

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* ( $\text{\AA}^2$ )

$$B_{\text{eq}} = (8\pi^2/3)\sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

|     | x           | y           | z           | $B_{\text{eq}}$ |
|-----|-------------|-------------|-------------|-----------------|
| Si1 | 0.19566 (4) | 0.65391 (4) | 0.21768 (3) | 1.31 (1)        |
| Si2 | 0.42230 (4) | 0.87138 (5) | 0.18621 (3) | 1.73 (1)        |
| Si3 | 0.05154 (4) | 0.76677 (5) | 0.32646 (3) | 1.75 (1)        |
| Si4 | 0.02440 (4) | 0.45092 (4) | 0.06946 (3) | 1.53 (1)        |
| Si5 | 0.29317 (5) | 0.51649 (5) | 0.31088 (3) | 1.85 (1)        |
| C21 | 0.3591 (2)  | 1.0206 (2)  | 0.1447 (1)  | 2.81 (5)        |
| C22 | 0.5281 (2)  | 0.7885 (2)  | 0.0883 (1)  | 2.81 (5)        |
| C23 | 0.5747 (2)  | 0.9919 (2)  | 0.3049 (1)  | 2.92 (5)        |
| C31 | -0.0789 (2) | 0.8337 (2)  | 0.2565 (1)  | 2.56 (5)        |
| C32 | -0.0830 (2) | 0.6129 (2)  | 0.3917 (1)  | 3.05 (5)        |
| C33 | 0.1959 (2)  | 0.9546 (2)  | 0.4278 (1)  | 2.85 (5)        |
| C41 | 0.1150 (2)  | 0.3009 (2)  | 0.0238 (1)  | 2.73 (5)        |
| C42 | -0.1737 (2) | 0.3359 (2)  | 0.1143 (1)  | 2.52 (5)        |
| C51 | 0.3738 (2)  | 0.6445 (2)  | 0.4469 (1)  | 2.96 (5)        |
| C52 | 0.4634 (2)  | 0.4799 (2)  | 0.2546 (2)  | 3.02 (6)        |
| C53 | 0.1286 (2)  | 0.3119 (2)  | 0.3149 (1)  | 2.82 (5)        |

Table 2. *Selected geometric parameters* ( $\text{\AA}$ ,  $^\circ$ )

|             |            |             |            |
|-------------|------------|-------------|------------|
| Si1—Si2     | 2.3467 (9) | Si3—C32     | 1.875 (2)  |
| Si1—Si3     | 2.3550 (9) | Si3—C33     | 1.874 (2)  |
| Si1—Si4     | 2.372 (1)  | Si4—Si4     | 2.374 (1)  |
| Si1—Si5     | 2.3604 (8) | Si4—C41     | 1.882 (2)  |
| Si2—C21     | 1.874 (2)  | Si4—C42     | 1.888 (2)  |
| Si2—C22     | 1.874 (2)  | Si5—C51     | 1.879 (2)  |
| Si2—C23     | 1.876 (2)  | Si5—C52     | 1.875 (2)  |
| Si3—C31     | 1.869 (2)  | Si5—C53     | 1.875 (2)  |
| Si2—Si1—Si3 | 109.04 (4) | C31—Si3—C32 | 107.70 (9) |
| Si2—Si1—Si4 | 115.02 (4) | C31—Si3—C33 | 107.10 (9) |
| Si2—Si1—Si5 | 107.38 (3) | C32—Si3—C33 | 107.89 (9) |
| Si3—Si1—Si4 | 111.92 (3) | Si1—Si4—Si4 | 116.80 (4) |
| Si3—Si1—Si5 | 105.94 (3) | Si1—Si4—C41 | 108.06 (6) |
| Si4—Si1—Si5 | 107.03 (4) | Si1—Si4—C42 | 105.25 (6) |
| Si1—Si2—C21 | 110.09 (6) | Si4—Si4—C41 | 108.54 (6) |
| Si1—Si2—C22 | 110.77 (7) | Si4—Si4—C42 | 109.76 (6) |
| Si1—Si2—C23 | 111.07 (7) | C41—Si4—C42 | 108.11 (9) |
| C21—Si2—C22 | 111.01 (9) | Si1—Si5—C51 | 110.82 (6) |
| C21—Si2—C23 | 107.02 (9) | Si1—Si5—C52 | 111.17 (7) |
| C22—Si2—C23 | 106.76 (9) | Si1—Si5—C53 | 111.64 (6) |
| Si1—Si3—C31 | 112.35 (6) | C51—Si5—C52 | 107.24 (9) |
| Si1—Si3—C32 | 111.29 (7) | C51—Si5—C53 | 107.01 (9) |
| Si1—Si3—C33 | 110.32 (6) | C52—Si5—C53 | 108.76 (9) |

