Crystallographic Studies and Physico-Chemical Properties of \( \pi \)-Electron Compounds. Part II. Crystal and Molecular Structure of 2,4-Dinitrobenzoic Acid (DNBA)

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The crystal structure of the title compound has been determined by single-crystal X-ray diffraction studies from 1043 reflections. The crystals are monoclinic with \( a = 6.2150(7) \) Å, \( b = 14.393(2) \) Å, and \( c = 9.487(1) \) Å, \( \beta = 97.175(9)^\circ \), space group \( P2_1/c \), and \( Z = 4 \). The structure was solved by direct methods and refined by full-matrix least-squares to a final \( R = 0.050 \).

The molecule are paired by hydrogen bonding between the carboxy-groups (O–H ... O 2.656(3) Å), the two halves of the dimer being related by a centre of symmetry. It was found that the planes of the two carboxy-groups in the dimer are separated by a distance 0.113 Å.

The significant difference between \( \alpha_{\text{COOH}} \) values for para substituted benzoic acids with \( \pi \)-electron withdrawing and -releasing substituents, 1.4(1)°, was found.

The Lippincott-Schroeder model\(^{29} \) was applied to describe the properties of the H-bridge in DNBA and six other, accurately determined, crystal structures of para-substituted benzoic acids.

The amplitudes of internal motion of the substituents are estimated in terms of the Dunitz and White model.\(^{29} \)

INTRODUCTION

Carboxylic acids are well known as convenient systems to study substituent effects\(^1 \) as well as to analyze the structure and properties of an H-bridge.\(^2,3,8 \) Recently it has been found\(^4 \) that the O···O distance in the H-bridge of \( p \)-substituted benzoic acids, which measures approximately the strength of H-bond, does not follow the Hammett rule. On the other hand, it is known that the internal angle at substituted carbon of the benzene ring varies roughly in a linear way with \( \alpha_1 \) or electronegativity of the substituent (the Domenicano rule).\(^5,6 \) This discrepancy between substituent effects on structural properties of exo- and endocyclic parameters of substituted benzenes was interpreted\(^4 \) in terms of packing forces which influence strongly exocyclic substituents of the system, overcoming more subtle intramolecular substituent effects. Hence, carboxylic acids are often intensively studied in order to test theories of the H-bridge\(^7,8 \) as well as to analyze packing forces.\(^9 \)

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Considering the known structures of \( p \)- and \( o \)-nitrobenzoic acids\(^{10,11,12} \), it was interesting to study DNBA in order to analyze the role played by the second \( \text{NO}_2 \) group in DNBA in comparison with the mononitro derivatives.

**EXPERIMENTAL**

Commercial DNBA (Fluka A. G.) was used. The crystals were obtained with two different shapes. Applying the diffusing crystallization technique with acetone as the diffusing solvent and benzene as the original solvent, the crystals grown were plates with \( \{110\}, \{010\} \) and \( \{012\} \) forms. By slow cooling a methanolic solution of DNBA, the crystals grown were prisms with \( \{010\}, \{110\} \) and \( \{001\} \) forms. The latter, which have a much more convenient shape for diffractometric measurements, were chosen for further studies.

**Crystallographic measurements**

Oscillation and Weissenberg photographs showed the crystal to be monoclinic. A pale yellow prismatic crystal of dimensions \( 0.23 \times 0.30 \times 0.40 \text{ mm} \) was used for intensity collection. The intensities were measured on a Syntex P21 four-circle computer-controlled diffractometer with \( \text{CuK}_{\alpha} \) radiation monochromated by graphite up to \( 2\theta = 115.0^\circ \). The cell constants were determined by the least-squares treatment of 15 reflexions with \( 2\theta \) values between 12.3 and 34.1°. The crystal data (at 20°C) are: \( \text{C}_7\text{H}_4\text{N}_2\text{O}_6, M = 212.12 \). Monoclinic, \( a = 6.2150(7), b = 14.393(2), c = 9.487(1) \text{ Å}, \beta = 97.175(9)^\circ \), \( V = 842 \text{ Å}^3 \), \( D_m = 1.67 \text{ g cm}^{-3} \) (flotation in aqueous KI), \( Z = 4 \), \( D_e = 1.670 \text{ g cm}^{-3} \). m. p.: 181–182°C, \( F(000) = 432 \). \( \text{CuK}_{\alpha} \) radiation \( (\lambda = 1.54178 \text{ Å}) \), \( f'(\text{CuK}_{\alpha}) = 13.4 \text{ cm}^{-1} \). Systematic absences \( 0k0 \) with \( k = 2n + 1 \) uniquely define the space group as \( P2_11/c \).

