# Reaction of 1,2-Bis(2-selenoxo-3-methyl-4-imidazolinyl)ethane (ebis) with TCNQ: Crystal Structure and Characterization of the Mixed-Valence Compound [2(ebis)$^{2+}$·ebis]·2[(TCNQ)$_3$$^{2-}$]

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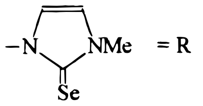
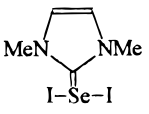
## Introduction

The quest for new molecular conductors and semiconductors has led to renewed interest in studies regarding the nature of the interaction between S or Se heterocycles containing $\pi$-delocalized electrons and suitable acceptors.[1] The conduction properties of the materials are strongly affected by the stacking mode of the donors and acceptors in the crystals and by the possible presence of peripheral chalcogen atoms, which can extend intermolecular interactions. We are presently investigating the reactions of molecules containing the heterocycles imidazoline-2-selone **1**−**3** depicted with acceptors of increasing strength. Minor modifications in the structure of the donors **1**−**3** yield different products with the same acceptor $I_2$, as shown by the isolated compounds **4**−**6**.[2] Moreover, using acceptors of increasing strength ($I_2$, IBr, and ICl), with the same donor (**1**) the variety of obtained products (**4**, **7**, **8**) is further increased.[3]



$CH_3$-R (**1**)
R-$CH_2$-R (**2**)
R-$(CH_2)_2$-R (ebis, **3**)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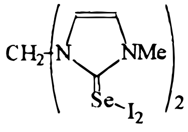
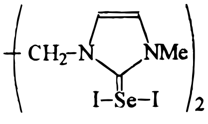

**(5)**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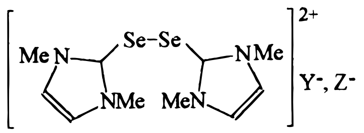
Y=Z=Br **(7)**
Y=Cl, Z=$I_3$ **(8)**

As a progression of this investigation to other acceptors, in this paper we report the characterization of the mixed-valence complex obtained with ebis (**3**) and tetracyanoquinodimethane (TCNQ).

## Experimental Section

The synthesis of ebis has been described elsewhere.[2] TCNQ, the solvents, and all other reagents described here were used as purchased from Aldrich. Upon addition of 30 mL of a $CH_3CN$ solution of TCNQ (47 mg) to 25 mL of a $CH_2Cl_2$ solution of **3** (40 mg, 1:2 ebis:TCNQ molecular ratio), a green solution was obtained. Lustrous dark-blue crystals suitable for X-ray diffraction studies were obtained by slow evaporation (2 weeks). Anal. Calcd for $C_{34}H_{22}N_{12}Se_2$: C, 53.98; H, 2.93; N, 22.22. Found: C, 54.07; H, 2.99; N, 22.22.

**Spectroscopic Measurements.** Nujol mull IR spectra (400−5000 $cm^{-1}$, resolution 2 $cm^{-1}$) were recorded on a Bruker IFS66 spectrometer. FT-Raman spectra (resolution $\pm 4$ $cm^{-1}$) of solid samples were recorded on a Bruker RFS100 FTR spectrometer, operating with an excitation frequency of 1064 nm (Nd:YAG laser). The power level of the laser source was 50 mW.

**Electrochemistry.** Cyclic voltammetry experiments were performed using a conventional three-electrode cell, consisting of a Pt counter electrode and a Pt micro working electrode *vs* SCE (saturated calomel electrode). The experiments were performed at room temperature in anhydrous $CH_2Cl_2$. The solution was $\sim 1 \times 10^{-3}$ mol dm$^{-3}$ in **3** with $Bu_4NBF_4$ ($\sim 1 \times 10^{-1}$ mol dm$^{-3}$) as supporting electrolyte. A flow of argon was passed through the solution prior to the scan. Data were recorded on a computer-controlled EG&G (Princeton Applied Research) Model 273 potentiostat−galvanostat using Model 270 electrochemical analysis software. The scan rate was 100 mV s$^{-1}$.

