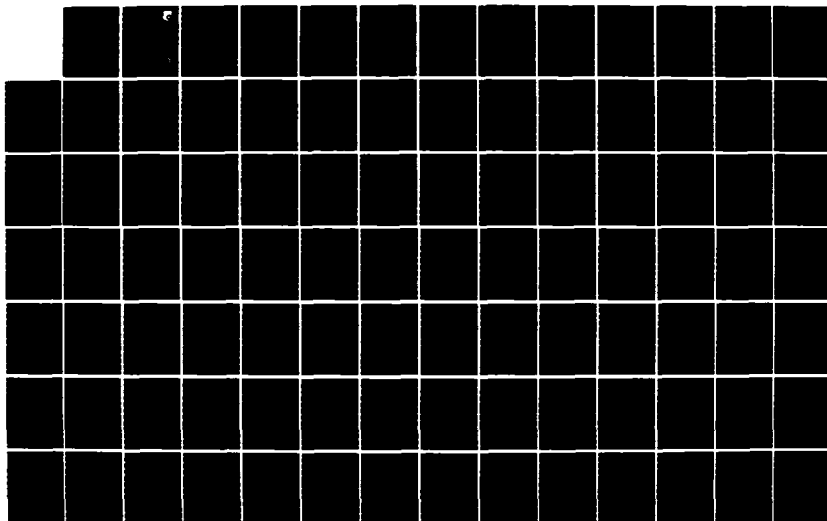


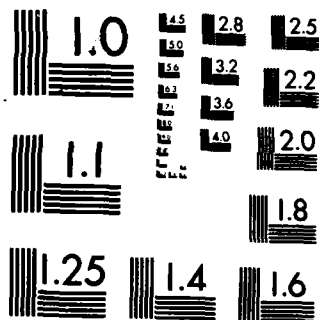
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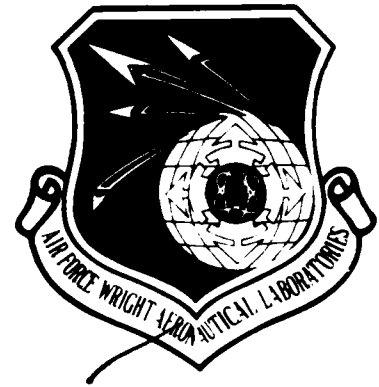
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ANALYSIS OF IMPURITY BAND FORMATION AND RELATED EFFECTS NEAR
THE P/N JUNCTION IN COMPENSATED GaAs and Si

L. Carlton Brown

University of Dayton
Research Institute
300 College Park
Dayton OH 45469-0001

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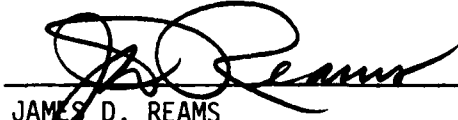


JOSEPH WISE, Technical Area Manager
Power Components Branch
Aerospace Power Division
Aero Propulsion Laboratory



E. T. MAHEFKEY, Chief
Power Components Branch
Aerospace Power Division
Aero Propulsion Laboratory

FOR THE COMMANDER



JAMES D. REAMS
Chief, Aerospace Power Division
Aero Propulsion Laboratory

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Analysis of Impurity Band Formation and Related Effects Near the P/N Junction in
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SUMMARY

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TASK TITLE; Analysis of Impurity Band Formation and Related Effects
Near the P/N Junction in Compensated GaAs and Si.

TASK OBJECTIVE; Utilizing the bandgap narrowing (BGN) model developed earlier by the author, the objective is to apply the model in studying concentration dependent changes near the P/N junction of semiconductor parameters that have a direct effect on current-voltage characteristics.

TASK DESCRIPTION; Based on statistical variations in neighboring impurity separations, free-carrier screening of impurity interaction energies, and statistical fluctuations in the local impurity concentration, the BGN model is to be used in studying variation across the P/N junction of several important characteristics including bandgap narrowing and edge tailing, impurity band tailing and merging with free carrier bands, Fermi-level, n-p type reversal due to fluctuations in local impurity density, which may influence recombination rate.

PREFACE

The work described in this report was conducted by the author in Columbus, Ohio under contract with The University of Dayton Research Institute during the period from July 1, 1985 to March 31, 1986. The program was sponsored by the Air Force Wright Aeronautical Laboratories, Wright-Patterson Air Force Base, Ohio. The Air Force Project Engineers were W. P. Rahilly and Joseph Wise (AFWAL/POOC).

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1. Introduction

Fabrication techniques, used in the production of photovoltaic devices such as solar cells, usually lead to high donor and acceptor concentrations, especially in compensated materials, sufficient to introduce substantial interactions between neighboring impurities. Because of these interactions, and also because of the electric screening effect of free charge carriers, the donor and acceptor energy levels are shifted with respect to the edge of the conduction or valence band, forming impurity bands and causing changes in the band gap. In addition to the obvious variations with temperature and impurity concentration, these effects also vary from region to region within the semiconductor material, due to the statistically random nature of dopant implantation, and vary with usage due to attendant changes in charge carrier density near the P/N junction.

A comprehensive analytical treatment of these effects is not feasible, primarily because the energy interactions between impurity ions and localized charge carriers constitute a many-body problem in quantum theory, but also because of the random statistical nature of the positions of impurity ions in the host lattice. Many investigators have been active [1 - 24] in various aspects of the overall problem, however, no treatment has been found in which energy levels of interacting impurities are calculated employing a screened potential energy. Some studies [16, 33] have been made with density matrix theory and potential energy screening leading directly to density-of-state data but these do not provide detailed information about individual energy levels needed for developing insight into the behavior of the semiconductor materials in question. In most studies, one or more of the above effects have been treated only qualitatively or not at all.

A compromise approach is used in the present study. In order to make the analysis feasible, only nearest-neighbor impurity ions are considered, but the energy levels are calculated with a screened potential interaction.

The resulting levels are then used, along with probability distributions to account for the random positions of the impurity ions, to calculate densities of state for each of the levels considered. In this way, the most important contributing influences, interactions between neighboring impurities, charge carrier potential screening, and random distances between impurities, are all treated quantitatively, thus providing a procedure for following changes in device characteristics due to changes in temperature, impurity concentration, compensation, and charge carrier densities.

In addition to the physical characteristics of the host material, the input parameters needed are temperature, donor concentration, and acceptor concentration. Before the energy levels can be calculated, the Fermi level, charge carrier density and screening factor are needed and must be estimated to provide this input. After the energy levels are then determined, they are used to recalculate the estimated values above and the energy levels recalculated. This procedure is repeated until a self-consistent set of values is obtained. The energy levels calculated are those for a pair of impurity ions separated by a distance, R , similar to the treatment of a diatomic molecule except that R is constant for a given pair, and also the localized carriers, bound to the ions, are assumed to be under the influence of a screened electric potential instead of the usual Coulomb potential. Levels are calculated for each of eight different systems involving pairs, donor-donor, donor-acceptor, and acceptor-acceptor with either one or two localized charge carriers. The levels are obtained for a range of values for the distance, R , to cover all possibilities needed for the statistically random distances found between nearest neighbors. The probability of finding a given R is then calculated as a function of R and used, along with the energy levels to obtain the probability of finding a given energy level as a function of energy.

These calculations are performed for a set of temperatures over values of interest and for a range of values of donor concentration as well as for acceptor concentration. The resulting information is presented in the form of graphic displays found in Appendix A.

2. Physical Model

Eight different physical systems are involved in the calculation of energy levels. Four of these form donor levels labeled E_1 , E_2 , E_3 , & E_4 , as follows: E_1 is the groundstate energy of a single electron bound to a pair of donor ions, abbreviated (DD)-; E_2 is the additional energy of the second electron bound to a donor pair with the first electron present, abbreviated (DD)-; E_3 is the groundstate energy of an electron bound to a donor-acceptor pair with no hole present, abbreviated (DA)-; E_4 is the energy of an electron bound to a donor-acceptor pair with a hole present, abbreviated (DA+)-. The other four systems form acceptor levels labeled H_1 , H_2 , H_3 , & H_4 , abbreviated (AA)+, (AA+)+, (AD)+, & (AD-)+, respectively. For the pair separation, R , large compared to the effective Bohr radius, the above systems reduce to isolated systems, for example, E_1 becomes the energy of one donor atom (electron present) and one donor ion, a total of one effective Rydberg for an electron. The binding energy of an isolated donor electron is not necessarily the same as that of a hole to an isolated acceptor. In this study, the isolated donor is taken as the unit of energy, one Rydberg, and the isolated acceptor is assumed to have a different groundstate hole energy in order to display in the results the consequences of an inequality. This introduces a corresponding inequality in the effective Bohr radii with that of the acceptor being different in inverse proportion to the energies. The ratio of these energies is an input parameter of the computer program.

The donor energy level calculations follow the procedures used in the treatment of the hydrogen molecule ion, H_2^+ , in the cases of E_1 levels, and the hydrogen molecule, H_2 , in determining E_{12} for two electrons, from which, $E_2 = E_{12} - E_1$, is found. A similar procedure is used for the acceptor levels and in both cases a variation procedure is used to minimize the energy obtained with s-state basis wavefunctions, the details are contained

in Appendices B and C. In the case of the donor-acceptor pair, a modified but similar calculation is developed to account for one positively and one negatively charged ion in the pair. Two variation parameters are used in order to obtain better approximations to the energies which are minimized with respect to a variation of both parameters. The details appear in Appendix B in which E_3 and E_4 are also called D_1 and D_2 . A similar method is used to obtain values for H_3 and H_4 .

In the hydrogen-like calculations, certain modifications are needed in order to properly represent the change from a hydrogen molecule in space to a hydrogen-like system in the crystal lattice:

- (1) The screened potential, $\pm 2 \exp(-\beta r)/r$, is used instead of the Coulomb potential, $\pm 2/r$, where β is the screening factor (also labeled B). The units are effective Bohr radii and effective Rydbergs for the isolated donor electron. The potential is assumed to be isotropic in order to keep the calculation manageable.
- (2) The dielectric constant, the electron effective mass, and the hole effective mass are assumed to be isotropic and are used to modify the Bohr radius and the Rydberg to their effective values in the lattice.
- (3) The potential energy term, $\pm 2/R$, between the impurity ions is not included in the Hamiltonian since the ion separation, R , is not a dynamic variable (in contrast with the hydrogen molecule). The value of R may vary from one ion pair to another, because of the random locations of impurities, but, in a given pair, the value of R is fixed.

For each of the values of temperature, donor and acceptor concentration considered, the eight energy levels are calculated for values of R covering a range up to eight Bohr radii in 32 steps. The first such calculation is based on a value of the screening factor, β , obtained from a simple estimate of the Fermi energy and the free charge carrier density using the Thomas-Fermi approximation for β . The resulting energy levels are then used to obtain an improved value for β based on the distribution of energy levels and their probability of occurrence (see Appendix B for details). The energy levels are then recalculated and this procedure is repeated until no further

changes occur in the value of β , thus assuring self-consistent results.

In the recalculation of the Fermi energy, E_F , and the screening factor, β , the charge balance equation, $n + N^- = p + N^+$, is used thus insuring the results to be valid for equilibrium conditions in bulk material. Also used in this step is the probability distribution function which describes the relative frequency of occurrence of different values of the distance, R , between neighboring impurity ions. The relation follows Poisson statistics, i.e., $P_k(cv) = ((cv)^k/k!) \exp(-cv)$, which in effect states that, if the average number of impurity ions expected in the volume, v , is given by cv , then the probability of finding, instead, the number, k , is given by the expression above. The validity of this formulation depends on only the facts that the position of an ion in the lattice is not dependent on the positions of the other ions and the number of impurity ions is much smaller than the number of lattice sites. The distribution of nearest neighbor impurity ion separations, R , can be deduced from this expression to be given by, $P(R,c')dR = 4\pi c'R^2 dR \exp(-4\pi c'R^3/3)$, where R is in units of Bohr radii and c' is the impurity concentration in the corresponding units, namely, $(\text{Bohr radii})^{-3}$.

In compensated semiconductors with a donor concentration of C_b in the bulk material, and an acceptor concentration of C_x diffused into the device from a surface value of C_s , the concentration, c' , in the probability above is derived from the total impurity concentration, $C_t = C_x + C_b$. The chance of finding D-D, D-A, & A-A pairs at distance R is then proportional to, q^2 , $2q(1-q)$, and $(1-q)(1-q)$, respectively, where $q = C_b/C_t$. The products of the probability above and these factors then provide the necessary information for weighting the different energy levels in the process of determining the contributions to the charge balance equation, above, and in generating the desired density-of-states data. More details of this process can be found in Appendix B.

Five temperatures were chosen for consideration in the computation, namely, 100 K, 200 K, 300 K, 400 K, and 500 K. For each of these values, five bulk (background) donor concentrations were selected. Their values

are $\text{Log } C_b = 15.5, 16, 16.5, 17, \text{ and } 17.5$, or $C_b = 3.16 \times 10^{15}, 10^{16}, 3.16 \times 10^{16}, 10^{17}, \text{ and } 3.16 \times 10^{17} \text{ cm}^{-3}$. For each of these cases, nine values of the variable acceptor concentration, C_x , were selected to cover a range of positions in the vicinity of the P/N junction. Figures 1 (a) and 1 (b) show typical concentration profiles across a P/N junction in which the $\text{Log } C_x$ is assumed to follow a parabolic decrease in magnitude starting at a value $\text{Log } C_s$ at the device surface, and the junction is assumed to be located at a distance of 0.3 or 0.4 microns from the surface.

The values of C_x and C_b are shown as dotted lines, C_t is shown as a dashed line and the net concentration, $C = |C_x - C_b|$, is shown as a solid line. The electrical characteristics of the device are closely related to the net concentration, C , however, those effects which result from closely spaced impurity ions also depend strongly on the total concentration, C_t . Nine numbers, 0 - 8, serve to mark the points on the curve, C , which follow from the selected values of C_x mentioned above. Actually, the values of C were chosen to be equal to C_b (0 and 8) or such that $\text{Log } C$ was less than $\text{Log } C_b$ by steps of 0.5 , 1.0 , 1.5 , and 2.0 , on each side of the junction, and the values of C_x then follow.

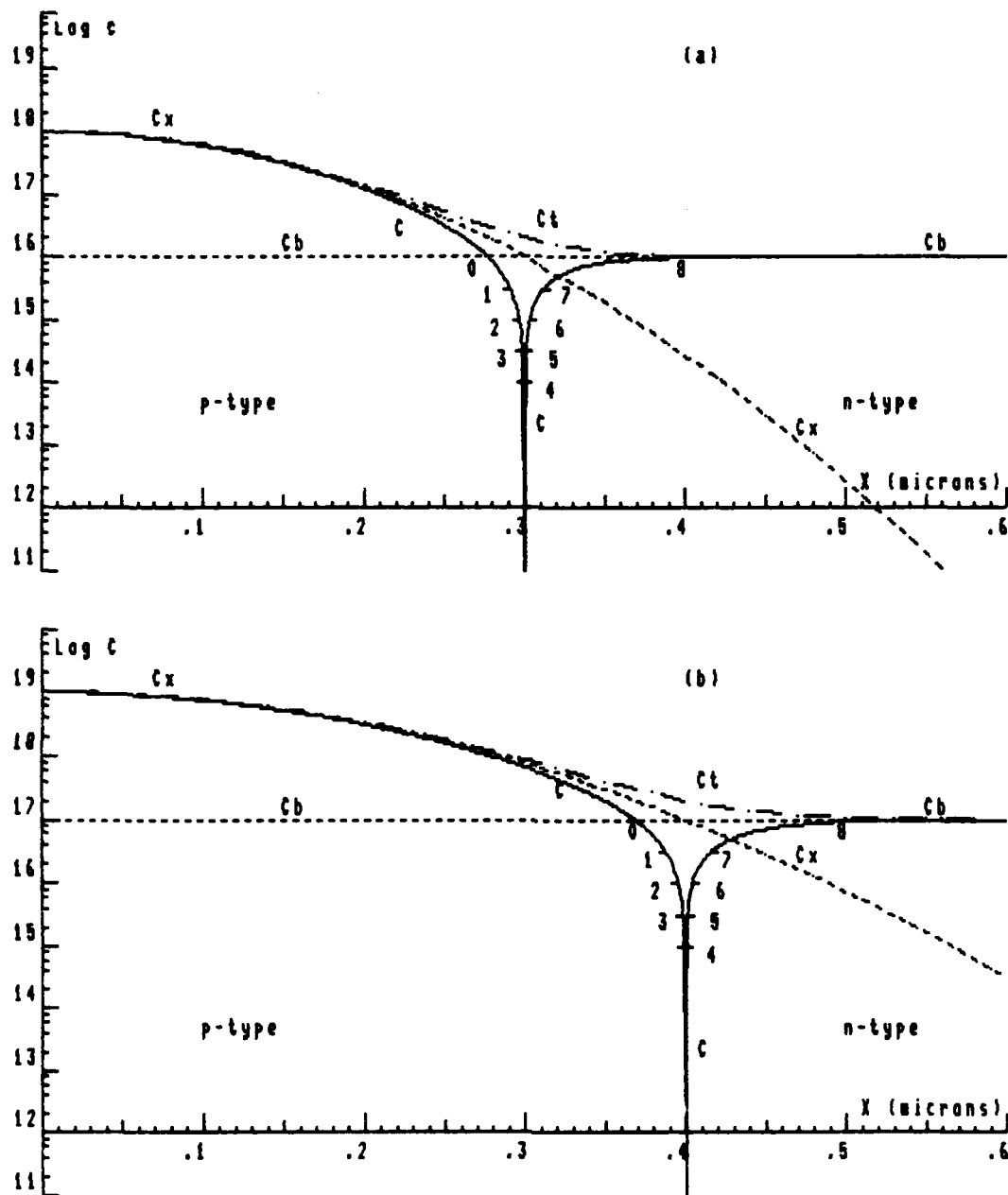


Fig. 1. Typical Concentration Profiles.

3. Discussion of Results

The numerical results obtained by the use of this model are presented in Appendix A in the form of graphic displays. Each figure consists of five displays, (a) Impurity Spacing Probability Distributions, (b) Donor Energy Levels, (c) Acceptor Energy Levels, (d) Densities of States for Conduction Band and Donor Levels, and (e) Densities of States for Acceptor Levels and Valence Band. Each Fig.(page) is based on input data for a single selection of temperature, T , donor, C_b , and acceptor, C_x , concentration. There are five temperatures treated, 100 K, 200 K, 300 K, 400 K, and 500 K. The first digit of the figure number is the first digit of the temperature.

For each temperature, there are five selections of background (or bulk) dopant level treated such that $\text{Log } C_b = 15.5, 16, 16.5, 17, \text{ and } 17.5$, where C_b is in units of cm^{-3} . C_b and C_x are also labeled C1 and C2. The second digit of the figure number has values 0, 1, 2, 3, and 4, corresponding to the values of $\text{Log } C_b$ above, respectively.

For each of these, nine values of the infused dopant, C_x , are chosen to form a profile of values across the P/N junction (see points labeled 0 - 8 shown in Fig. 1, Typical Concentration Profiles). These labels correspond to the last digit in the figure numbers. The points 0, 1, 2, and 3 are chosen so that $\text{Log } C$ is less than $\text{Log } C_b$ by values of 0.0, 0.5, 1.0 and 1.5, where $C = C_x - C_b$. The point labeled 4 is at $C = C_b - C_x = 10^{10}$.

Points 5, 6 and 7 provide values of $\text{Log } C$ less than $\text{Log } C_b$ by 1.5, 1.0 and 0.5, respectively, with $C = C_b - C_x$, and point 8 sets $\text{Log } C$ almost equal to $\text{Log } C_b$, (less than C_b by 10^{-6}). The input values of Temp., $\text{Log } C_b$, $\text{Log } C$, and $\text{Log } C_x$ are shown in the inset of display (b) of each figure along with the calculated values of $\text{Log } n$ and $\text{Log } p$, the free carrier densities.

The calculated Fermi energy, E_F , and the screening factor, β , are shown in the inset of display (c). Also shown are corrected values of the isolated donor energy, E_D , (depends on β) and the gap energy, E_V (depends on T).

In the first display of each figure, labeled (a) Impurity Spacing Distribution, the upper curve represents the probability distribution of R vs R , in units of the isolated donor Bohr radius, arbitrarily normalized to a peak height of unity for plotting convenience. The total area under this curve is proportional to the total number of impurity pairs and is divided into three areas, DD, DA, and AA, proportional to the number of donor-donor, donor-acceptor, and acceptor-acceptor pairs, respectively. The areas between these curves and their general positions along the R axis provide required information for weighting the energy levels vs R in displays (b) and (c).

Spacing between impurities is often estimated by the rule $d = C_t^{-1/3}$. It is interesting to note that this value is too large by almost 85 %, i.e., d is larger than R_m , the most probable value of R (peak of curve in (a)), by a factor of 1.845, and that the position of d on the curve is sufficiently far to the right of the peak, R_m , that 98.5 % of the nearest-neighbor pairs are more closely spaced than d . Only 1.5 % have larger spacing.

In compensated semiconductor materials with concentration profiles such as those shown in Fig. 1, the donor and acceptor concentrations are equal at the junction. In this case the relative probabilities, DD, DA, and AA are in proportion to $\frac{1}{2}$; $\frac{1}{2}$; $\frac{1}{2}$. At points away from the junction, DA numbers continue to dominate until the concentration ratio exceeds 2 ; 1 (refer to Section 2 and to Appendix B).

The part of the probability distribution labeled DD applies to the donor energy levels, E1 and E2, shown in display (b), the first and second electron energies in a donor-donor pair. The distribution labeled DA is applicable both to E3 and E4 in (b) and also to H3 and H4 in (c). The AA part applies to hole energy levels H1 and H2 in (c).

The position of the peak in the impurity separation distribution is determined by the total impurity concentration, $C_t = C_x + C_d$. As this concentration is increased, from one example to another, the position of the peak moves toward lower values of R , thus changing the section of an energy level curve, in (b) or (c), that is applicable for a given example.

Energy Levels

Four levels are shown in display (b) Donor Energy Levels. Of these, E1 and E3 are the most likely and next most likely to be occupied by a localized electron since they are single electron systems and E1 is the deeper of the two. Level E2 does not come into existence unless level E1 is already occupied by an electron. Level E4 comes into existence only if the DA pair is already occupied by a hole. Thus levels E1 and E3 are the donor states of primary importance in applications falling near room temperature. Levels E2 and E4 become important at low temperatures when E1 and H3 are largely occupied. A similar discussion applies to the hole levels. H2 and H4 exist only if H1 and E3 are occupied.

As the free carrier densities n and/or p increase, either due to an increase in temperature or because of an increase in the net concentration $C = |C_x - C_b|$, the value of the screening factor, β , increases. This makes the screening range, $1/\beta$, smaller so that neighboring systems interact more weakly and localized carriers are more weakly bound to impurity ions. In other words, all levels become shallower, at all values of R . This trend is clearly evident in the figures, especially at higher concentrations.

In displays (a), (b), and (c), the units used in the horizontal axes are the same, the Bohr radius of an isolated donor electron. The hole states have been assumed to have larger Bohr radii so that the energy level curves in (c) appear expanded in the horizontal direction. Similarly the unit of energy, effective Rydberg, is the same in both (b) and (c), but, since the hole binding energy was assumed to be smaller, the hole levels appear compressed in the vertical direction as compared with the electron levels.

As R increases, the levels E2 and E4 (also H2 and H4) approach their final common value, E_D (screened atom value), at much smaller values of R than in the case of E1 and E3 (or H1 and H3). At R greater than two or three Bohr radii there is no further change in the E2, E4, H2, or H4 levels. The odd numbered, one electron or one hole levels have not yet converged to E_D even at eight Bohr radii in most cases. Since the even numbered levels are

the most active at low temperatures and the odd ones are dominant at the usual operating temperatures of solar cells it would seem that test data obtained at low temperatures should be projected with caution into room temperature applications.

Two ionized donor impurities, separated by a distance, R , form a double potential well with a barrier at the midpoint of R . If the energy of an electron, localized at the well, is above the potential barrier, the electron is not restricted to one of the ion sites. On the other hand, if the electron level is below the barrier potential, transport from one site to the other requires a tunneling process involving time constants of sufficient length to diminish contributions to conductivity. The expression for the barrier height is given by $V_b = -8 \exp(-\beta R/2)/R$ in the usual units. This function is plotted in graphic (b) as a dotted curve. It is significant that, although the donor energy, E_1 (also E_2), moves to lower levels as R decreases, the barrier energy, V_b , moves to lower levels at a greater rate, crossing E_1 at about six Bohr radii and moving substantially lower as the ion separation becomes smaller. This behavior can be viewed as an indicator of the onset of impurity conduction. When the bulk of the donor pairs are closer than the critical R , as shown by the distribution DD in (a), the donor state electrons are no longer strictly localized. The exact condition at which this happens becomes a problem in percolation theory. Electrons with levels somewhat below the barrier level probably contribute to the so-called hopping conduction which has a temperature dependence suggesting the tunneling process. Note that the curve, V_b , shifts in position from one example to another because of the dependence on the screening factor, β .

The screening factor, β , also plays a role in reducing the energy gap. The energy needed to ionize a donor or an acceptor or to form an electron-hole pair is partly the result of short range forces, such as exchange interactions and ion core penetration, and partly due to the long range Coulomb or screened Coulomb forces. The short range forces are largely responsible for the differences in the binding energies of

different impurity ions. The additional contribution of the long range forces is essentially the same for all, including the electron-hole pair. The calculated energy levels displayed in Appendix A show that the donor and acceptor binding energies go to zero as the value of β increases, due to the screening effect in the long range Coulomb forces. In view of this and the remarks above, it follows that the long range part of the energy of the electron-hole pair is also reduced by an amount paralleling the donor energy reduction as β increases. Consequently, the energy gap will show a reduction with increasing β in addition to changes for other reasons.

Densities of States

The density of states distributions in displays (d) and (e) follow from the probability distributions in (a) of the form, $P(R)$, and the energy levels in (b) and (c) of the form, $E(R)$. A numerical routine is used to transform $P(R)$ and $E(R)$ into the form $P(E)$ which is the required density of states, S . A separate transformation is performed for each energy level with the appropriate probability distribution to form displays (d) and (e) where each distribution peak has the same label as the corresponding energy level. Chart (d) contains the donor state distributions, along with the conduction band density-of-states data, plotted with $\log S$ as the vertical axis and the energy, E , measured from the intrinsic conduction band edge in effective donor Rydbergs, as the horizontal axis. Chart (e) contains the acceptor state distributions and the density-of-states data for the valence band. The horizontal axis is in this case referred to the edge of the intrinsic valence band and labeled $E - E_v$. The units are effective donor Rydbergs. The units of S are cm^{-3} per effective Rydberg.

The distributions of primary importance, E1, E3, H1, H3, and the conduction and valence band states are displayed with a solid line style. The curves E2, E4, H2, and H4 are shown with a dotted line. Additional distributions show, with dashed lines, filled states, i.e., those states in the bandgap that are occupied by localized electrons or holes and those states in the conduction or valence bands that are occupied by carrier

electrons or holes.

The upper and lower portions of the bandgap are shown in (d) and (e) with an expanded scale since there is no need for displaying the central part. The portion not shown varies between figures based on different temperatures since the value of E_v in intrinsic material depends upon the temperature. This value is shown both at the zero position of (e), marked E_v , and in the inset data in (d). In those cases where the Fermi energy is within the range of E displayed, the position is marked by a vertical dotted line labeled E_F . In all cases E_F is given in the inset data of (d) referenced to the conduction band edge.

The shapes and positions of the distributions in (d) and (e) as well as their changes with concentration and temperature reveal quite clearly the influence of neighboring impurity interactions and of charge screening in producing substantial, and in many cases undesirable, modifications in the characteristics of semiconductor materials and in diodes such as those used in solar energy conversion.

One of the most important aspects of these effects is that they are inherent in the nature of the materials. They are still present in crystals of the highest quality containing the specified dopants of the greatest purity.

In the asymmetric distribution of the energy level, E_1 , (also H_1) of an electron at a donor pair, $(DD)^-$, there is an impurity band tail that extends toward the center of the bandgap by values up to four Rydbergs in the case of donor pairs. Clusters of three, four or more donors were not considered here in order to keep the calculation manageable. In real devices, such clusters can be expected, perhaps with lower probability, and in those cases the tail can be expected to extend much farther into the gap. Electrons will be localized in such pairs or clusters at deeper levels with greater probability, thus causing them to act as deep traps exactly as the deep traps due to undesirable chemical impurities.

In the case of the distribution corresponding to the energy level, E_3 , (also H_3) associated with a donor-acceptor pair with a localized electron,

(DA)-, the impurity band tail is again present but asymmetric in the reverse sense to E1, with the tail extending toward the conduction band. Of course this reflects the fact that a neighboring acceptor ion causes an electron to be bound more weakly to a donor ion. At increasing concentrations, the tail extends to the conduction band and then shifts to become a tail of the conduction band extending into the bandgap. Near the junction, such levels exceed the E1 levels in frequency of occurrence roughly by a factor of two and are more likely to support impurity band conduction. Under these conditions, the distributions, E3 and H3, are acting to shift the effective edges of both the conduction band and the valence band into the bandgap, thus narrowing the gap substantially.

Several effects caused by changes in temperature are displayed in the density of states charts. In addition to the inherent increase in bandgap with decreasing temperature, present even in intrinsic materials, there is a decrease in free carrier concentration which, in turn, causes a decrease in β , the screening constant, resulting in a general shift away from the band edges of the distribution peaks. In addition, as carriers become localized, the one electron and one hole levels, E1, E3, H1, and H3, become filled, shifting emphasis to the E2, E4, H2, and H4, second particle levels. Under these conditions, the distributions displayed with dotted lines are the valid ones to consider and, being much less broadened and more nearly placed at the unperturbed dopant energy levels, appear to belong to a more nearly ideal semiconductor material with low dopant concentration.

The distributions for one particle states (solid line, odd numbers) and those for second particles (dotted line, even numbers) are each plotted at their maximum density values even though the second particle states exist only to the extent that the one particle states are occupied, and the one particle states are diminished in number to the extent that the second particle states are occupied.

For purposes of keeping the calculation manageable, various device circuit conditions, e.g., open circuit, short circuit, etc. were not treated. The Fermi energy, screening factor, and carrier densities were

obtained from a thermal equilibrium condition in bulk material. In the space charge region and in the depletion region these parameters will be modified slightly with the net result that changes across the junction take place less rapidly and over larger displacements depending on the width of the depletion region, a function of junction bias.

p-n Fluctuations

The calculations made in this investigation emphasize statistically random variations in impurity separations which take place over distances ranging from a few $\text{\AA}$ up to a few hundred $\text{\AA}$, i.e., from the host lattice constant up to a few effective Bohr radii. With larger distance scales the effects of random fluctuations decrease in magnitude, however, at distances of the order of the width of the depletion region, these effects may still be substantial.

The Poisson relation $P_k(cv) = \{(cv)^k/k!\} \exp(-cv)$ introduced above, which states the probability of finding k impurities in the volume, v , if the average (mean) number is cv , has the property of exhibiting a peak value at $k = cv$ and also has a standard deviation, $s = (cv)^{1/2}$, which serves as a measure of the distribution width. It is useful here to define a fractional standard deviation, $f = s/cv = (cv)^{-1/2}$, the ratio of the standard deviation to the mean value. The basic quantities treated in the relation are numbers and their magnitude depends on size of the volume under consideration. For example, with $c = 10^{16} \text{ cm}^{-3}$, if $v = 10^{-12} \text{ cm}^3$ then $cv = 10^4$ and $f = 1\%$; if $v = 10^{-14}$, $cv = 100$ and $f = 10\%$, etc.

The relations can be put in more familiar terms by calculating the deviations in concentration in cm^{-3} as $D_c = cf$, remembering that the v which appears in $f = (cv)^{-1/2}$ is the actual volume under consideration and c is the concentration in cm^{-3} . Then $D_c = (c)^{1/2}(v)^{-1/2} = (c/v)^{1/2}$.

For the example shown in Figure 1 (a), near the junction C_x and C_b are approximately 10^{16} . If the width of the depletion region is about 0.1 microns then the volume, v , can be taken to be 0.001 microns^3 or 10^{-15} cm^3 . Then $D_c = 3.16 \times 10^{15}$ each for C_x and C_b and, since deviations in C_x and C_b are independent, they are large enough as compared with

the net concentration, $C = |C_x - C_b|$, to cause random fluctuations in the local position of the junction surface about the mean position and produce small closed regions or p-n anomalies near the junction in which the p-n type is reversed from normal. In Figure 1 (b), C_x and C_b are about 10^{17} near the junction. In this case, for the same v , the fractional s.d. is $f = 10\%$, and $D_c = 10^{16}$, again larger than C_{net} near the junction.

These types of situations can be expected in cases where the total concentration is high in the vicinity of the junction. The question that arises is what effects they may have on recombination rates, efficiency, and power losses.

4. Summary

The model used in calculations for this investigation, known as the BGN model, incorporates statistically random spacing between neighboring dopant positions in a GaAs or Si host, impurity band formation due to interactions of neighboring donors and acceptors, screened Coulomb-like potential energy based on the Thomas-Fermi approximation involving charge carrier densities, effects due to the higher concentrations used in compensated materials, and computing techniques designed to achieve accuracy and self-consistency in the process.

The results of the calculations, displayed in the form of quantitative plots in Appendix A, show a number of effects that substantially agree with experimental knowledge of these semiconductor systems.

(1) Donor and acceptor energy levels show broadening with increasing total dopant concentration and shifting toward bandgap edges with increasing charge carrier concentrations.

(2) Donor-donor and acceptor-acceptor neighbor interactions cause an asymmetrical impurity level broadening by introducing an impurity band tail reaching deep into the bandgap.

(3) Donor-acceptor neighbor interactions produce asymmetric impurity band broadening with tails extending toward the bandgap edges at moderate concentrations. At higher concentrations and/or higher charge carrier densities, the tail moves to the bandgap edge and becomes a conduction or valence band tail that is a primary source of bandgap narrowing.

(4) Four sources of bandgap narrowing are identified in addition to the temperature dependent effect known to be present in the host intrinsic material. In addition to the band edge tails described in (3) above, the electron-hole pair creation requires less energy with the screened potential and, in the depletion region, electrons with energy levels lower than the intrinsic conduction band but higher than the potential barrier, V_b , may

become mobile, thus lowering the effective bandgap edge. Holes behave in a similar way at the valence band edge.

(5) Impurity band broadening effects are primarily due to increasing values of total concentration, $C_x + C_b$, although electrical effects are controlled by the net concentration, $|C_x - C_b|$, in compensated materials. Thus, broadening is greater in compensated materials than in electrically similar uncompensated materials.

(6) The more closely spaced pairs or clusters of donors or of acceptors have levels in the bandgap sufficiently deep to act as if they are a deep level variety of chemical impurity traps.

(7) At low temperatures, with most of the carriers localized and the free carrier screening effect removed, the active dopant energy level distributions appear sharp and unperturbed as if the impurities were dilute and non-interacting, even at relatively high concentrations. At normal operating (room) temperatures or higher, different sets of dopant energy levels become active and screening effects are restored, resulting in impurity band broadening, bandgap narrowing, band edge tailing, etc. Low temperature data should be projected into room temperature applications with caution.

(8) In compensated materials near the location of the P/N junction, statistical fluctuations in concentration are sufficiently large to produce random shifts in junction position about the mean as well as anomalous cells with inverted p-n type which may contribute to recombination rates.

(9) The calculation reveals an anomalous behavior at lowered temperatures resembling that of a solidstate phase transition. At a critical temperature which varies with host material and with impurity concentration, two contrasting stable conditions are possible. In one the carriers are localized, screening is removed and dopant energy levels are well separated from the band edge. In the other the carriers are ionized, screening is restored and the levels merge with the band edge. If a device, such as a photodiode in the first state, received a strong burst of radiation, it appears that it would be locked in the second state until the temperature

were lowered sufficiently to definitely return the system to the first state. Further investigation of this type of behavior is recommended.