The \( \Theta - 2\Theta \) scan technique was employed at a scan rate varying from 2.01 to 29.30° \( \text{min}^{-1} \) in \( 2\theta \).

The intensities were measured for 1130 unique reflexions, of which 1043 were classified as observed. A reflexion was considered as unobserved if \( I_{\text{obs}} < 1.960 \sigma(I) \), where \( \sigma(I) \) was calculated from the counting statistics. Lorentz and polarization factors were applied but no correction was made for absorption or extinction.

**Structure Solution and Refinement**

The crystal structure was solved by the direct multisolution method with the MULTAN program\(^{13} \) using 133 \( E^2 \)'s \( \geq 1.50 \) for which 983 \( \Sigma_2 \) relationships were generated.

A six-cycles refinement of the non-hydrogen atom coordinates by full-matrix least-squares procedures with individual isotropic thermal parameters unit weights gave \( R = 0.168 \); the CRYLSQ program in the XRAY 70 system\(^{14} \) was used with minimization of \( \Sigma w (|F_o| - |F_c|)^2 \). Subsequently, the quantities \( 1/\sigma^2(F_o) \), where \( \sigma(F_o) \) was as defined by Stout and Jensen,\(^{15} \) were used to weigh the least-squares differences for the observed data.

The vibrational model was then changed to an anisotropic one and five subsequent cycles of least-squares refinement were attempted; \( R \) was reduced to 0.080. The next six cycles of refinement, with H-atom positions calculated geometrically by using the XANADU program\(^{16} \) resulted in \( R = 0.052 \) and \( R_w = 0.087 \).

A difference Fourier map revealed distinctly the position of the carboxylic H-atom. Finally, the coordinates and isotropic temperature factors of the H-atom in the carboxylic group were refined in six additional cycles of refinement. The analysis was based on scattering factors for neutral atoms taken from International Tables for X-ray Crystallography.\(^{17} \) Refinement converged with \( R = 0.050 \) and \( R_w = 0.059 \).

The average shift/error value at the end of the refinement procedure was 0.003. The computations were performed on a CDC 6600 (CYBER-72) computer.
The final fractional coordinates from the last cycle of the least-squares refinement of non-hydrogen atoms (including the H-atom involved in an H-bond) are given in Table I*.

**TABLE I**

Fractional Coordinates ($\times 10^4$) for Non-hydrogen Atoms (Including, However, the H Atom ($\times 10^3$) Involved in an H-bond). Estimated Standard Deviations from the Final Full-matrix Least-squares Cycle are Given in Parentheses

<table>
<thead>
<tr>
<th>Atom</th>
<th>$x$</th>
<th>$y$</th>
<th>$z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>7543(5)</td>
<td>2958(2)</td>
<td>646(3)</td>
</tr>
<tr>
<td>C2</td>
<td>8203(5)</td>
<td>2058(2)</td>
<td>386(3)</td>
</tr>
<tr>
<td>C3</td>
<td>7208(5)</td>
<td>1283(2)</td>
<td>856(3)</td>
</tr>
<tr>
<td>C4</td>
<td>5453(5)</td>
<td>1436(2)</td>
<td>1581(3)</td>
</tr>
<tr>
<td>C5</td>
<td>4690(5)</td>
<td>2306(2)</td>
<td>1850(4)</td>
</tr>
<tr>
<td>C6</td>
<td>5753(5)</td>
<td>3070(2)</td>
<td>1370(4)</td>
</tr>
<tr>
<td>C7</td>
<td>8684(5)</td>
<td>3330(2)</td>
<td>282(3)</td>
</tr>
<tr>
<td>O1</td>
<td>10564(4)</td>
<td>3945(1)</td>
<td>994(3)</td>
</tr>
<tr>
<td>O2</td>
<td>7767(4)</td>
<td>4397(1)</td>
<td>-553(2)</td>
</tr>
<tr>
<td>N1</td>
<td>9998(4)</td>
<td>1906(2)</td>
<td>-474(3)</td>
</tr>
<tr>
<td>O3</td>
<td>10886(4)</td>
<td>1156(2)</td>
<td>-411(3)</td>
</tr>
<tr>
<td>O4</td>
<td>10471(5)</td>
<td>2549(2)</td>
<td>-1203(3)</td>
</tr>
<tr>
<td>N2</td>
<td>4318(5)</td>
<td>619(2)</td>
<td>2061(3)</td>
</tr>
<tr>
<td>O5</td>
<td>4943(5)</td>
<td>-143(2)</td>
<td>1738(3)</td>
</tr>
<tr>
<td>O6</td>
<td>2849(5)</td>
<td>747(2)</td>
<td>2770(4)</td>
</tr>
<tr>
<td>HO1</td>
<td>1124(5)</td>
<td>454(2)</td>
<td>79(4)</td>
</tr>
</tbody>
</table>