**Conductivity Measurements.** Conductivity measurements were made on pellets (thickness 0.5 mm, diameter 12 mm) with the two-point probe method.

**Crystallographic Data Collection and Structure Determination.** A selected crystal of **11** was placed on a Siemens AED diffractometer using Ni-filtered Cu K$\alpha$ radiation. The structure was solved and refined using the computer programs SHELX-76[4] and SHELX-86.[5] All hydrogen atoms were placed at their geometrically calculated positions (C−H 0.96 Å) and refined by "riding" on the corresponding atoms with unique isotropic thermal parameters [$U = 0.0515(113)$ Å$^2$]. All non-hydrogen atoms were refined anisotropically. The main crystallographic data are summarized in Table 1, and the atomic coordinates of the non-hydrogen atoms are listed in Table 2.

## Results and Discussion

Dark-blue, shining crystals of analytical formula ebis·2TCNQ are isolated from a $CH_2Cl_2$/$CH_3CN$ solution of the reagents in a 1:2 ebis:TCNQ molecular ratio.

X-ray diffractometric studies show that this compound (see compound **11** of Scheme 1) can be described as a tetracation, formed by one molecule of the neutral ligand and two dications bearing a Se−Se bridge (Figure 1), and two anions, each of which is formed by a triad of TCNQ molecules bearing two negative charges. We previously isolated this dication by reduction of **6** with metallic tellurium.[3] The synthetic procedures are summarized in Scheme 1.

Figure 2 shows the projection of the structure of [2(ebis)$^{2+}$·ebis]·2[(TCNQ)$_3$$^{2-}$] along *b*. The crystal structure consists of homologous layers of alternating cations and anions parallel to the *ab* plane. The trimeric tetracation is composed of one neutral centrosymmetric molecule of ebis and two dications ebis$^{2+}$, mutually related by the symmetry center, owing to the Se(11)···Se(13$^i$) interaction [2.959(2) Å] between each selenium

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[†] Università degli Studi di Parma.

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(1) Ferraro, J. R.; Williams, J. M. *Introduction to Synthetic Electrical Conductors*; Academic Press: New York, 1987.

(2) Bigoli, F.; Deplano, P.; Devillanova, F. A.; Mercuri, M. L.; Pellinghelli, M. A.; Lippolis, V.; Trogu, E. F. *Gazz. Chim. Ital.* **1994**, *124*, 445.

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(4) Sheldrick, G. M. SHELX 76: Programs for Crystal Structure Determination. University of Cambridge, U.K., 1976.

(5) Sheldrick, G. M. SHELX 86: Program for the Solution of Crystal Structures. Universität Göttingen, Germany, 1986.

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**Table 1.** Crystallographic Data[a]

| | |
|---|---|
| empirical formula: $C_{102}H_{66}N_{36}Se_6$ | fw = 2269.64 |
| $a = 10.219(7)$ Å | space group: $P\bar{1}$ (No. 2) |
| $b = 13.909(6)$ Å | $T = 22$ °C |
| $c = 17.775(5)$ Å | $\lambda = 1.541\ 838$ Å |
| $\alpha = 78.93(2)°$ | $\rho_{obsd} = 1.59$ g cm$^{-3}$ |
| $\beta = 88.69(2)°$ | $\rho_{calcd} = 1.574$ g cm$^{-3}$ |
| $\gamma = 75.07(2)°$ | $\mu = 32.76$ cm$^{-1}$ |
| $V = 2395(2)$ Å$^3$ | $R(F_o) = 0.0698$ |
| $Z = 1$ | $R_w(F_o) = 0.0819$ |

[a] $R = \sum|\Delta F|/\sum|F_o|$; $R_w = [\sum w(\Delta F)^2/\sum wF_o^2]^{1/2}$.

