# X-ray powder diffraction data for N-[4-(aminocarbonyl)phenyl]-4-[2-[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]diazenyl]-benzamide, a β-form of pigment yellow 181

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X-ray powder diffraction data, unit-cell parameters and space group for the $\beta$-form of pigment yellow 181, $C_{25}H_{21}N_7O_5$, are reported [$a = 22.556(6)$ Å, $b = 4.9684(9)$ Å, $c = 21.318(6)$ Å, $\beta = 109.492(4)°$, unit-cell volume $V = 2252,1$ Å$^3$, $Z = 4$, space group $P2_1/c$]. All measured lines were indexed and are consistent with the $P2_1/c$ space group. No detectable impurities were observed.
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Key words: X-ray powder diffraction, $\beta$-form of pigment yellow 181

## I. INTRODUCTION

The $\beta$-form of pigment yellow 181 (P.Y. 181, $C_{25}H_{21}N_7O_5$, Figure 1) belongs to a family of industrialy important benzimidazolone pigments (van de Streek *et al.*, 2009). It is a reddish-yellow pigment with good heat stability and lightfastness (Herbst and Hunger, 2004). Its yellow colour closely resembles the colour of wood, so enables its application in the manufacture of laminate and other wood-effect products. P.Y. 181 is known to exist in several polymorphs (Schmidt and Mehltretter, 2008), of which the $\beta$- polymorph has the most favourable properties, and it is therefore this polymorph that is prepared industrially. Pidcock *et al.* (2007) reported detailed synthesis of the compound and its crystal structure determined from laboratory powder diffraction data.

## II. EXPERIMENTAL

The title compound (Figure 1) was obtained as a gift from the company Synthesia, a.s., Pardubice, Czech Republic.

The diffraction pattern for the title compound was collected at room temperature using an X'Pert PRO $\theta$-$\theta$ powder diffractometer with parafocusing Bragg-Brentano geometry and Cu $K\alpha$ radiation ($\lambda = 1.5418$ Å, generator setting: 40 kV, 30 mA). An ultrafast X'Celerator detector was employed to collect XRD data over the angular range from 7 to 70°$2\theta$ with a step size of 0.017°$2\theta$ and a counting time of 81.28 s/step. Data evaluation were performed using the software package HIGHSCORE PLUS V 2.2e PANALYTICAL, Almelo, Netherlands.

Automatic indexing of the experimental XRD pattern was done using DICVOL04 (Boultif and Louër, 2004).

## III. RESULTS

The experimental powder diffraction pattern is depicted in Figure 2. Automatic indexing results obtained by DICVOL04 show that the title compound is monoclinic with space group $P2_1/c$ and unit-cell parameters: $a = 22.556(6)$ Å, $b = 4.9684(9)$ Å, $c = 21.318(6)$ Å, $\beta = 109.492(4)°$, unit-cell volume $V = 2252,1$ Å$^3$, $Z = 4$. The figures of merits are $F_{30} = 12.1$ (0.0134, 185) (Smith and Snyder, 1979) and $M_{20} = 5.1$ (de Wolff, 1968). All lines were indexed and are consistent with the $P2_1/c$ space group (Table I).

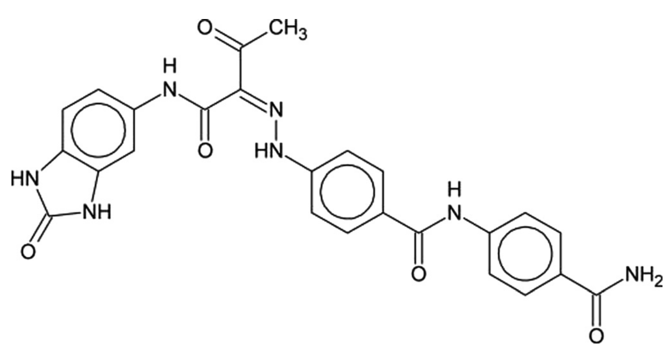


Figure 1. Structural formula of the title compound, $C_{25}H_{21}N_7O_5$.