The space group was determined from packing considerations and a statistical analysis of intensity distribution. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1986). Program(s) used to refine structure: *TEXSAN* (Molecular Structure Corporation, 1989).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BK1051). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## (Z)-{4-[1-Cyano-3-(diethyliminio)-1-propenyl]phenyl}dicyanomethanide, a Novel 'Blue Window' Zwitterionic Molecule for Non-Linear Optics

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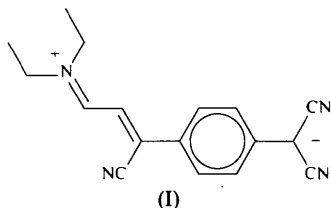
## Abstract

The crystal structure of the title compound,  $\text{C}_{17}\text{H}_{16}\text{N}_4$ , (1), has been elucidated. The molecule is shown to be planar with a highly delocalized  $\pi$  system between the two zwitterionic charge centres. This rationalizes the strong solution dipole moment exhibited by this molecule (45 D) and its high measured first hyperpolarizability ( $190 \times 10^{-30}$  e.s.u.). The electronic spectrum of the molecule consists of strong transitions in the visible region between 500 and 700 nm, but with an absence of absorption to either side. The unusually low optical absorption between 450 and 470 nm suggests that the description 'blue window material' may be applied in relation to frequency doubling applications

## Comment

There are now numerous organic non-linear optical materials showing large second-order non-linearities (Prasad & Williams, 1991). The basic structural requirements for second-order molecules have been known

since the early 1970's when second-harmonic generation was observed from crystals of 3-nitroaniline (Southgate & Hall, 1971). This molecule exemplifies the general class in having a dipolar conjugated structure where the optical excitation involves redistribution of  $\pi$  charge along the conjugated chain between substituents of differing electron affinity. The two major application areas foreseen utilize either the electro-optic effect or second-harmonic generation. In the former case, the colour of the materials is a less restrictive factor since electro-optic effects are usually needed at 1.3 or 1.5  $\mu\text{m}$ , where organic materials are often transparent. For second-harmonic generation, the important wavelengths for transparency lie below 500 nm and molecules where the lowest energy transition is below 400 nm have commensurately lower non-linearities. The molecular first hyperpolarizability,  $\beta_{ijk}$ , scales with the cube of the wavelength of the longest absorption peak (if only two levels, the ground and first excited state are considered), but this benefit is often lost in the increase in absorption of the harmonic radiation. The new molecule (I), whose crystal structure is reported here, has been shown to have a large dipole moment in solution, a high measured hyperpolarizability and excellent transparency between 400 and 500 nm, thus making it an important candidate for second-harmonic generation using anomalous-dispersion phase matching (Cahill, Singer & King, 1989).



The purpose of the structure determination was to establish the nature of the conjugation and molecular environment in the crystalline state in order to rationalize the high dipole moment that has been observed. Fig. 1 shows the molecular structure and the atomic numbering scheme. The bond lengths suggest that the six-membered ring [C(6)–C(11)] is quinoid in nature rather than aromatic. The molecule (I) forms a fully conjugated  $\pi$  system, from the  $sp^2$  N atom, N(17), to C(3), showing a marked shortening of the formal C–C single bonds and a lengthening of the C=C double bonds; therefore (I) cannot be rationalized as a particular canonical form. The mean deviation of the conjugated plane is only 0.02 Å. The molecule is zwitterionic in nature; this is confirmed by the shortness of the C(16)–N(17) bond (1.32 Å) and the bond angles around N(17), all of which are between 117.4 and 122.6°. Because of this, N(17) is considered to be positively charged. The formal negative charge is best considered to be delocalized across the quinoidal ring.