APPENDIX A

Diagrams of Calculated Results

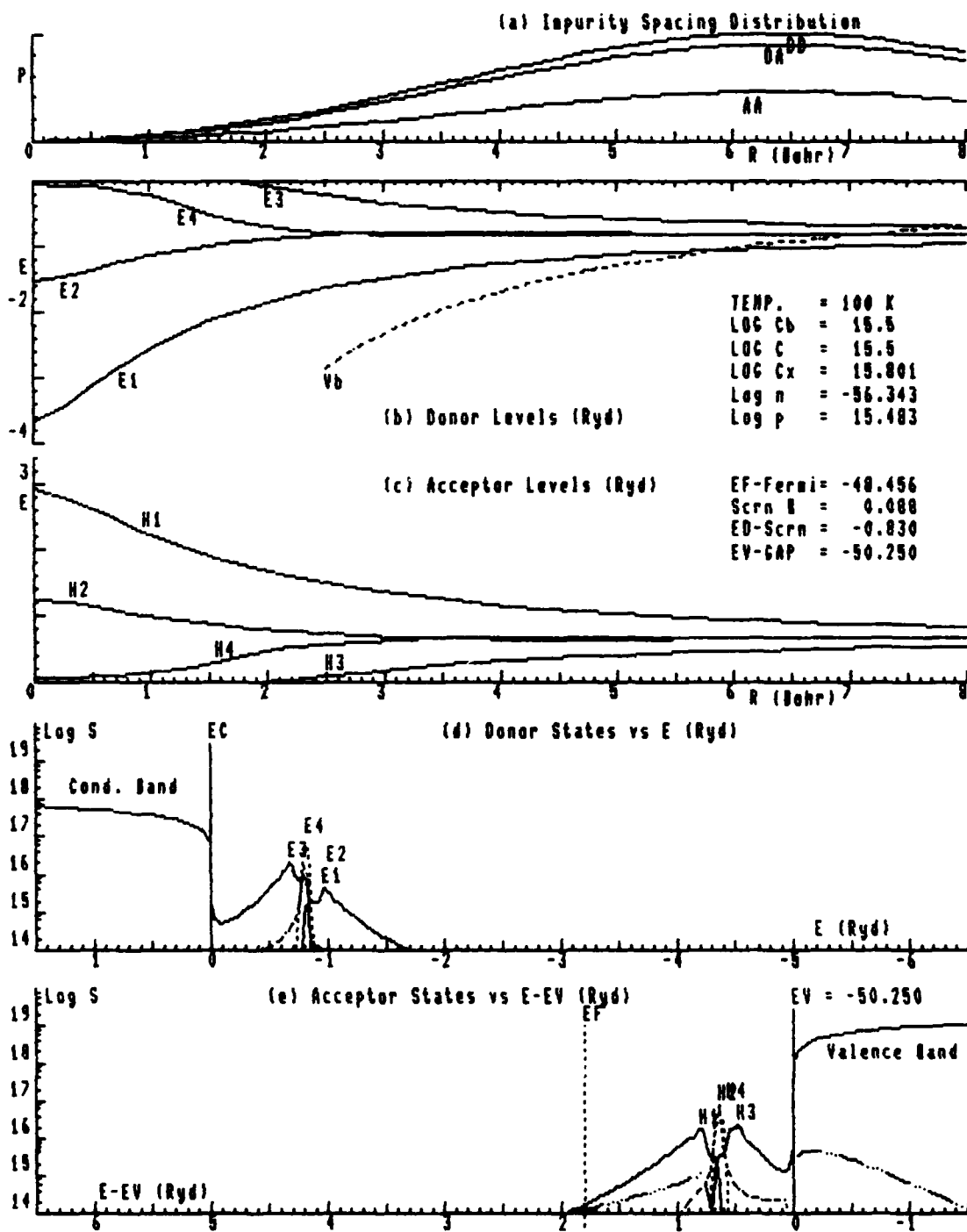


Fig. A 100. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

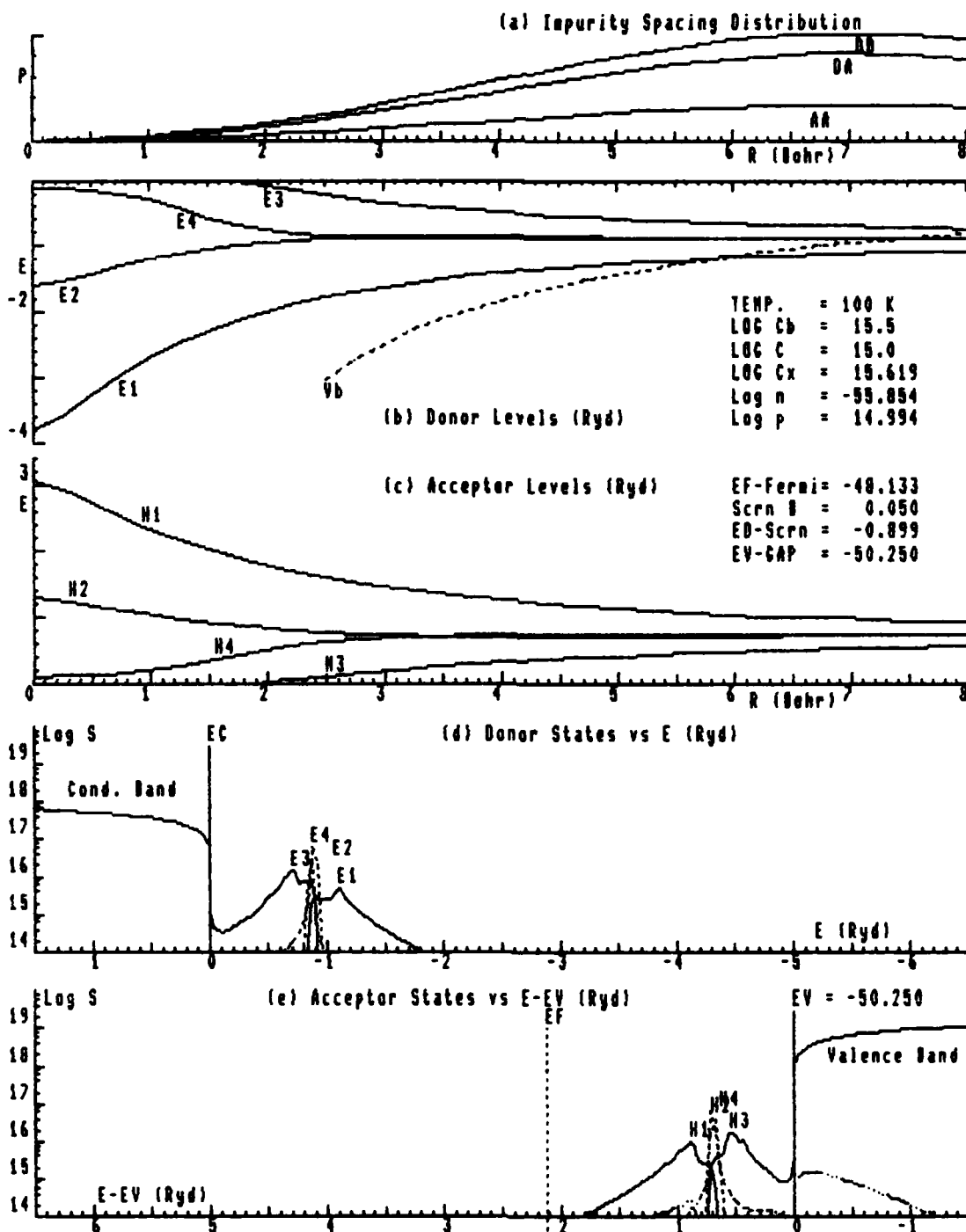


Fig. A 101. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

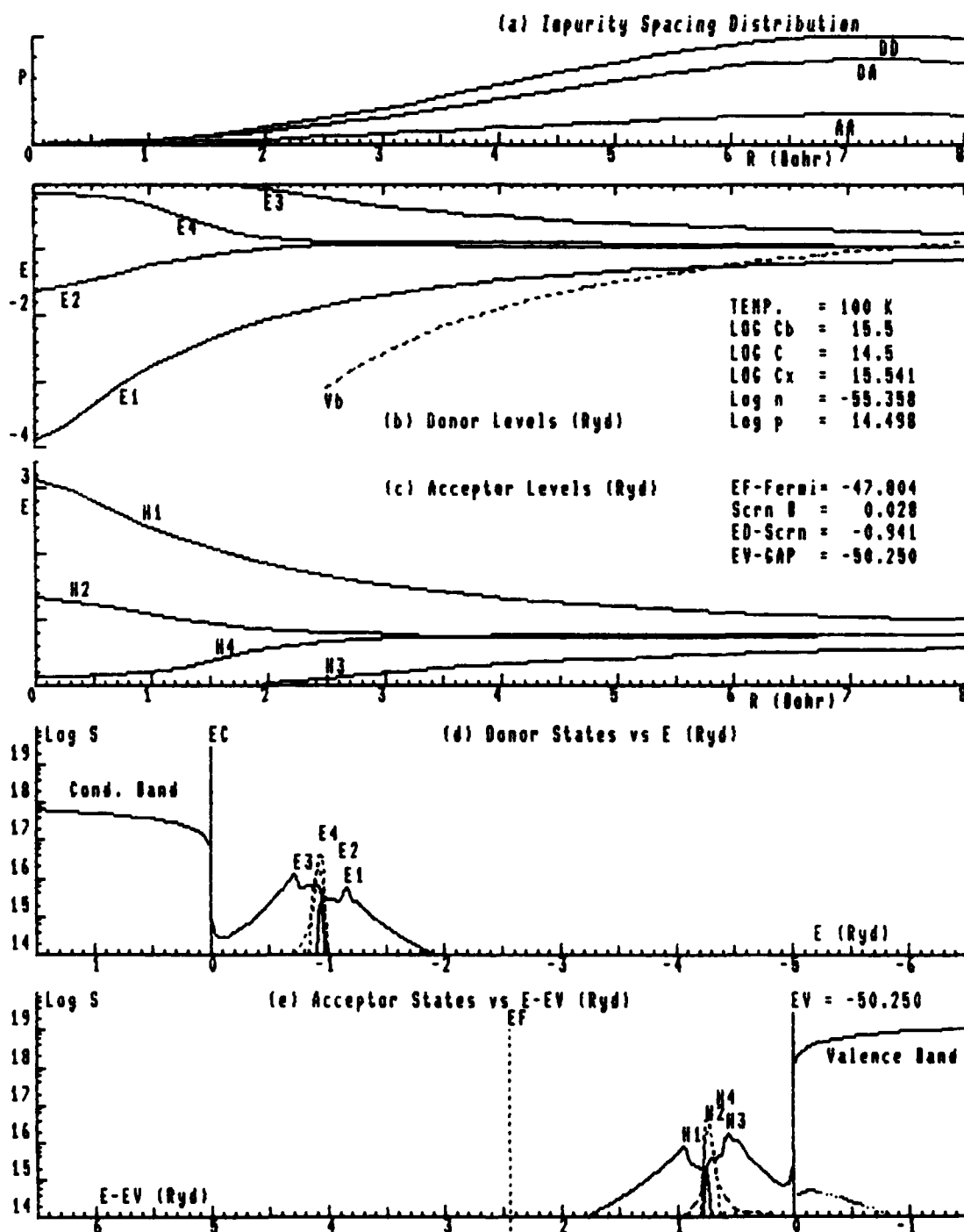


Fig. A 102. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

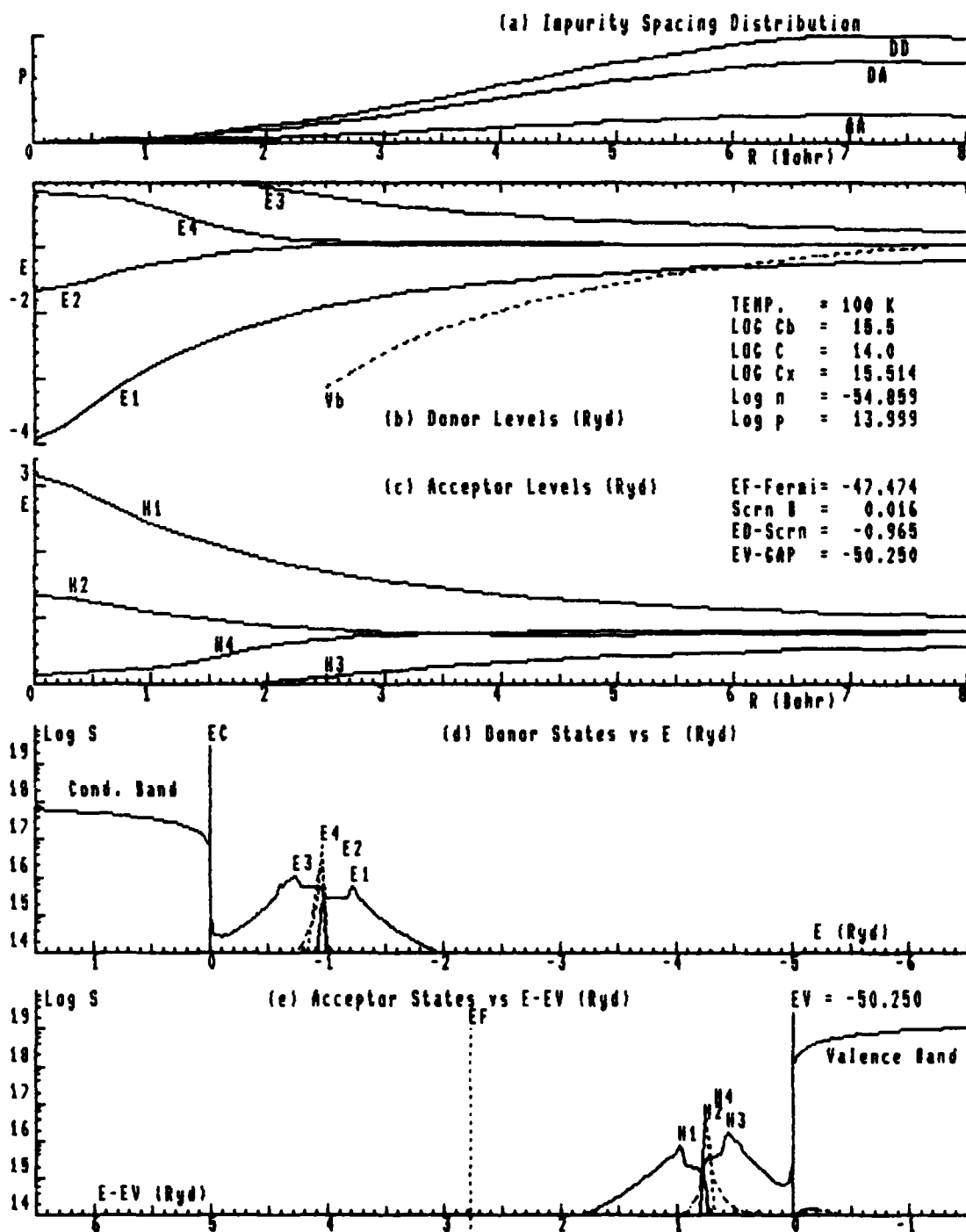


Fig. A 103. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

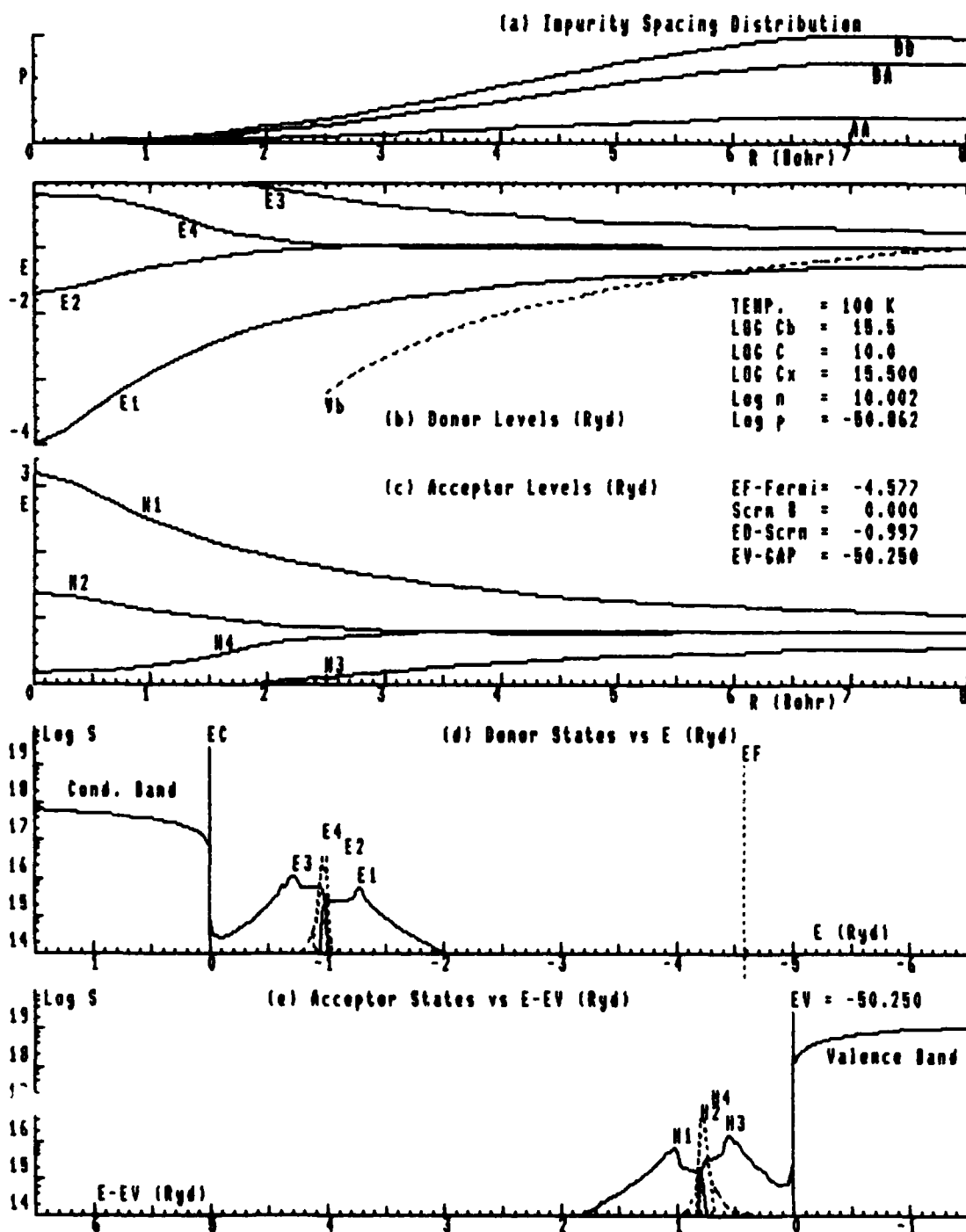


Fig. A 104. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

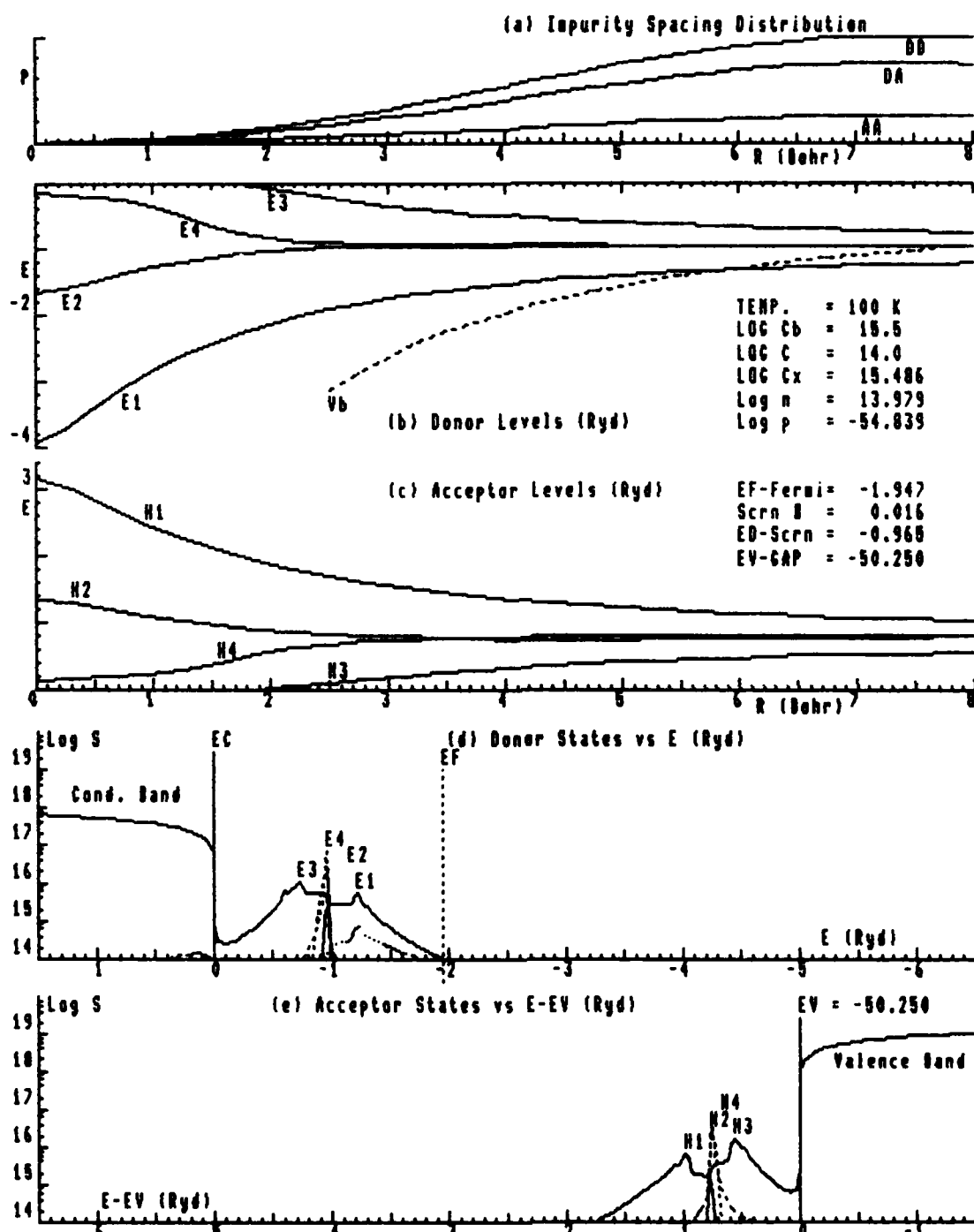


Fig. A 105. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

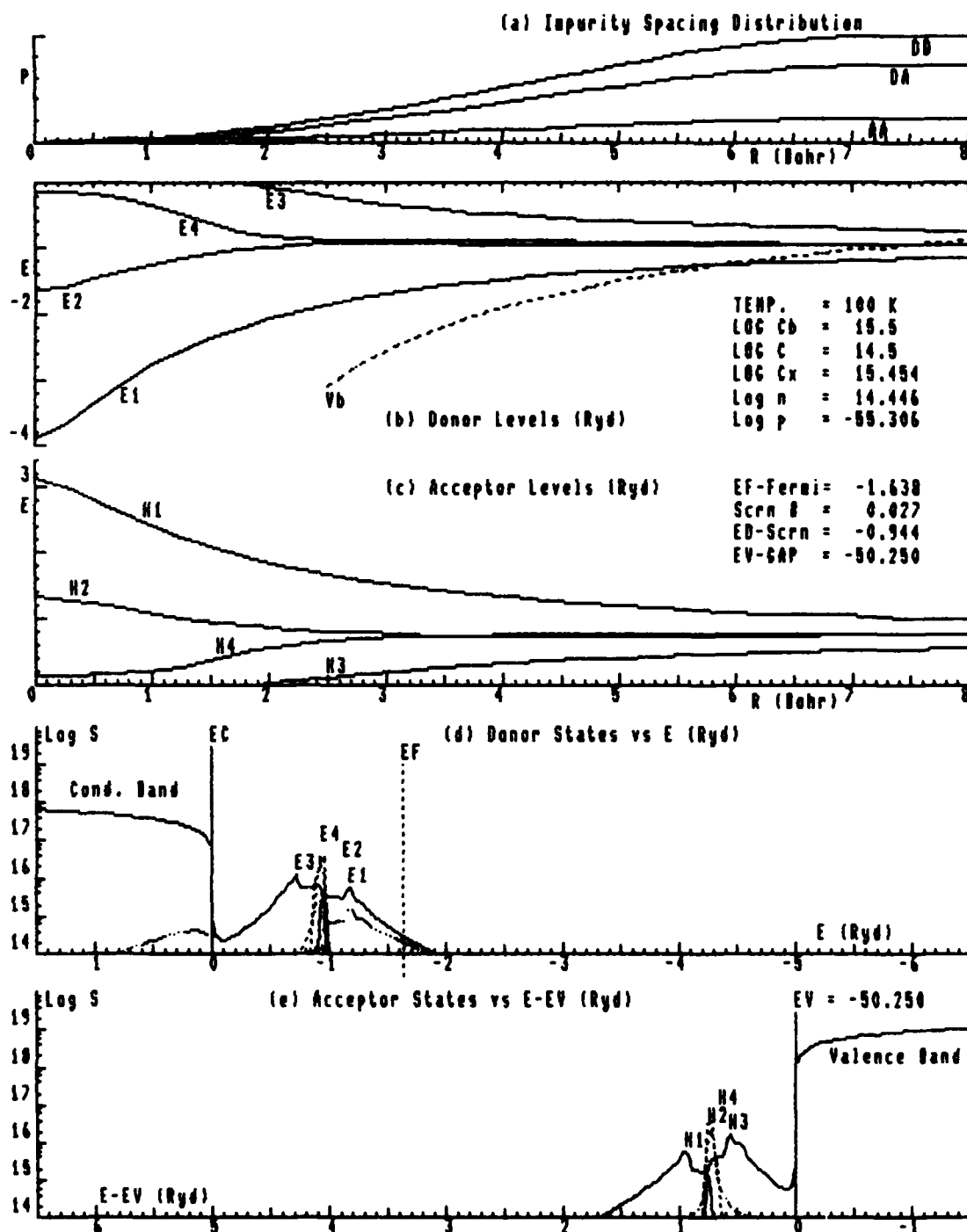


Fig. A 106. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

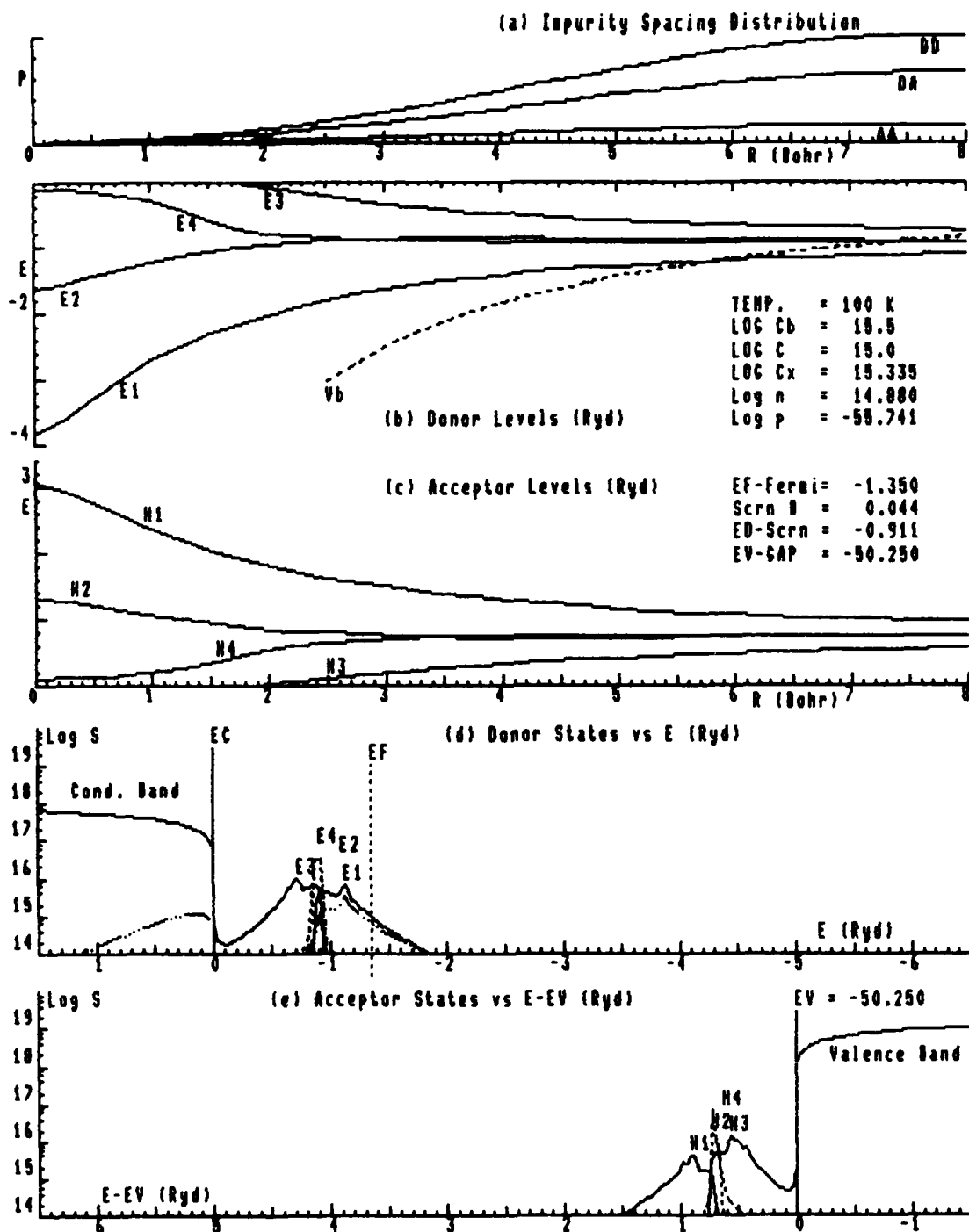


Fig. A 107. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

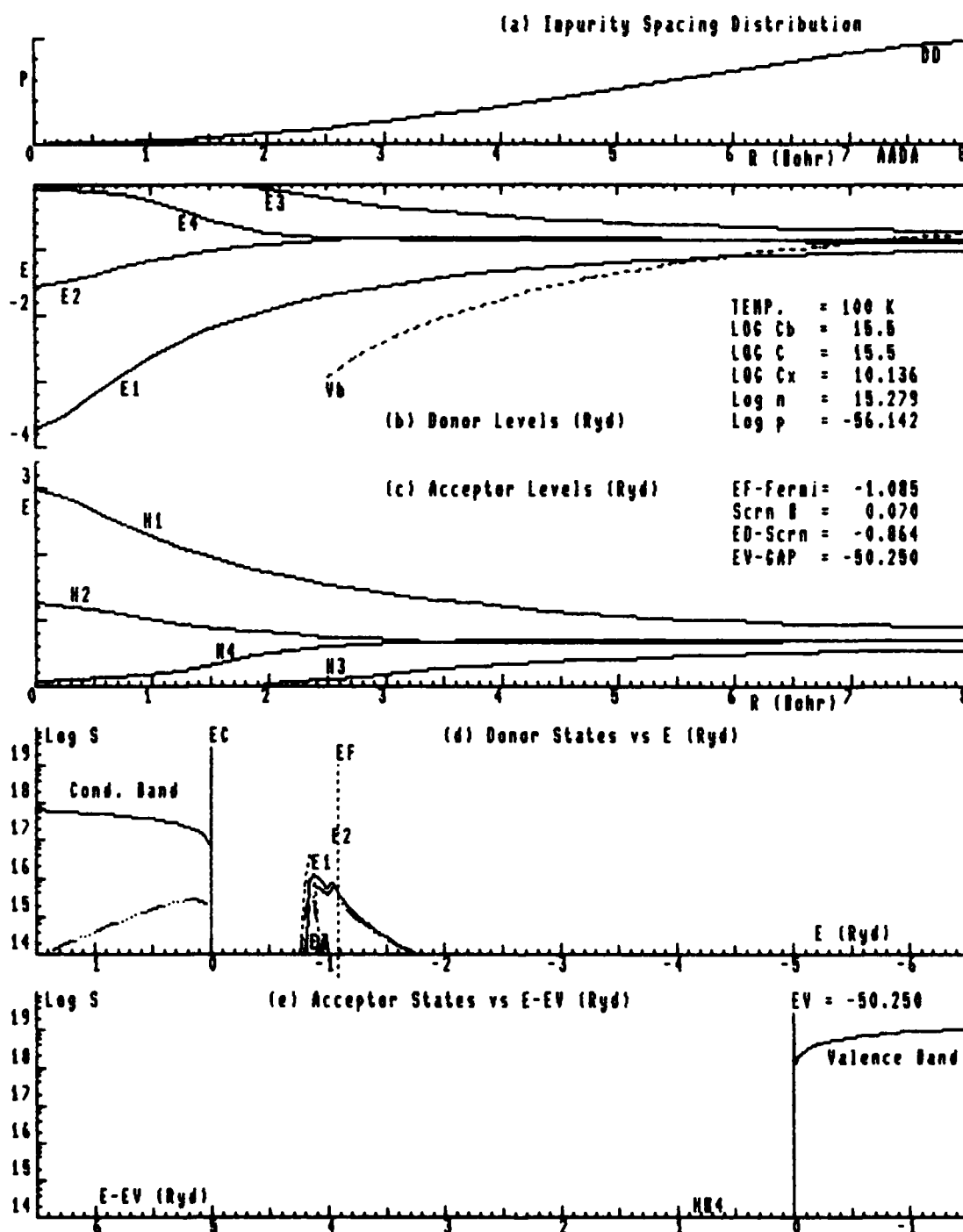


Fig. A 10B. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

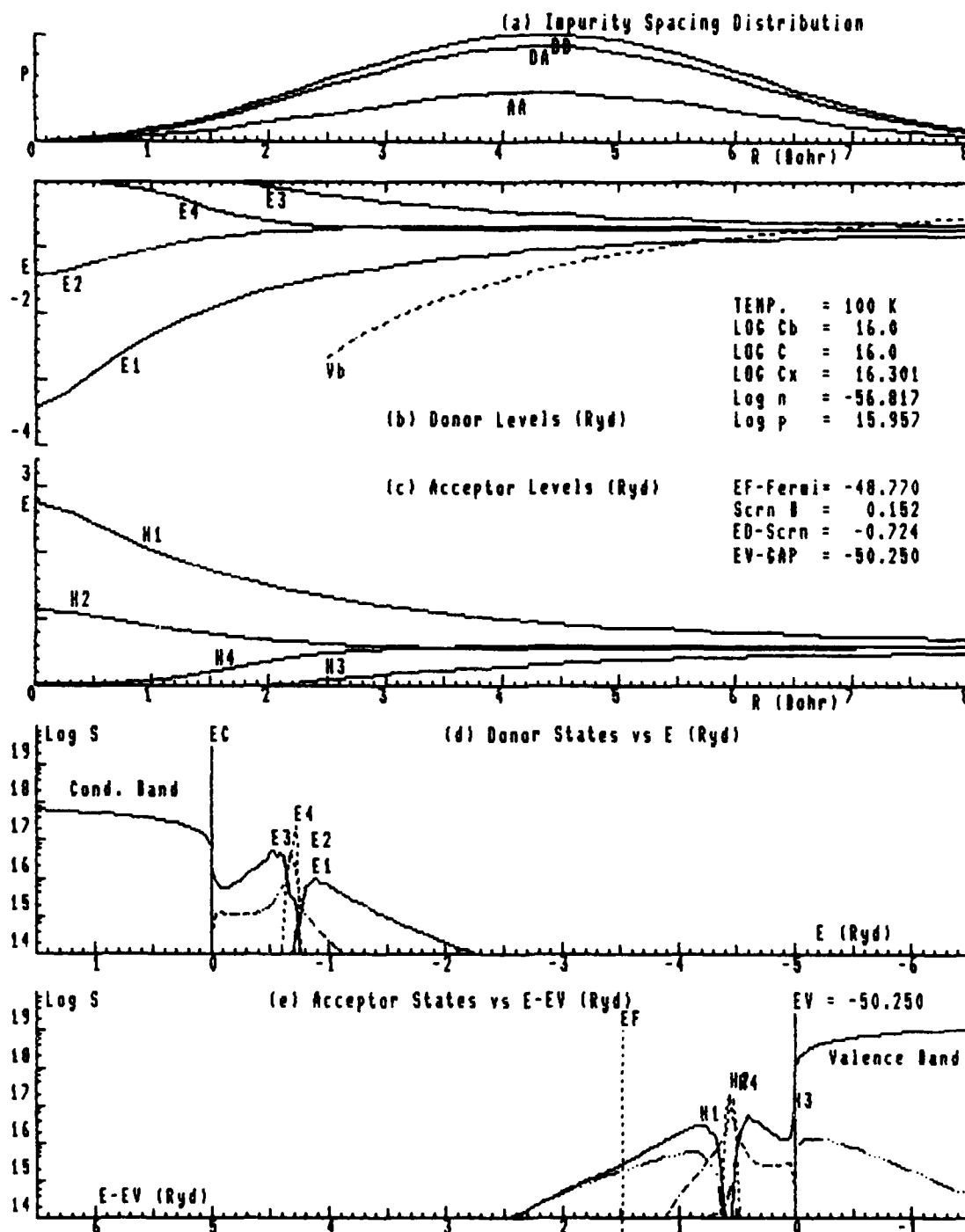


Fig. A 110. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

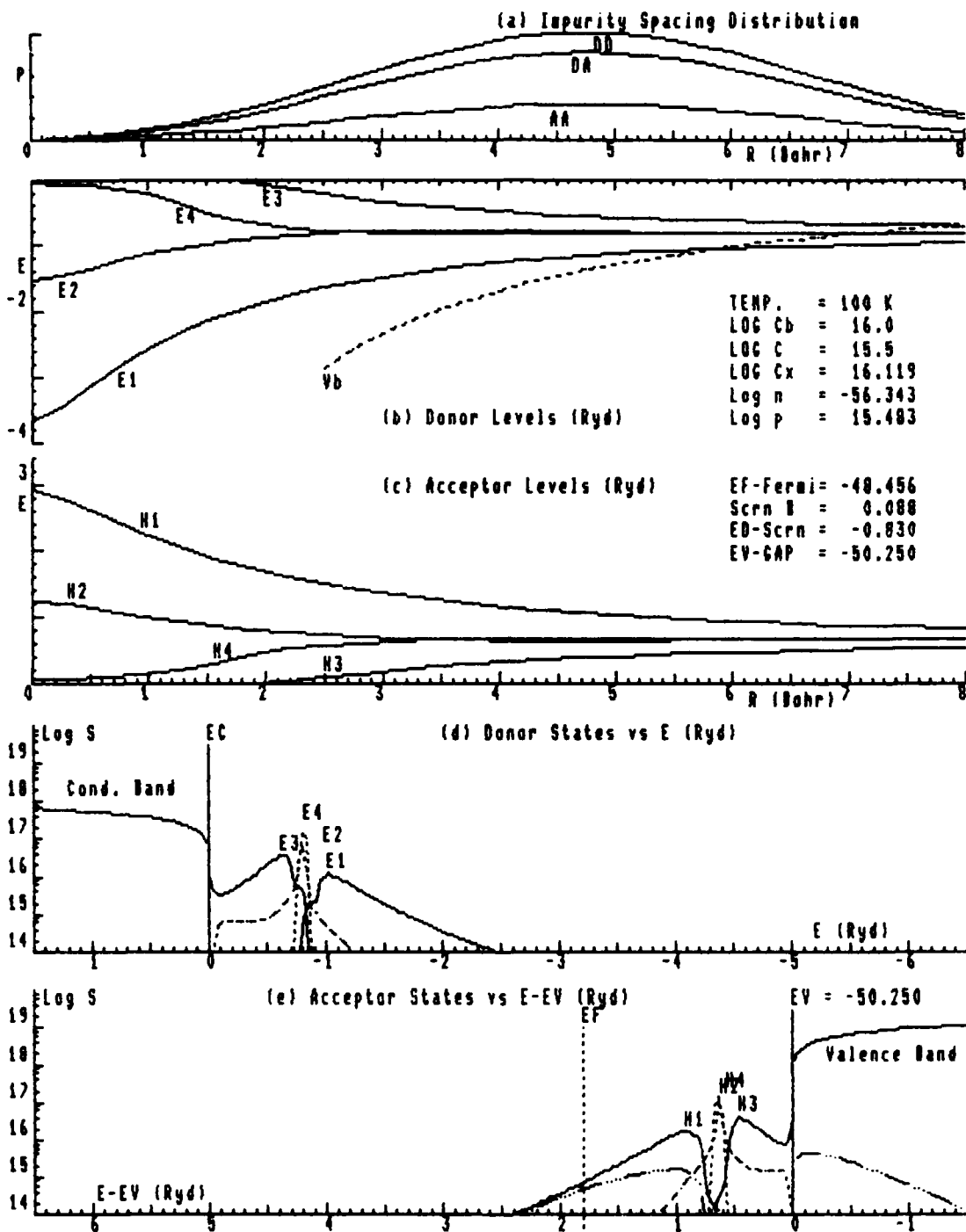


Fig. A 111. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

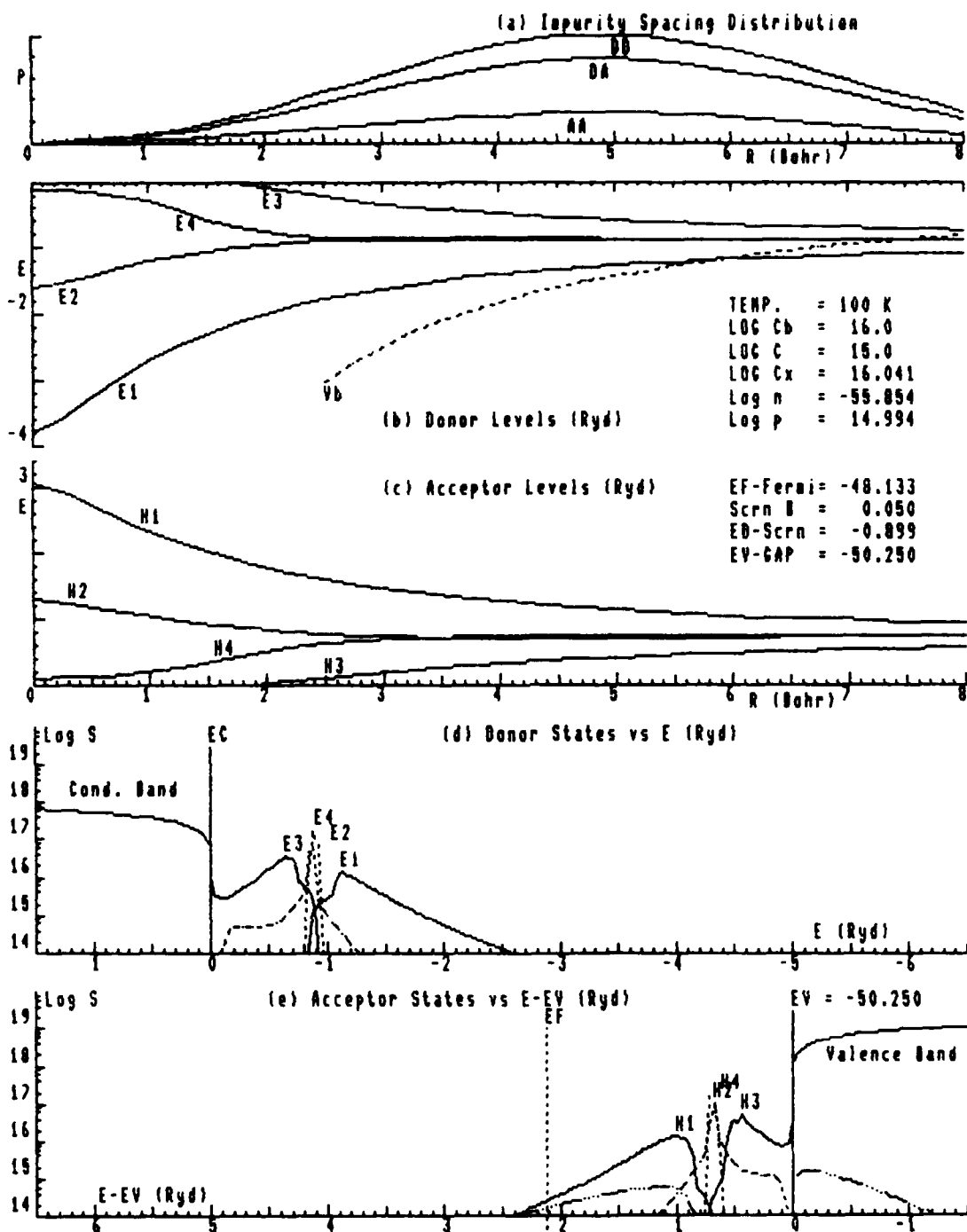


Fig. A 112. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

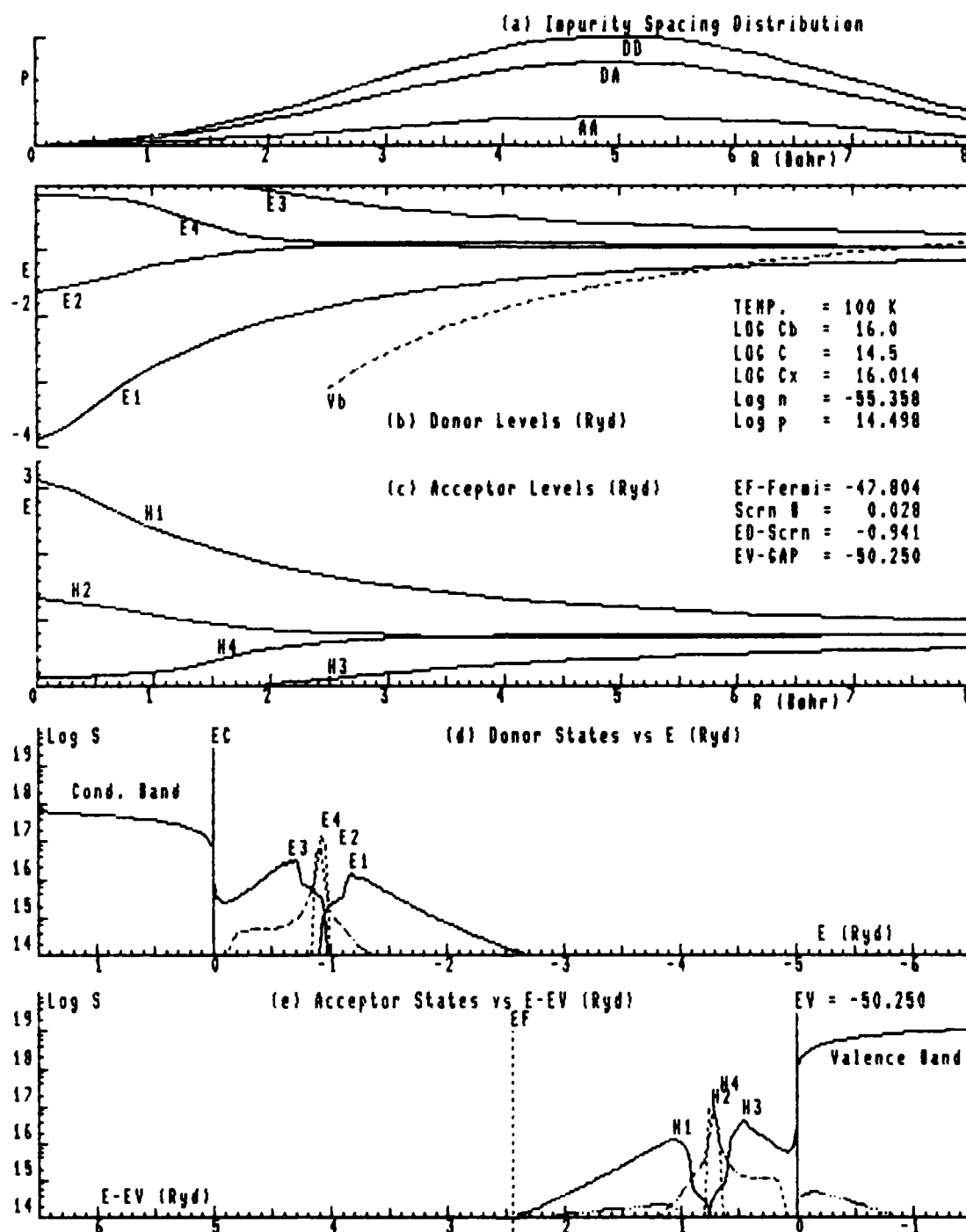


Fig. A 113. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA+)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