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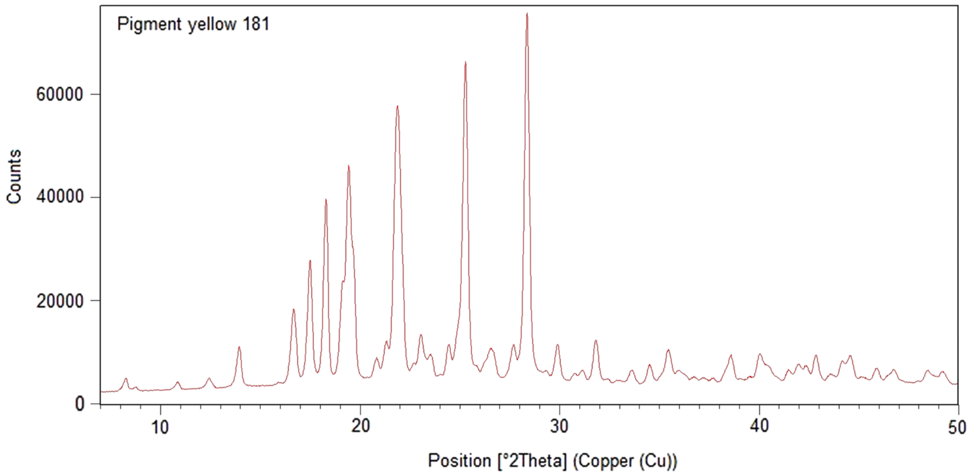


Figure 2. (Color online) X-ray powder diffraction pattern of the title compound, $C_{25}H_{21}N_7O_5$, using Cu $K\alpha$ radiation ($\lambda = 1.5418$ Å).

TABLE I. Indexed X-ray powder diffraction data for the title compound, $C_{25}H_{21}N_7O_5$. Only the peaks with $I_{rel}$ of 1 or greater are presented [$a = 22.556(6)$ Å, $b = 4.9684(9)$ Å, $c = 21.318(6)$ Å, $\beta = 109.492(4)°$, unit-cell volume $V = 2252{,}1$ Å$^3$, $Z = 4$, space group $P2_1/c$]. All lines were indexed and are consistent with the $P2_1/c$ space group.

