ | 3·056 (5) |
| | | N(1)–O(4)–H(2‴) | 157 | O(4)–H(2‴) | 2·48 (60) |
| | | N(1)–O(4)–N‴ | 141·7 | O(4)–N‴ | 2·927 (4) |

lines in Fig. 3(*b*). Since the phenoxide oxygen, which is one of the acceptors, lies on a twofold axis, it takes part in two equal hydrogen bondings, over H(1) and H(1) ($\frac{1}{2}-x,y,\bar{z}$). O(2) is neighboured by H(1) and H(2) ($\bar{x},\frac{1}{2}-y,-\frac{1}{2}+z$), while O(4) has only one hydrogen atom, H(2) ($x,\frac{1}{2}-y,-\frac{1}{2}+z$), of the ammonium ion close enough for hydrogen bonding.

Among the distances between atoms of different picrate ions in the crystals, the only short one in the direction approximately normal to the benzene ring is between C(1) and O(4) ($x,\frac{1}{2}-y,-\frac{1}{2}-z$) and O(4) ($\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}+z$), this being 3·206 Å in potassium picrate and 3·278 Å tn ammonium picrate.

All computations in this investigation have been performed on the IBM 360/50 computer at the University of Bergen Computer Facility. The programs used are written by the author and he wishes to take the opportunity to thank the computer staff for their assistance and advice.

### References

ALBRECHT, G. A. & COREY, R. B. (1939). *J. Amer. Chem. Soc.* **61**, 1087.

COPPENS, P. & SCHMIDT, G. M. J. (1964). *Acta Cryst.* **17**, 222.

DONOHUE, J. (1952). *J. Phys. Chem.* **56**, 502.

EICHHORN, E. L. (1956). *Acta Cryst.* **9**, 787.

FULLER, W. (1959). *J. Phys. Chem.* **63**, 1705.

HANSON, A. W. (1964). *Acta Cryst.* **17**, 559.

*International Tables for X-ray Crystallography* (1962). Vol. III. p. 202. Birmingham: Kynoch Press.

LARSON, G. & NAHRINGBAUER, I. (1968). *Acta Cryst.* B**24**, 666.

LINGAFELTER, E. C. & DONOHUE, J. (1966). *Acta Cryst.* **20**, 321.

MANOJLOVIĆ, L. (1968). *Acta Cryst.* B**24**, 326.

MANOJLOVIĆ, L. & SPEAKMAN, J. C. (1968). *Acta Cryst.* B**24**, 323.

MARSH, R. E. (1958). *Acta Cryst.* **11**, 654.

MUGNOLI, A. & MARIANI, C. & SIMONETTI, M. (1965). *Acta Cryst.* **19**, 367.

ROLLETT, J. S. (1965). *Computing Methods in Crystallography.* Oxford: Pergamon Press.

*Tables of Interatomic Distances and Configuration in Molecules and Ions* (1958, 1965). London: The Chemical Society.

TROTTER, J. (1959). *Acta Cryst.* **12**, 605.

TRUEBLOOD, K. N., GOLDISH, E. & DONOHUE, J. (1961). *Acta Cryst.* **14**, 1009.

ZACHARIASSEN, W. H. (1963). *Acta Cryst.* **16**, 1139.

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*Acta Cryst.* (1969). B**25**, 1460

# Zur Kristall- und Molekülstruktur des Octamethyl-tetraamidodiphosphono-2,3-butadien-1,3

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(*Eingegangen am* 4. *März* 1968 *und wiedereingereicht am* 20. *August* 1968)

Octamethyltetra-amino-2,3-diphosphinylbuta-1,3-diene, $CH_2:C[PO(NMe_2)_2].C[PO(NMe_2)_2]:CH_2$, crystallizes in the triclinic space group $P1$ ($C_1^1$) with unit-cell dimensions $a=8·7240$, $b=8·3414$, $c=6·3356$ Å; $\alpha=98·154°$, $\beta=85·601°$, $\gamma=105·513°$, and with $Z=1$. The crystal structure was determined by interpretation of the three-dimensional Patterson synthesis with aid of minimum functions and refined by isotropic and anisotropic least-squares methods. The hydrogen positions were determined by three-dimensional Fourier synthesis and also refined by least-squares methods. The final $R_1$ value was 0·074 (0·063 for observed intensities only). The molecule inclines to a *trans*-configuration. But the centrosymmetry around the C–C bond is considerably distorted, presumably because of the packing of the molecules. The bonding lengths are discussed. Only the N–C bond lengths differ significantly amongst themselves. The average value of the C–H distance is lower than the value determined by other methods. The other bond lengths are normal.

## Einleitung

Das Octamethyl-tetraamido-diphosphono-2,3-butadien-1,3 wurde im anorganisch-wissenschaftlichen Labor der Farbenfabriken Bayer AG von R. Schliebs dargestellt. Neben einer Bestätigung der Molekülkonstitution (mittelständige Anlagerung der beiden Phosphoratome) interessierte der gesamte sterische Aufbau des Moleküls, zumal P–N-Bindungen bislang vorwiegend in Ringstrukturen untersucht wurden.

## Experimentelles

Die zu untersuchende Substanz kristallisiert aus Aceton in säuligen, durchsichtigen Einkristallen, die wegen leichter Hygroskopie in Röhrchen aus Lindemannglas eingeschlossen wurden. Für die röntgenographische Untersuchung wurden Kristalle mit einem angenäherten Durchmesser von 0,15–0,20 mm ausgewählt. Es wurde Nickel-gefilterte Cu *Kα*-Strahlung verwendet. Die Absorption wurde nicht berücksichtigt.