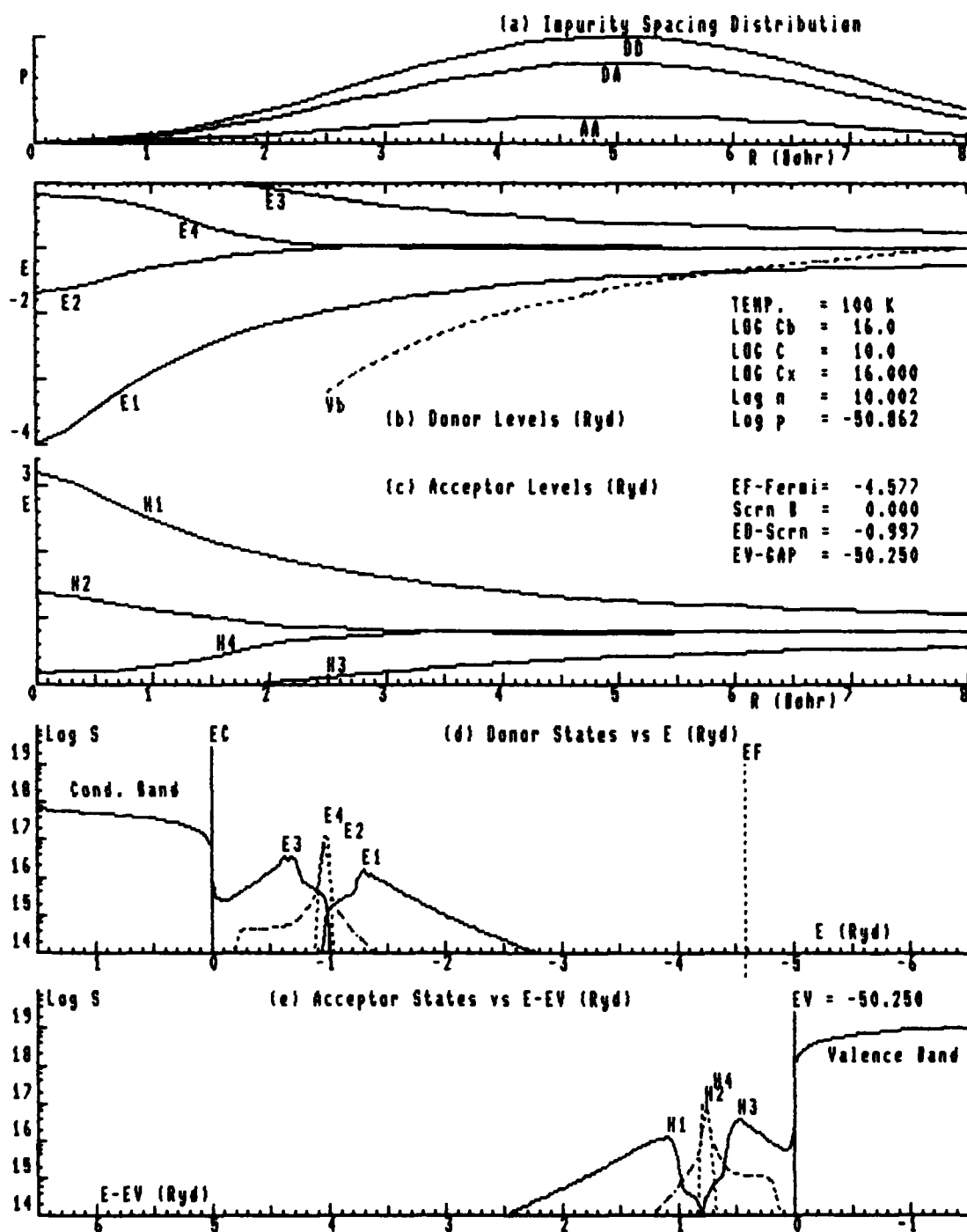


Fig. A 114. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

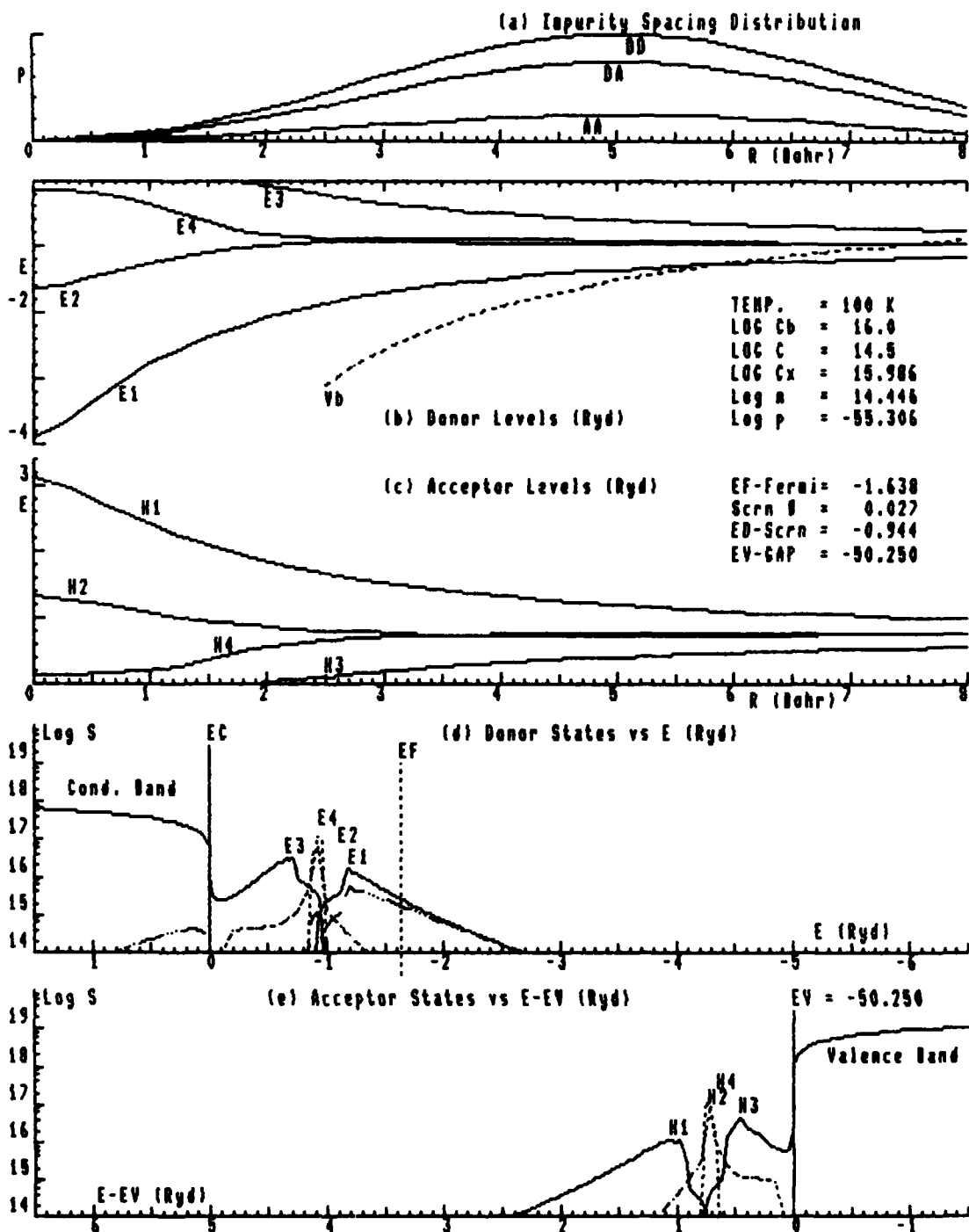


Fig. A 115. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

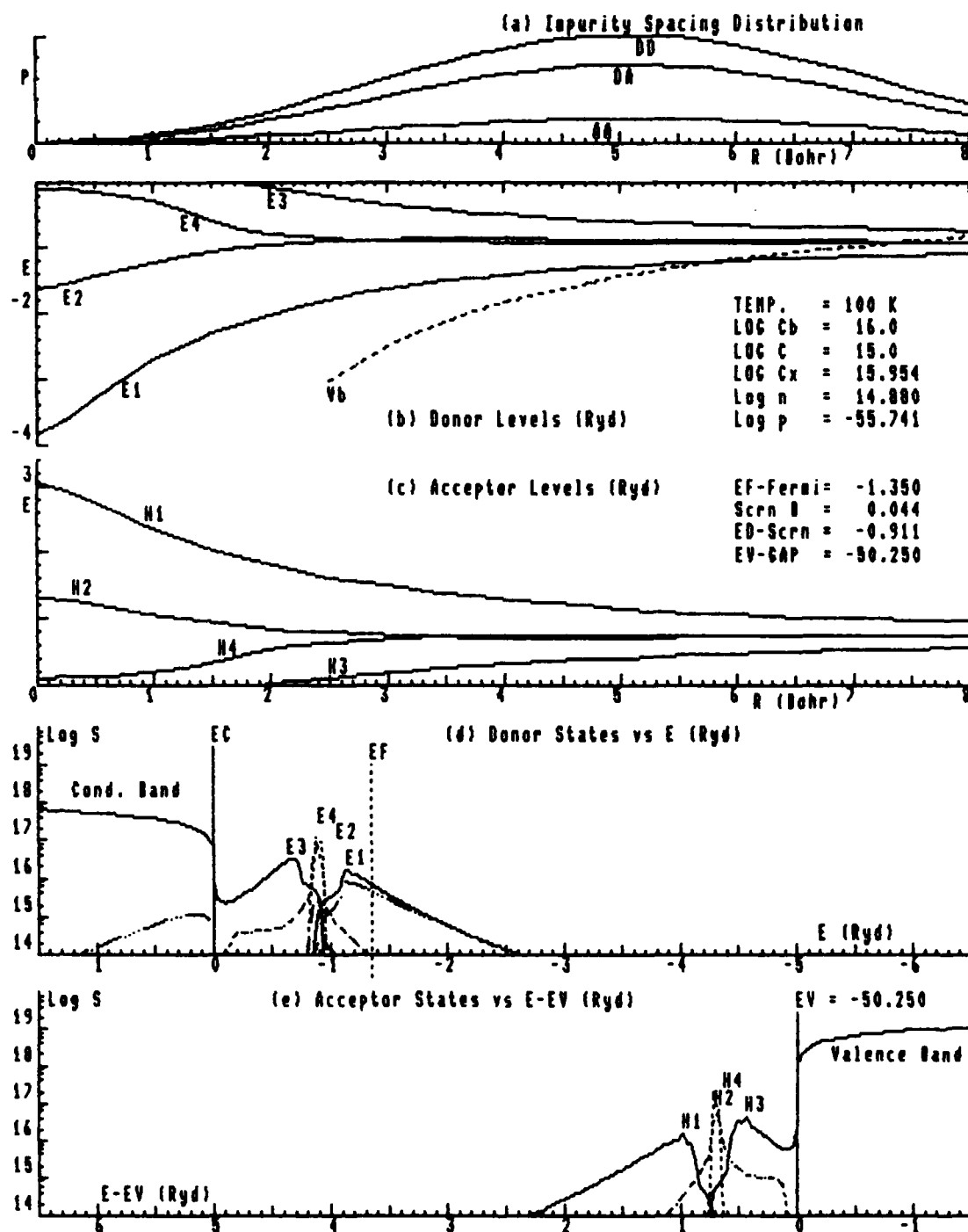


Fig. A 116. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

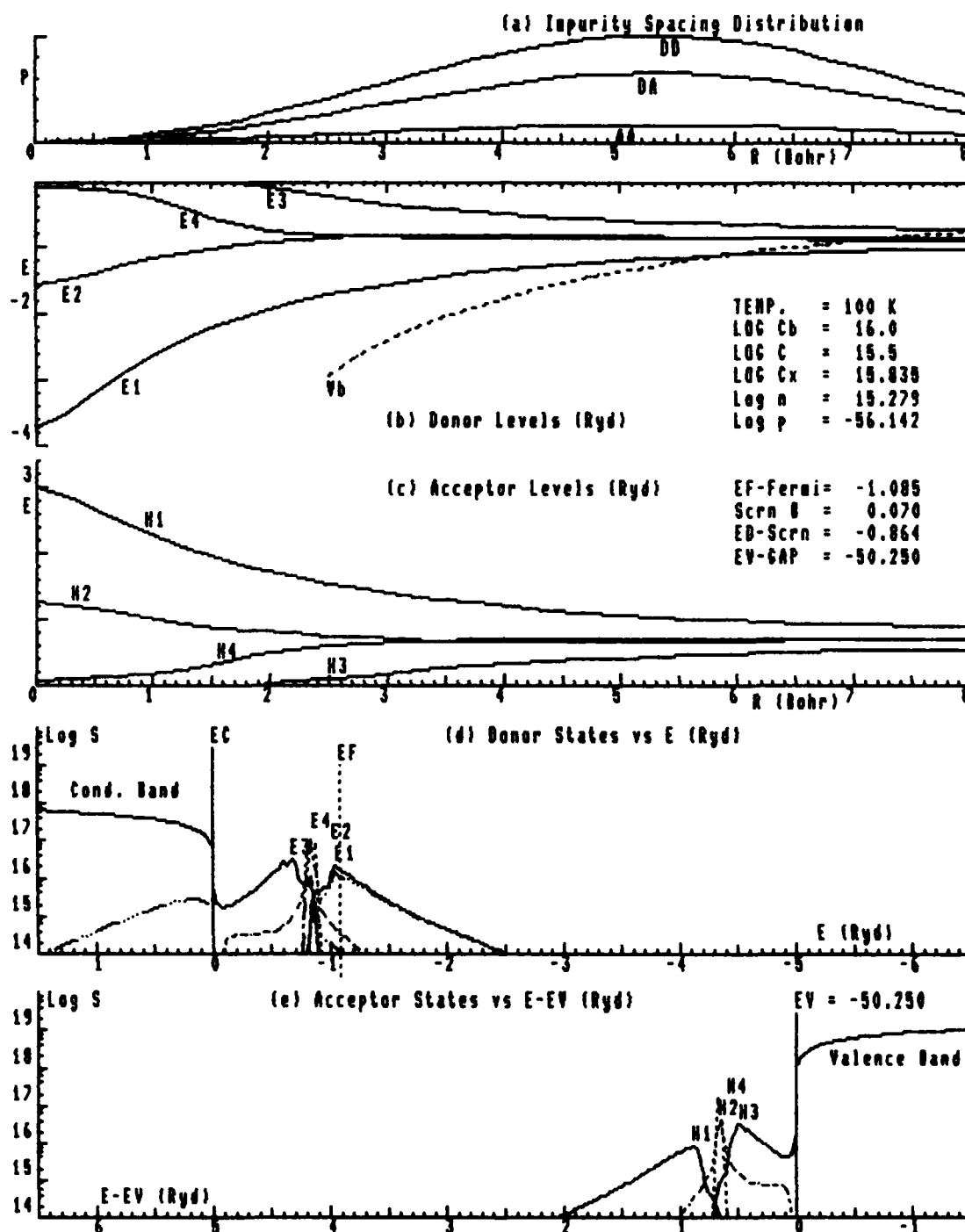


Fig. A 117. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

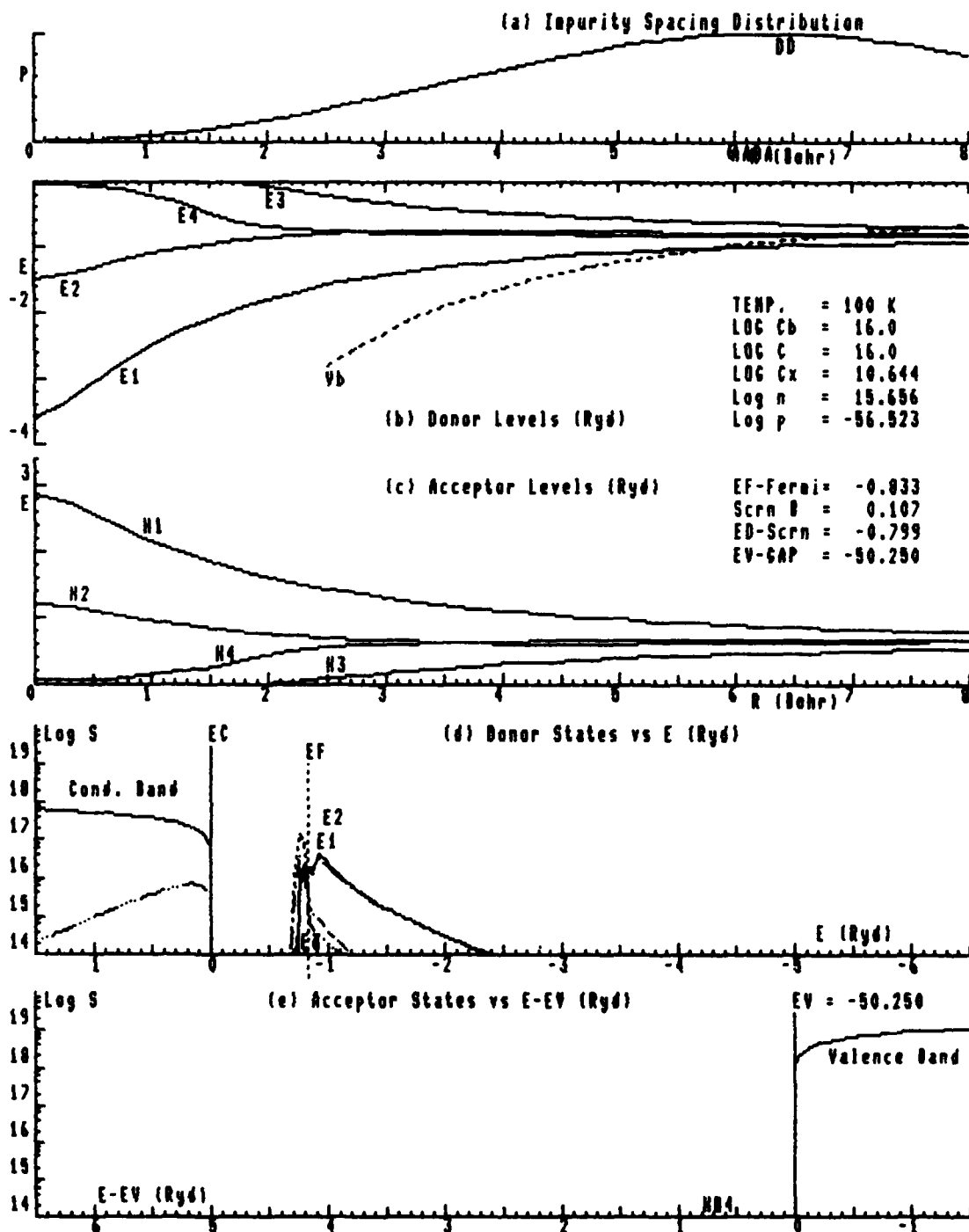


Fig. A 11B. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

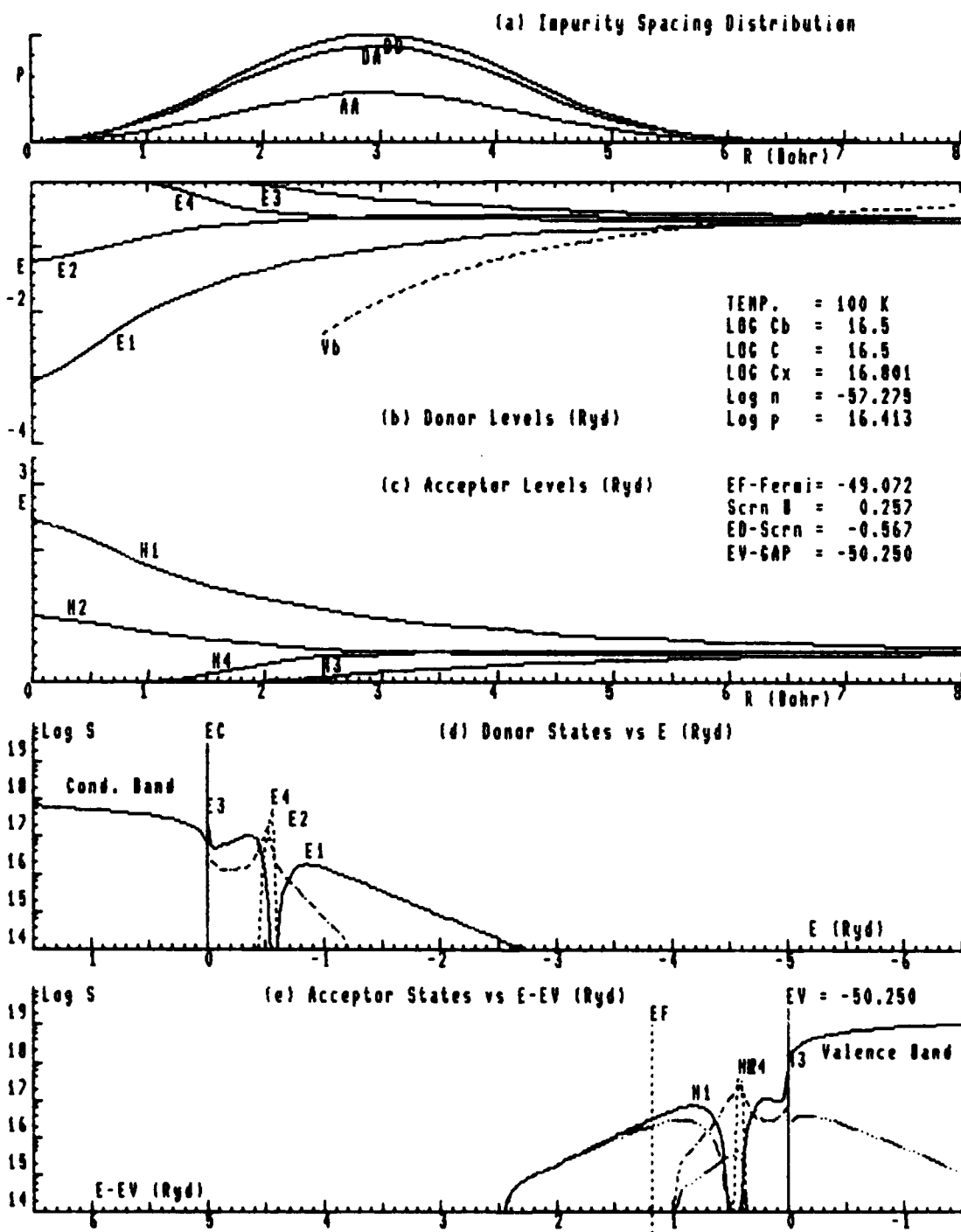


Fig. A 120. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

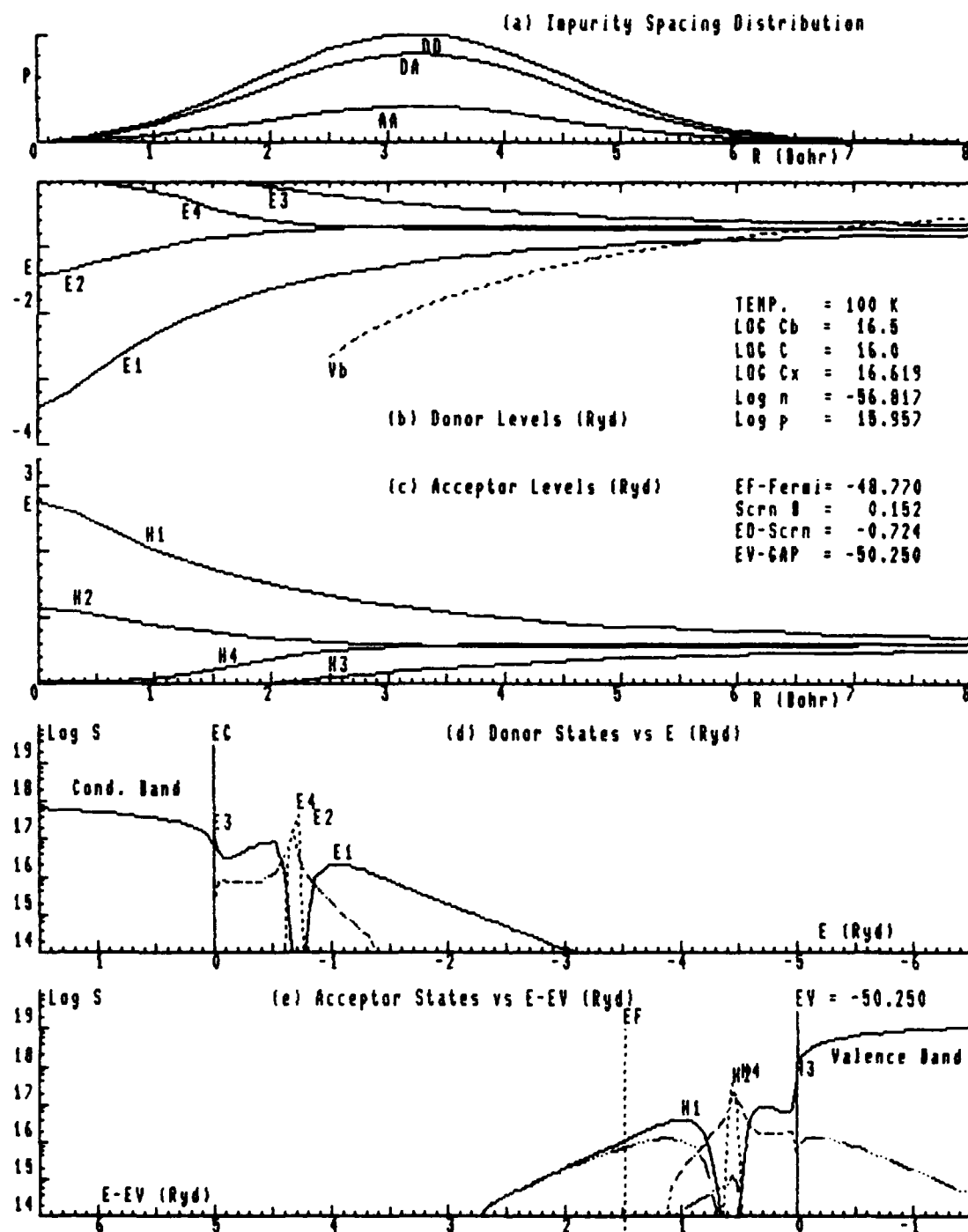


Fig. A 121. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA+)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

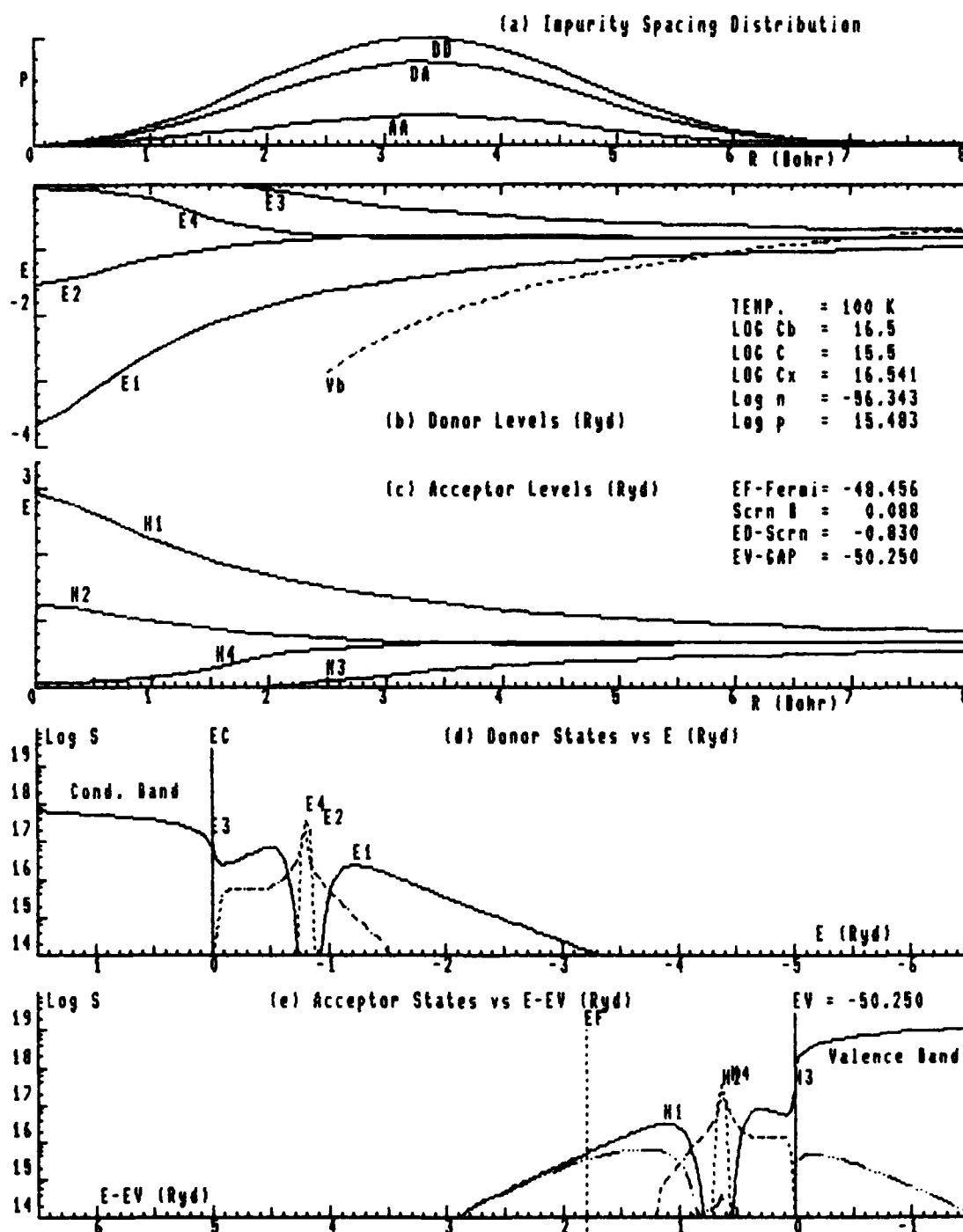


Fig. A 122. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA+)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