| $2\theta_{obs}$ (deg) | $d_{obs}$ (Å) | $I_{obs}$ | $h$ | $k$ | $l$ | $2\theta_{cal}$ (deg) | $d_{calc}$ (Å) | $\Delta 2\theta$ (deg) |
|---|---|---|---|---|---|---|---|---|
| 8.274 | 10.678 | 4 | 2 | 0 | 0 | 8.309 | 10.632 | −0.045 |
| 8.747 | 10.102 | 1 | 0 | 0 | 2 | 8.794 | 10.047 | −0.054 |
| 10.861 | 8.139 | 2 | 1 | 0 | 2 | 10.913 | 8.100 | −0.039 |
| 12.438 | 7.111 | 3 | 3 | 0 | 0 | 12.478 | 7.088 | −0.023 |
| 13.948 | 6.344 | 11 | 2 | 0 | 2 | 13.990 | 6.325 | −0.019 |
| 15.947 | 5.553 | 1 | 4 | 0 | −2 | 16.039 | 5.522 | −0.032 |
| 16.674 | 5.312 | 21 | 4 | 0 | 0 | 16.663 | 5.316 | 0.004 |
| 17.494 | 5.066 | 34 | 3 | 0 | 2 | 17.540 | 5.052 | −0.013 |
| 18.291 | 4.846 | 50 | 1 | 1 | 0 | 18.323 | 4.838 | −0.008 |
| 19.142 | 4.633 | 28 | 1 | 1 | 1 | 19.177 | 4.624 | −0.008 |
| 19.431 | 4.564 | 59 | 1 | 0 | 4 | 19.448 | 4.561 | −0.004 |
| 19.703 | 4.502 | 32 | 2 | 1 | 0 | 19.707 | 4.501 | −0.001 |
| 20.821 | 4.263 | 6 | 2 | 1 | 1 | 20.807 | 4.266 | 0.003 |
| 21.319 | 4.164 | 11 | 4 | 0 | 2 | 21.341 | 4.160 | −0.004 |
| 21.870 | 4.061 | 75 | 3 | 1 | 0 | 21.828 | 4.068 | 0.008 |
| 22.154 | 4.009 | 29 | 2 | 1 | −3 | 22.166 | 4.007 | −0.002 |
| 22.706 | 3.913 | 5 | 2 | 1 | 2 | 22.741 | 3.907 | −0.006 |
| 23.054 | 3.855 | 13 | 3 | 1 | 1 | 23.102 | 3.847 | −0.008 |
| 23.516 | 3.780 | 7 | 1 | 1 | 3 | 23.467 | 3.788 | 0.008 |
| 24.038 | 3.699 | 2 | 4 | 1 | −2 | 24.077 | 3.693 | −0.006 |
| 24.453 | 3.637 | 10 | 4 | 1 | 0 | 24.504 | 3.630 | −0.007 |
| 24.898 | 3.573 | 13 | 3 | 0 | 4 | 24.889 | 3.575 | 0.001 |
| 25.278 | 3.520 | 87 | 5 | 0 | 2 | 25.297 | 3.518 | −0.003 |
| 25.856 | 3.443 | 4 | 4 | 1 | 1 | 25.896 | 3.438 | −0.005 |
| 26.329 | 3.382 | 10 | 4 | 0 | −6 | 26.276 | 3.389 | 0.007 |
| 26.556 | 3.354 | 14 | 0 | 0 | 6 | 26.594 | 3.349 | −0.005 |
| 27.690 | 3.219 | 10 | 7 | 0 | −2 | 27.676 | 3.221 | 0.002 |
| 28.362 | 3.144 | 100 | 2 | 1 | 4 | 28.408 | 3.139 | −0.005 |
| 29.306 | 3.045 | 3 | 6 | 0 | 2 | 29.362 | 3.039 | −0.006 |
| 29.893 | 2.987 | 10 | 1 | 1 | 5 | 29.938 | 2.982 | −0.004 |
| 30.759 | 2.905 | 2 | 5 | 1 | −5 | 30.778 | 2.903 | −0.002 |
| 31.138 | 2.870 | 3 | 3 | 1 | −6 | 31.146 | 2.869 | −0.001 |
| 31.808 | 2.811 | 11 | 8 | 0 | −2 | 31.796 | 2.812 | 0.001 |
| 32.384 | 2.762 | 1 | 8 | 0 | −4 | 32.403 | 2.761 | −0.002 |
| 32.929 | 2.718 | 1 | 6 | 1 | −5 | 32.907 | 2.720 | 0.002 |
| 33.683 | 2.659 | 3 | 5 | 1 | 3 | 33.688 | 2.658 | 0.000 |
| 34.512 | 2.597 | 8 | 1 | 0 | −8 | 34.502 | 2.597 | 0.001 |
| 35.458 | 2.530 | 9 | 7 | 1 | −5 | 35.442 | 2.531 | 0.001 |
| 35.960 | 2.495 | 3 | 9 | 0 | −2 | 36.000 | 2.493 | −0.003 |
| 36.359 | 2.469 | 2 | 1 | 2 | 0 | 36.383 | 2.467 | −0.002 |
| 36.732 | 2.445 | 2 | 8 | 1 | −2 | 36.693 | 2.447 | 0.003 |
| 37.184 | 2.416 | 1 | 1 | 2 | −2 | 37.153 | 2.418 | 0.002 |