[Se(13$^i$) and Se(13)] of ebis with the adjacent selenium [Se(11) and Se(11$^i$)] of the dication. The structural data for the dication are very similar to those observed for $[C_{10}H_{14}N_4Se_2]I_3{\cdot}{}^1/_2I_4$ (**9**).[3] The Se(11)−Se(12) bond length 2.451(2) Å is longer than the sum of covalent radii[6] and longer than the bond length in the bis(selenourea) dication (2.380 Å),[7] while it is comparable to those in other similar Se−Se dications reported by us (in the range 2.409−2.440 Å).[3] Longer bond distances are found in tris(selenourea) dications.[8] In the three reported dications of tris(selenourea), the $Se_1{-}Se_2{-}Se_3$ distances are asymmetrical, $d(Se_1{-}Se_2)$ ranging from 2.597 to 2.640 Å and $d(Se_2{-}Se_3)$ from 2.717 to 2.664 Å. Interestingly the sum of the $Se_1{-}Se_2{-}Se_3$ distances (∼5.3 Å) is similar to that found in the moiety under discussion (∼5.4 Å).[9] These geometrical features and the approximately linear Se(12)−Se(11)···Se(13$^i$) arrangement are in agreement with a donor−acceptor interaction, where both Se atoms of a neutral molecule act as donors and one Se atom of each dication acts as an acceptor (hypervalent 10-Se-3). A three-center two-electron bond type[8] has been used to describe this kind of coordination geometry in the above cited tris(selenourea) dications where the almost linear $Se_1{-}Se_2{-}Se_3$ fragments are less asymmetric than in the present case. The Se−Se moieties can indeed behave as acceptors even toward different kinds of donors (X) as shown by du Mont *et al.*[10] in the bis(diphenyldiselenane)−bis(diiodine) $[(R_2Se_2{\cdot}I_2)_2]$, and by us in some halides of dications bearing the same Se−Se bridge.[3] In $(R_2Se_2{\cdot}I_2)_2$, the features of the linear Se−Se···I arrangement produced as a consequence of the weaker interaction[11] [$d$(Se···I) = 3.588 Å], have been taken as characteristic of an adduct of an $I_2$ donor with a hypervalent (10-Se-3) acceptor selenium atom. The linear Se−Se···X groups in the salts described by us[3] show even longer Se−Se and shorter Se−X distances than in the previous example, indicating, as expected, that the interaction is stronger with halide donors than with $I_2$.

Pressed-pellet conductivity of **11** is $1.0 \times 10^{-2}$ S cm$^{-1}$ at room temperature. Although single-crystal, temperature-dependent measurements are required to properly characterize the conductivity properties, the conductivity value at room temperature suggests that ebis·2TCNQ is a semiconductor. From the structural data it appears that electrical conductivity is mainly due to the TCNQ stacks. The TCNQ molecules are in fact stacked plane-to-plane in groups of three (Table 3, Figure 2) along *a*, and in each triad the molecules are mutually shifted in the direction of *c* in such a way that the quinonoid double bond

**Table 2.** Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic $U$ (×10$^4$), Defined as One-Third of the Trace of the Orthogonalized $\mathbf{U}_{ij}$ Tensor, for the Non-Hydrogen Atoms, with Esd's in Parentheses