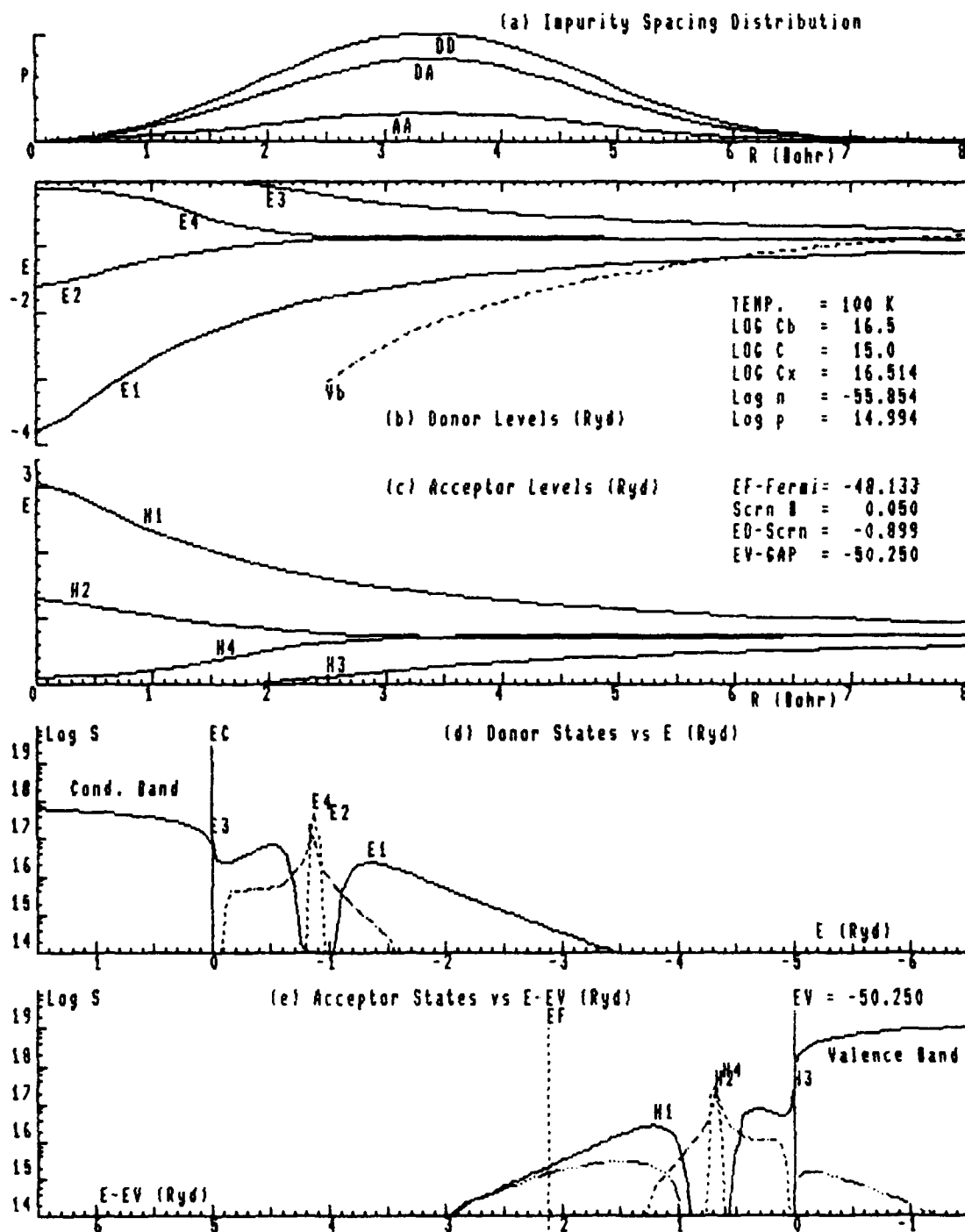


Fig. A 123. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

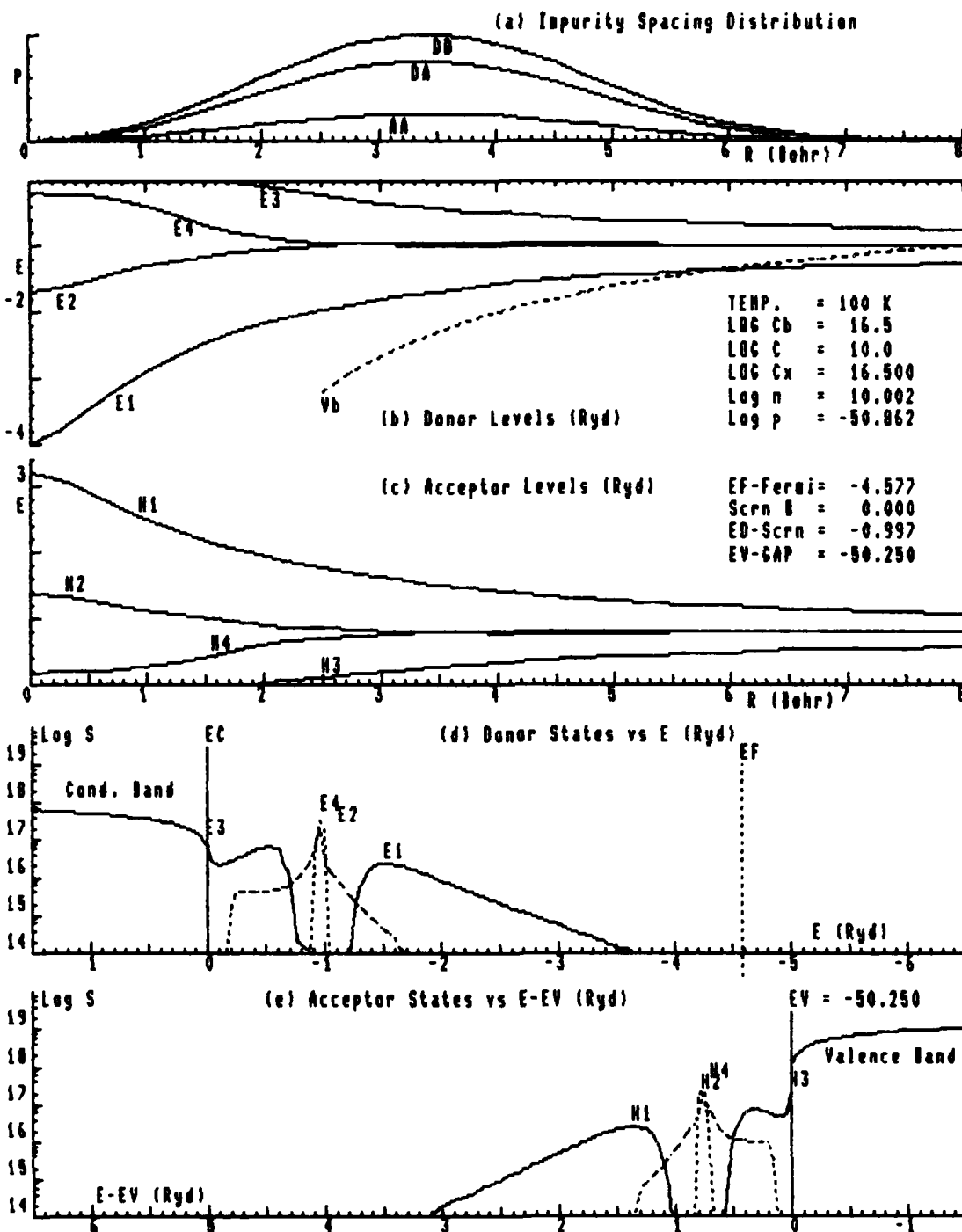


Fig. A 124. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

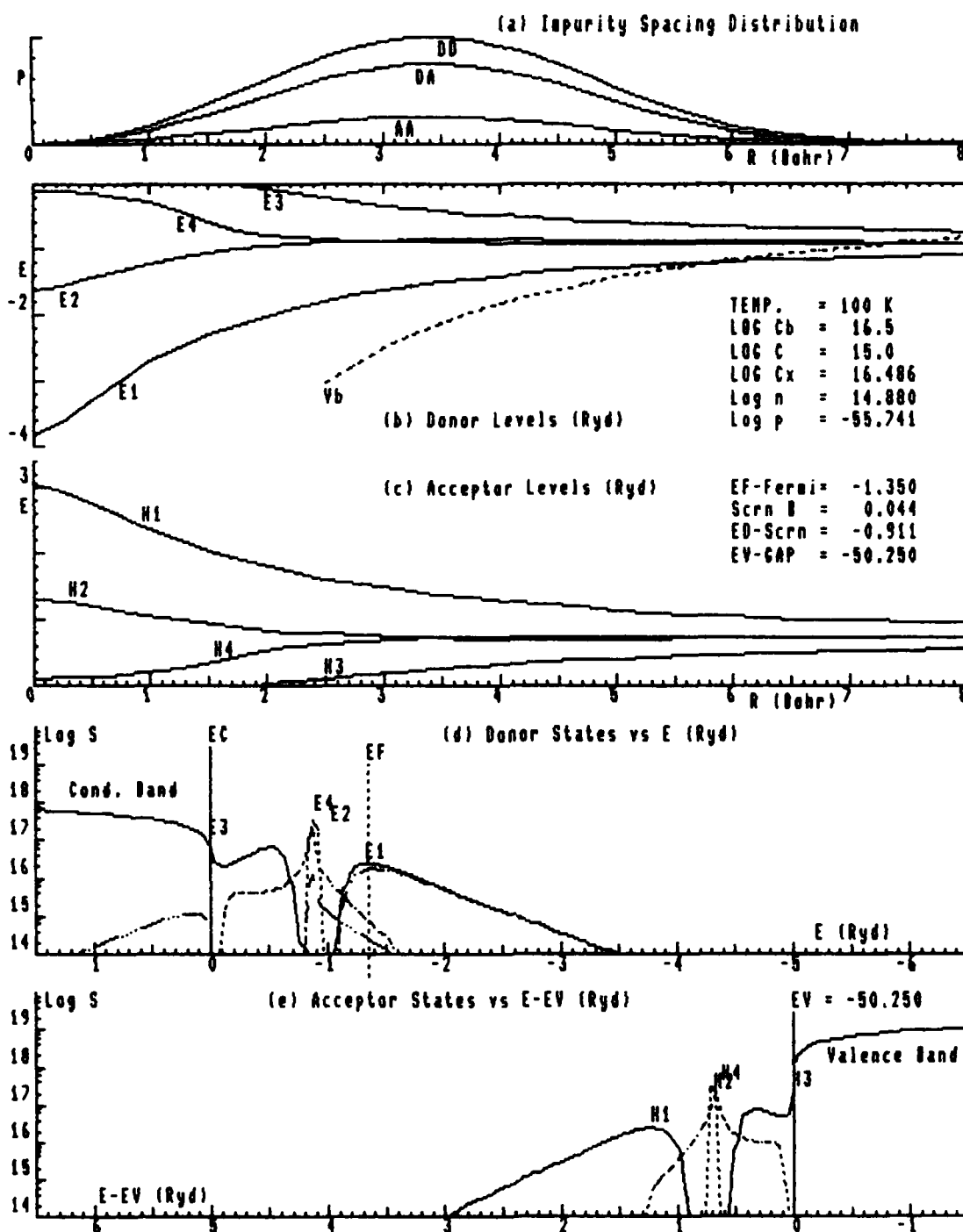


Fig. A 125. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

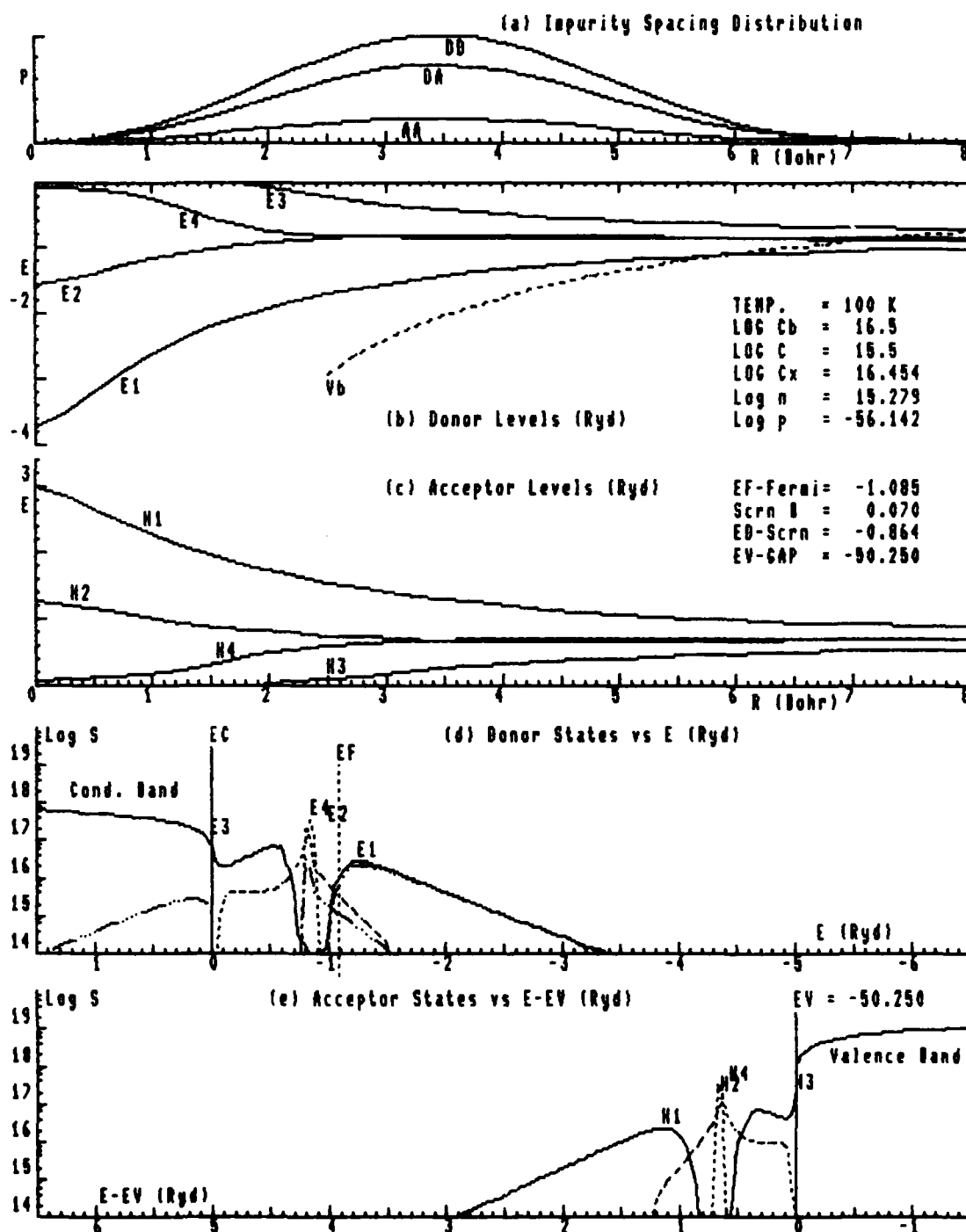


Fig. A 126. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

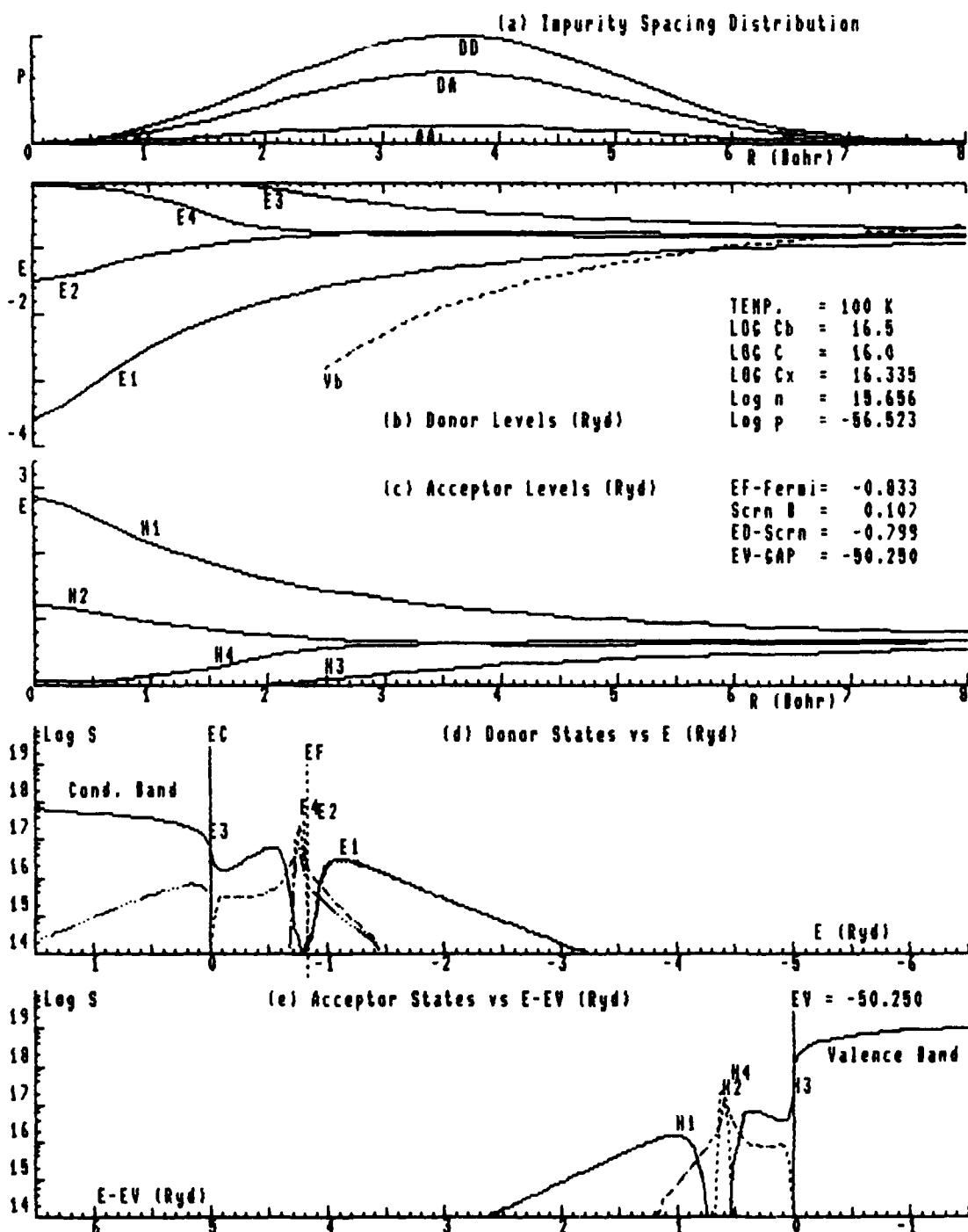


Fig. A 127. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

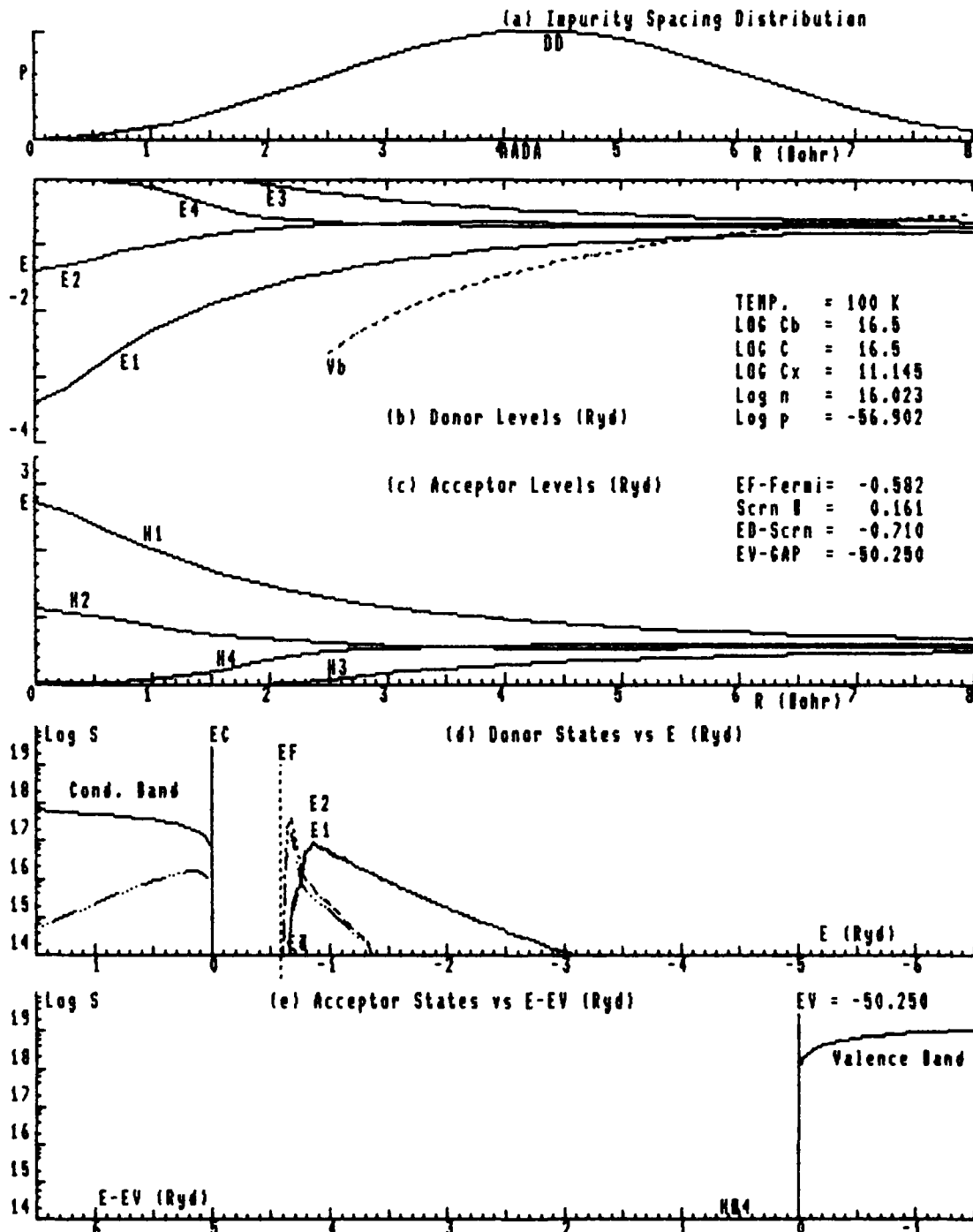


Fig. A 128. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

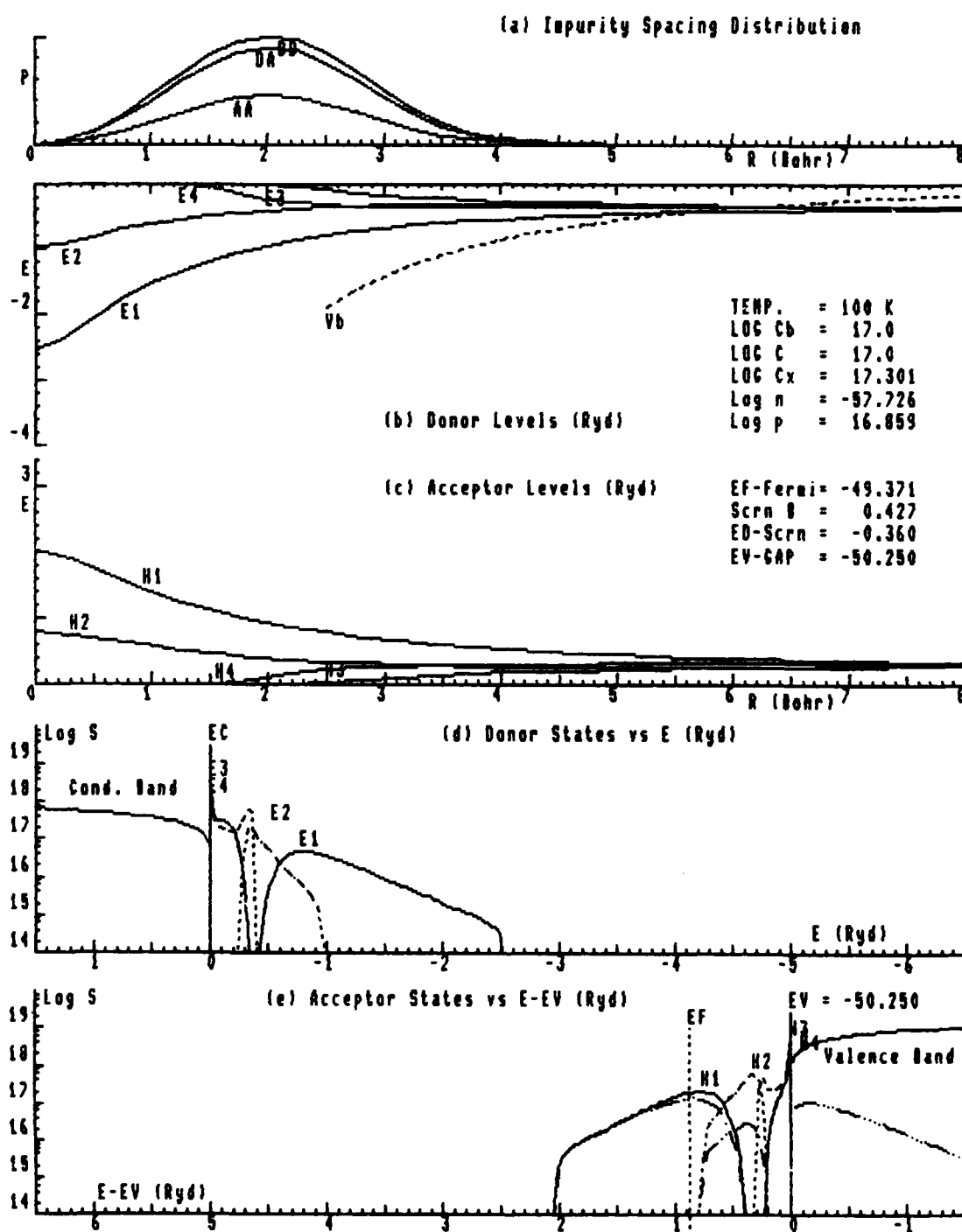


Fig. A 130. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

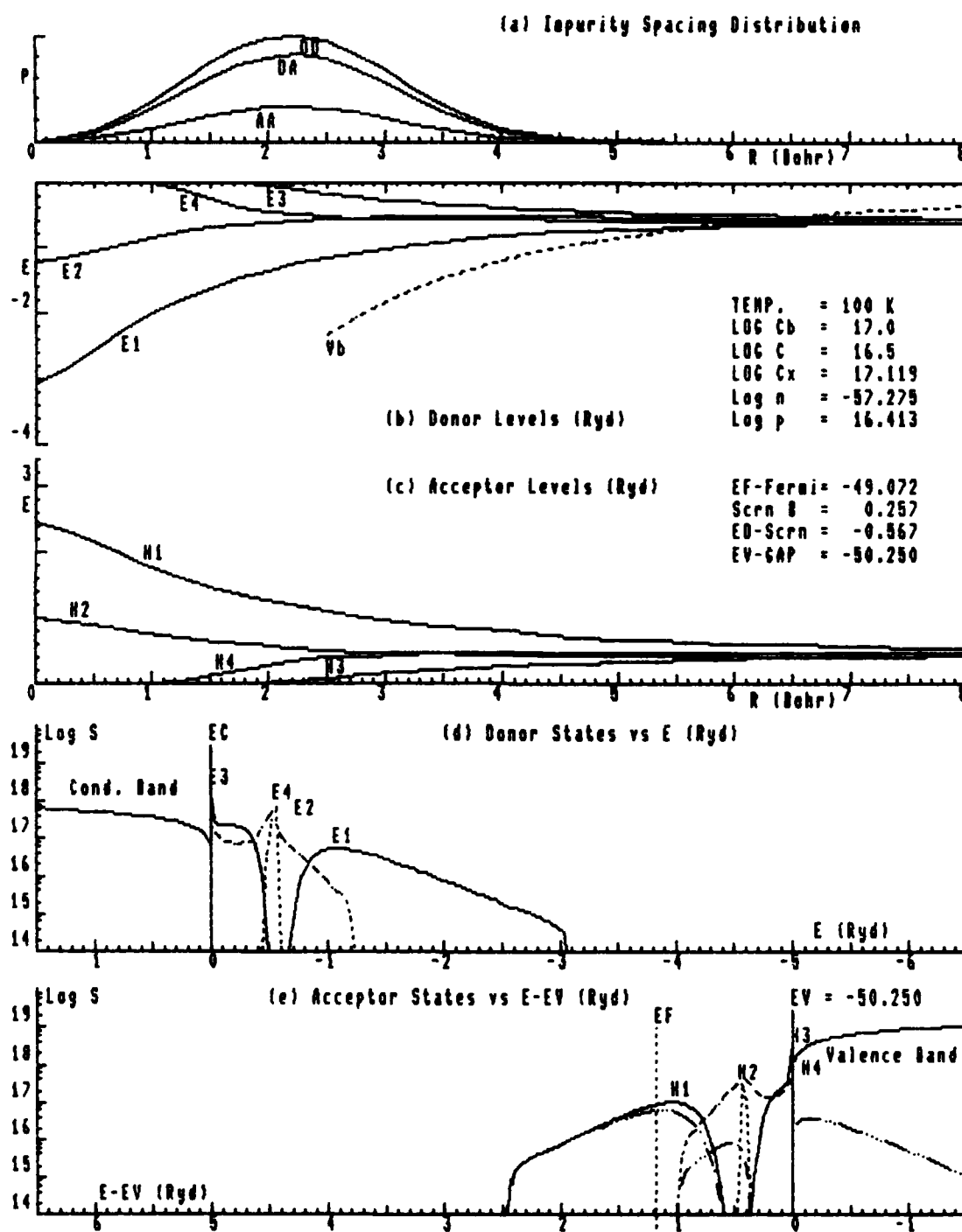


Fig. A 131. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

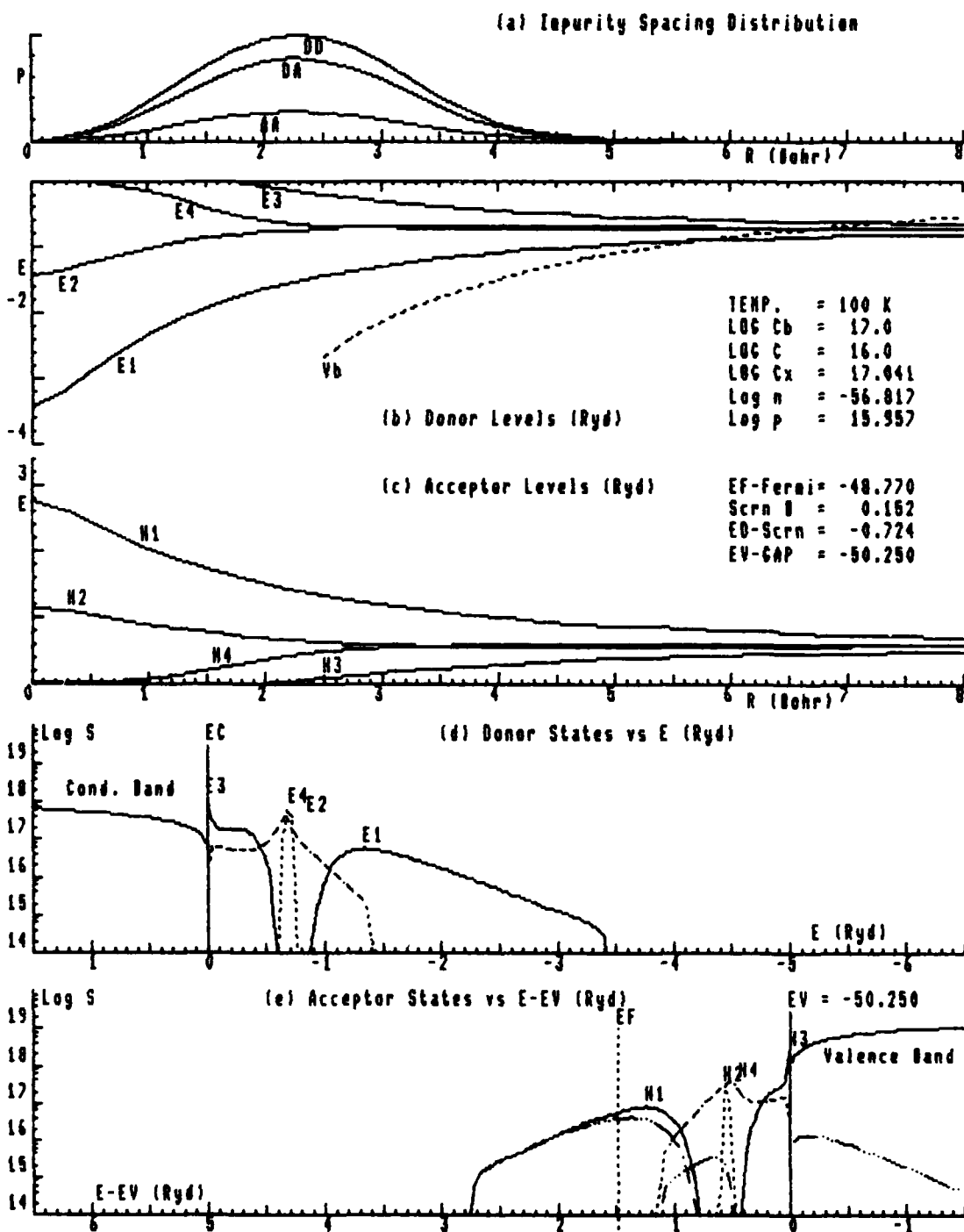


Fig. A 132. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

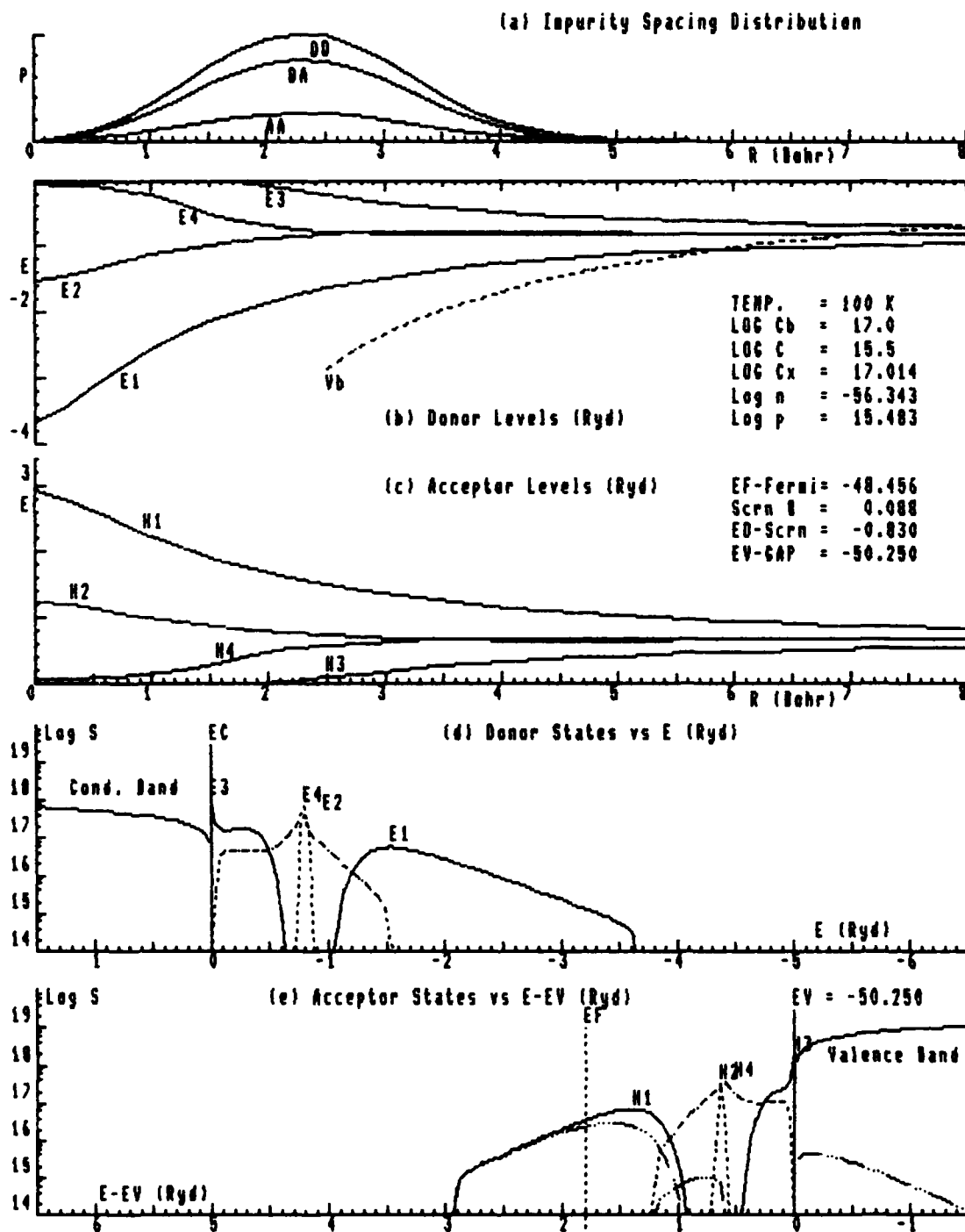


Fig. A 133. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

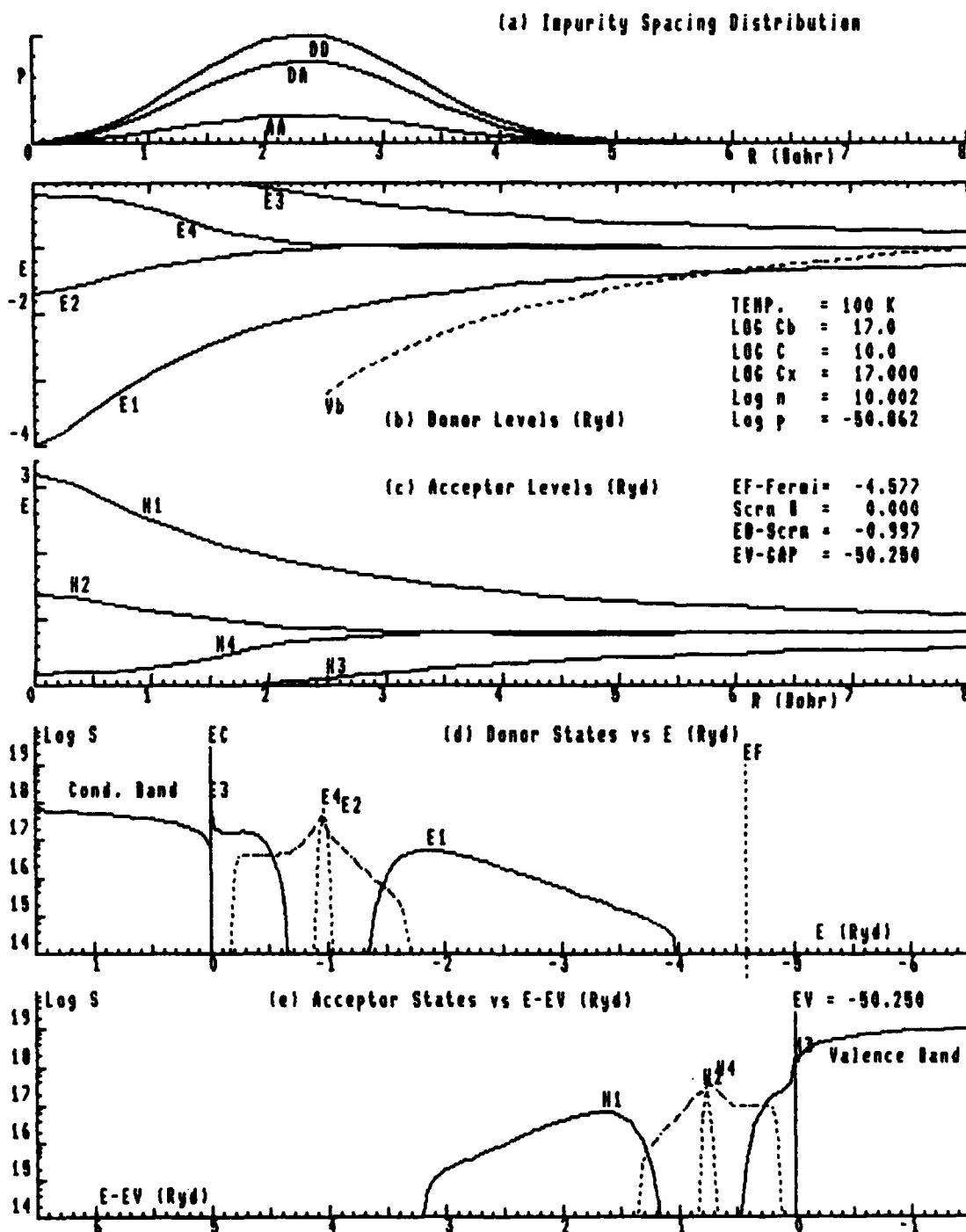


Fig. A 134. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

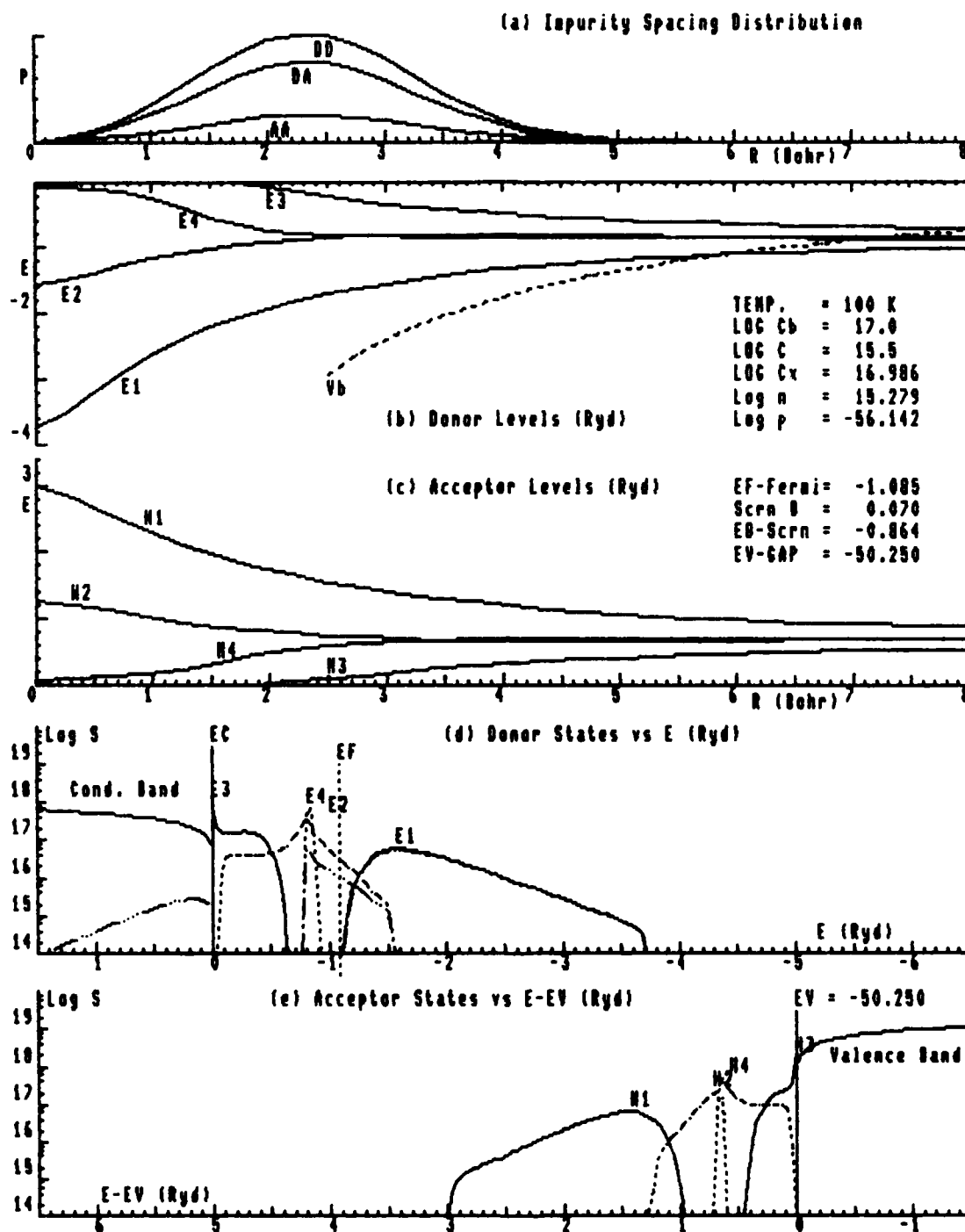


Fig. A 135. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

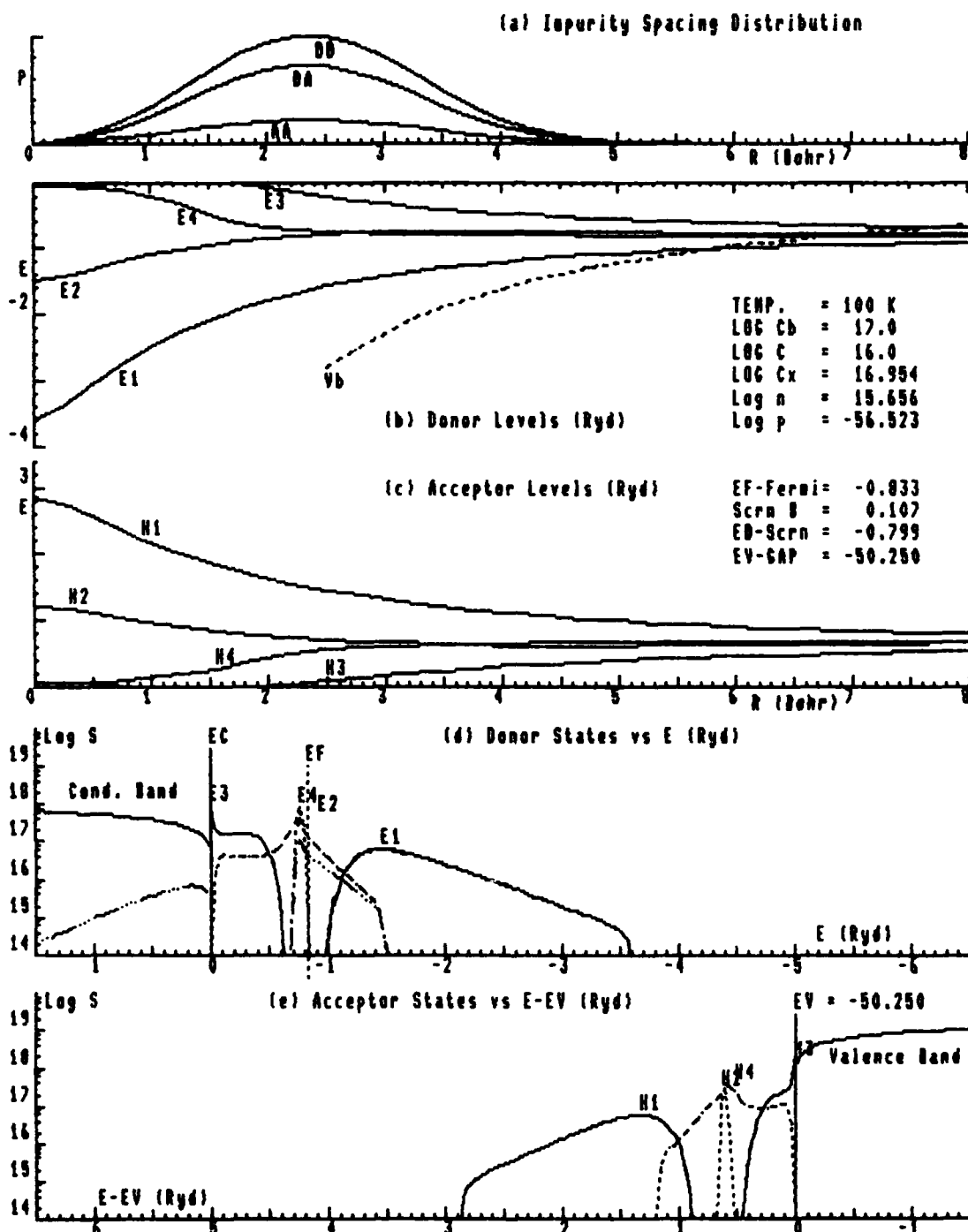


Fig. A 136. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

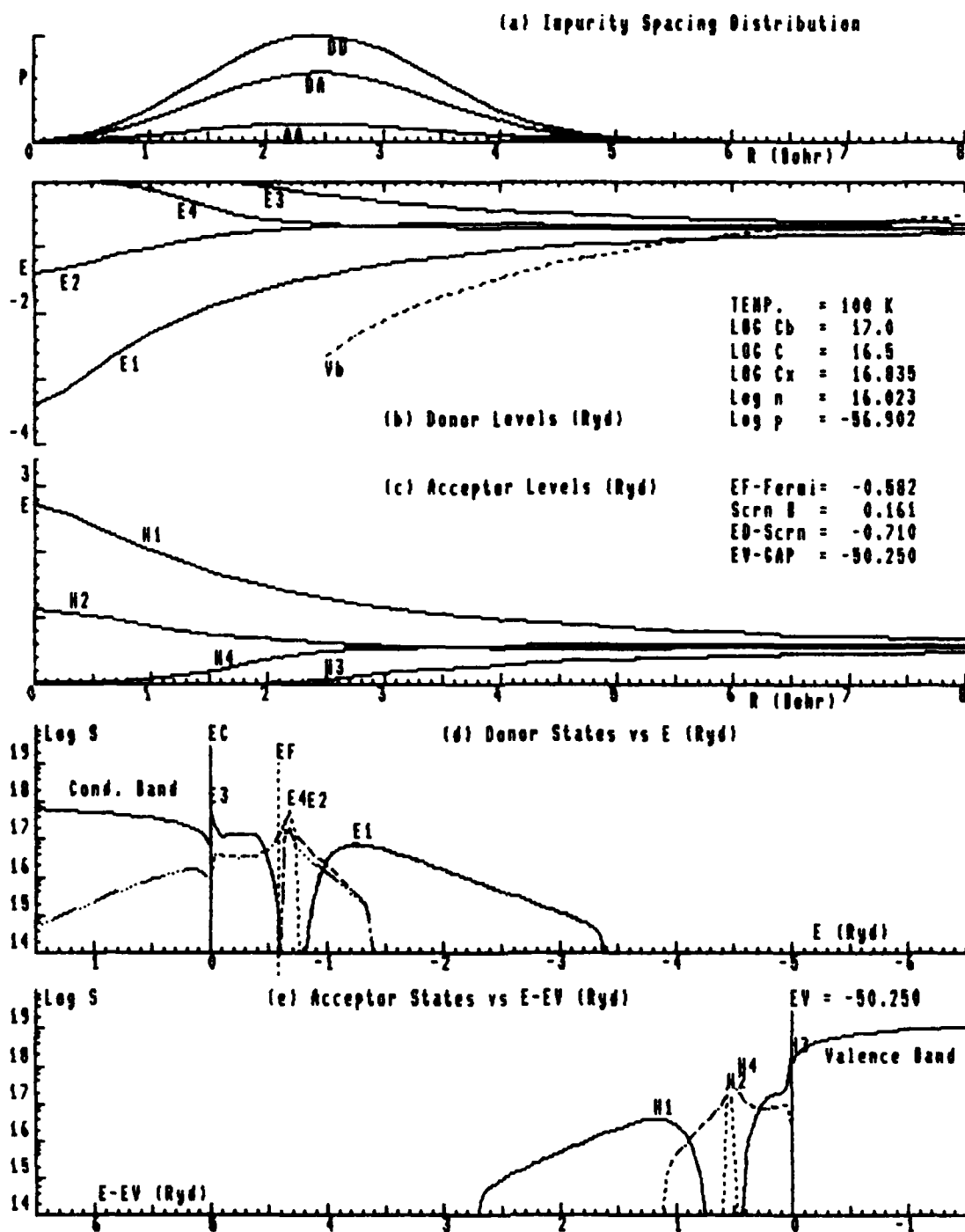


Fig. A 137. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

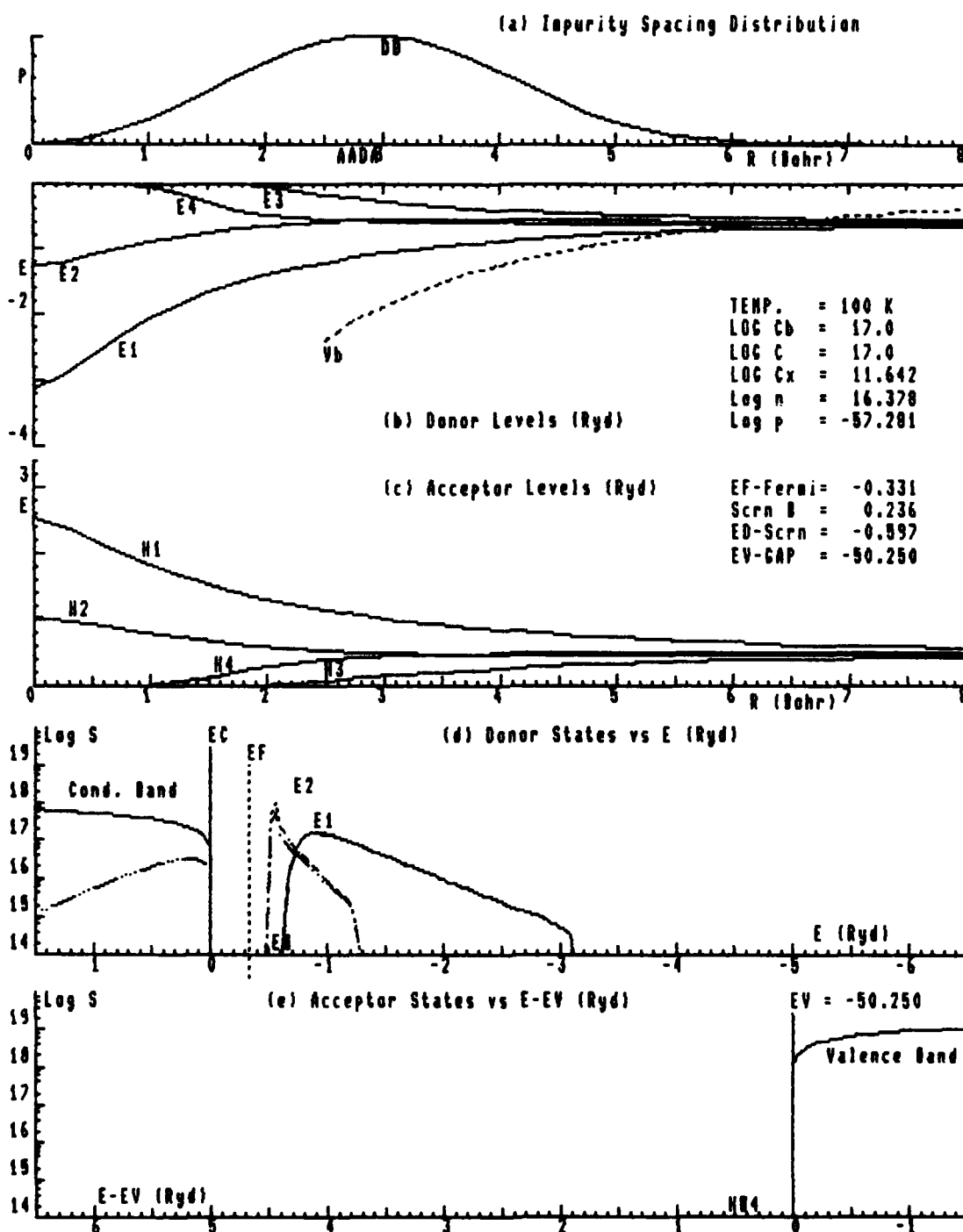


Fig. A 138. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

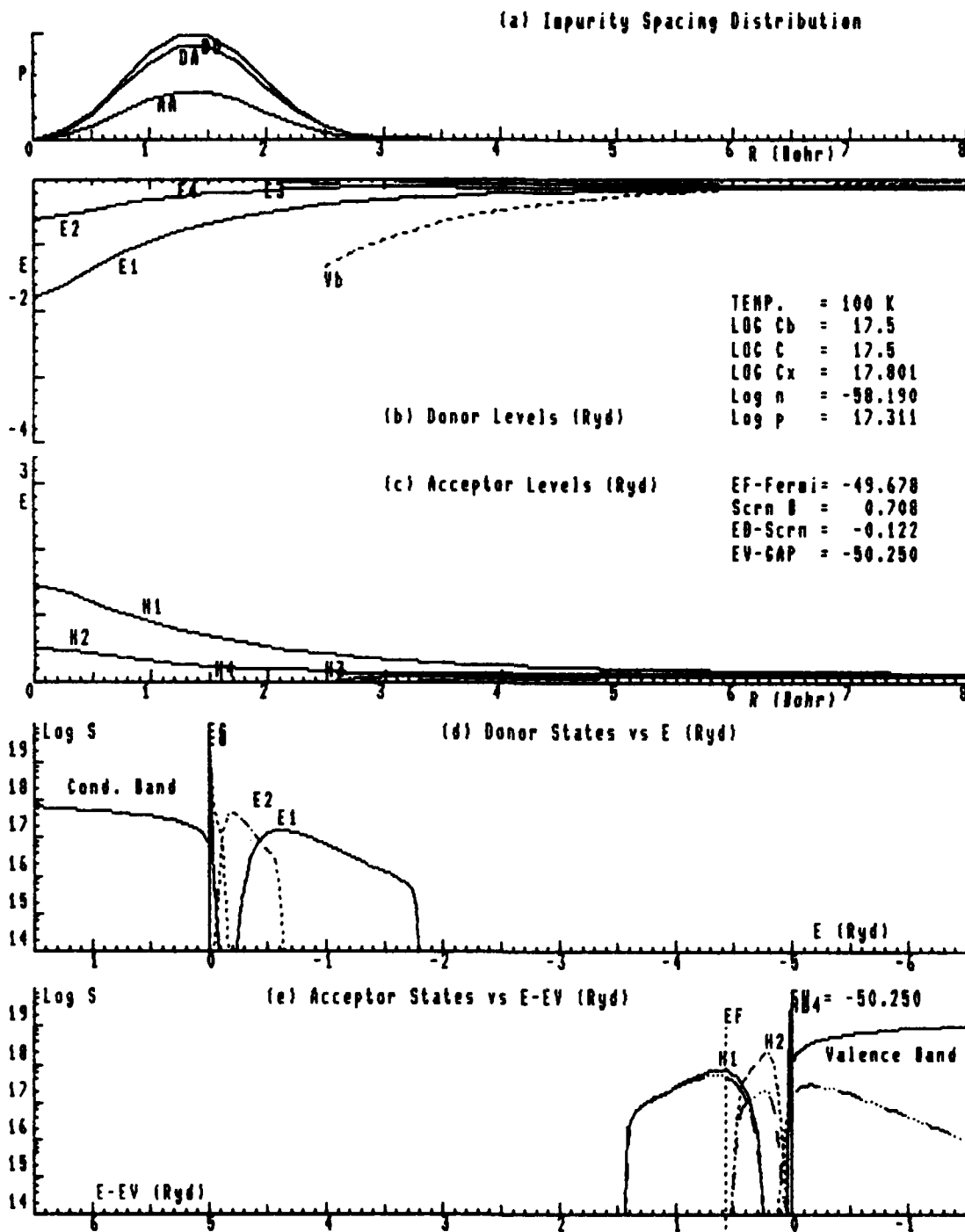


Fig. A 140. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

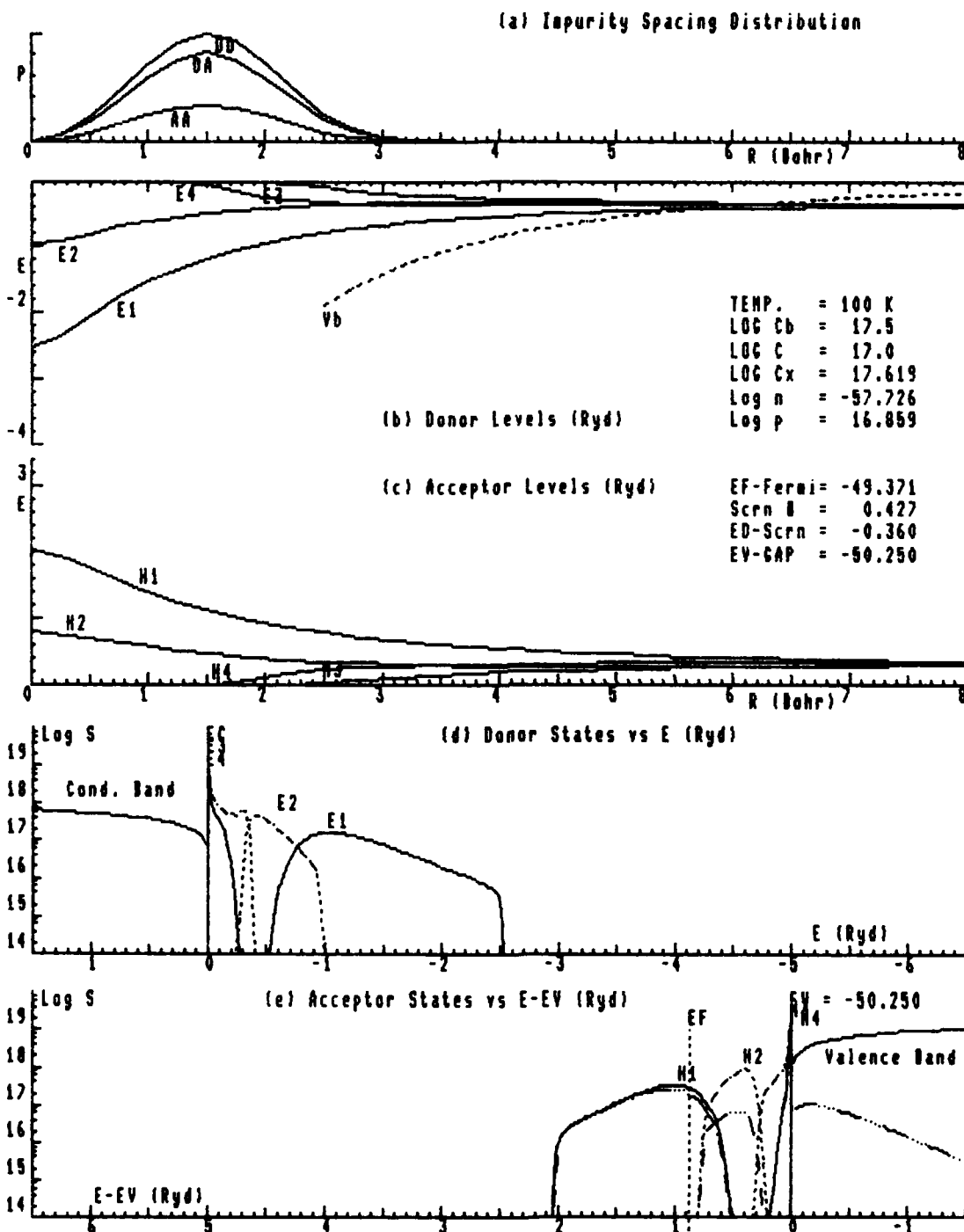


Fig. A 141. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

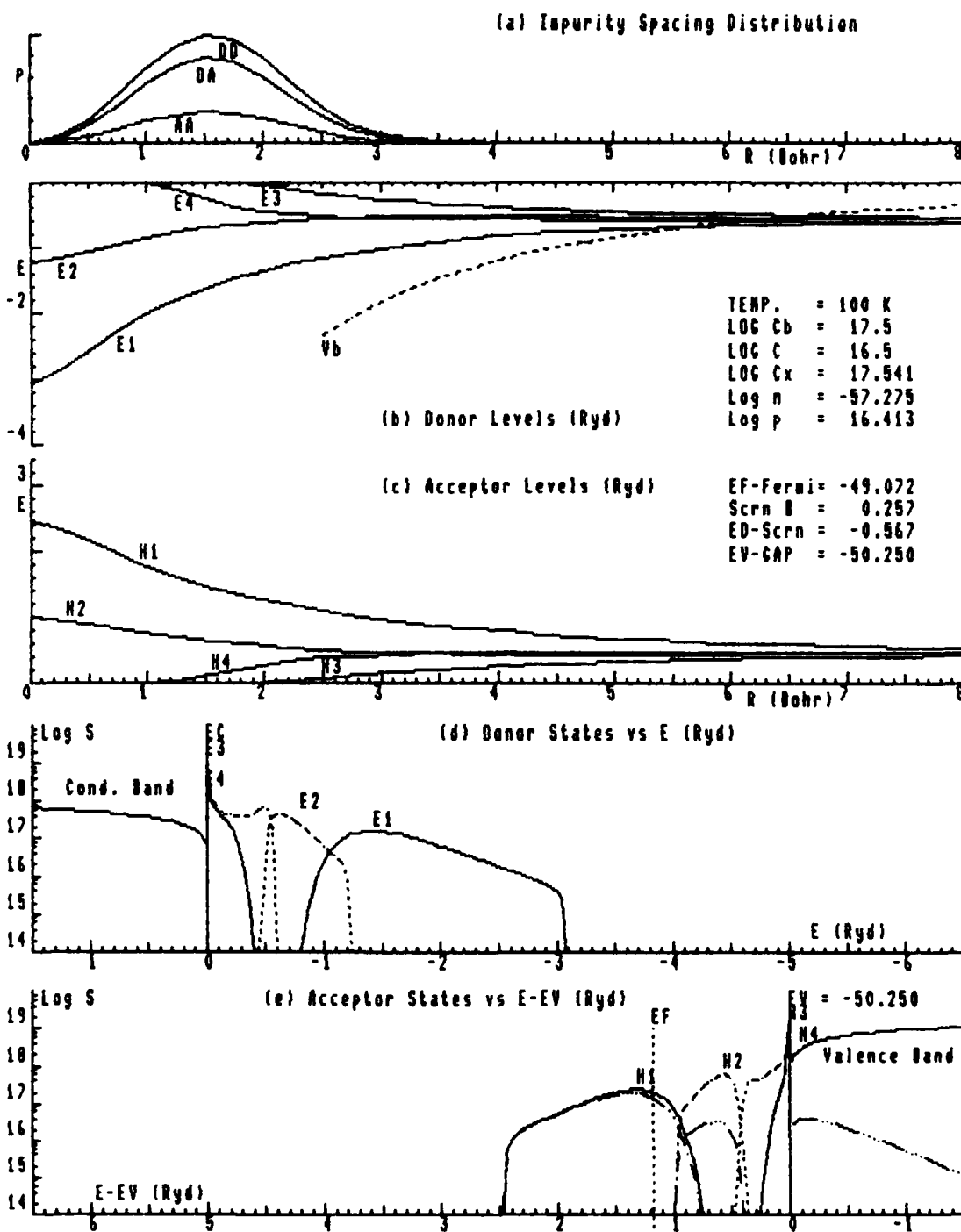


Fig. A 142. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

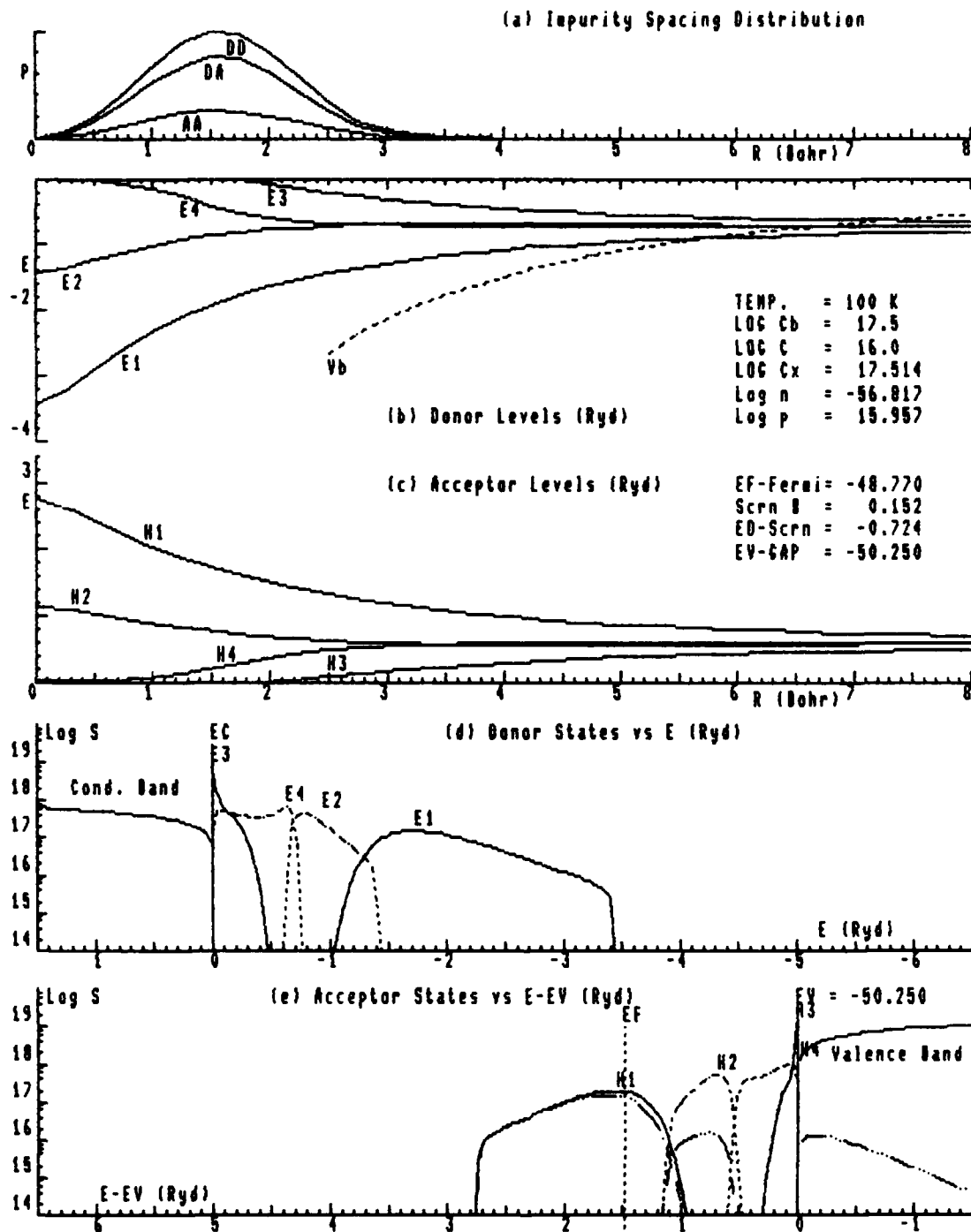


Fig. A 143. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(LA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