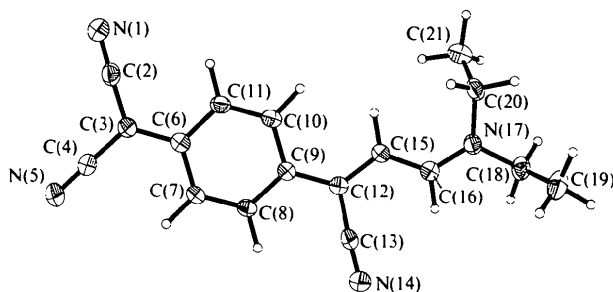


Fig. 1. View of (I), with non-H atoms labelled.

Non-bonding interactions, as described in a paper by Taylor & Kennard (1982), are observed between H(10) and N(14<sup>i</sup>) [H(10)···N(14<sup>i</sup>) = 2.59, C(10)···N(14<sup>i</sup>) = 3.42 Å, C–H···N<sup>i</sup> = 141°], N(1) and H(202) [H(202)···N(1<sup>ii</sup>) = 2.47, C(20)···N(1<sup>ii</sup>) = 3.45 Å, C–H···N<sup>ii</sup> = 161°], and H(201) and N(5<sup>iii</sup>) [H(201)···N(5<sup>iii</sup>) = 2.55, C(20)···N(5<sup>iii</sup>) = 3.55 Å, C–H···N<sup>iii</sup> = 167°] [symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $-x - 1, 1 - y, 1 - z$ ; (iii)  $x, y, z - 1$ ]. These rationalize the slight deviations from linearity of the C–C–N bond angles.

The remainder of the structure is unremarkable. The C≡N triple bonds are not significantly lengthened by the conjugated  $\pi$  system and the ethyl groups exhibit expected tetrahedral angles.

Within the lattice, the molecules form dimeric stacks in the *b* direction, such that the molecular dipoles align in opposing fashion (see Fig. 2). The intermolecular

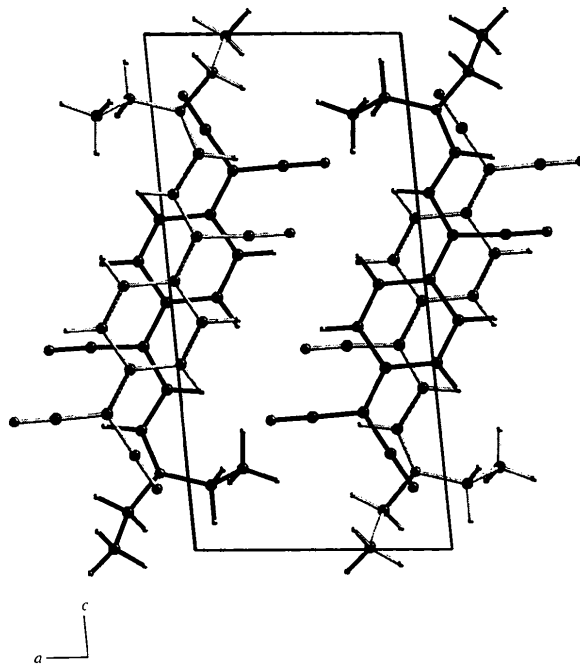


Fig. 2. View of the stacking down the *b* axis; the opposite dipoles are aligned and the stacking maximizes ring–bond overlap.

separation is 3.35 Å. Such stacking is similar to that for a related zwitterionic molecule (Metzger, Heimer & Ashwell, 1984), and shows a common bond–ring packing arrangement that is often observed in TCNQ salts and related molecules. The stacks are translated relative to one another. This minimizes unfavourable dipole interactions and facilitates 12-fold close packing in the crystal (see Fig. 3).