| atom | *X*/*a* | *Y*/*b* | *Z*/*c* | $U_{eq}$, Å$^2$ |
|---|---|---|---|---|
| Se(11) | 1230.2(11) | 8455.3(8) | 5541.5(6) | 464(4) |
| Se(12) | −1128.1(11) | 8865.3(8) | 5940.4(6) | 517(5) |
| Se(13) | 5870.9(12) | 2347.9(11) | 4756.9(7) | 743(6) |
| N(11) | 1746(8) | 6582(6) | 6630(4) | 457(31) |
| N(21) | 2299(7) | 7726(6) | 7100(4) | 456(32) |
| N(12) | −1240(7) | 6940(6) | 5581(4) | 433(32) |
| N(22) | −2422(7) | 8227(6) | 4784(4) | 425(31) |
| N(13) | 5724(9) | 3820(7) | 5722(7) | 647(42) |
| N(23) | 5982(8) | 2321(7) | 6372(5) | 502(35) |
| C(11) | 1778(8) | 7556(6) | 6493(5) | 325(31) |
| C(21) | 2621(10) | 6849(8) | 7640(6) | 571(45) |
| C(31) | 2278(11) | 6120(8) | 7334(5) | 549(44) |
| C(41) | 1190(10) | 6195(8) | 6055(6) | 829(51) |
| C(51) | 2401(11) | 8717(8) | 7201(6) | 620(48) |
| C(12) | −1650(9) | 7975(7) | 5414(5) | 401(36) |
| C(22) | −2526(9) | 7379(7) | 4536(5) | 443(39) |
| C(32) | −1801(10) | 6573(8) | 5018(5) | 476(41) |
| C(42) | −468(7) | 6366(6) | 6236(4) | 226(27) |
| C(52) | −3133(10) | 9278(7) | 4438(6) | 593(45) |
| C(13) | 5907(9) | 2865(7) | 5641(6) | 492(42) |
| C(23) | 5854(12) | 2958(10) | 6878(7) | 698(59) |
| C(33) | 5710(13) | 3880(11) | 6491(9) | 887(72) |
| C(43) | 5712(12) | 4669(10) | 5088(9) | 952(69) |
| C(53) | 6241(11) | 1215(8) | 6568(7) | 791(57) |
| N(1A) | −2295(11) | 4167(8) | 361(6) | 815(50) |
| N(2A) | −1424(11) | 865(8) | 861(5) | 775(49) |
| N(3A) | −1083(9) | 4092(7) | −4281(5) | 559(38) |
| N(4A) | −79(10) | 800(7) | −3801(5) | 613(42) |
| C(1A) | −1281(9) | 2484(7) | −913(5) | 359(34) |
| C(2A) | −1416(9) | 3399(7) | −1463(5) | 429(37) |
| C(3A) | −1179(10) | 3374(7) | −2214(5) | 430(38) |
| C(4A) | −815(9) | 2464(7) | −2488(5) | 372(35) |
| C(5A) | −666(9) | 1545(7) | −1938(5) | 390(36) |
| C(6A) | −909(10) | 1570(7) | −1193(5) | 399(36) |
| C(7A) | −1559(10) | 2518(7) | −152(6) | 429(38) |
| C(8A) | −1966(11) | 3423(9) | 142(6) | 537(45) |
| C(9A) | −1493(11) | 1590(8) | 416(6) | 509(45) |
| C(10A) | −661(10) | 2467(7) | −3270(5) | 414(37) |
| C(11A) | −858(10) | 3357(8) | −3825(5) | 426(38) |
| C(12A) | −303(10) | 1538(8) | −3564(5) | 452(40) |
| N(1B) | 3038(11) | 658(7) | −2387(5) | 694(45) |
| N(2B) | 2033(11) | 3826(7) | −2954(5) | 724(47) |
| N(3B) | 1290(12) | 882(8) | 2237(5) | 870(56) |
| N(4B) | 534(10) | 4180(8) | 1746(5) | 688(46) |
| C(1B) | 1998(9) | 2355(7) | −1108(5) | 356(34) |
| C(2B) | 2137(9) | 1463(7) | −530(5) | 399(36) |
| C(3B) | 1902(9) | 1514(7) | 204(5) | 384(35) |
| C(4B) | 1475(9) | 2472(7) | 460(5) | 359(34) |
| C(5B) | 1362(10) | 3375(7) | −117(5) | 402(37) |
| C(6B) | 1590(9) | 3321(7) | −856(5) | 365(34) |
| C(7B) | 2220(10) | 2298(7) | −1875(5) | 420(38) |
| C(8B) | 2684(10) | 1352(7) | −2133(5) | 415(38) |
| C(9B) | 2125(11) | 3169(7) | −2454(5) | 472(41) |
| C(10B) | 1226(9) | 2509(7) | 1227(5) | 404(37) |
| C(11B) | 1279(11) | 1618(8) | 1789(6) | 514(45) |
| C(12B) | 816(10) | 3450(9) | 1498(5) | 479(43) |
| N(1C) | 3297(10) | 4238(7) | 3121(5) | 679(45) |
| N(2C) | 4253(9) | 977(7) | 3642(5) | 605(40) |
| N(3C) | 4827(12) | 4151(7) | −1532(6) | 837(52) |
| N(4C) | 5813(12) | 870(8) | −1038(6) | 887(57) |
| C(1C) | 4183(9) | 2557(7) | 1827(5) | 377(35) |
| C(2C) | 4073(9) | 3467(7) | 1263(5) | 391(36) |
| C(3C) | 4333(10) | 3449(7) | 526(6) | 415(37) |
| C(4C) | 4734(9) | 2517(7) | 252(5) | 372(34) |
| C(5C) | 4837(10) | 1616(7) | 809(5) | 435(37) |
| C(6C) | 4576(9) | 1634(7) | 1551(5) | 393(35) |
| C(7C) | 3953(10) | 2598(7) | 2600(5) | 398(36) |
| C(8C) | 3600(11) | 3523(8) | 2885(5) | 458(41) |
| C(9C) | 4102(10) | 1683(8) | 3180(6) | 453(40) |
| C(10C) | 5018(10) | 2512(8) | −515(5) | 454(40) |
| C(11C) | 4896(11) | 3413(9) | −1068(6) | 575(48) |
| C(12C) | 5446(11) | 1607(9) | −793(6) | 548(48) |