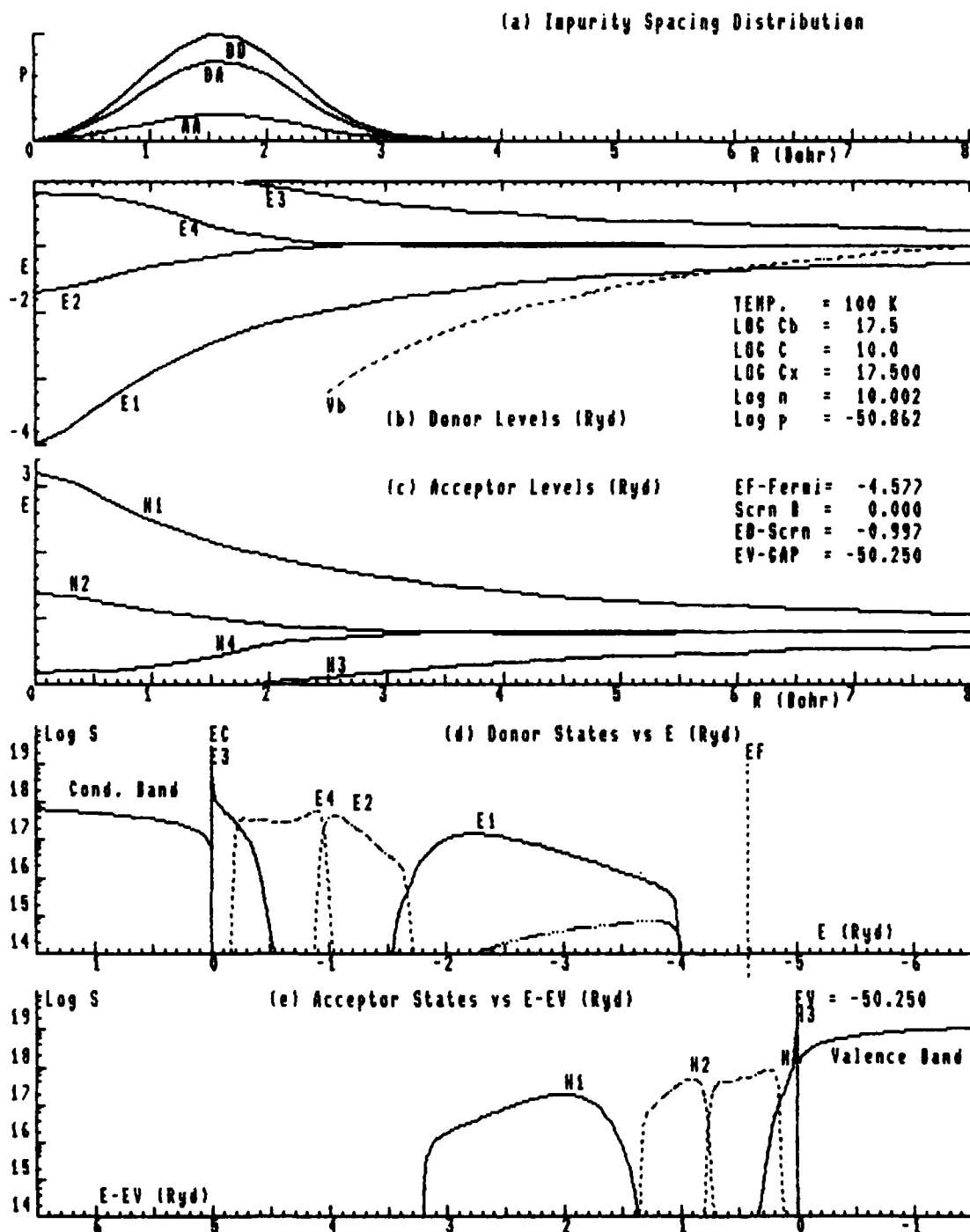


Fig. A 144. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

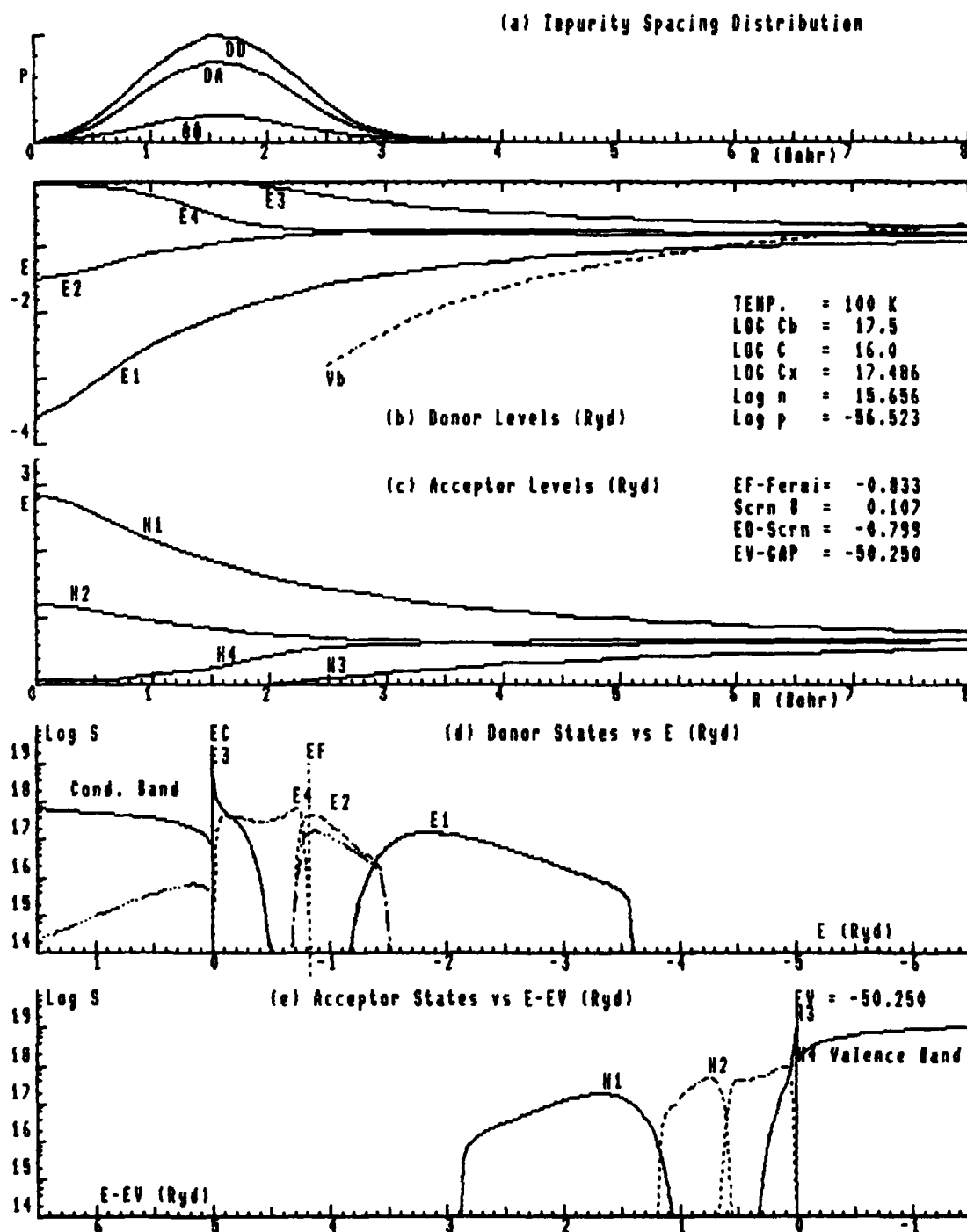


Fig. A 145. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

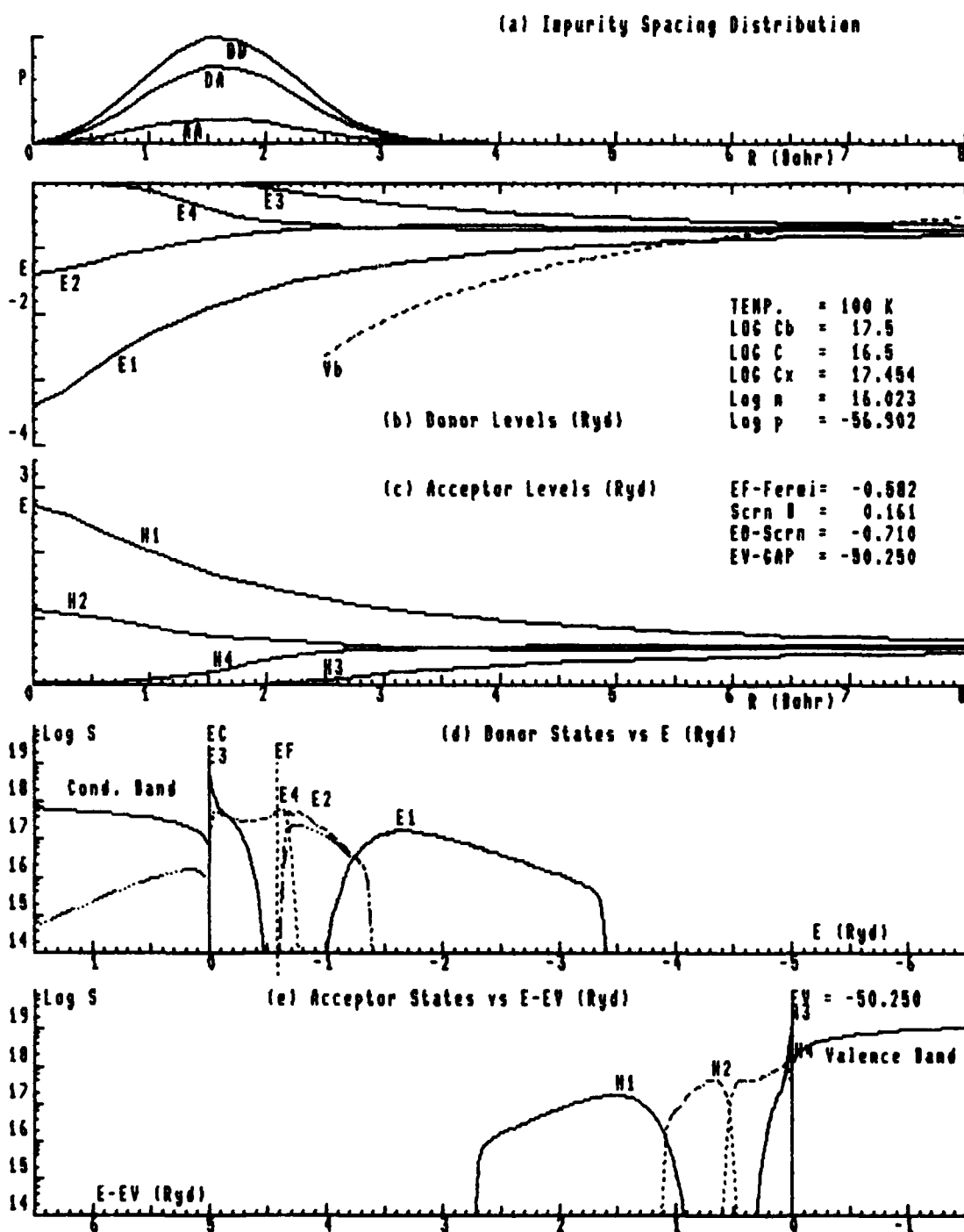


Fig. A 146. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

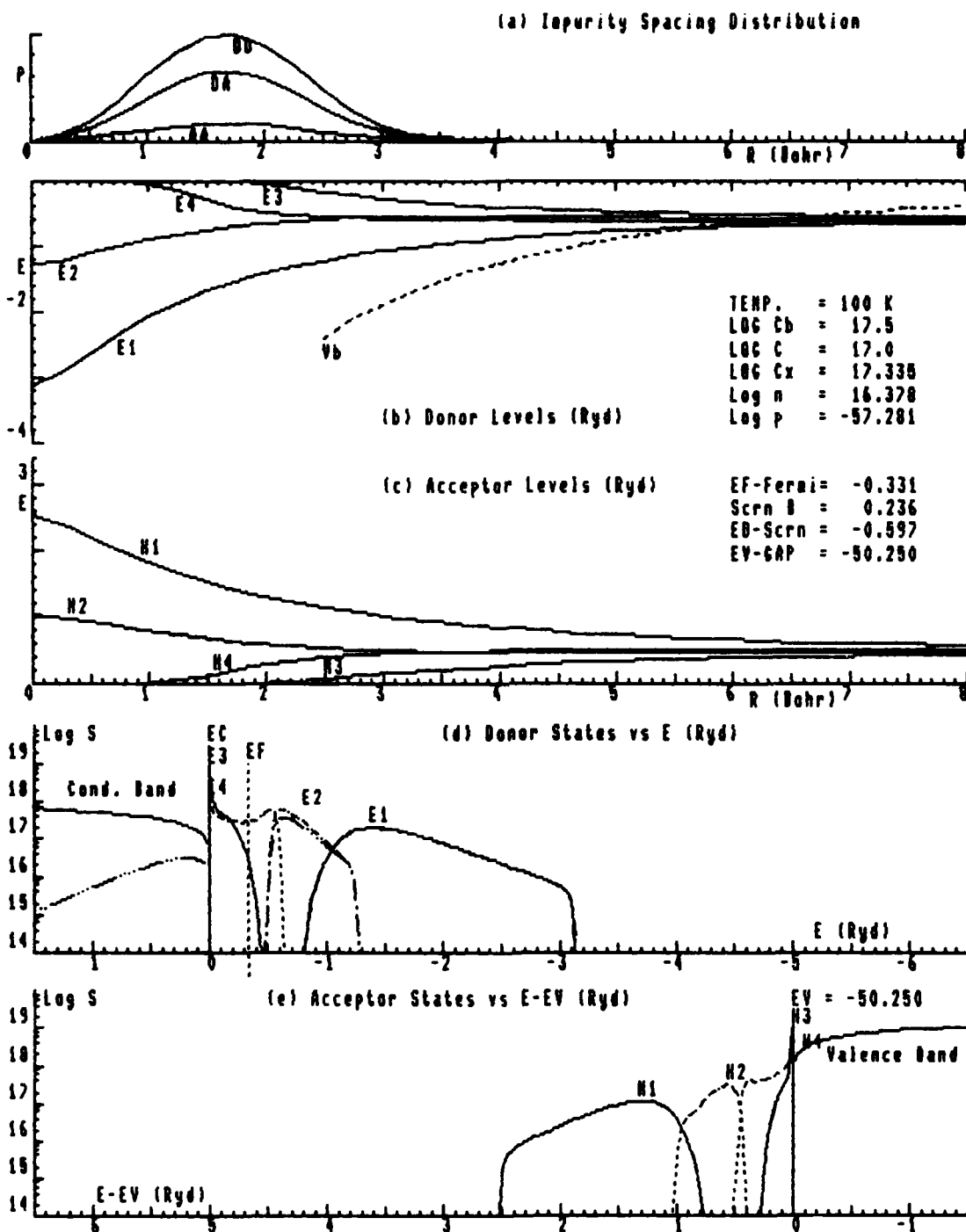


Fig. A 147. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD-)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA+)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