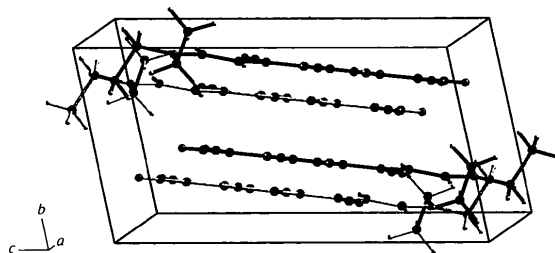


Fig. 3. A view of the translation of the dimeric stacks relative to one another.

**Experimental**

The compound was synthesized at the Department of Physics, University of Durham (Szablewski, 1994).

*Crystal data*

C<sub>17</sub>H<sub>16</sub>N<sub>4</sub>  
*M<sub>r</sub>* = 276.34  
 Triclinic  
*P* $\bar{1}$   
*a* = 7.221 (2) Å  
*b* = 7.262 (1) Å  
*c* = 14.670 (2) Å  
 $\alpha$  = 76.970 (10)°  
 $\beta$  = 82.280 (10)°  
 $\gamma$  = 79.400 (10)°  
*V* = 733.2 (2) Å<sup>3</sup>  
*Z* = 2  
*D<sub>x</sub>* = 1.252 Mg m<sup>-3</sup>

Mo *K*α radiation  
 $\lambda$  = 0.71073 Å  
 Cell parameters from 25 reflections  
 $\theta$  = 9.0–11.7°  
 $\mu$  = 0.077 mm<sup>-1</sup>  
*T* = 150 (2) K  
 Rectangular plate  
 0.5 × 0.2 × 0.1 mm  
 Emerald green

*Data collection*

Rigaku AFC-6S four-circle diffractometer  
 Repeated constant speed  $\omega$ -2 $\theta$  scans  
 Absorption correction: empirical  
*T<sub>min</sub>* = 0.974, *T<sub>max</sub>* = 1.000  
 2816 measured reflections  
 2592 independent reflections  
 1709 observed reflections  
 [*I* > 2σ(*I*)]

*R<sub>int</sub>* = 0.0301  
 $\theta_{\text{max}}$  = 25.89°  
*h* = -8 → 8  
*k* = -8 → 0  
*l* = -17 → 17  
 3 standard reflections monitored every 150 reflections  
 intensity decay: none

*Refinement*

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.0417  
*wR*(*F*<sup>2</sup>) = 0.0729

( $\Delta/\sigma$ )<sub>max</sub> < 0.001  
 $\Delta\rho_{\text{max}}$  = 0.202 e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}}$  = -0.160 e Å<sup>-3</sup>

*S* = 1.280  
 2588 reflections  
 202 parameters  
 Only coordinates of H atoms refined  
 $w = 1/[\sigma^2(F_o^2) + 0.2000P + 0.2500\sin\theta/\lambda]$   
 where  $P = 0.33333F_o^2 + 0.66667F_c^2$

Extinction correction: none  
 Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å<sup>2</sup>)