**RESULTS**

The atom-labelling scheme and the anisotropic thermal ellipsoids of the DNBA molecule are shown in Figure 1. Bond lengths and angles are shown in Figure 2. The shortest intermolecular distances (less than 3.4 Å) are listed in

Figure 1. Thermal ellipsoid plot (ORTEP, Johnson***) showing vibration ellipsoids at the 50% probability level.

* Thermal parameters (Table II), positions of hydrogen atoms (Table III) and comparison of observed and calculated structure factors are available on request.
Figure 2. The number scheme for the atoms together with bond lengths (Å) and angles (°). The bond lengths in the upper line are corrected for libration.

Table IV. Table V gives the least-squares planes for the atoms C1 through C6, (plane 1), C1, C7, O1, O2 (plane 2), C2, N1, O3, O4 (plane 3) and C4, N2, O5, O6 (plane 4). The angles between the above-mentioned planes are listed in Table VI. Figure 3 represents a projection of the unit cell along the \{001\} direction.

**TABLE IV**

*Table V and Table VI are available on request.*
DISCUSSION

(i) Geometry of the Ring

Two parameters, valence angles and bond lengths, describe the geometry of the benzene ring. It is usually considered that both are affected by substituents. Following the Walsh rule the C—C bonds adjacent to the substituted carbon atom are shortened when the substituent is electron withdrawing. In the DNBA-molecule all substituents are of this character and the shortening of CC-bond lengths in the ring is expected. In fact C2C3, C3C4 and C4C5-bonds are considerably shorter than the others, as shown clearly in Figure 2. In consequence the mean bond length for ring bonds is \( R = 1.387 \) Å, whereas for benzene \( R = 1.392 \) Å, for the X-ray measurements corrected for libration.

Both nitro groups influence the endocyclic angle at substituted carbon atoms in nearly the same way yielding \( \alpha = 123.4^\circ \) and 122.9°; these values are in good agreement with other data for the nitro group: \( \alpha = 123.7^\circ \) for o-nitrobenzoic acid and \( \alpha = 123.3^\circ \) and \( \alpha = 122.6^\circ \) for p-nitrobenzoic acid.

Following Domenicano et al. the valence angle at the carbon atom substituted by COOH should be about 120° for unsubstituted and para-substituted benzoic acids. In the DNBA molecule \( \alpha_{COOH} = 117.9^\circ \). Similar values are observed for: o-nitrobenzoic acid with \( \alpha \) (at COOH) = 116.2°, o-N,N-dimethyl-aminobenzoic acid and o-aminobenzoic acid for which \( \alpha = 117.0^\circ \) and 118.0°. Our finding and those mentioned above may be partially explained in terms of intramolecular interactions between non-bonded atoms in the o-substituent and the carboxyl group. In most of those systems the closest contacts between the interacting atoms of ortho-substituents are lower or much lower than the sum of the Van der Waals radii. In the case of DNBA the closest contacts are \( R(O_1 \cdots O_3) = 2.891 \) Å and \( R(O_1 \cdots C_7) = 2.648 \) Å whereas the sums of Van der Waals radii for these contacts are 3.04 Å and 3.22 Å respectively.
Due to the interactions described above, the X substituent repels the COOH group yielding a larger $a'$-angle. As a consequence the sp$^2$-hybridization at the C-atom is perturbed, leading in turn to a decrease of two other angles $\alpha$ and $\alpha''$:

$\text{COOH}$

Hence $\alpha$ becomes lower as a result of steric hindrance of the ortho-substituent.