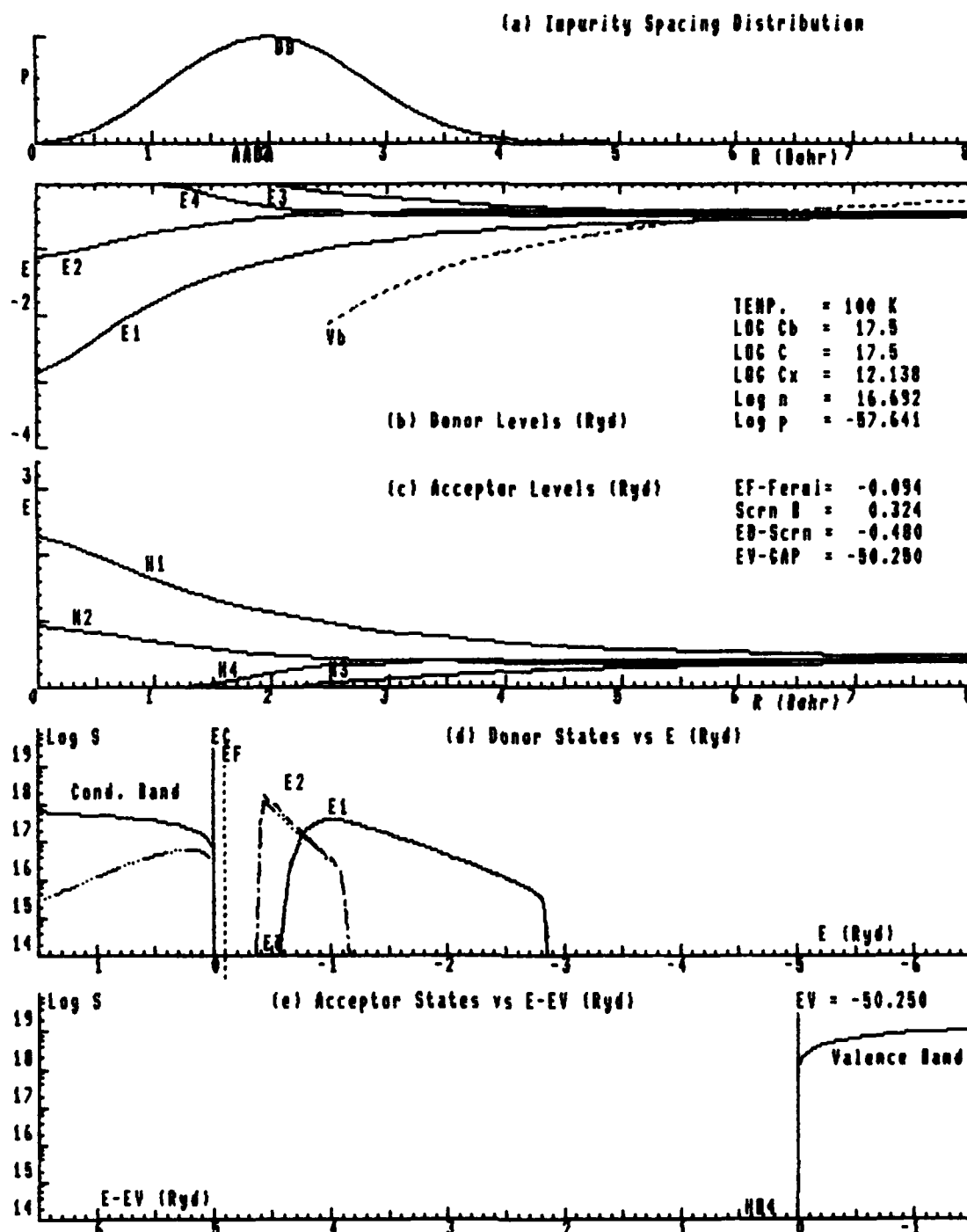


Fig. A 148. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

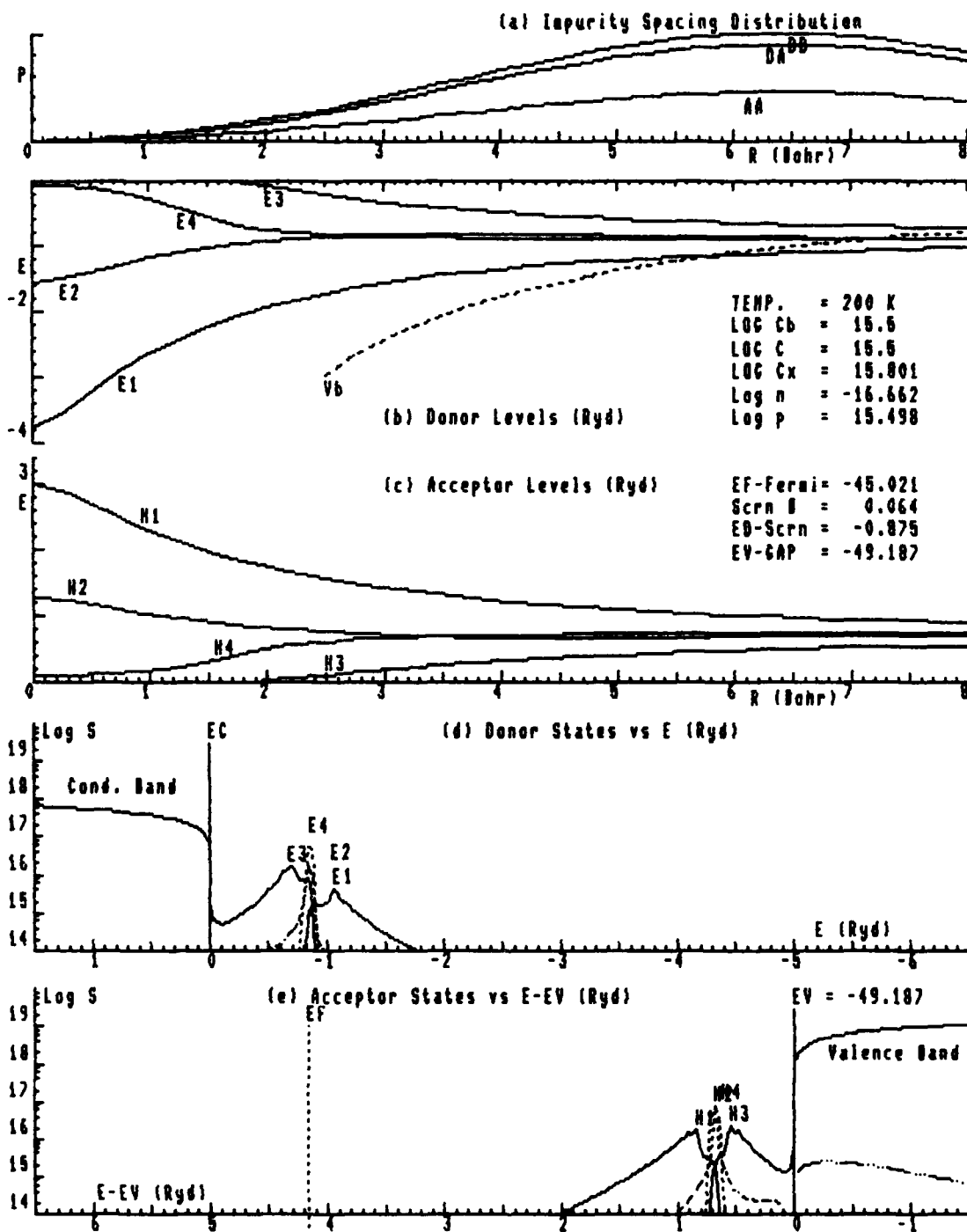


Fig. A 200. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

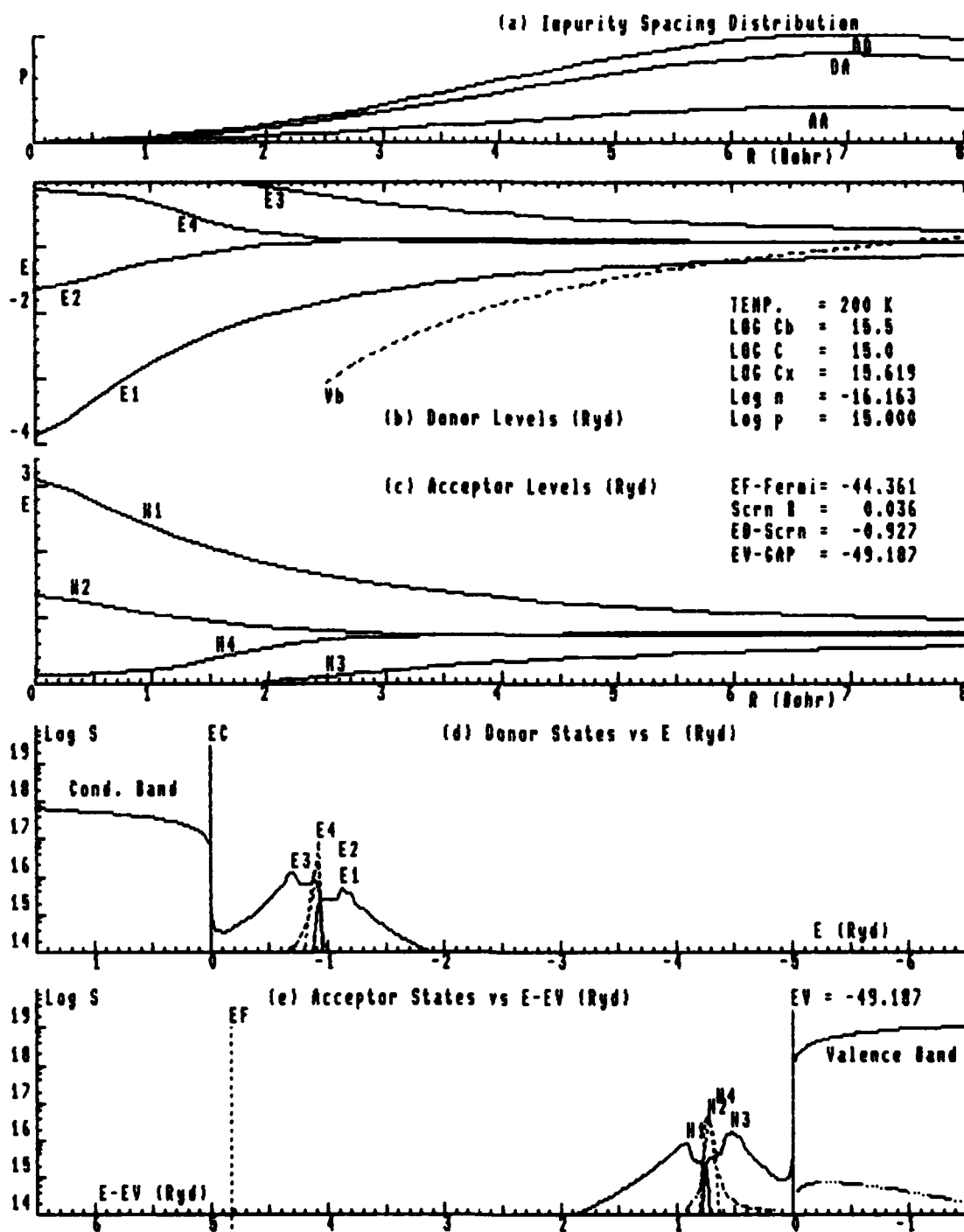


Fig. A 201. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

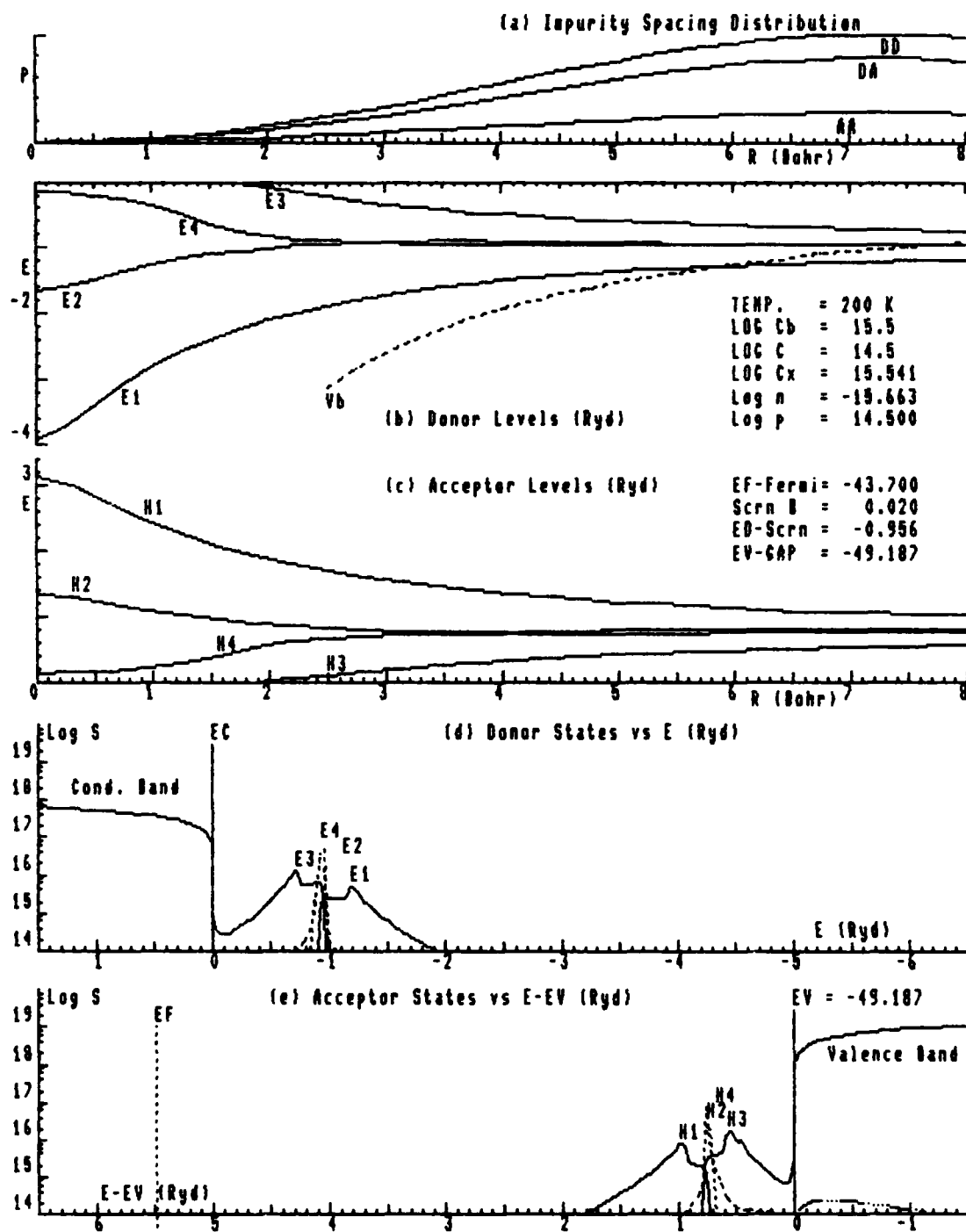


Fig. A 202. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

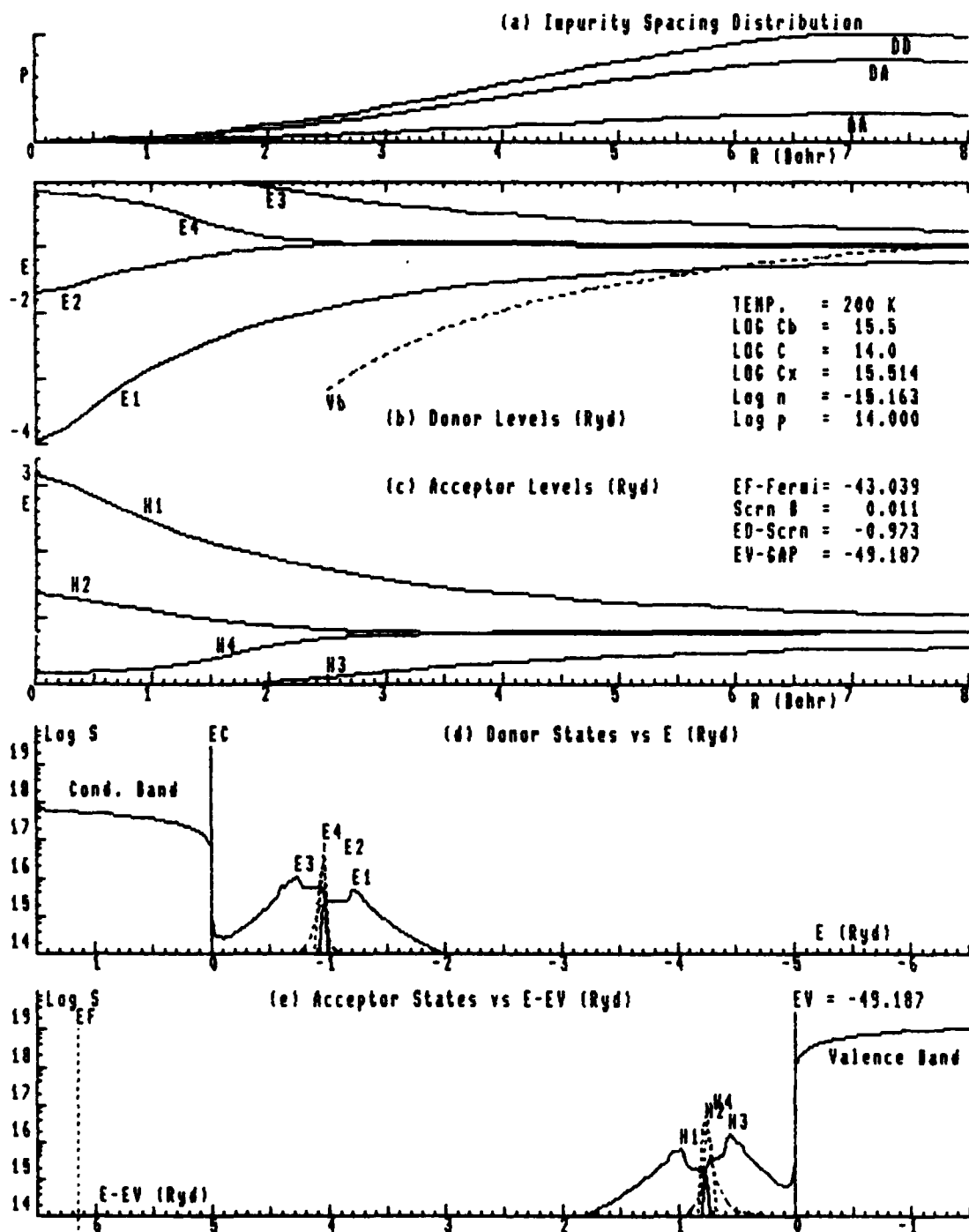


Fig. A 203. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

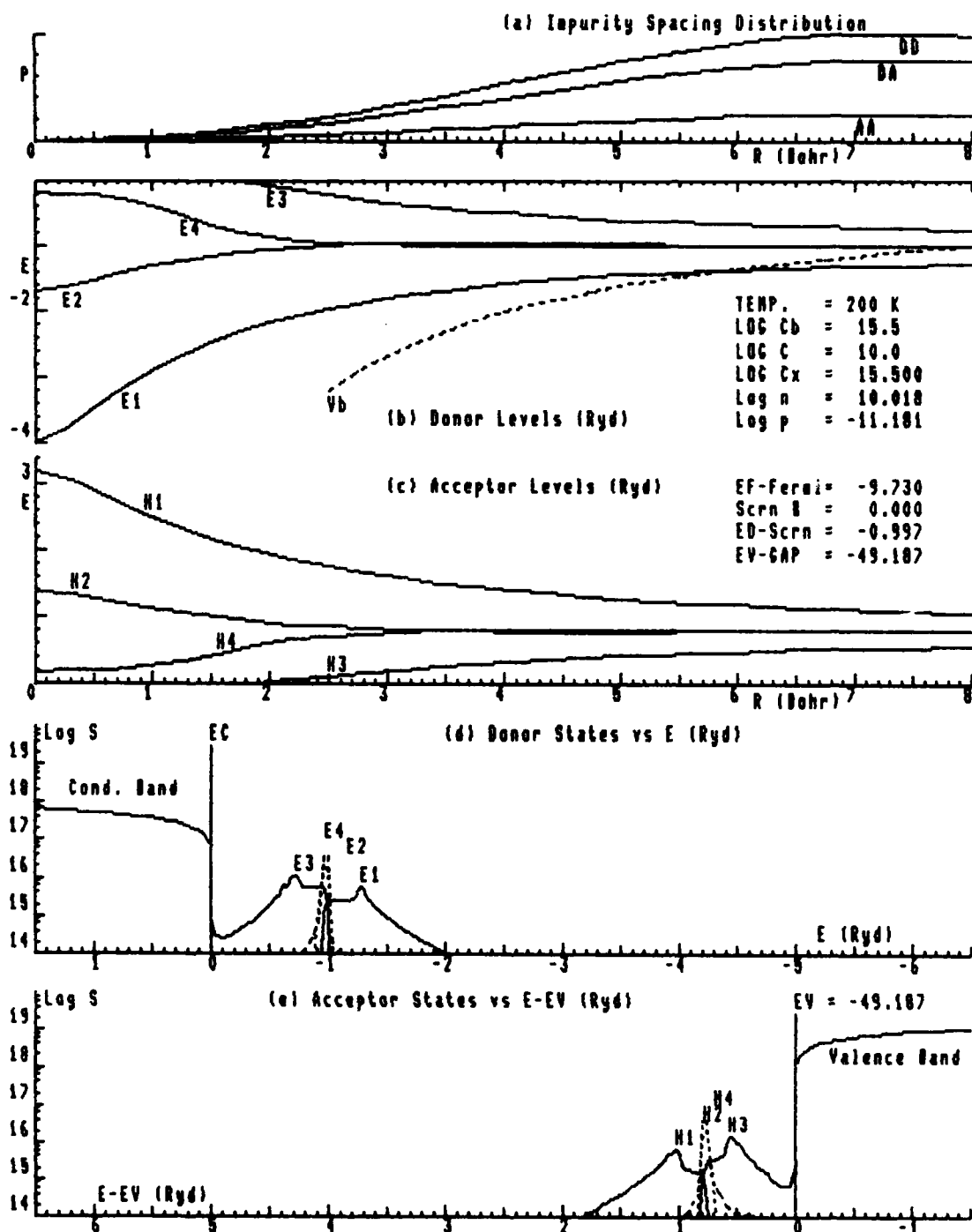


Fig. A 204. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

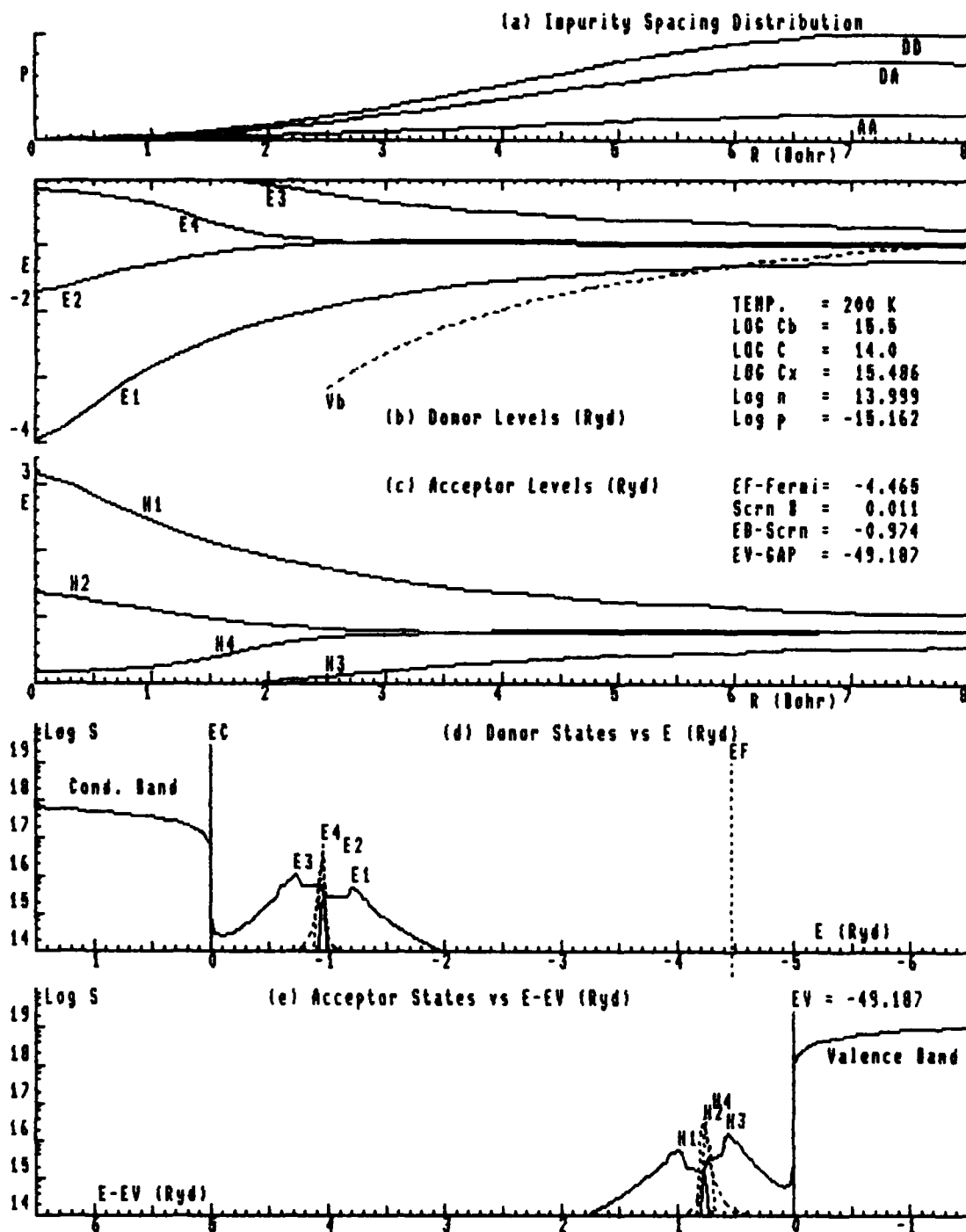


Fig. A 205. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

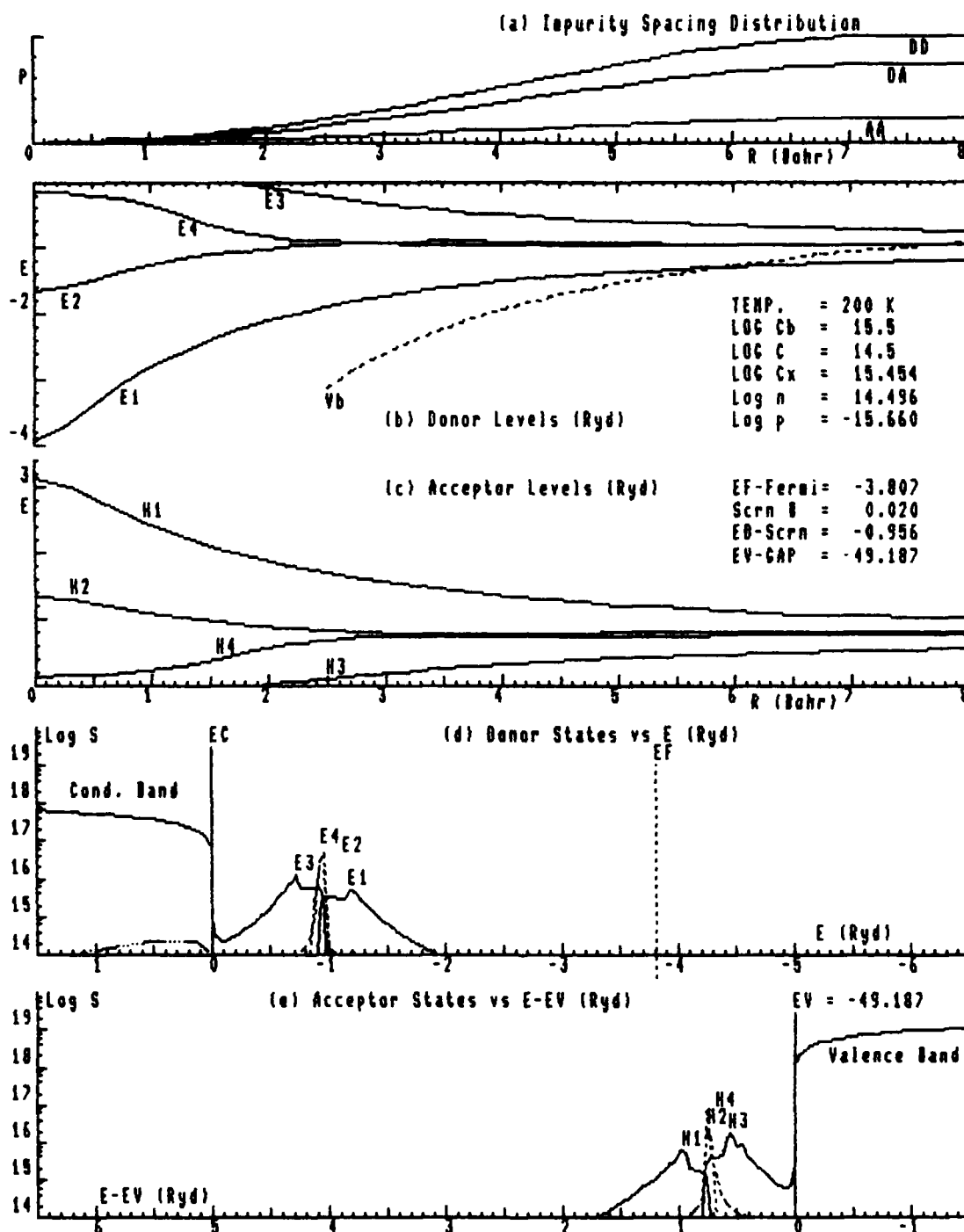


Fig. A 206. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

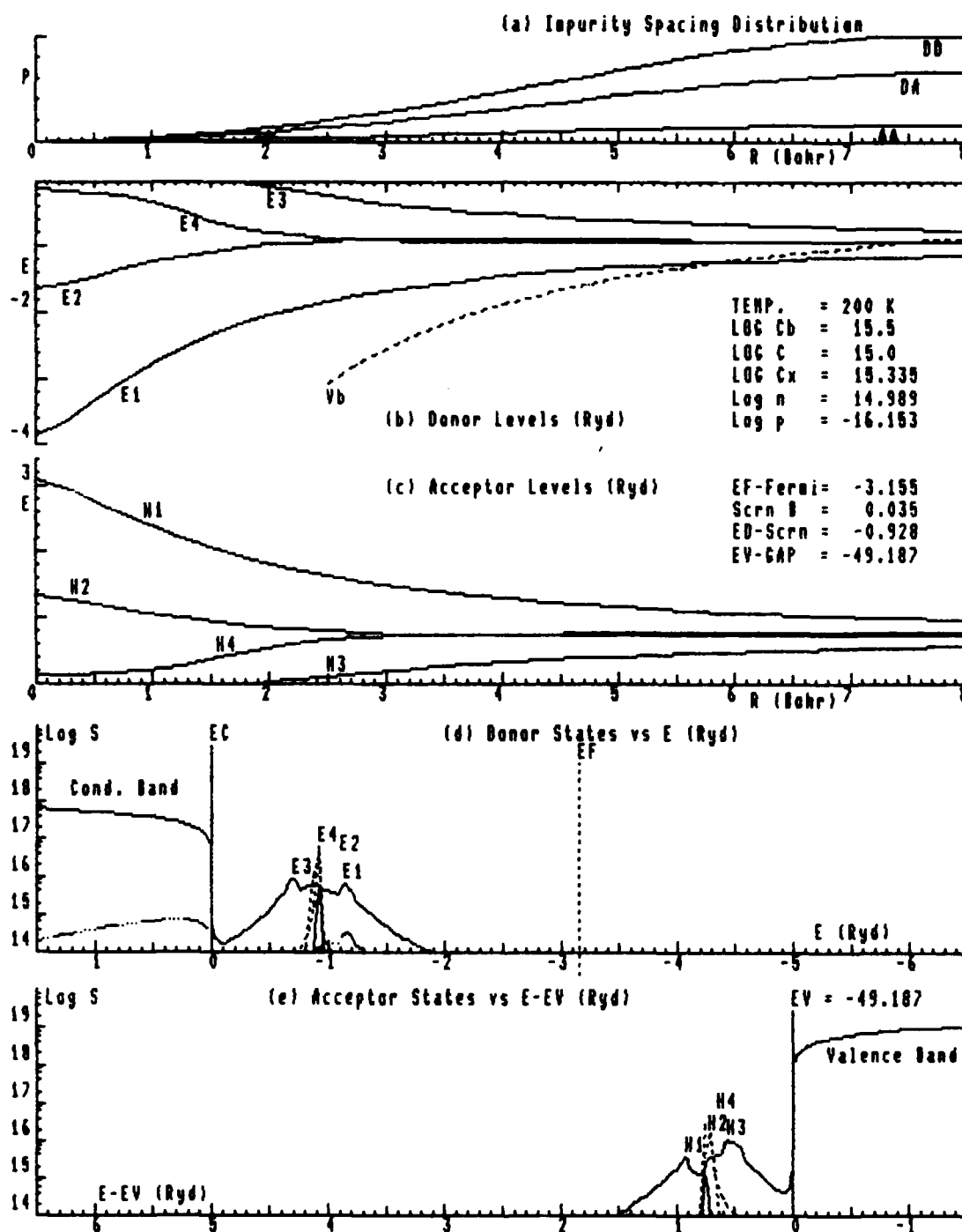


Fig. A 207. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

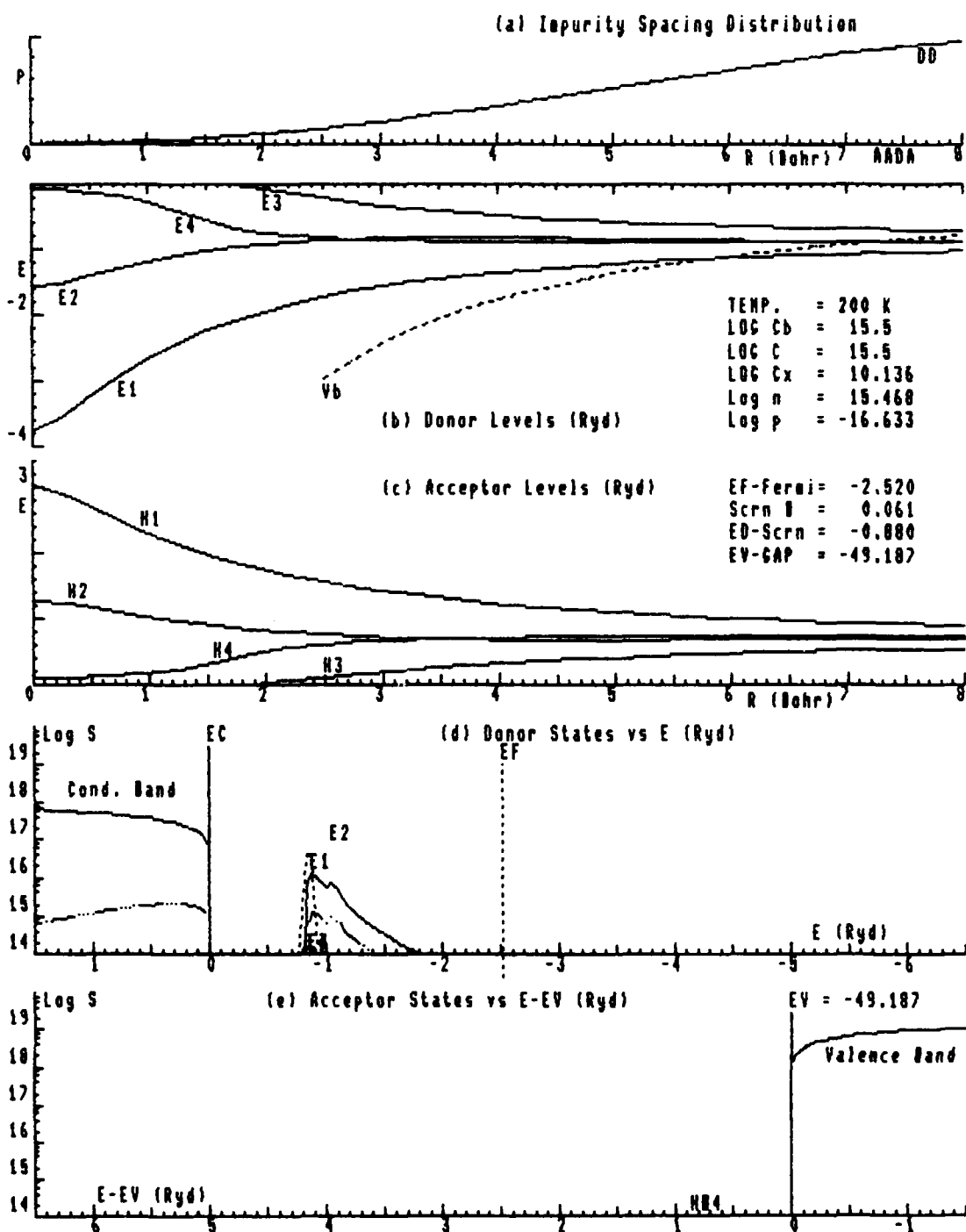


Fig. A 208. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

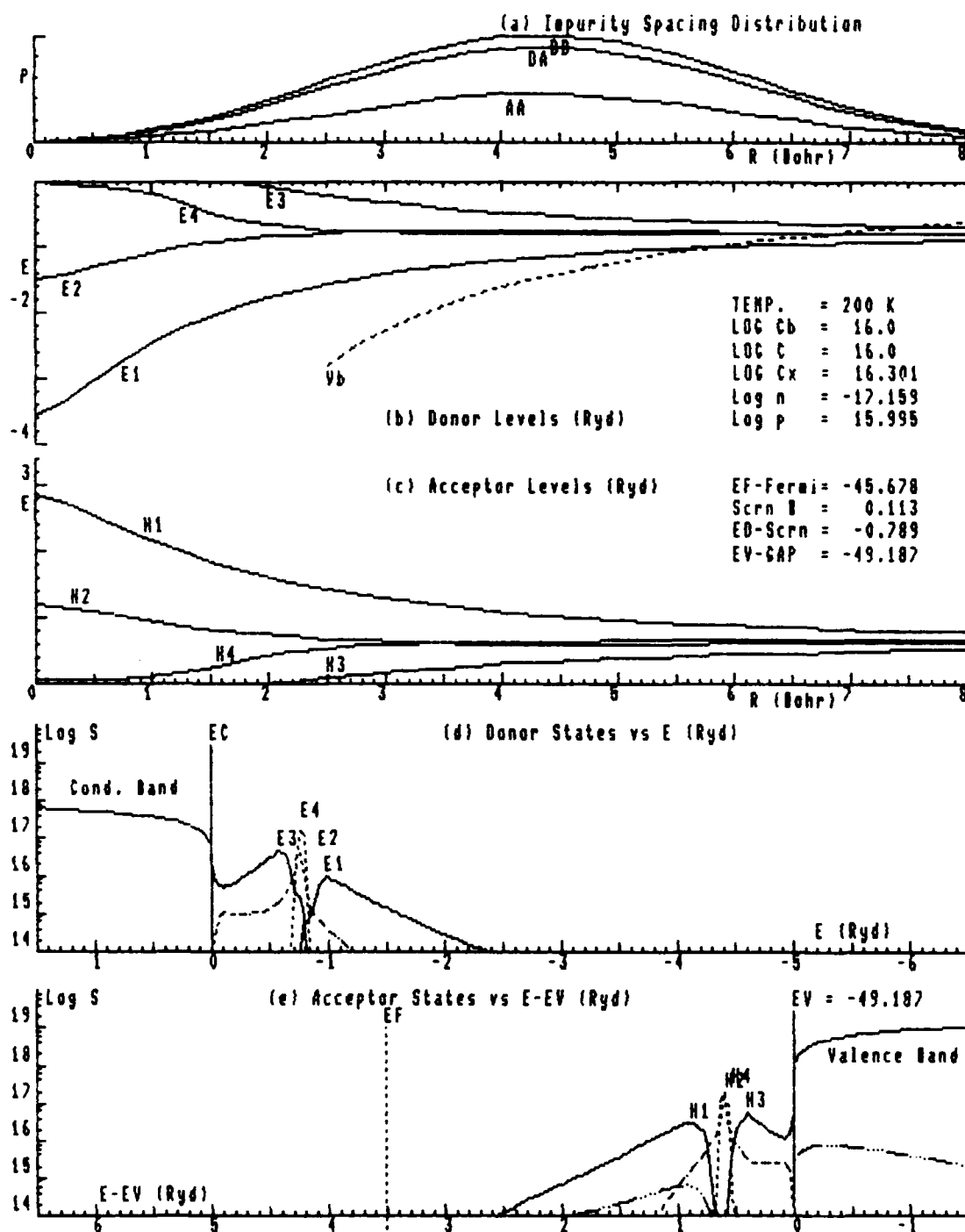


Fig. A 210. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

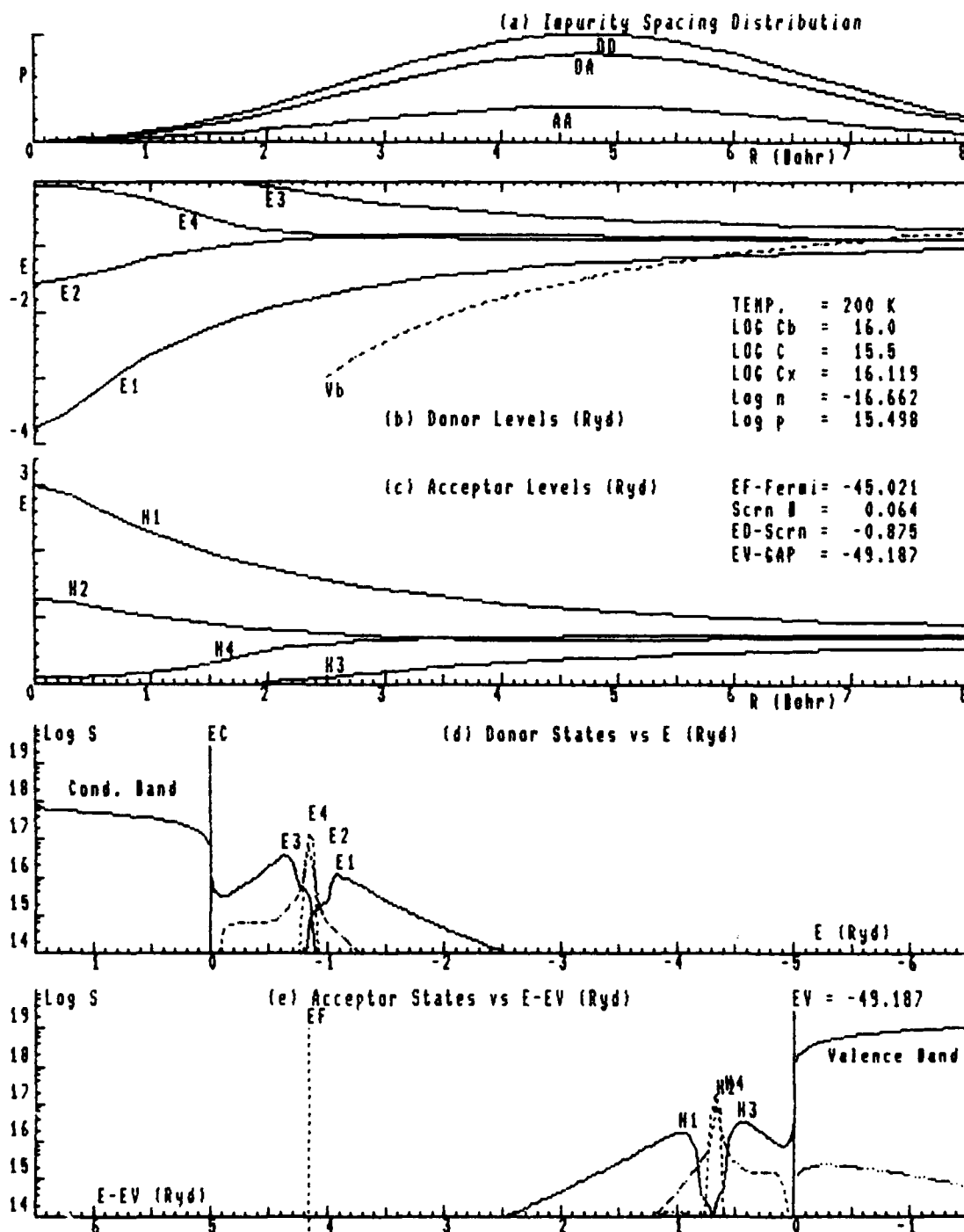


Fig. A 211. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

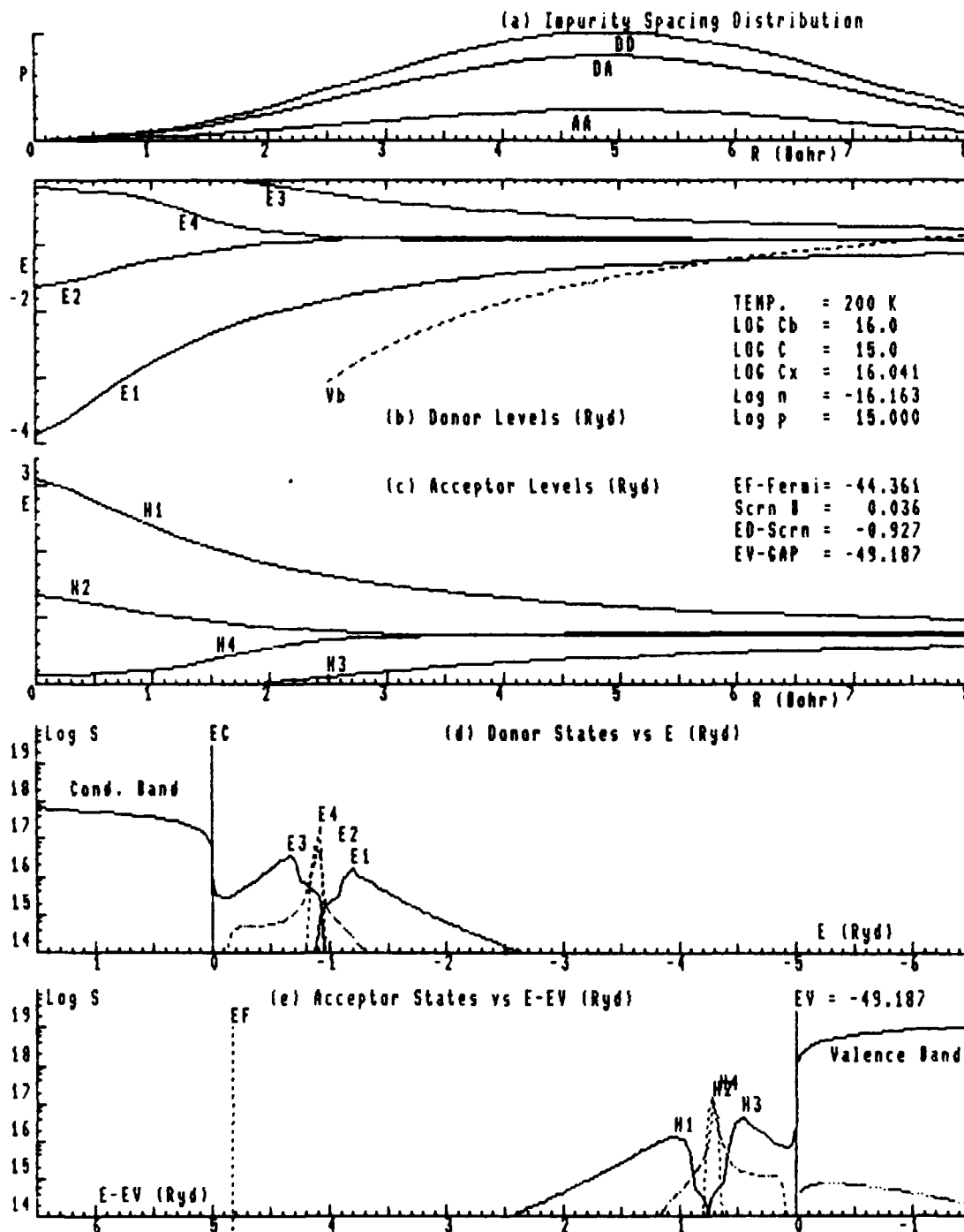


Fig. A 212. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA+)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