$$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*a_i \cdot a_j$$

|       | <i>x</i>    | <i>y</i>   | <i>z</i>     | <i>U<sub>eq</sub></i> |
|-------|-------------|------------|--------------|-----------------------|
| N(1)  | -0.6559 (3) | 0.4289 (3) | 0.74852 (13) | 0.0448 (5)            |
| C(2)  | -0.4926 (3) | 0.3955 (3) | 0.74316 (14) | 0.0310 (5)            |
| C(3)  | -0.2921 (3) | 0.3543 (3) | 0.73463 (13) | 0.0253 (5)            |
| C(4)  | -0.2013 (3) | 0.3549 (3) | 0.81468 (14) | 0.0280 (5)            |
| N(5)  | -0.1273 (3) | 0.3526 (3) | 0.88030 (12) | 0.0381 (5)            |
| C(6)  | -0.1874 (3) | 0.3181 (3) | 0.64966 (13) | 0.0227 (4)            |
| C(7)  | 0.0132 (3)  | 0.2805 (3) | 0.64052 (14) | 0.0249 (5)            |
| C(8)  | 0.1121 (3)  | 0.2435 (3) | 0.55867 (13) | 0.0241 (5)            |
| C(9)  | 0.0195 (3)  | 0.2440 (3) | 0.47906 (13) | 0.0212 (4)            |
| C(10) | -0.1810 (3) | 0.2822 (3) | 0.48821 (14) | 0.0252 (5)            |
| C(11) | -0.2802 (3) | 0.3168 (3) | 0.57009 (13) | 0.0255 (5)            |
| C(12) | 0.1240 (3)  | 0.2062 (3) | 0.39376 (13) | 0.0233 (4)            |
| C(13) | 0.3288 (3)  | 0.1607 (3) | 0.39281 (13) | 0.0253 (5)            |
| N(14) | 0.4914 (3)  | 0.1275 (3) | 0.38767 (12) | 0.0360 (5)            |
| C(15) | 0.0497 (3)  | 0.2128 (3) | 0.31042 (13) | 0.0249 (5)            |
| C(16) | 0.1645 (3)  | 0.1597 (3) | 0.23282 (13) | 0.0248 (5)            |
| N(17) | 0.1100 (2)  | 0.1666 (2) | 0.14989 (11) | 0.0274 (4)            |
| C(18) | 0.2484 (3)  | 0.1027 (3) | 0.07522 (14) | 0.0330 (5)            |
| C(19) | 0.3159 (3)  | 0.2695 (3) | 0.00435 (15) | 0.0432 (6)            |
| C(20) | -0.0853 (3) | 0.2446 (3) | 0.12588 (14) | 0.0327 (5)            |
| C(21) | -0.2167 (3) | 0.0956 (4) | 0.1578 (2)   | 0.0437 (6)            |

Table 2. Selected geometric parameters (Å, °)

|                  |           |                   |           |
|------------------|-----------|-------------------|-----------|
| N(1)—C(2)        | 1.155 (3) | C(10)—C(11)       | 1.363 (3) |
| C(2)—C(3)        | 1.418 (3) | C(12)—C(15)       | 1.388 (3) |
| C(3)—C(6)        | 1.420 (3) | C(12)—C(13)       | 1.453 (3) |
| C(3)—C(4)        | 1.421 (3) | C(13)—N(14)       | 1.150 (2) |
| C(4)—N(5)        | 1.157 (2) | C(15)—C(16)       | 1.399 (3) |
| C(6)—C(7)        | 1.417 (3) | C(16)—N(17)       | 1.316 (2) |
| C(6)—C(11)       | 1.425 (3) | N(17)—C(18)       | 1.476 (2) |
| C(7)—C(8)        | 1.367 (3) | N(17)—C(20)       | 1.478 (2) |
| C(8)—C(9)        | 1.421 (3) | C(18)—C(19)       | 1.516 (3) |
| C(9)—C(10)       | 1.417 (3) | C(20)—C(21)       | 1.523 (3) |
| C(9)—C(12)       | 1.427 (2) |                   |           |
| N(1)—C(2)—C(3)   | 178.8 (2) | C(11)—C(10)—C(9)  | 121.2 (2) |
| C(2)—C(3)—C(6)   | 121.6 (2) | C(10)—C(11)—C(6)  | 121.6 (2) |
| C(2)—C(3)—C(4)   | 116.7 (2) | C(15)—C(12)—C(9)  | 126.3 (2) |
| C(6)—C(3)—C(4)   | 121.7 (2) | C(15)—C(12)—C(13) | 116.4 (2) |
| N(5)—C(4)—C(3)   | 179.0 (2) | C(9)—C(12)—C(13)  | 117.2 (2) |
| C(7)—C(6)—C(3)   | 121.6 (2) | N(14)—C(13)—C(12) | 176.9 (2) |
| C(7)—C(6)—C(11)  | 117.2 (2) | C(12)—C(13)—C(16) | 121.5 (2) |
| C(3)—C(6)—C(11)  | 121.2 (2) | N(17)—C(16)—C(15) | 126.4 (2) |
| C(8)—C(7)—C(6)   | 121.0 (2) | C(16)—N(17)—C(18) | 119.9 (2) |
| C(7)—C(8)—C(9)   | 121.8 (2) | C(16)—N(17)—C(20) | 122.6 (2) |
| C(10)—C(9)—C(8)  | 117.2 (2) | C(18)—N(17)—C(20) | 117.4 (2) |
| C(10)—C(9)—C(12) | 121.5 (2) | N(17)—C(18)—C(19) | 112.1 (2) |
| C(8)—C(9)—C(12)  | 121.4 (2) | N(17)—C(20)—C(21) | 112.0 (2) |