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(6) Pauling, L. *The Nature of the Chemical Bond*, 3rd ed.; Cornell University Press: New York, 1960.

(7) Chiesi Villa, A.; Nardelli, M.; Vidoni, M. E. *Acta Crystallogr.* **1970**, *B26*, 1504.

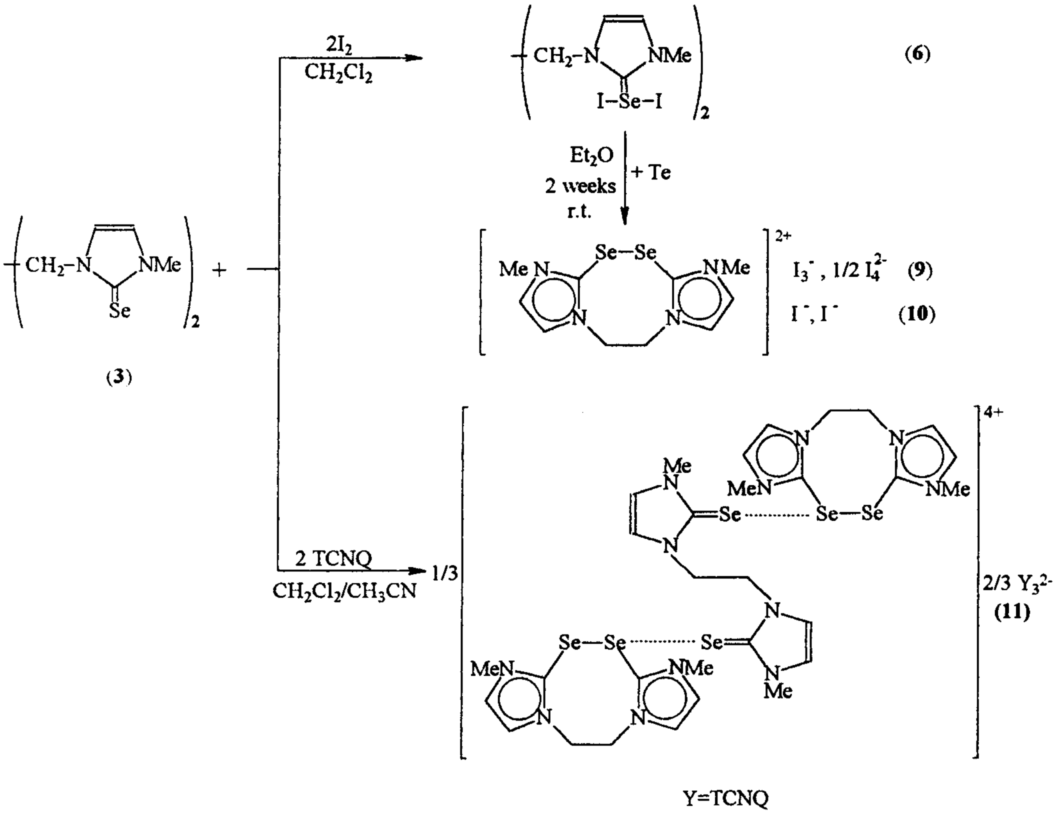
(8) Hauge, S. *Acta Chem. Scand.* **1979**, *A33*, 317.