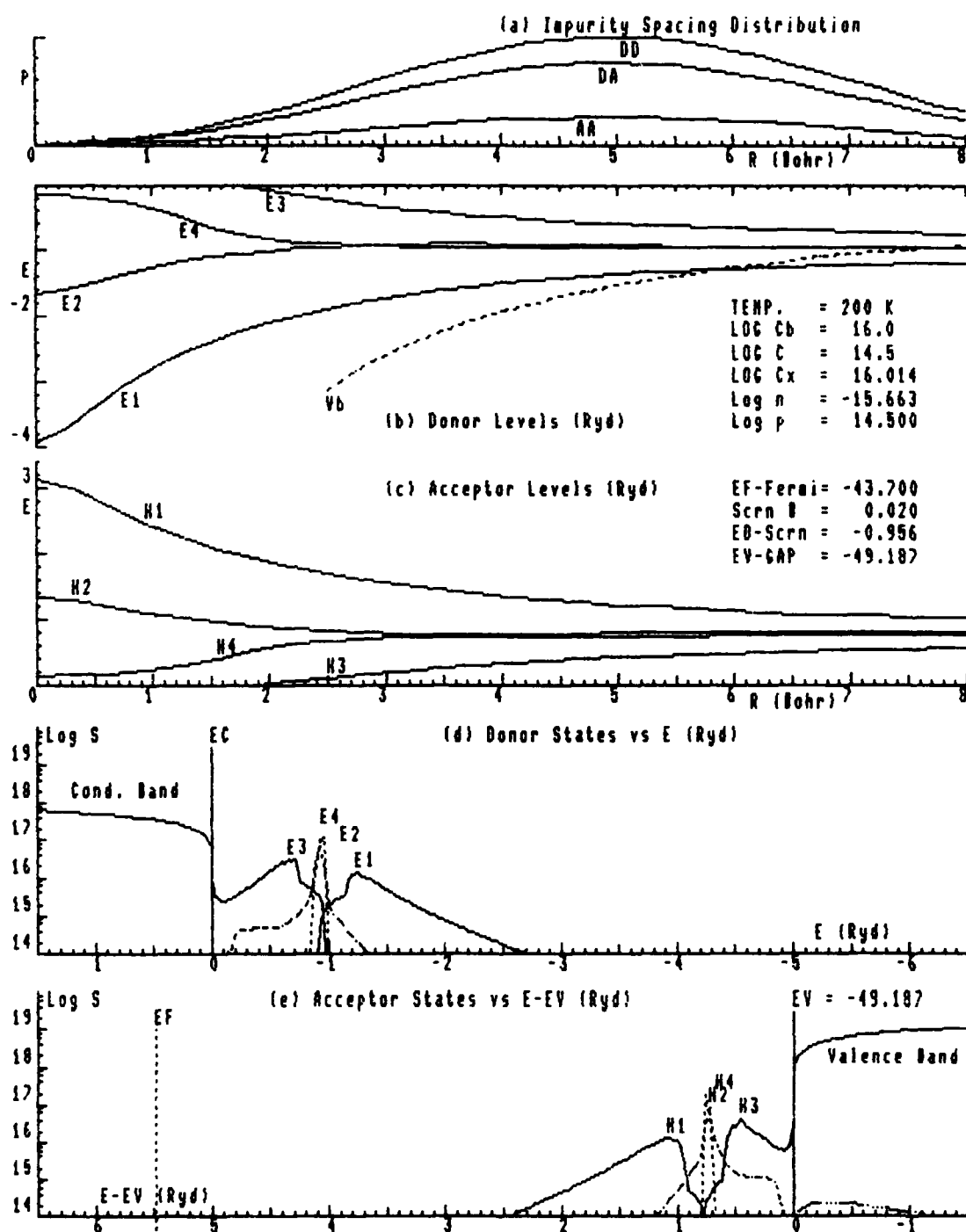


Fig. A 213. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

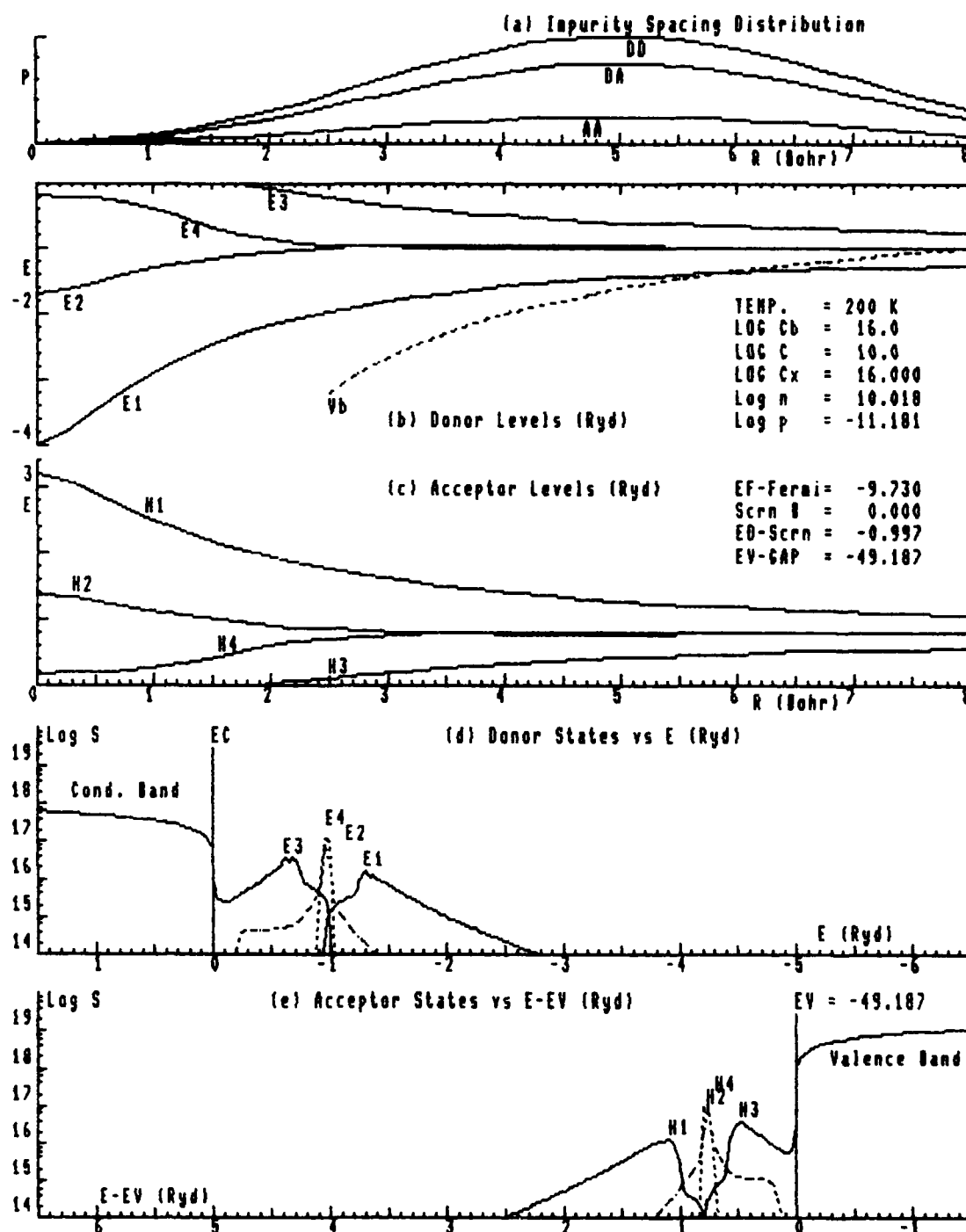


Fig. A 214. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

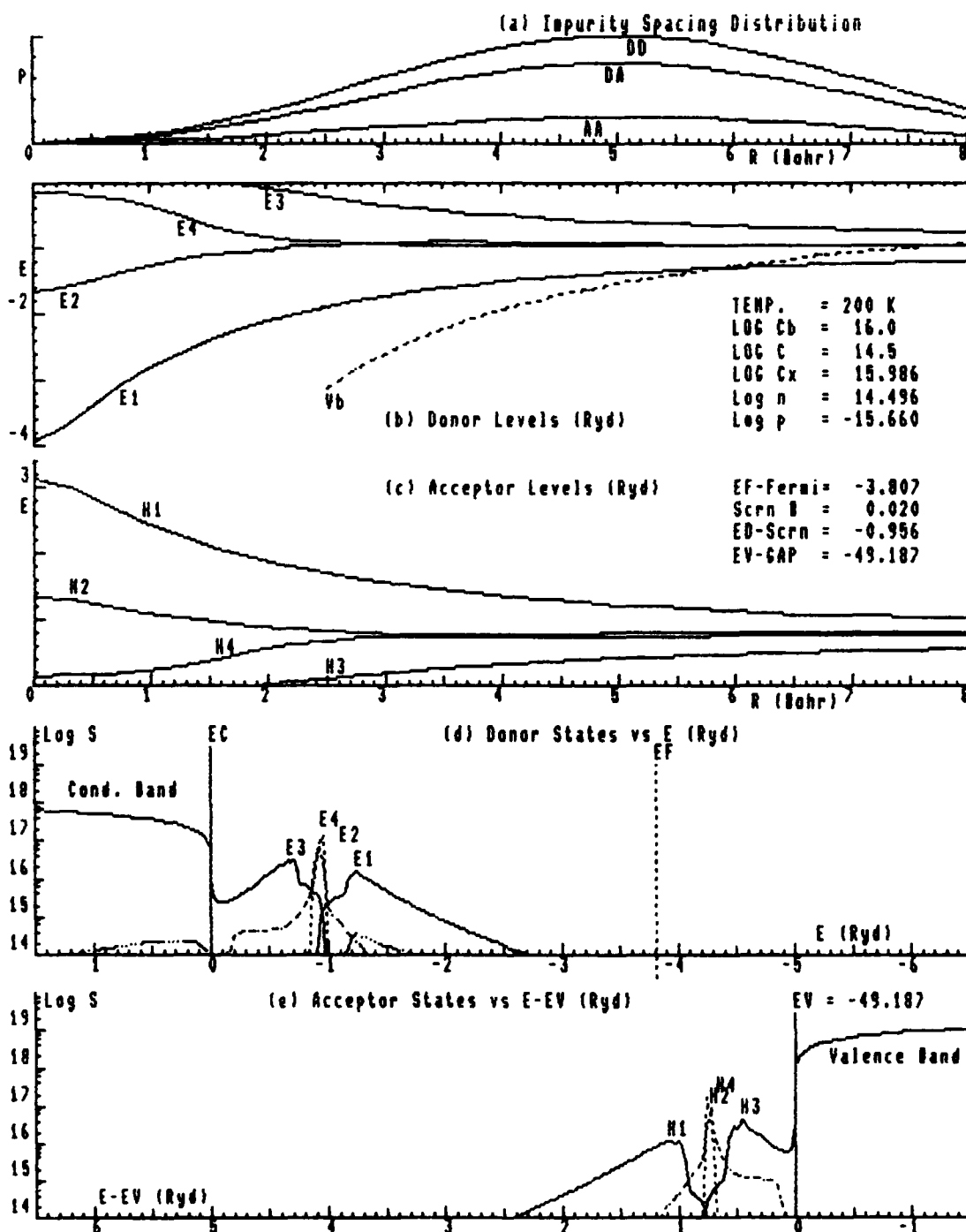


Fig. A 215. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

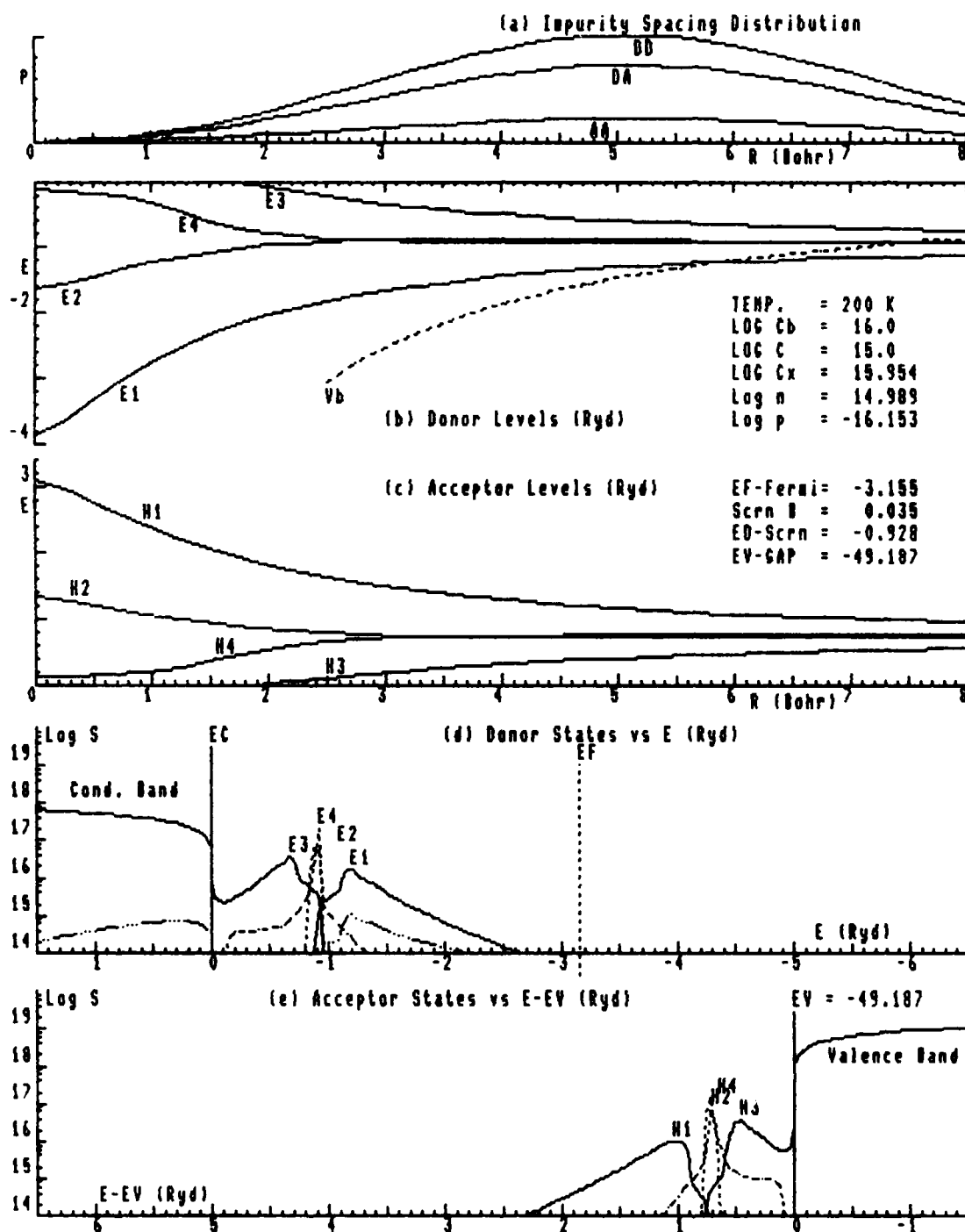


Fig. A 216. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

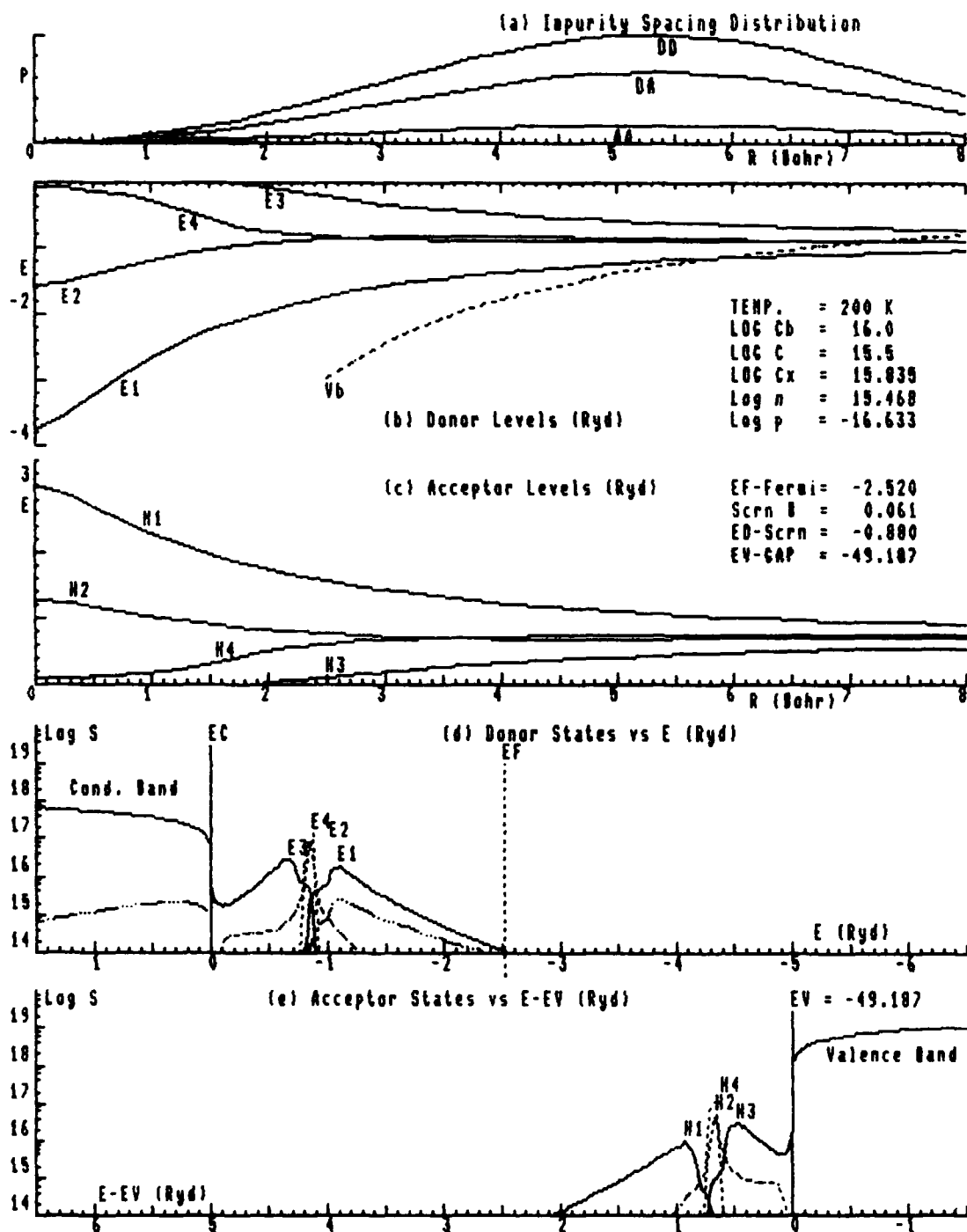


Fig. A 217. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

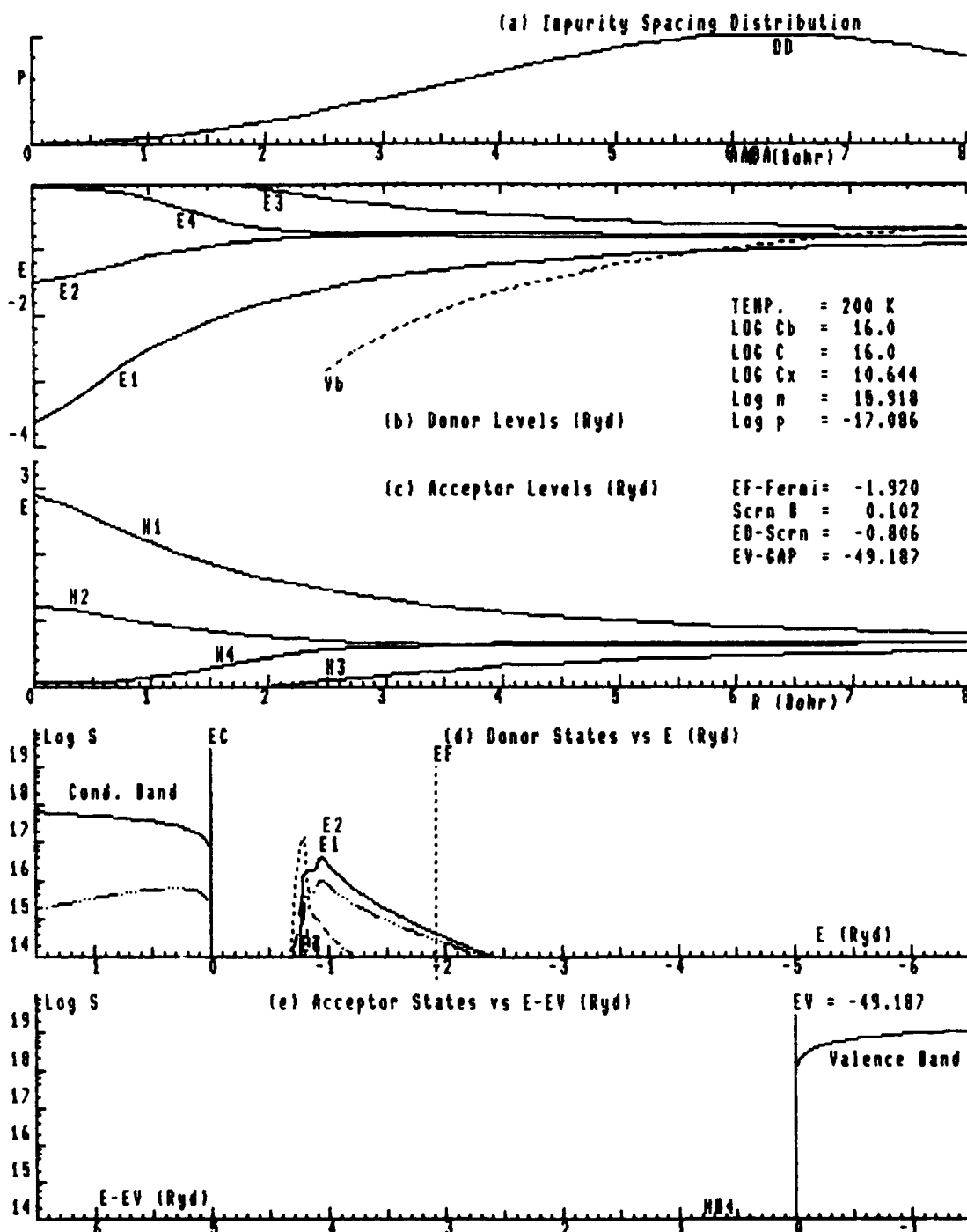


Fig. A 218. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

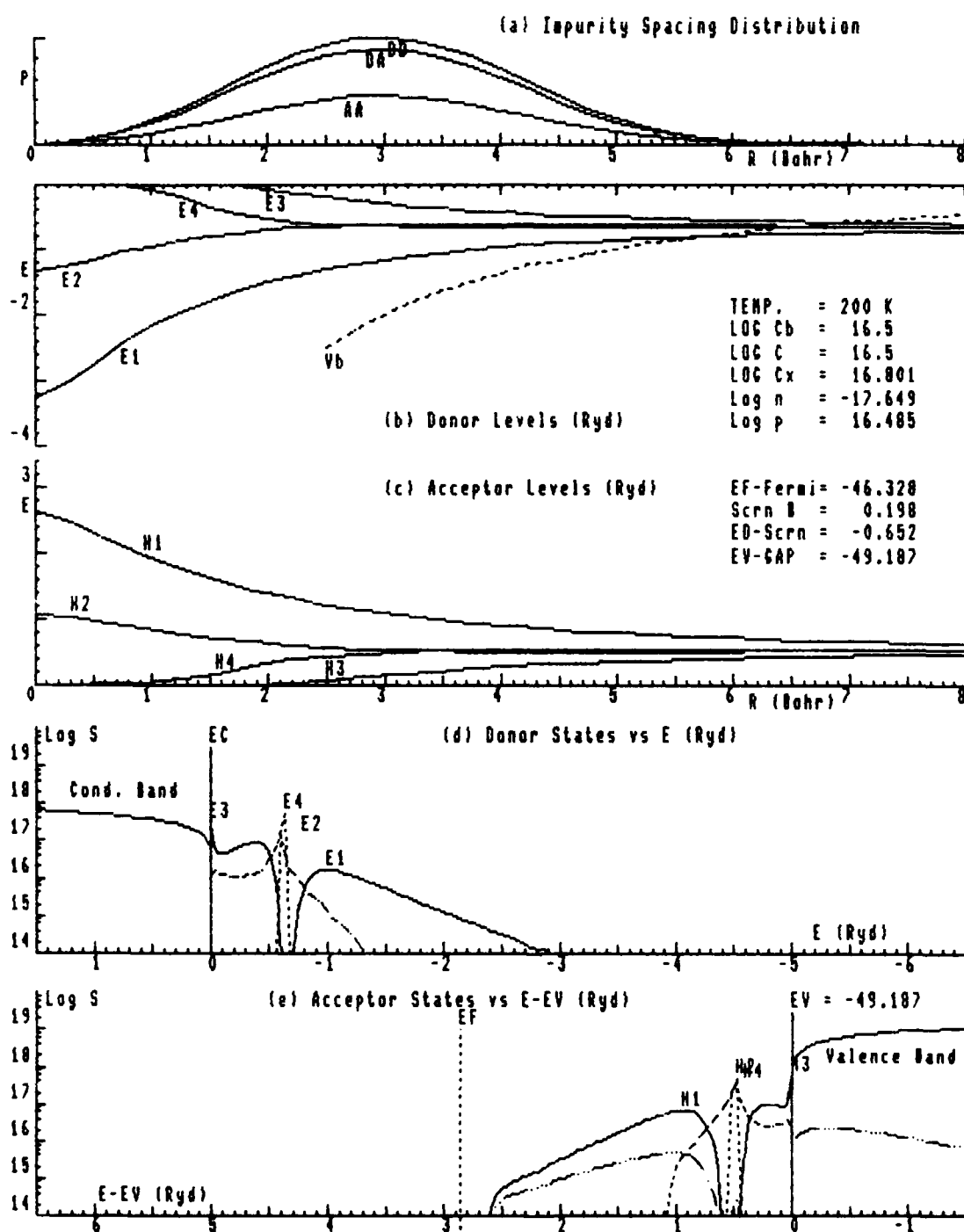


Fig. A 220. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

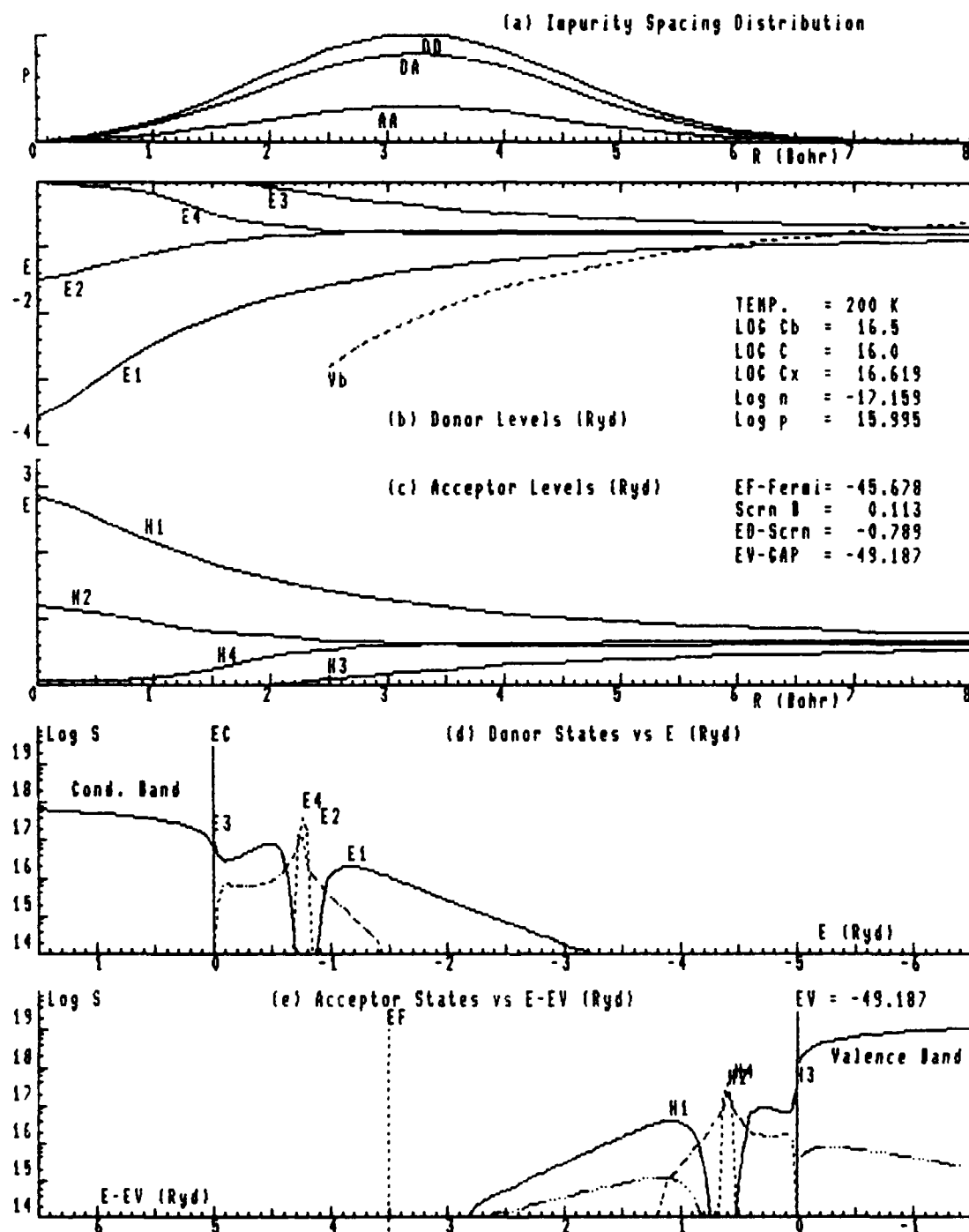


Fig. A 221. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

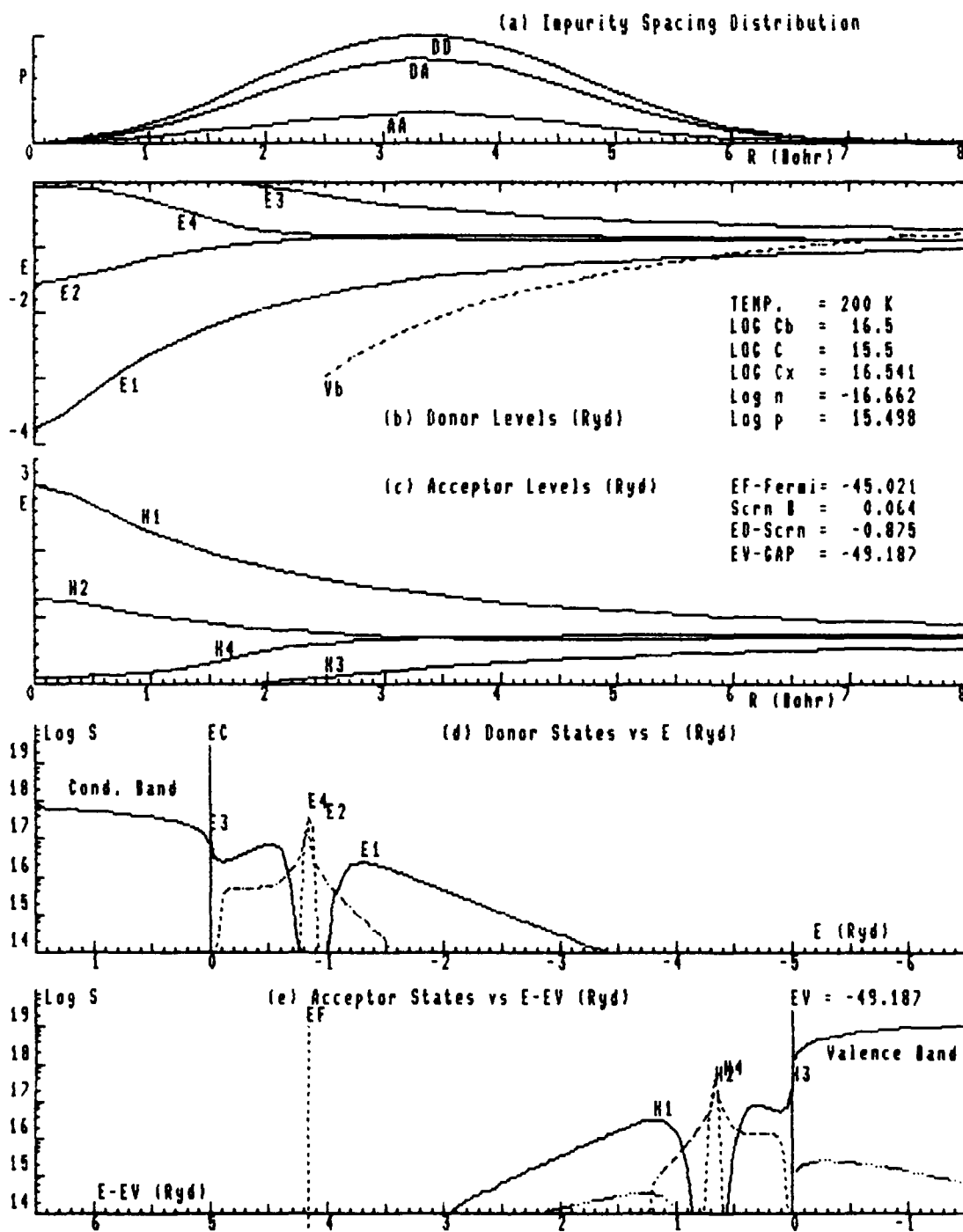


Fig. A 222. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

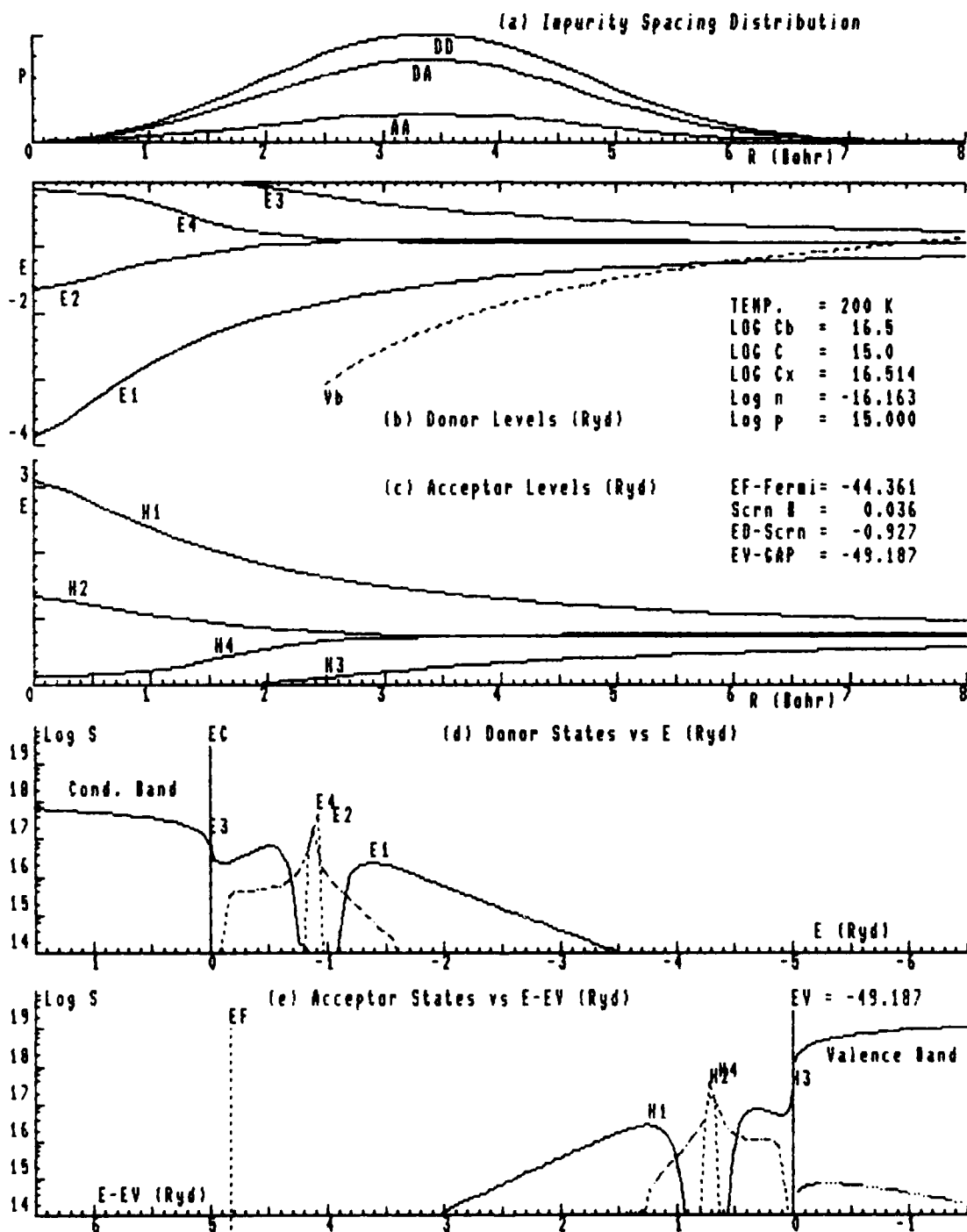


Fig. A 223. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, v< E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

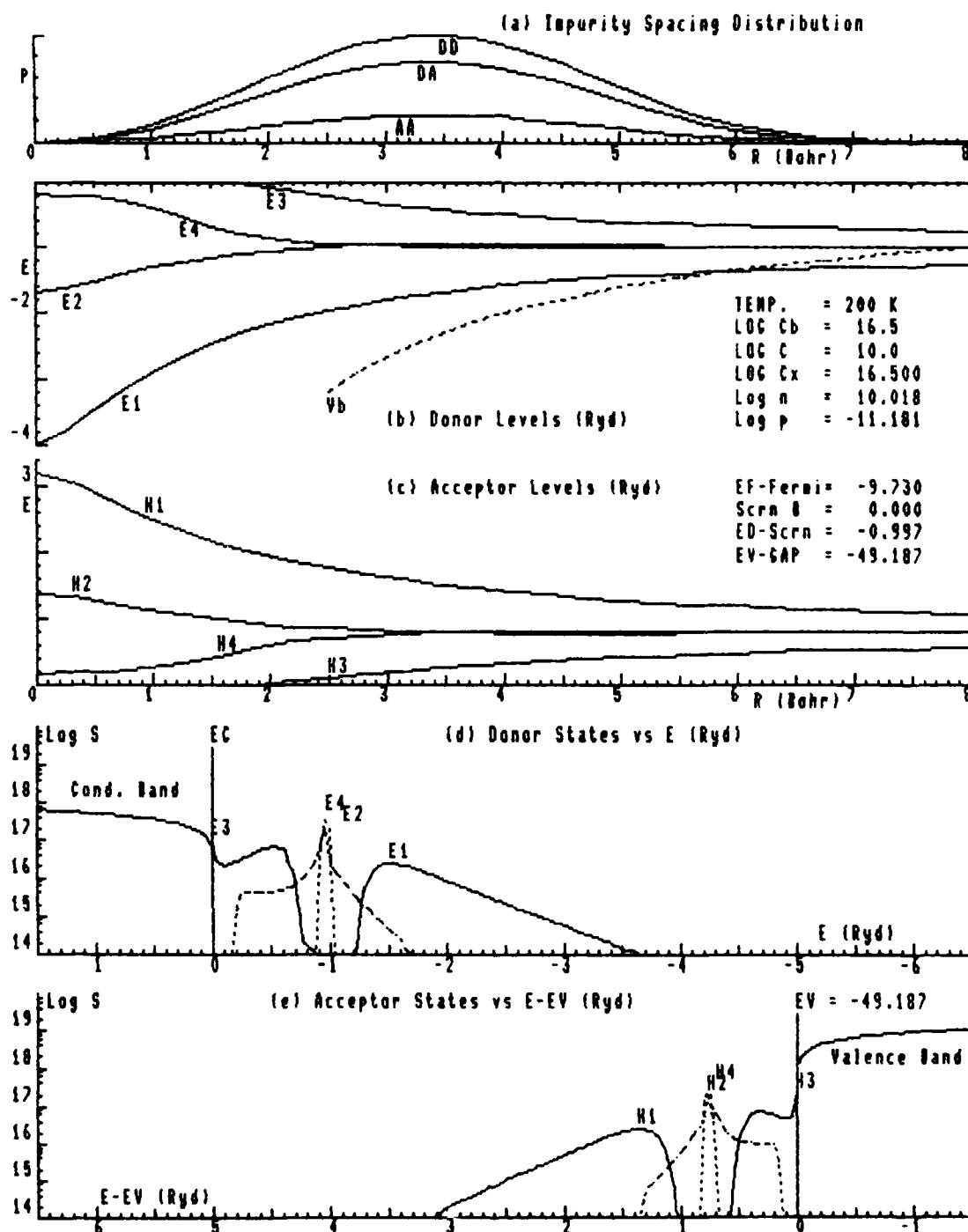


Fig. A 224. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

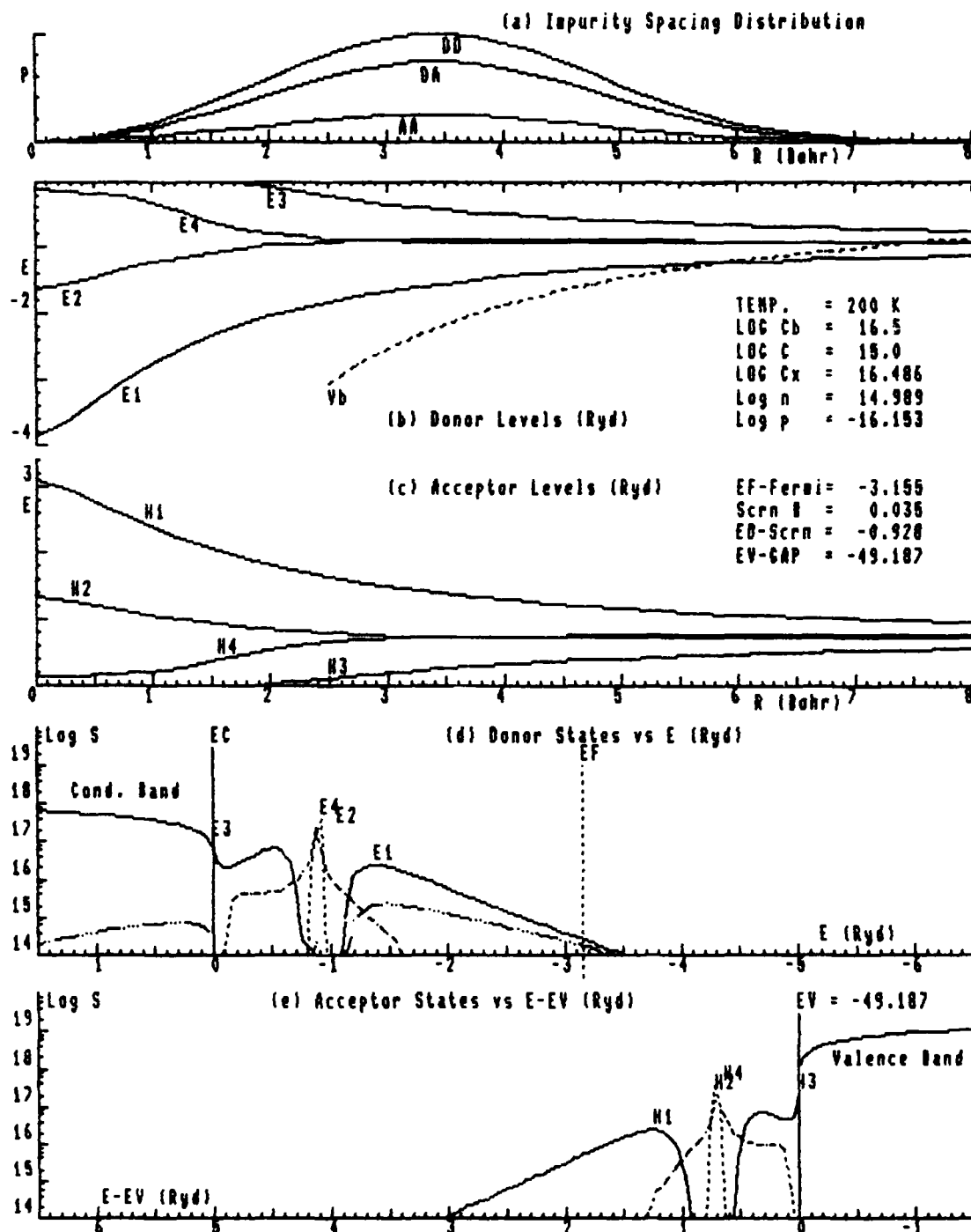


Fig. A 225. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

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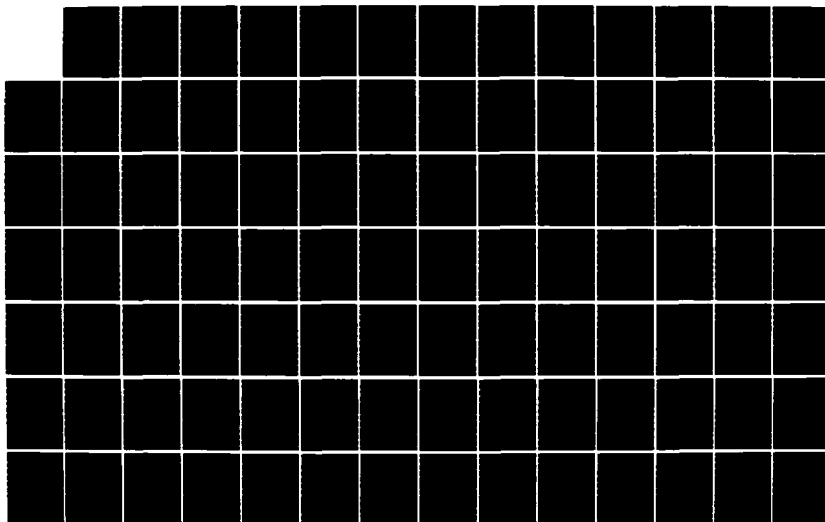
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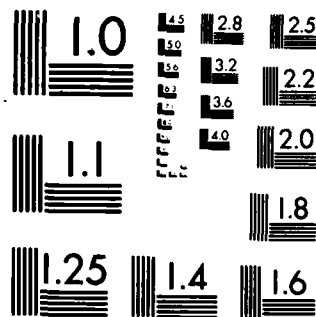
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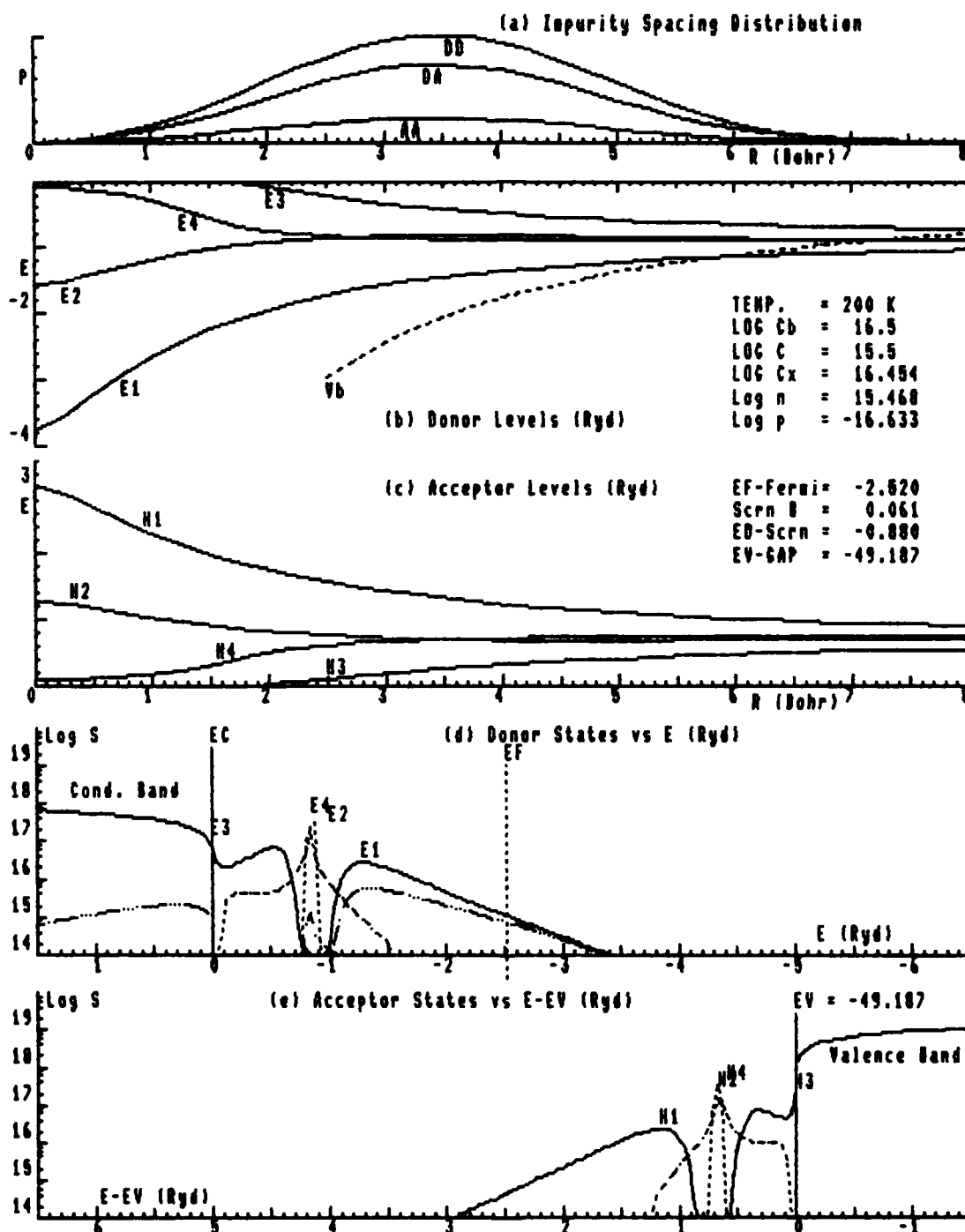