| 37.671 | 2.386 | 1 | 6 | 1 | −7 | 37.698 | 2.384 | −0.002 |
| 38.314 | 2.347 | 3 | 3 | 1 | −8 | 38.309 | 2.348 | 0.000 |
| 38.572 | 2.332 | 7 | 2 | 2 | −3 | 38.568 | 2.332 | 0.000 |
| 39.079 | 2.303 | 1 | 1 | 1 | −8 | 39.102 | 2.302 | −0.001 |
| 39.527 | 2.278 | 2 | 2 | 1 | 7 | 39.513 | 2.279 | 0.001 |
| 40.035 | 2.250 | 8 | 4 | 2 | 0 | 40.030 | 2.251 | 0.000 |
| 40.515 | 2.225 | 4 | 0 | 2 | 4 | 40.476 | 2.227 | 0.002 |
| 41.476 | 2.175 | 3 | 9 | 1 | −5 | 41.475 | 2.175 | 0.000 |
| 41.976 | 2.151 | 5 | 5 | 2 | −3 | 41.976 | 2.151 | 0.000 |
| 42.332 | 2.133 | 4 | 9 | 1 | 0 | 42.324 | 2.134 | 0.000 |
| 42.840 | 2.109 | 7 | 5 | 0 | −10 | 42.851 | 2.109 | 0.000 |
| 43.583 | 2.075 | 2 | 7 | 1 | 4 | 43.578 | 2.075 | 0.000 |
| 44.164 | 2.049 | 6 | 4 | 2 | 3 | 44.191 | 2.048 | −0.001 |
| 44.555 | 2.032 | 7 | 8 | 1 | 3 | 44.516 | 2.034 | 0.002 |
| 45.158 | 2.006 | 2 | 2 | 2 | 5 | 45.154 | 2.006 | 0.000 |
| 45.958 | 1.973 | 3 | 6 | 2 | −5 | 45.947 | 1.974 | 0.000 |
| 46.485 | 1.952 | 2 | 10 | 0 | 2 | 46.468 | 1.953 | 0.001 |
| 46.735 | 1.942 | 4 | 7 | 1 | 5 | 46.763 | 1.941 | −0.001 |
| 47.953 | 1.896 | 1 | 2 | 1 | 9 | 47.931 | 1.896 | 0.001 |
| 48.430 | 1.878 | 3 | 0 | 2 | −7 | 48.418 | 1.878 | 0.000 |
| 49.175 | 1.851 | 3 | 6 | 2 | 3 | 49.200 | 1.850 | −0.001 |
| 50.323 | 1.812 | 2 | 8 | 1 | −10 | 50.336 | 1.811 | 0.000 |
| 51.013 | 1.789 | 1 | 10 | 0 | −10 | 51.029 | 1.788 | 0.000 |
| 51.535 | 1.772 | 1 | 8 | 2 | 1 | 51.539 | 1.772 | 0.000 |
| 52.050 | 1.756 | 1 | 9 | 2 | −4 | 52.063 | 1.755 | 0.000 |
| 52.355 | 1.746 | 1 | 2 | 0 | −12 | 52.356 | 1.746 | 0.000 |
| 53.636 | 1.707 | 0 | 13 | 0 | −2 | 53.637 | 1.707 | 0.000 |
| 54.518 | 1.682 | 1 | 6 | 1 | 8 | 54.519 | 1.682 | 0.000 |
| 55.184 | 1.663 | 1 | 10 | 2 | −2 | 55.211 | 1.662 | −0.001 |
| 56.181 | 1.636 | 1 | 13 | 0 | 0 | 56.187 | 1.636 | 0.000 |
| 57.226 | 1.609 | 1 | 2 | 3 | −3 | 57.215 | 1.609 | 0.000 |
| 57.623 | 1.598 | 1 | 14 | 0 | −6 | 57.626 | 1.598 | 0.000 |
| 58.765 | 1.570 | 4 | 11 | 2 | −5 | 58.764 | 1.570 | 0.000 |
| 60.399 | 1.531 | 0 | 8 | 2 | −10 | 60.393 | 1.532 | 0.000 |
| 61.717 | 1.502 | 0 | 10 | 2 | −9 | 61.709 | 1.502 | 0.000 |
| 62.238 | 1.490 | 0 | 9 | 0 | 8 | 62.229 | 1.491 | 0.000 |
| 63.402 | 1.466 | 1 | 1 | 3 | 6 | 63.399 | 1.466 | 0.000 |
| 64.822 | 1.437 | 0 | 15 | 1 | −4 | 64.813 | 1.437 | 0.000 |

TABLE I. (*Continued*).

| $2\theta_{obs}$ (deg) | $d_{obs}$ (Å) | $I_{obs}$ | $h$ | $k$ | $l$ | $2\theta_{cal}$ (deg) | $d_{calc}$ (Å) | $\Delta 2\theta$ (deg) |
|---|---|---|---|---|---|---|---|---|
| 65.643 | 1.421 | 0 | 8 | 1 | 9 | 65.637 | 1.421 | 0.000 |
| 67.854 | 1.380 | 0 | 16 | 0 | −8 | 67.839 | 1.380 | 0.000 |
| 68.850 | 1.363 | 1 | 3 | 3 | 7 | 68.851 | 1.363 | 0.000 |


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