Data solution yielded all non-H atoms. H atoms were placed at geometrically calculated positions and then allowed to ride with temperature factors fixed at 1.5 times that of their parent atom. The methyl H atoms were located using the ring Fourier method available in *SHELXL93* (Sheldrick, 1993). Refinement employed the full-matrix least-squares method.

Cell refinement, data collection and data reduction: *TEXSAN* (Molecular Structure Corporation, 1989). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s)

used to refine structure: *SHELXL93*. Molecular graphics: *JACKAL* (Cockcroft, private program). Software used to prepare material for publication: *SHELXL93*.

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Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: HU1101). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## (1*R*)-4,5-Benzocyclodeca-4-ene-2,6-diyn-1-yl 2,3,4,6-Tetra-*O*-acetyl-β-D-glucopyranoside and 4,5-Benzocyclodeca-4-ene-2,6-diyn-1-one

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## Abstract

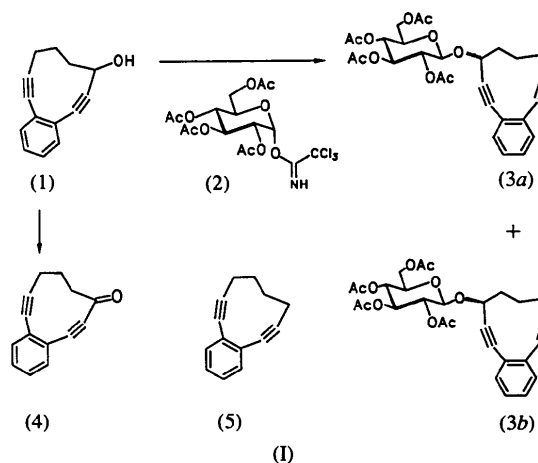
The title compounds, C<sub>28</sub>H<sub>30</sub>O<sub>10</sub> and C<sub>14</sub>H<sub>10</sub>O, have been synthesized during the course of a program designed to prepare molecules with DNA-cleaving prop-

erties. The geometry of the strained benzodiyne system has been determined, the *S* configuration at the propargylic center established and the orientation of the sugar unit in relation to the aglycon defined. The results are compared with those for other derivatives. The molecular packing is governed by normal van der Waals interactions.

## Comment

The glycosylated enediyne antibiotics such as calicheamicins and esperamicins have recently attracted a great deal of attention because of the potential antitumor properties of the enediyne moiety (Nicolaou & Dai, 1991; Lee, Ellestad & Borders, 1991). The carbohydrate domain is in part responsible for the sequence-selective double-stranded cleavage of various oligonucleotide targets by positioning the drug in the minor groove (Aiyar, Danishefsky & Crothers, 1992; Nicolaou, Tsay, Suzuki & Joyce, 1992). We undertook the preparation of simple models (Crévisy & Beau, 1991), including glycosylated congeners (I. Dancy & J.-M. Beau, unpublished results), compounds which may help to understand the mode-of-action of these substances.

Glucosylation of racemic benzodiyinol (1) by the α-imidate (2) under the conditions of Schmidt (1986) provided the easily separated diastereomeric β-glucosides (3*a*) and (3*b*) according to the scheme below.



The structure of crystalline isomer (3*a*) was studied in order to establish the configuration at the propargylic center, to determine the structural parameters of the strained benzodiyne system and to define the orientation of the sugar unit in relation to the aglycon. The crystal structure of benzodiynone (4) is also reported for comparison.

The chemical reactivity of the ene(benzo)diyne systems can be correlated, to a first approximation, with the distance between the remote acetylenic C atoms, a measure of the molecular strain in the ground state