This effect is apparent while applying the additivity rule of substituent effect on the ring geometry. Applying the most recent angular parameters$^{25}$ for NO$_2$ and COOH the results obtained are given on the scheme below (calculated data in parentheses):

Only calculated value for $\alpha_{\text{COOH}}$ differs distinctly from its experimental value. This result supports our suggestion on mechanism of interactions for o-substituents.

Another problem arises when looking at $\alpha_{\text{COOH}}$ for para-substituted benzoic acids. According to Domenicano et al.$^{13}$ the mean value of the internal angle $\alpha_{\text{COOH}}$ at the ipso carbon of the ring is 119.8° for five para-substituted benzoic acids. Colapietro et al.$^{26,27}$ have studied the molecular geometries of several para-substituted benzoic acids. Their comparison has shown small structural effect of the para-substituent on the $\alpha_{\text{COOH}}$ angle. Actually the geometries of almost 20 molecules of para-substituted benzoic acids are available. More detailed analysis of the problem leads to the result that $\alpha_{\text{COOH}}$ for para-substituted benzoic acids with $\sigma$-electron-withdrawing substituents equals to 120.2(1)° whereas for $\sigma$-electron-releasing substituted acids $\alpha_{\text{COOH}} = 118.8(1)$°. The difference is significant and indicates the importance of intramolecular interactions between the COOH-group and the para-substituent. Hence it should be stated that a substituent in para-position does influence the $\alpha_{\text{COOH}}$ and this effect depends on the electronic properties of the substituent.

(ii) Geometry of Substituents

The geometry of the substituents may be discussed in terms of their bond lengths and valence angles as well as of dihedral angles between the planes of the substituents and that of the benzene ring. Within experimental error the NO$_2$ groups in DNBA possess axial symmetry in agreement with the data.
for p-nitrobenzoic acid,\textsuperscript{10} but in opposition to the geometry of the NO\textsubscript{2} group in o-nitrobenzoic acid\textsuperscript{12} where the geometry deviates considerably from axial symmetry. As seen in Table IV, the intermolecular contacts between oxygen atoms in NO\textsubscript{2} groups with other atoms are almost equal to or longer than the sum of the Van der Waals radii and hence axial symmetry of both NO\textsubscript{2} groups is found, as expected. The only slightly shorter contact between O and C is 3.196(4) Å in comparison with the sum of Van der Waals radii of these atoms, 3.22 Å.\textsuperscript{24} This interaction is not reflected in a change of the N—O bond length, but only in the r.m.s. thermal motion amplitude of the oxygen atom. Another consequence of both overcrowded o-substituents is the considerable displacement of C\textsubscript{7} and N\textsubscript{1} atoms, by 0.126 Å and −0.099 Å, respectively, measured relatively to the plane of the ring. For o-nitrobenzoic acid the first figure is 0.209 Å\textsuperscript{12} whereas for p-nitrobenzoic acid it is −0.019 Å.\textsuperscript{10}

The latter finding means almost coplanarity of the ring- and carboxyl group-planes in p-nitrobenzoic acid.

The intra- and intermolecular interactions are the reason for mutual orientations of planes of the ring and of all substituents. The relevant data are collected in Table VI.

(iii) Application of the Lippincott-Schroeder Model to DNBA and Several p-Substituted Benzoic Acids

The geometry of the hydrogen bond determined by X-ray diffraction analysis can be applied in estimations of such properties as the energy, force constants for OH and OH···O vibrations as well as charge density at oxygen atoms. This has been accomplished for DNBA and several p-substituted benzoic acids within the semiempirical model of the hydrogen bond introduced by Lippincott and Schroeder.\textsuperscript{28,29}

The results of the analysis are presented in Table VII. Columns 2—4 show the geometry of the H-bridge. Column 5 contains the energies, $V_{\text{exp}}$, of the H-bridge: these values tend to increase with a decrease of the O···O distance.