(9) The values of the C−Se distances are those of a normal single covalent C(sp$^2$)−Se bond. The structural data of the imidazoline rings indicate a strong $\pi$-delocalization (6$\pi$ electrons).

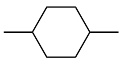
(10) Kubiniok, S.; du Mont, W. W.; Pohl, S.; Saak, W. *Angew. Chem., Int. Ed. Engl.* **1988**, *27*, 431.

(11) The stronger interaction is due to the usual Se-donor/diiodine-acceptor interaction.

**Scheme 1**



of one molecule is almost placed above the ring of the adjacent one, as observed in the majority of TCNQ salts.[12] The resulting chains of triads show a zigzag shape. The intermolecular separation between the TCNQ molecules in the triad is in the range 3.25(1)−3.36(1) Å and is longer than 3.50 Å between triads.[13] The dihedral angles between the mean-weighted planes of the molecule in the triad range from 0.3(2) to 1.7(1)°. As usual, the TCNQ molecules are not exactly planar. The values of the dihedral angle between the least-squares planes of the



and $C(CN)_2$ fragments are in the range 2.0(5)−7.0(5)°.

The similarity among the bond distances and angles of the TCNQ in the triad (Table 3) suggests that there is no charge localization and that the negative charge (2 e) is evenly distributed within the triad. However, the significant digits of the obtained TCNQ bond lengths are not sufficient to allow a more precise estimate of the average charge on the TCNQ molecule.[14] We have therefore undertaken a vibrational study on **11** since vibrational spectroscopy has proved to be a powerful tool in investigating molecular conductors and semiconductors.[15] Figure 3 shows the powder IR spectrum, which is dominated by a strong absorption corresponding to the charge-transfer transition along the TCNQ stack. The vibrational absorptions are superimposed on the electronic absorption, but above 1000 $cm^{-1}$ they appear as identations in the continuous single-electron absorption. This is a well-known phenomenon related to the electron−phonon coupling.[16] The vibrational modes coupled to the electron system in fact produce a normal absorption when their frequency is below the semiconducting gap and Fano interferences (identations) when above. The IR data therefore confirm that **11** is a semiconductor with a gap of approximately 1000 $cm^{-1}$ (~ 0.12 eV). The average charge $\rho$ on TCNQ sites is often estimated from the frequency of the Raman-active $a_g$ $\nu_4$ mode, approximately described as wind and ring C=C stretching,[17] which is known to exhibit a linear dependence on

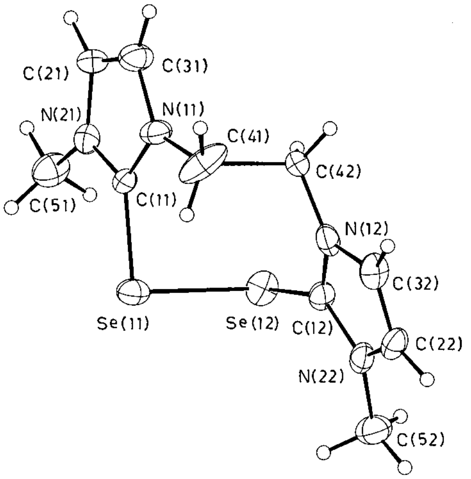


**Figure 1.** Molecular structure of the dication $(ebis)^{2+}$. Selected bond lengths (Å) and angles (deg): Se(11)−Se(12) 2.451(2), Se(11)−C(11) 1.90(1), Se(12)−C(12) 1.87(1), $N-C_{ring}$ in the range 1.30(1)−1.40(1), $N-C_{exo}$ in the range 1.41(1)−1.47(1); C(11)−Se(11)−Se(12) 90.9(3), C(12)−Se(12)−Se(11) 94.7(3).

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(12) Perlstein, J. H. *Angew. Chem., Int. Ed. Engl.* **1977**, *16*, 519.

(13) The interactions between anions and cations are of the type Se···N, Se···C, C···N, and C···C ranging from 3.15(2) to 3.72(1) Å.

(14) Flandrois, S.; Chasseau, D. *Acta Crystallogr.* **1977**, *B33*, 2744. Umland, T. C.; Allie, S.; Kuhlmann, T.; Coppens, P. *J. Phys. Chem.* **1988**, *92*, 6456.

(15) Pecile, C.; Painelli, A.; Girlando, A. *Mol. Cryst. Liq. Cryst.* **1989**, *171*, 69.

(16) Rice, M. J.; Pietronero, L.; Bruesch, P. *Solid State Commun.* **1977**, *21*, 757.

(17) Girlando, A.; Pecile, C. *Spectrochim. Acta* **1973**, *29A*, 1859.

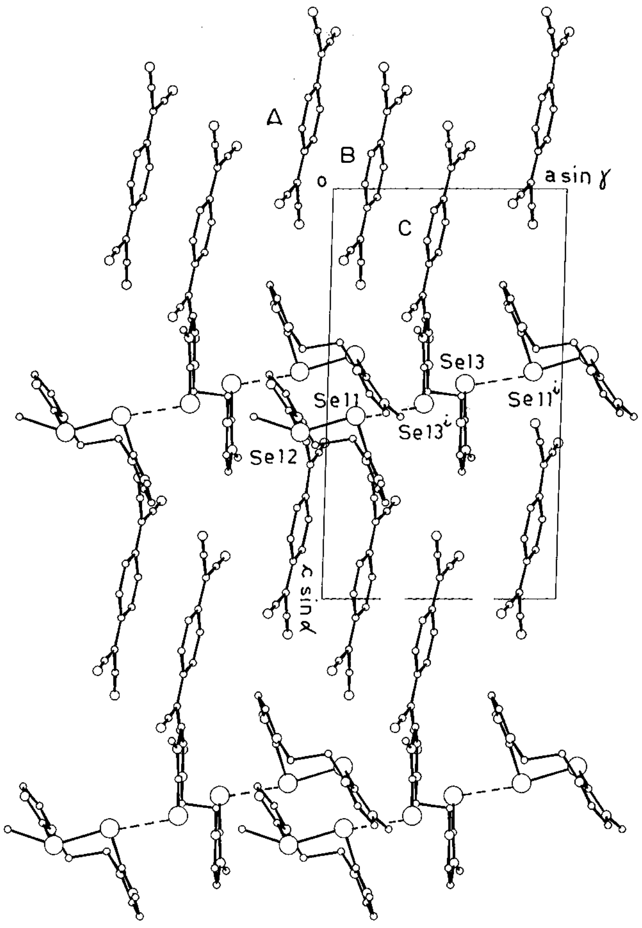
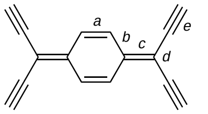


**Figure 2.** Projection of the structure of $[2(\text{ebis})^{2+}\cdot\text{ebis}]\cdot2[(\text{TCNQ})_3{}^{2-}]$ along *b*.