Column 6 contains the charge-density values at oxygen atoms whereas columns 7—8 present the force constants $k_{O-O}$ and $k_{O-H}$. Column 9 lists the calculated frequencies of OH vibration ($\nu_{\text{OH}}$) involved in the H-bridge.

Apart from the information contained in Table VIII, it is worth mentioning that COOH groups in the dimer of DNBA are parallel, but they do not lie in the same plane. The perpendicular distance between the planes is 0.113 Å. This finding was also observed by Jeffrey\textsuperscript{30} for many carboxylic systems and it was interpreted in terms of intermolecular forces.

(iv) Torsional Motions of Substituents

When analyzing the values of atomic root-mean-square amplitudes of vibration of the atoms in the p-NO\textsubscript{2} group along the principal axes of the thermal ellipsoids, one can observe a significant difference between the r.m.s. amplitudes of vibration of both oxygen atoms. This appears to be due to the difference in the intermolecular contact for the two atoms. One of them O\textsubscript{5}···C\textsubscript{6} is equal to 3.196 Å, and is shorter than the sum of Van der Waals radii 3.22 Å.\textsuperscript{24} For O\textsubscript{3} ($\langle u^2 \rangle^{1/2} = 0.22$ Å compared with the value 0.29 Å for O which is not surrounded by such close contacts. For the ortho-NO\textsubscript{2} group
<table>
<thead>
<tr>
<th>Acid</th>
<th>O...O (Å)</th>
<th>O−H (Å)</th>
<th>O−H...O (°)</th>
<th>$V_{\text{exp}}$ (\text{kcal/mol})</th>
<th>Charge (e\textsuperscript{−})</th>
<th>$k_{\text{O−H}}$ (\text{(10}^5 \times \text{dyna. cm}^{-1}\text{)})</th>
<th>$k_{\text{O...O}}$ (cm\textsuperscript{-1})</th>
<th>$\gamma_{\text{OH}}$ (cm\textsuperscript{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-Nitrobenzoic\textsuperscript{16}</td>
<td>2.660(2)</td>
<td>1.04(2)</td>
<td>177(2)</td>
<td>−8.85</td>
<td>0.251</td>
<td>0.876</td>
<td>4.232</td>
<td>2714.4</td>
</tr>
<tr>
<td>(A) p-n-Butoxybenzoic\textsuperscript{36}</td>
<td>2.600(3)</td>
<td>1.08\textsuperscript{L}</td>
<td>179</td>
<td>−10.35</td>
<td>0.288</td>
<td>1.586</td>
<td>2.959</td>
<td>2269.8</td>
</tr>
<tr>
<td>(B) p-n-Butoxybenzoic\textsuperscript{36}</td>
<td>2.652(3)</td>
<td>0.98\textsuperscript{L}</td>
<td>166</td>
<td>−7.34</td>
<td>0.222</td>
<td>0.561</td>
<td>6.126</td>
<td>3264.6</td>
</tr>
<tr>
<td>p-Fluorobenzoic\textsuperscript{37}</td>
<td>2.618(2)</td>
<td>1.11(4)</td>
<td>176(3)</td>
<td>−7.87</td>
<td>0.292</td>
<td>1.676</td>
<td>2.146</td>
<td>1928.9</td>
</tr>
<tr>
<td>p-Methoxybenzoic\textsuperscript{38}</td>
<td>2.632(2)</td>
<td>1.00(4)</td>
<td>172(3)</td>
<td>−8.90</td>
<td>0.241</td>
<td>0.774</td>
<td>5.421</td>
<td>3068.7</td>
</tr>
<tr>
<td>Cinnamic\textsuperscript{39}</td>
<td>2.630</td>
<td>1.01</td>
<td>175</td>
<td>−9.35</td>
<td>0.249</td>
<td>0.866</td>
<td>5.075</td>
<td>2971.3</td>
</tr>
<tr>
<td>$\beta$-(p-chlorophenyl) propionic\textsuperscript{40}</td>
<td>2.645(3)</td>
<td>0.93(4)</td>
<td>177(3)</td>
<td>−5.35</td>
<td>0.210</td>
<td>0.456</td>
<td>7.227</td>
<td>3548.3</td>
</tr>
<tr>
<td>DNBA</td>
<td>2.656(3)</td>
<td>0.98(3)</td>
<td>174(3)</td>
<td>−7.71</td>
<td>0.227</td>
<td>0.600</td>
<td>6.023</td>
<td>3237.8</td>
</tr>
</tbody>
</table>

- thermally corrected values are based on a riding model.
there are no shorter contacts than the sum of Van der Waals radii, and the r.m.s. thermal motion amplitudes for both oxygens in this group are axially symmetric within experimental error: \((<\mathbf{u}^2>)^2 = 0.25\) and 0.27 Å.

More detailed analysis of the thermal motion of the substituents was carried out by the use of Huber-Buser\(^{24}\) THMB computer program based upon the theory of Dunitz and White.\(^{23}\) This theory allows the analysis of thermal motions of the substituents treated as internally rigid, librating usually around the bond relative to the rigid moiety of the ring. An agreement between the calculated and experimentally determined anisotropic temperature factors was tested by using the reliability factor\(^{33}\) \(R_{wu} = \frac{[\sum W_{ij}(|U_{ij}|^2 - |U_{ij}\text{obs.}|^2)]^{1/2}}{\sum W_{ij} |U_{ij}|^2}\) where \(U_{ij}\) is the contravariant component of mean square atomic motion tensor (in Å\(^2\)) whereas \(w_{ij} = (\sigma_{ij})^2\) with \(\sigma_{ij}\) being standard deviation of \(U_{ij}\). A hypothesis for improving the agreement between the calculated anisotropic temperature factors for the non-rigid body model and those determined experimentally for the rigid body model was verified by the Hamilton R-ratio test.\(^{34}\) The value of \(R_{wu}^2/R_{wu}\) is 1.209 with the number of degrees of freedom 72. Hence, the difference between \(R_{wu}\) and \(R_{wu}\) is significant at the level of 0.05.

The r.m.s. thermal motion amplitude has the lowest value for the COOH group, 4.9°; due to overcrowding as well as to the H-bond effect in dimers of the two NO\(_2\) groups in the DNBA molecule the ortho-group exhibits a smaller value of r.m.s. group libration amplitude, 8.2°, in comparison with more sterically free p-group for which it equals to 9.7°. The \(R_{wu}\) for DNBA is 0.115, \(\Delta U_{ij} = 0.0053\) and \(\langle\sigma_{ij}\rangle_{av} = 0.0046\). In comparison, for the COOH group in p-nitrobenzoic acid,\(^{11}\) which is involved in H-bonding but is not sterically hindered the r.m.s. value is as large as 9°.

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**REFERENCES**


**SAŽETAK**

Kristalografsko istraživanje i fizičko-kemijska svojstva \ensuremath{\pi}\,-elektronskih spojeva. Kristalna i molekulska struktura 2,4-dinitrobenzojeve kiseline (DNBA)

T. Wieckowski i T. M. Krygowski

Kristalna struktura 2,4-dinitrobenzojeve kiseline (DNBA) određena je metodom difrakcije rendgenskih zraka na monokristalu sa 1043 refleksa. Kristali su monoklinski, \(a = 6,2150(7), b = 14,393(2)\) i \(c = 9,487(1)\) Å, \(\beta = 97,175(9)^{o}\), prostorna grupa \(P2_1/c\) i \(Z = 4\). Struktura je riješena direktnim metodama i utočnjena metodom najmanjih kvadrata do konačnog \(R = 0,050\).

Molekule su spojene u parove preko centrosimetričnih vodikovih veza među karboksilnim grupama (O—H...O 2,656(3) Å). Nađeno je da je razmak među ravnina karboksilnih skupina u dimeru 0,113 Å. Nađena je snažnja razlika (1,4(1)°) među vrijednostima \(\alpha_{COOH}\) za para-supstituiranu benzojevu kiselinu sa supstituentima koji privlače i onima koji oslobađaju \(\sigma\)-elektrone.

Za opis svojstava vodikovog mosta u DNBA i šest drugih, točno određenih, kristalnih struktura para-supstituirane benzojeve kiseline primijenjen je Lippincott-Schroederov model.

Amplitude internog gibanja supstituenata analizirane su upotrebom modela Dunitza i Whitea.