**Table 3.** Mean Bond Lengths (Å) of the TCNQ Molecules



| | *a* | *b* | *c* | *d* | *e* |
|---|---|---|---|---|---|
| TCNQ (A) | 1.34(1) | 1.41(1) | 1.40(1) | 1.43(2) | 1.15(2) |
| TCNQ (B) | 1.36(1) | 1.42(1) | 1.39(1) | 1.44(2) | 1.15(2) |
| TCNQ (C) | 1.34(1) | 1.44(1) | 1.39(1) | 1.43(1) | 1.14(2) |

the degree of charge transfer.[18] The Raman spectra of **11** only show a peak at 1413 cm$^{-1}$ in the spectral region of interest. This finding again suggests a charge of about 0.7 uniformly distributed on TCNQ. However, it should be remembered that for trimerized stacks the Raman frequencies can be perturbed by electron−phonon coupling,[19] so that a precise and safe determination of $\rho$ requires the collection of additional data, as for instance single-crystal polarized IR spectra. At present, we can only conclude that the charge is delocalized to an extent certainly greater than, for instance, in $Cs_2(TCNQ)_3$, where $\rho = 0.14$ and 0.93 for centric and noncentric TCNQ molecules, respectively.[16]

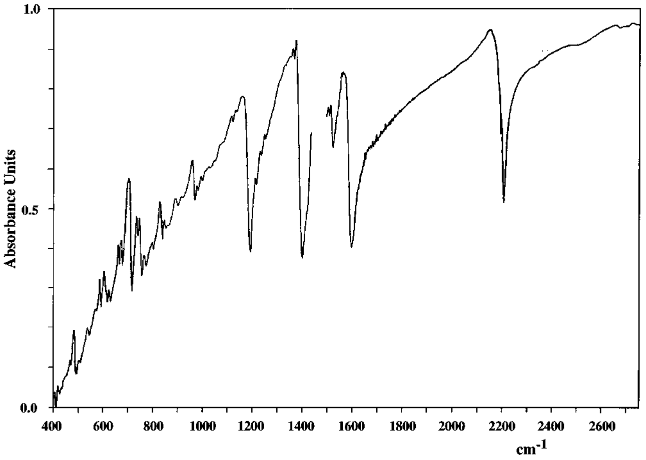


**Figure 3.** Infrared spectrum of $[2(\text{ebis})^{2+}\cdot\text{ebis}]\cdot2[(\text{TCNQ})_3{}^{2-}]$ (Nujol mull). The Nujol absorption around 1460 cm$^{-1}$ has been omitted for clarity.

As cited in the Introduction, ebis yields the neutral derivative **6** when it reacts with diiodine[2] and the dication containing a Se−Se bridge[3] (compounds **9** and **10**) with the reaction reported in Scheme 1. In the present study, we have found that this donor yields a mixed-valence product when it reacts with TCNQ. To better investigate the redox properties of ebis, an electrochemical study was carried out in $CH_2Cl_2$ solutions. Cyclic voltammograms started at 0.00 V potential, scanned in the positive potential direction and reversed at +1.0 and −0.2 V to the starting potential, show two oxidation peaks (at +0.50 and +0.66 V) and one reduction peak (+0.04 V). The fact that the oxidation and reduction peak separation is much greater than 60 mV indicates that these systems undergo irreversible electron transfer. To check whether the reduction peak is related to the oxidation peaks or whether it is due to an independent reduction, cyclic voltammograms were also recorded by initiating the sweep in the negative direction, starting at 0.00 V potential. Absence of the reduction peak indicates that it is related to the oxidation peaks. The two oxidation peaks could be related to a two-step process involving the oxidation of one Se atom, which interacts with the unoxidated Se atom. The formed intermediate then undergoes a second oxidation to give a Se−Se dication similar to those obtained by chemical oxidation (**7**, **8**).

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**Supporting Information Available:** Tables SI−SIV, listing the detailed crystallographic data, bond lengths and angles, atomic coordinates for the hydrogen atoms, and anisotropic thermal parameters for the non-hydrogen atoms (6 pages). Ordering information is given on any current masthead page.

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