Fig. A 226. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

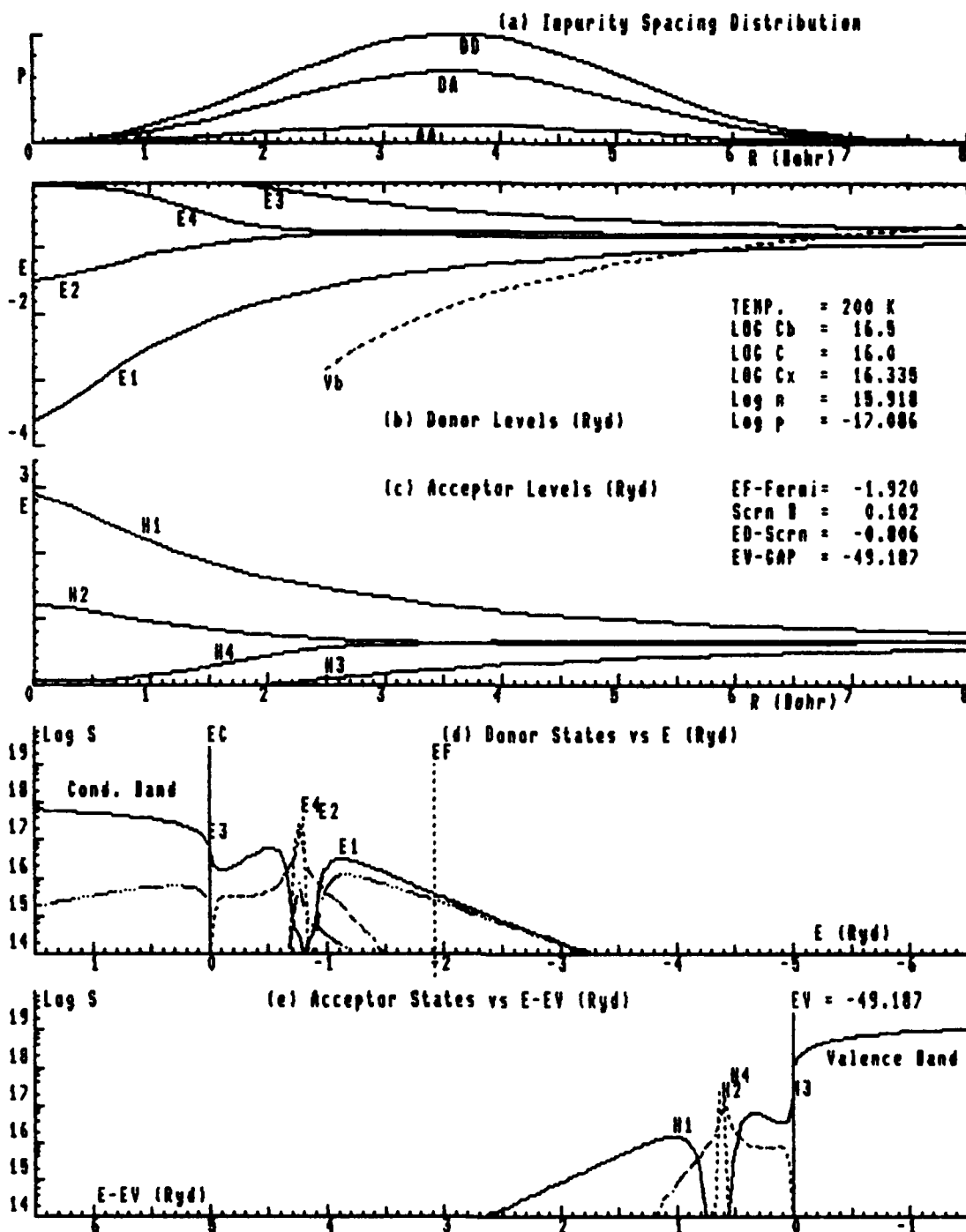


Fig. A 227. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

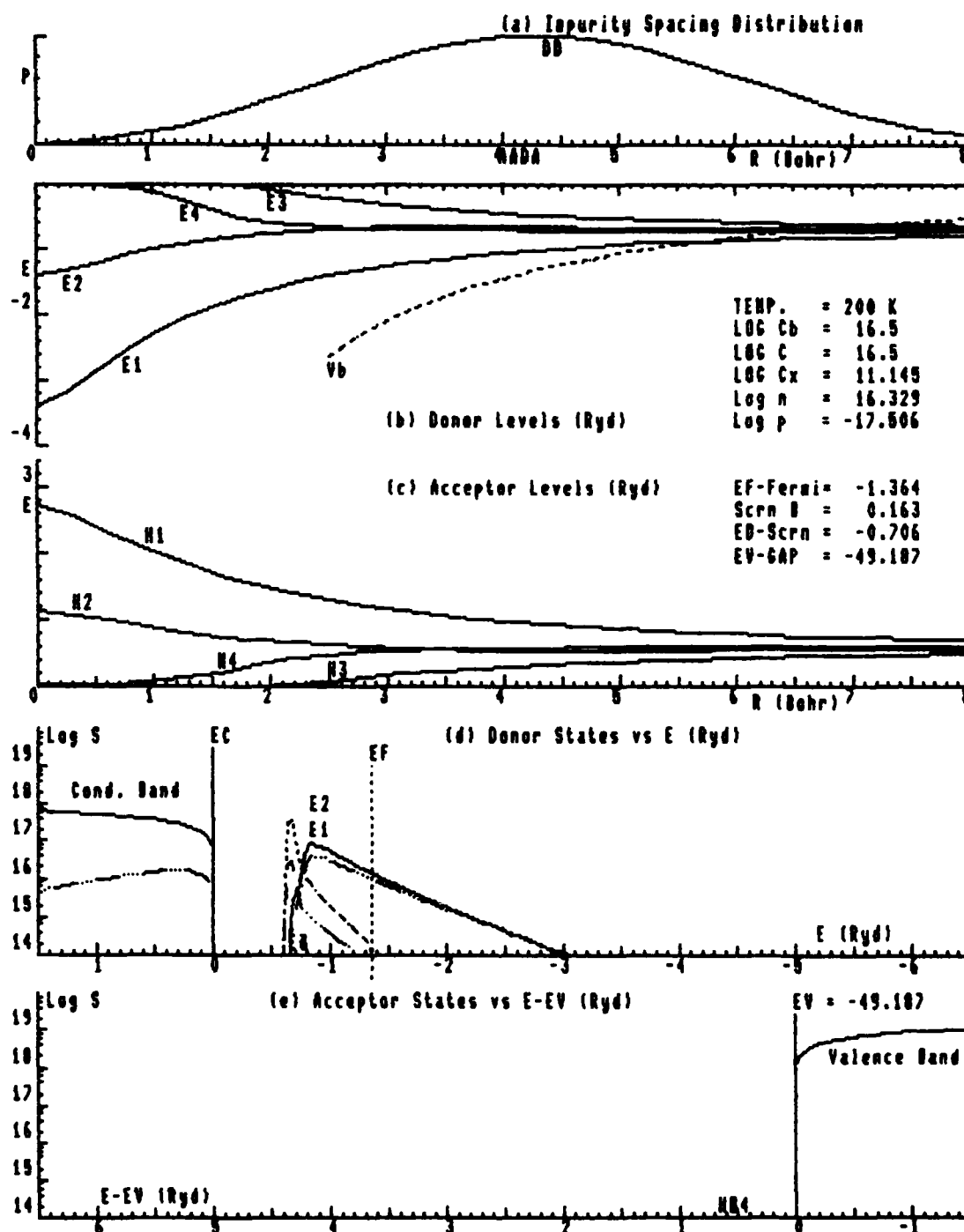


Fig. A 228. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

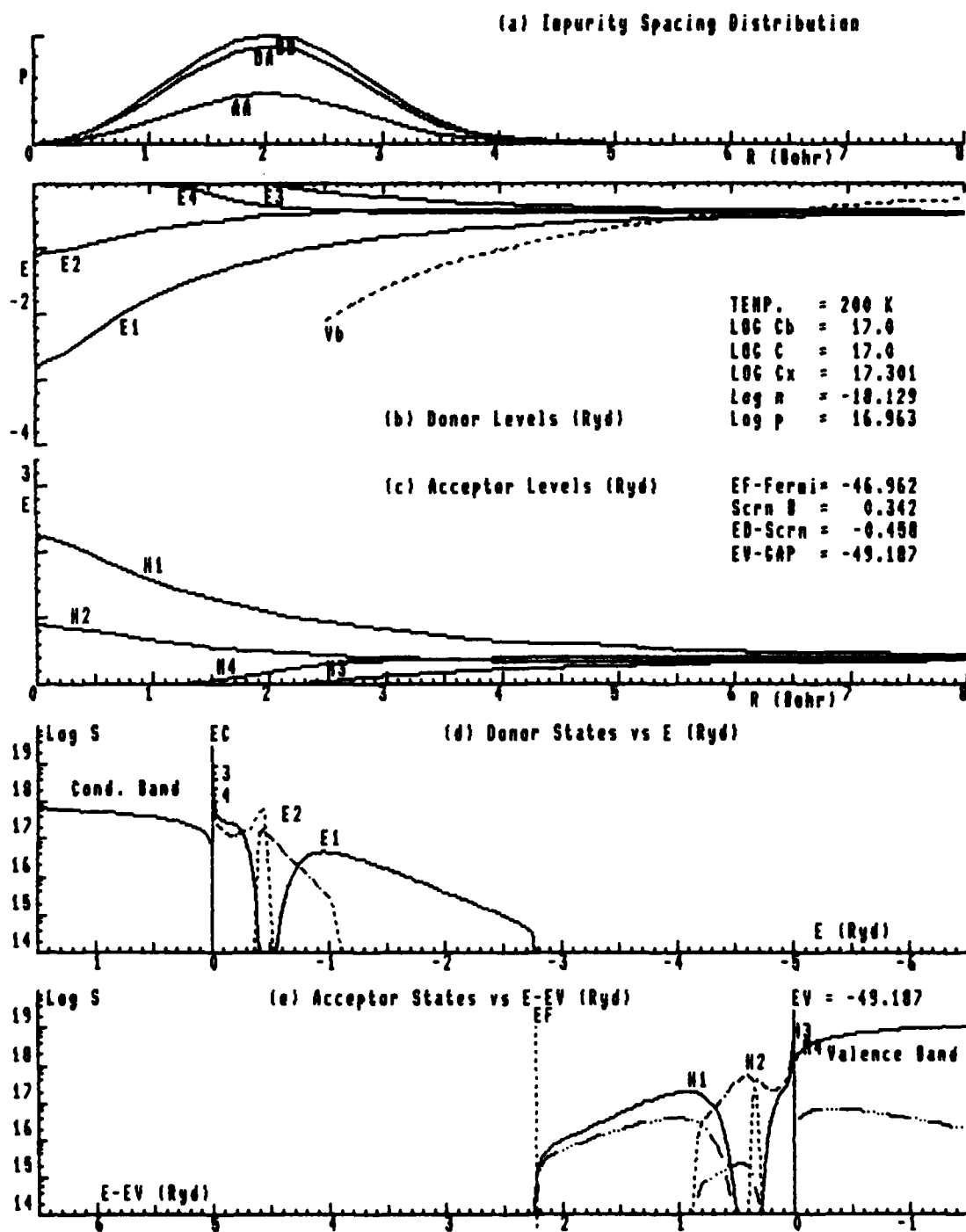


Fig. A 230. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

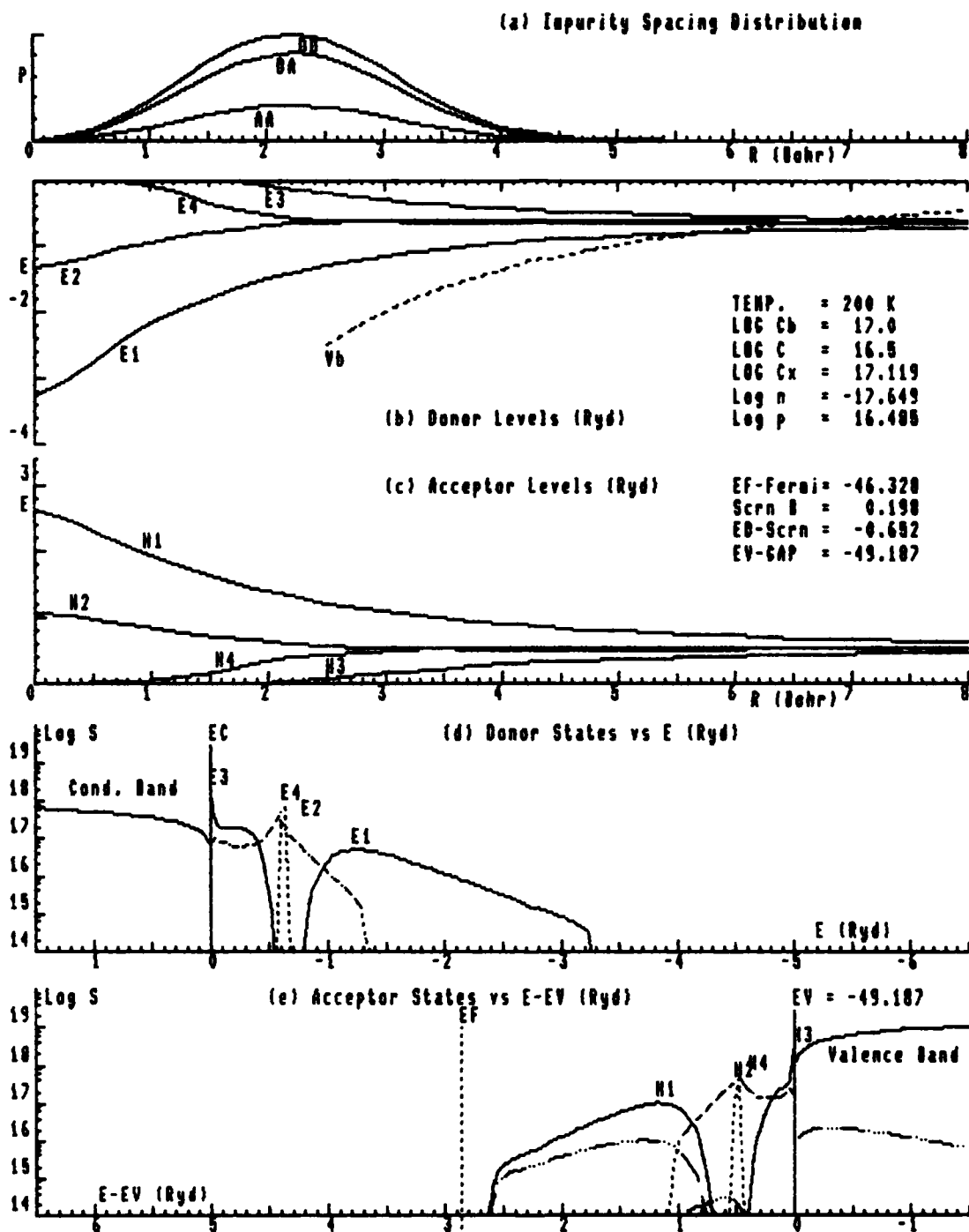


Fig. A 231. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

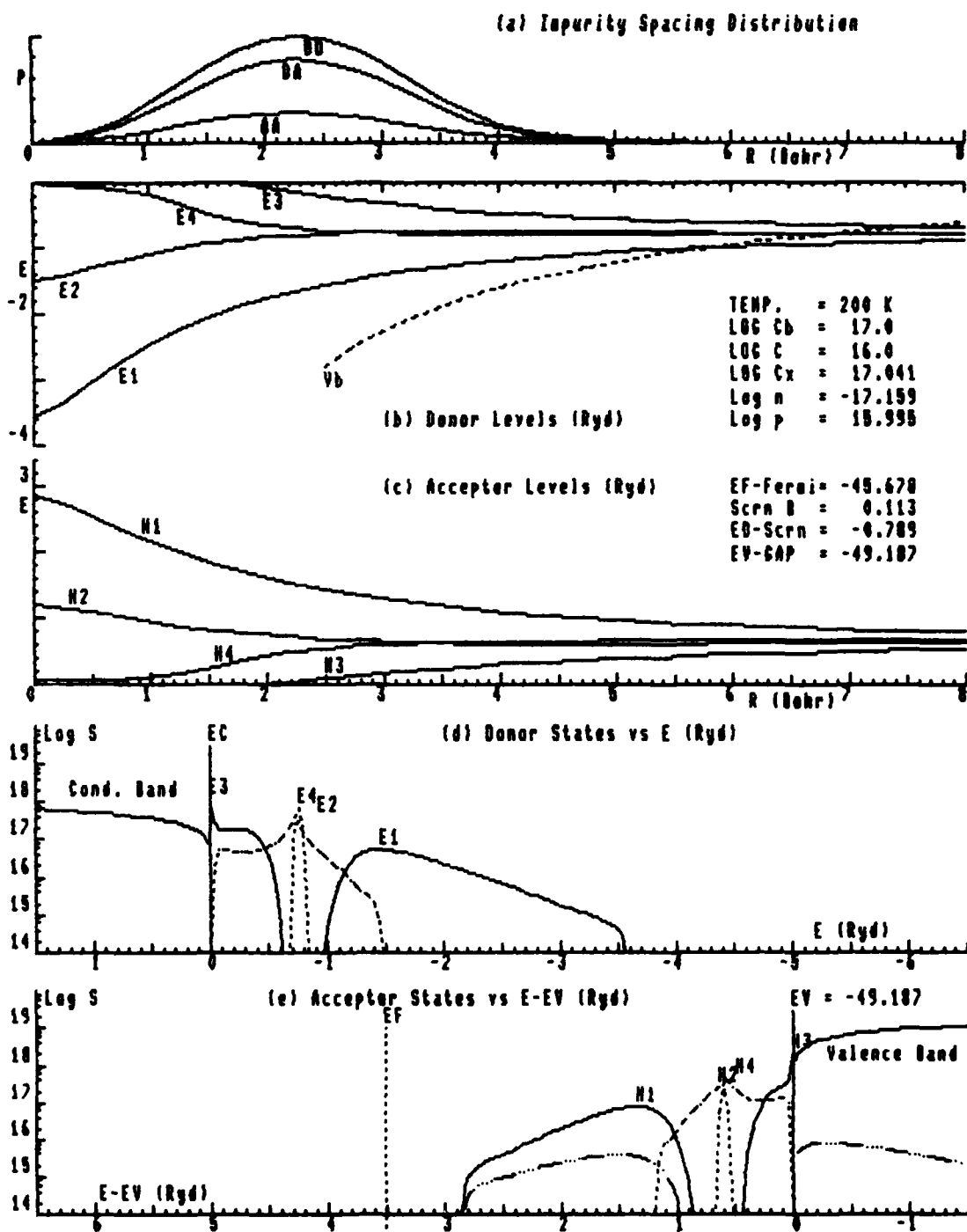


Fig. A 232. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

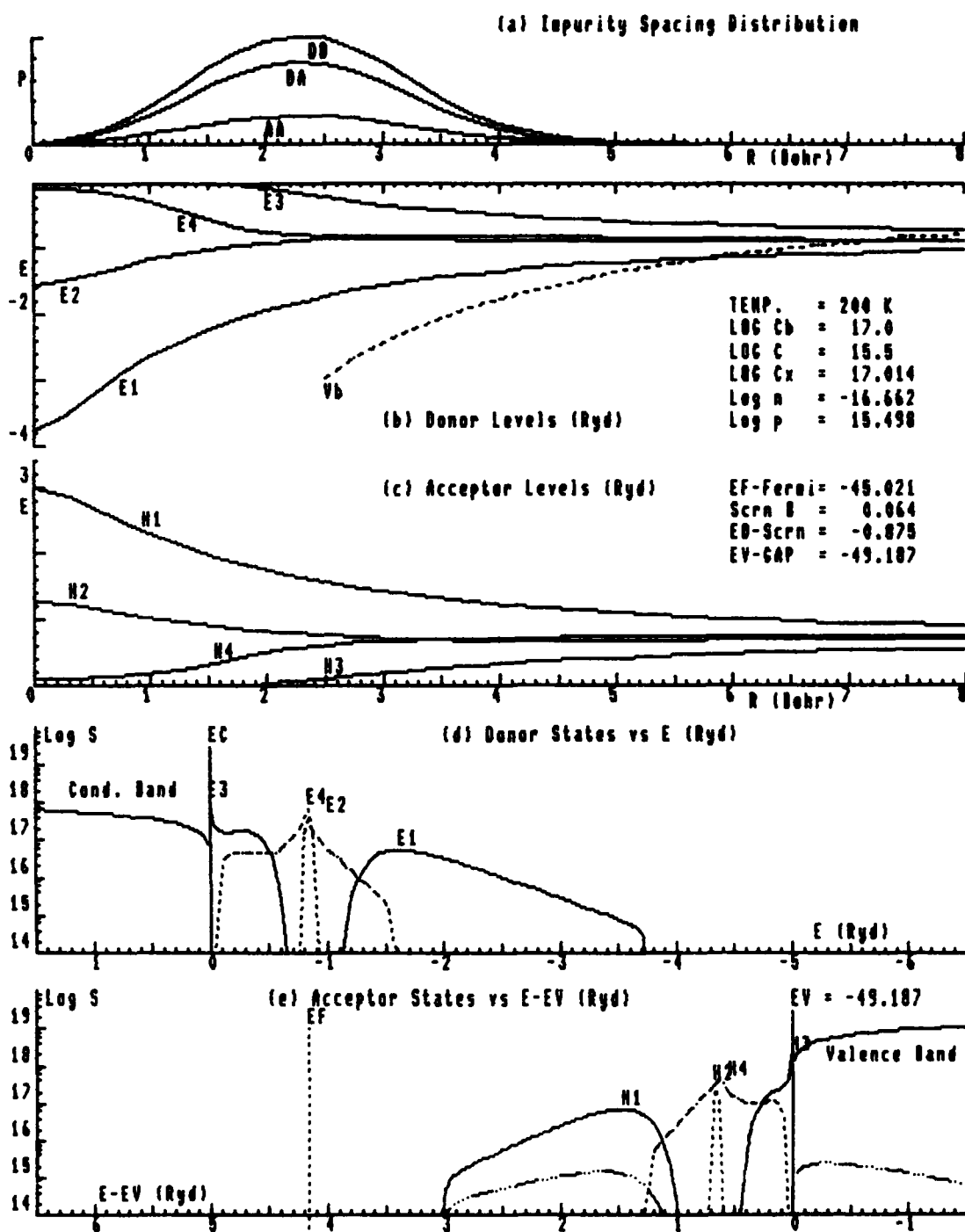


Fig. A 233. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

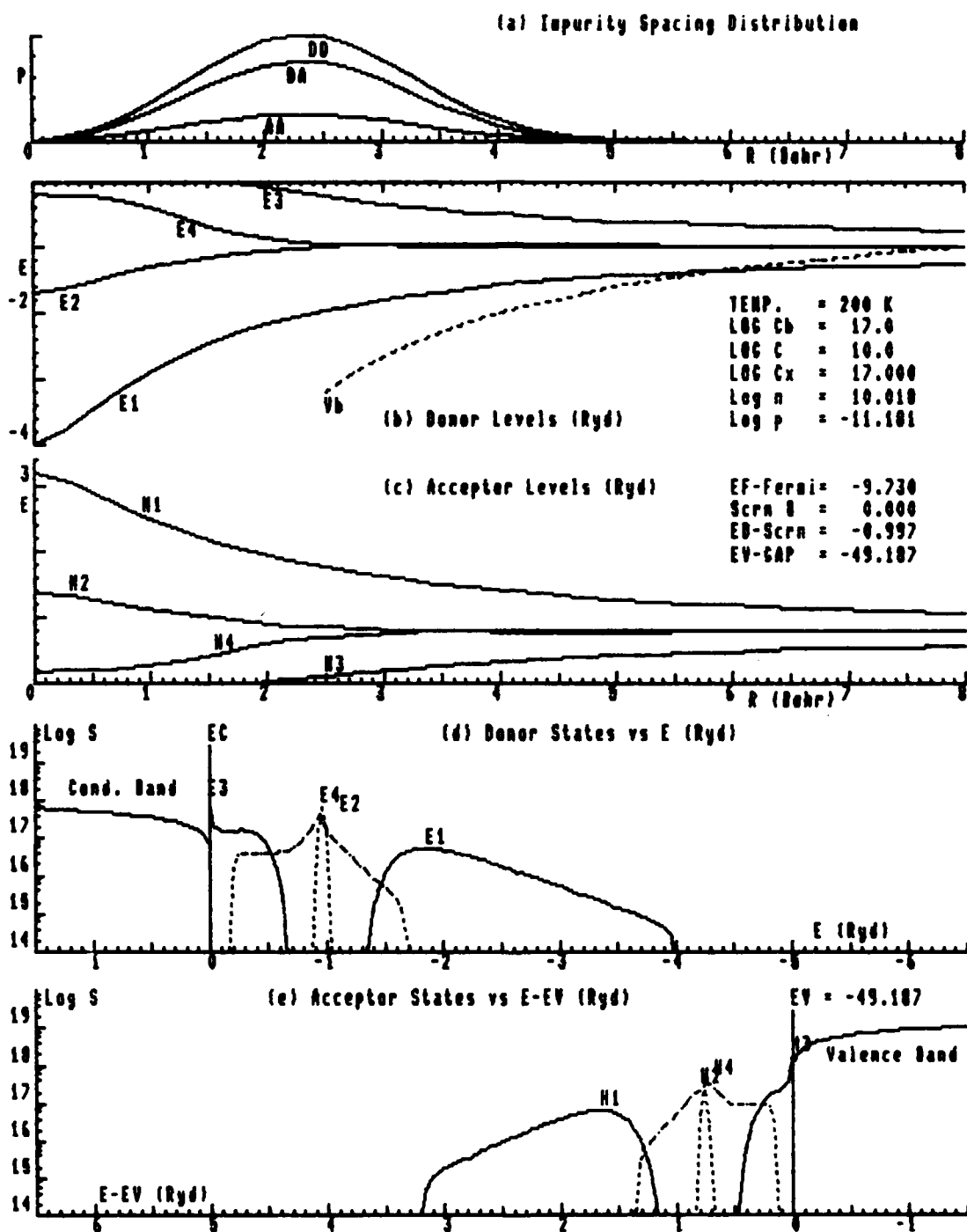


Fig. A 234. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

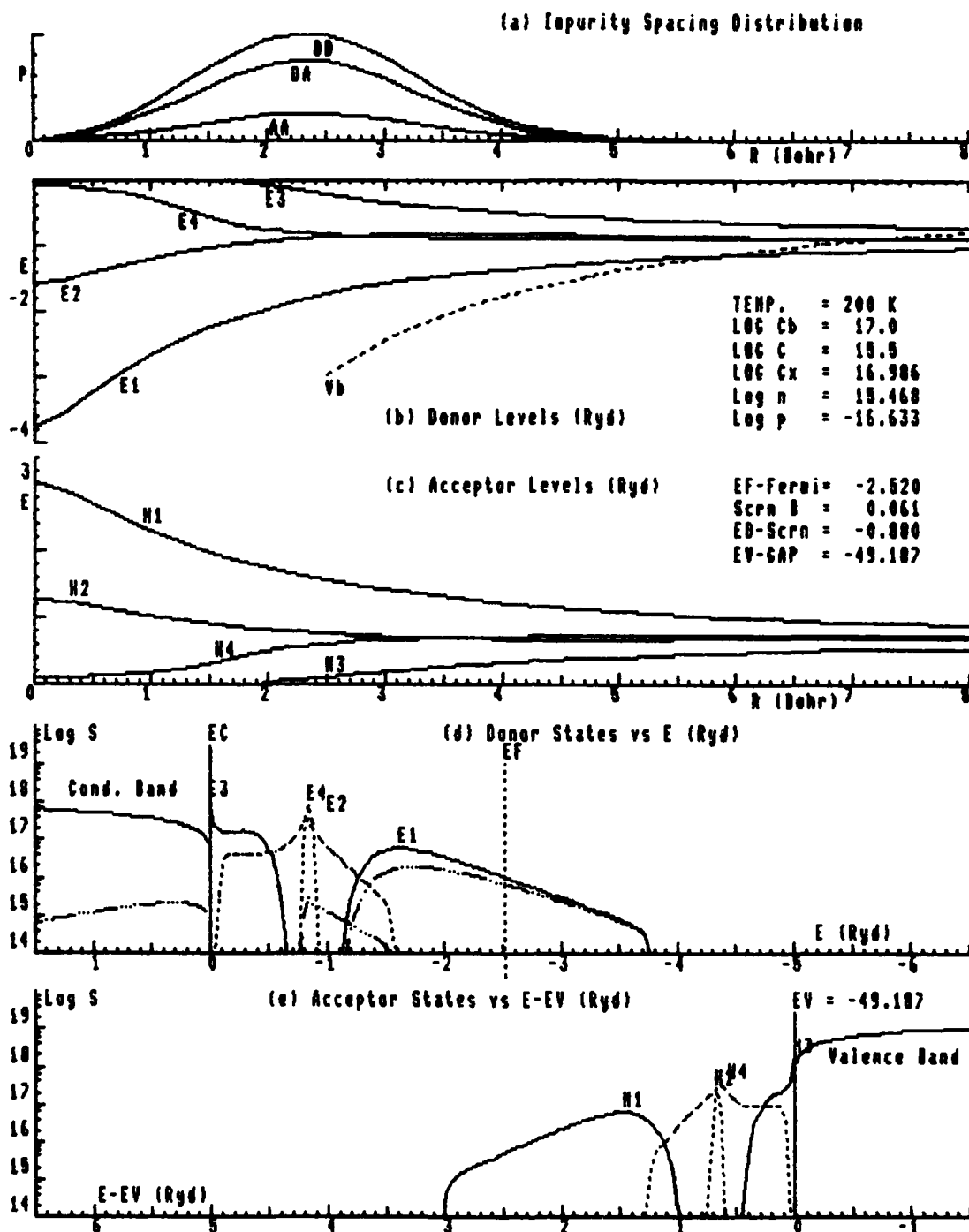


Fig. A 235. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

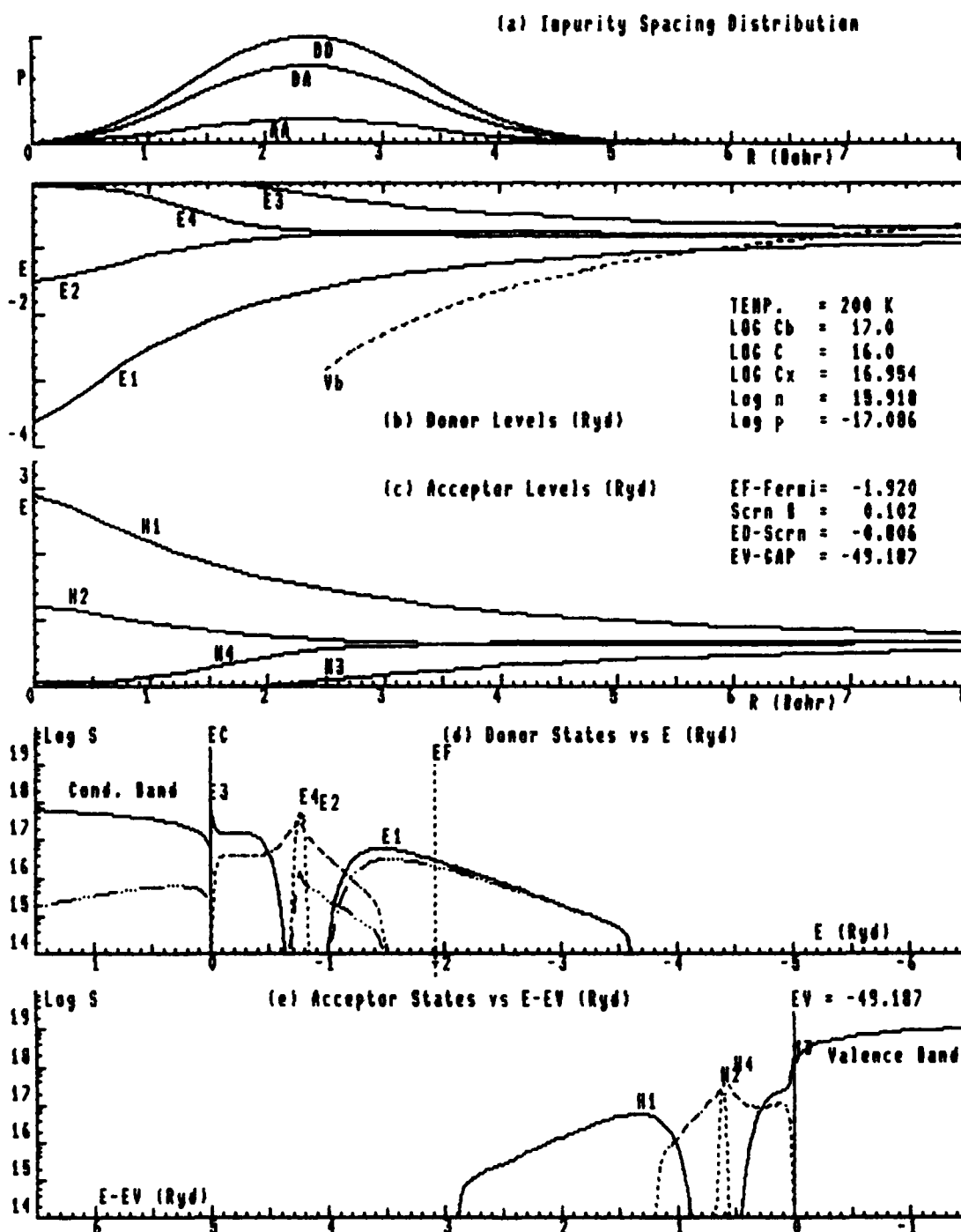


Fig. A 236. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

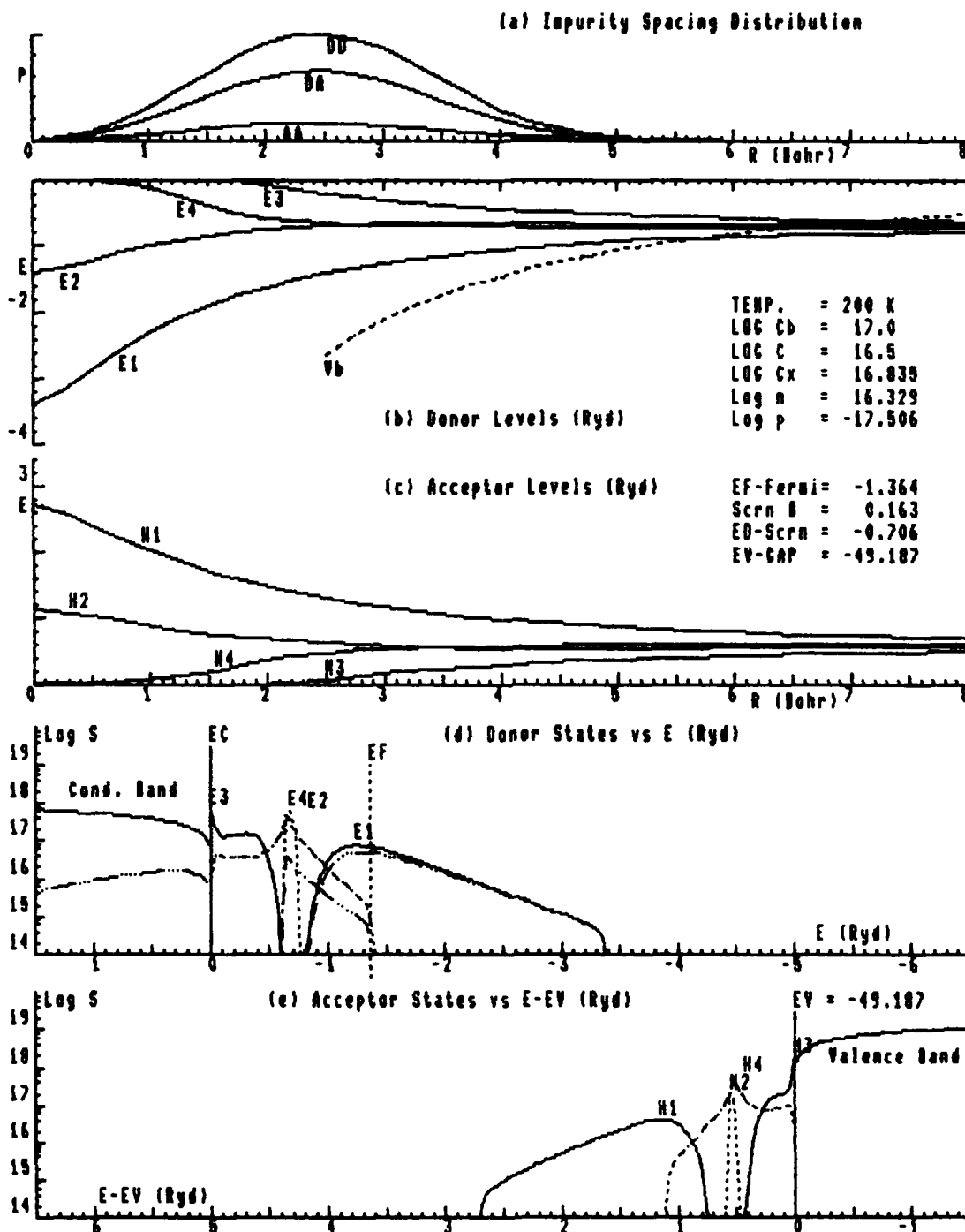


Fig. A 237. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

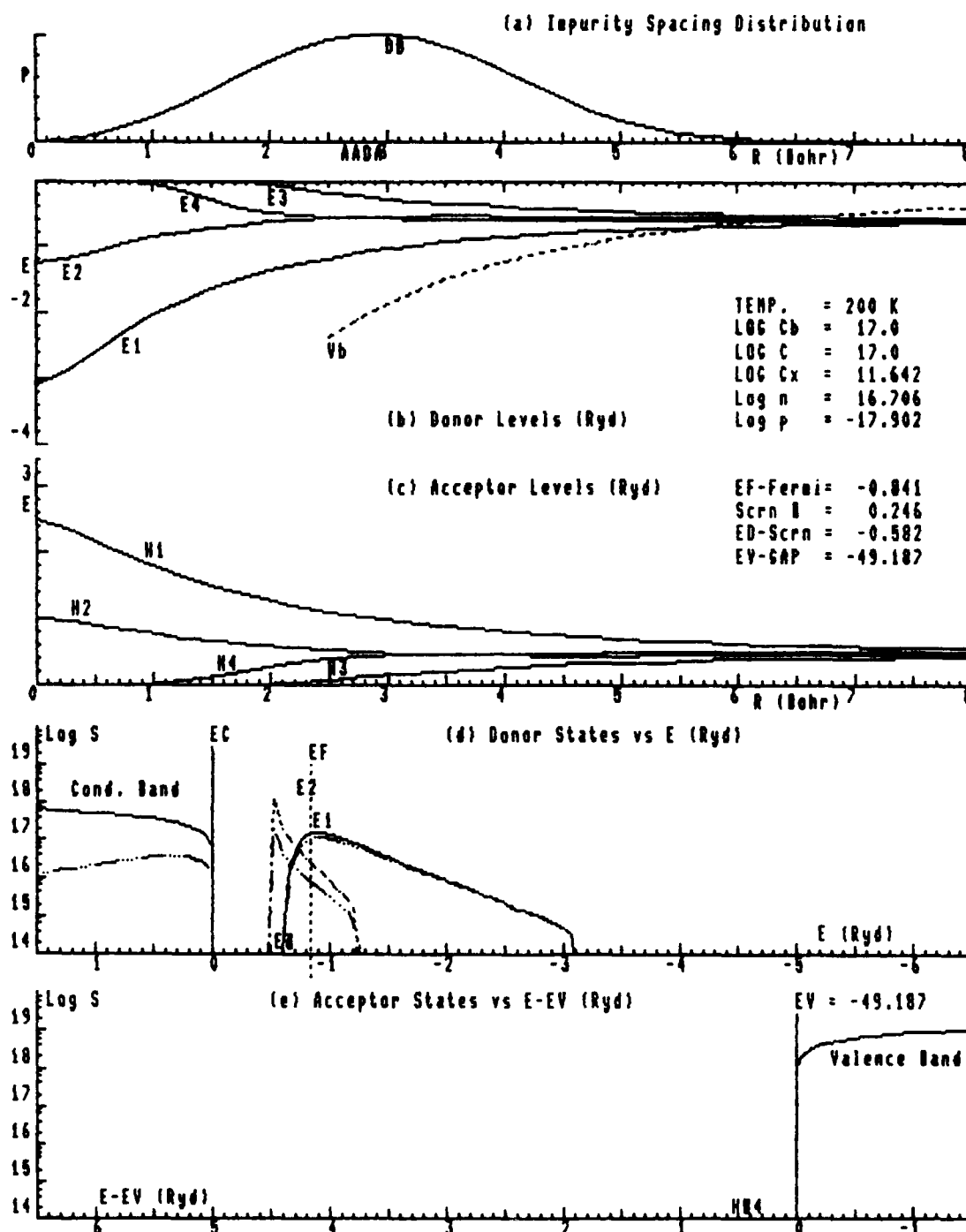


Fig. A 238. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

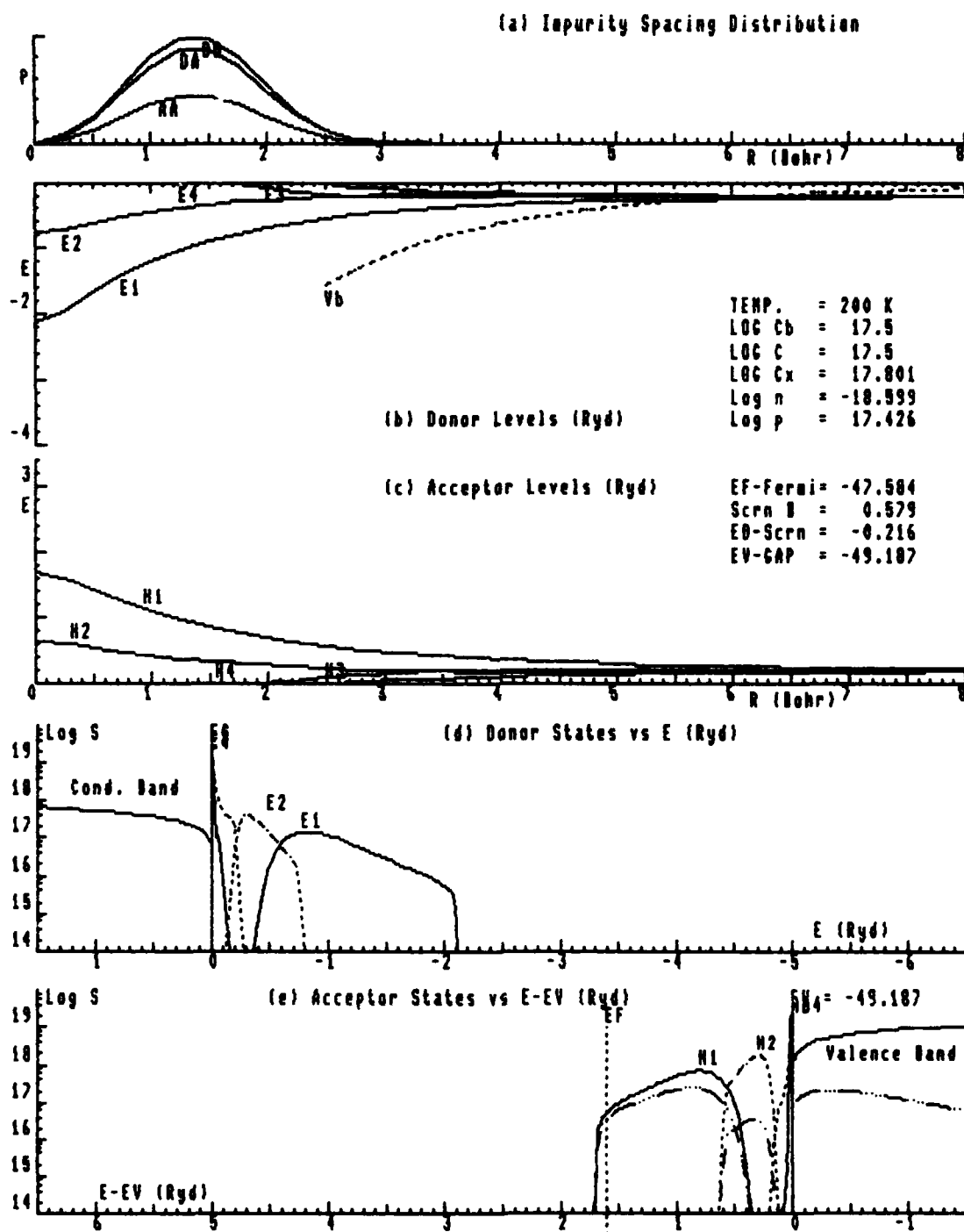


Fig. A 240. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

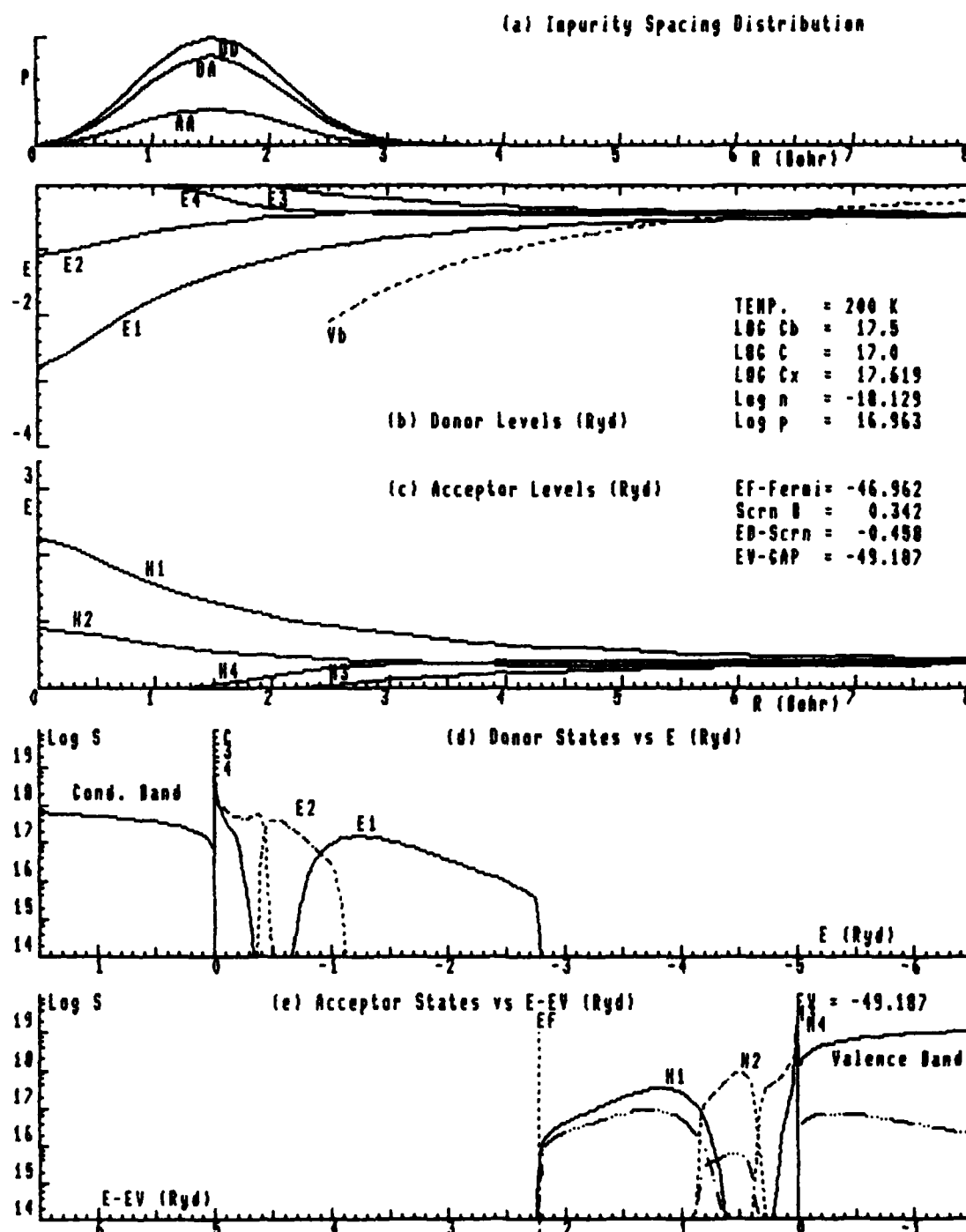


Fig. A 241. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

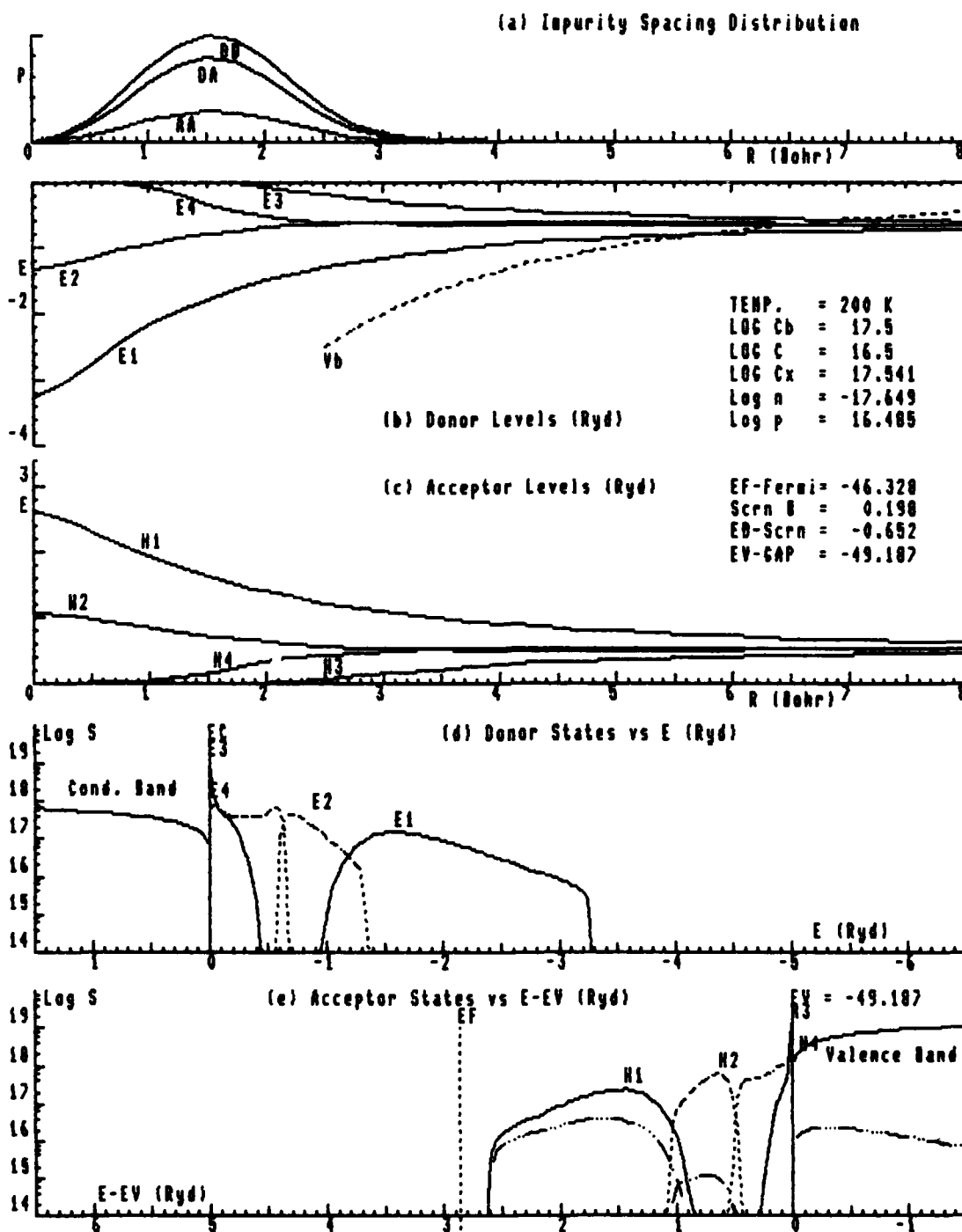


Fig. A 242. (a) Probability, $AA + DA + DD$, of Pairs vs R
 (b) Donor Energy $E1; (DD)^-, E2; (DD)^-, E3; (DA)^-, E4(DA)^-$ vs R
 (c) Acceptor En. $H1; (AA)^+, H2; (AA)^+, H3; (AD)^+, H4(AD)^+$ vs R
 (d) Densities of Donor States, $E1, E2, E3$, & $E4$, vs E
 (e) Densities of Acceptor States, $H1, H2, H3$, & $H4$ vs $E-EV$.

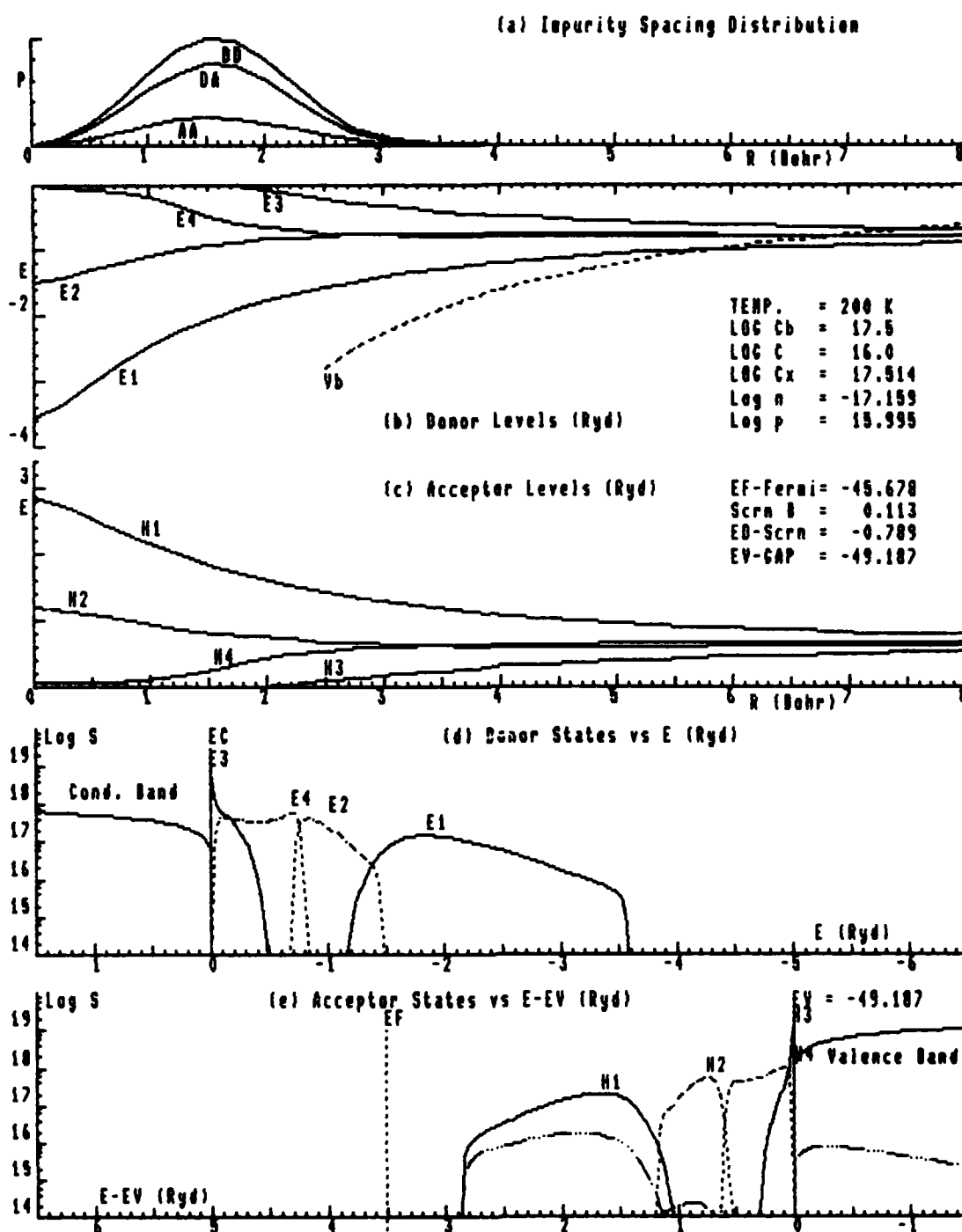


Fig. A 243. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

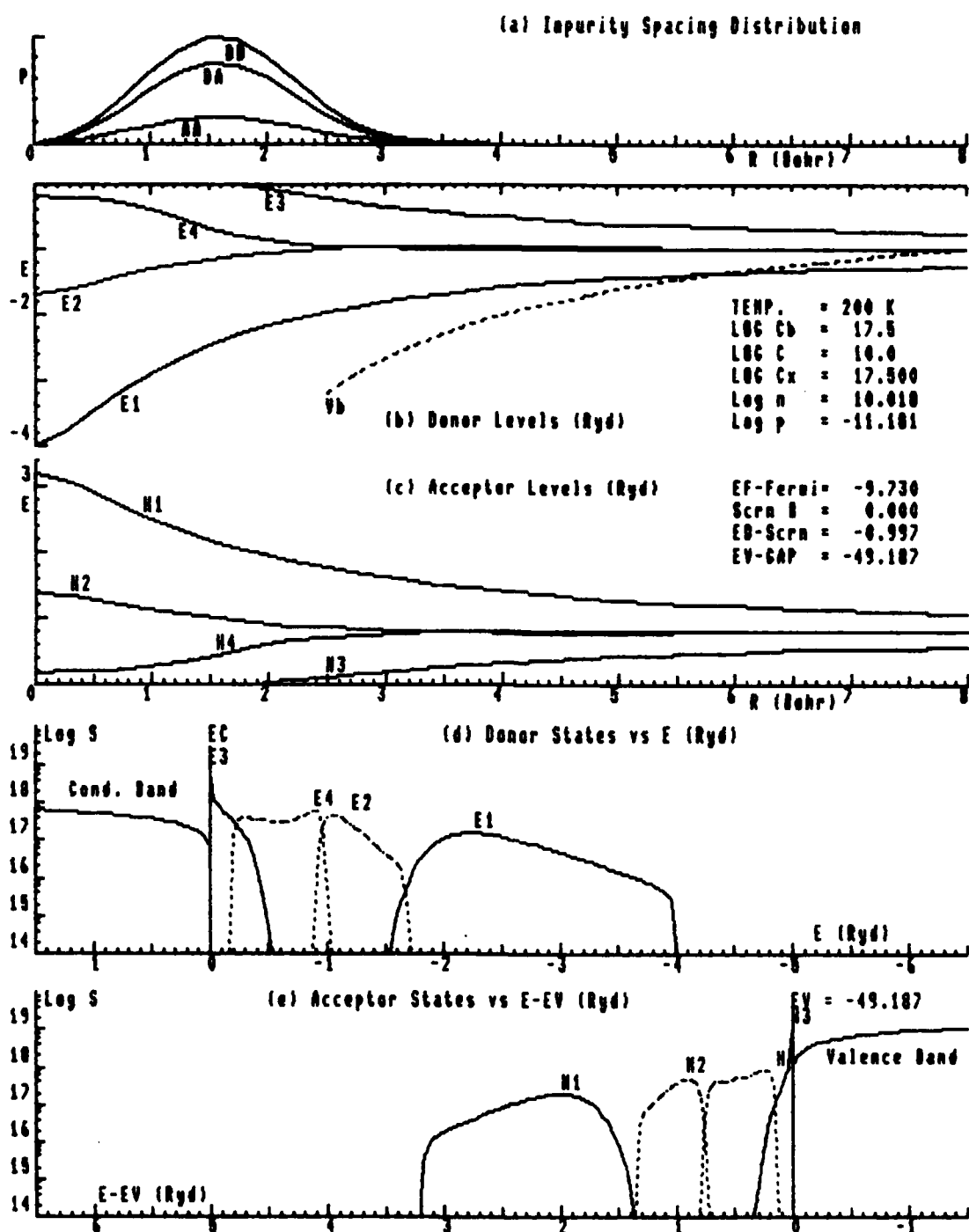


Fig. A 244. (a) Probability, $AA + DA + DD$, of Pairs vs R
 (b) Donor Energy $E_1; (DD)^-, E_2; (DD)^-, E_3; (DA)^-, E_4; (DA)^-$ vs R
 (c) Acceptor En. $H_1; (AA)^+, H_2; (AA)^+, H_3; (AD)^+, H_4; (AD)^+$ vs R
 (d) Densities of Donor States, E_1, E_2, E_3 , & E_4 , vs E
 (e) Densities of Acceptor States, H_1, H_2, H_3 , & H_4 vs $E-EV$.

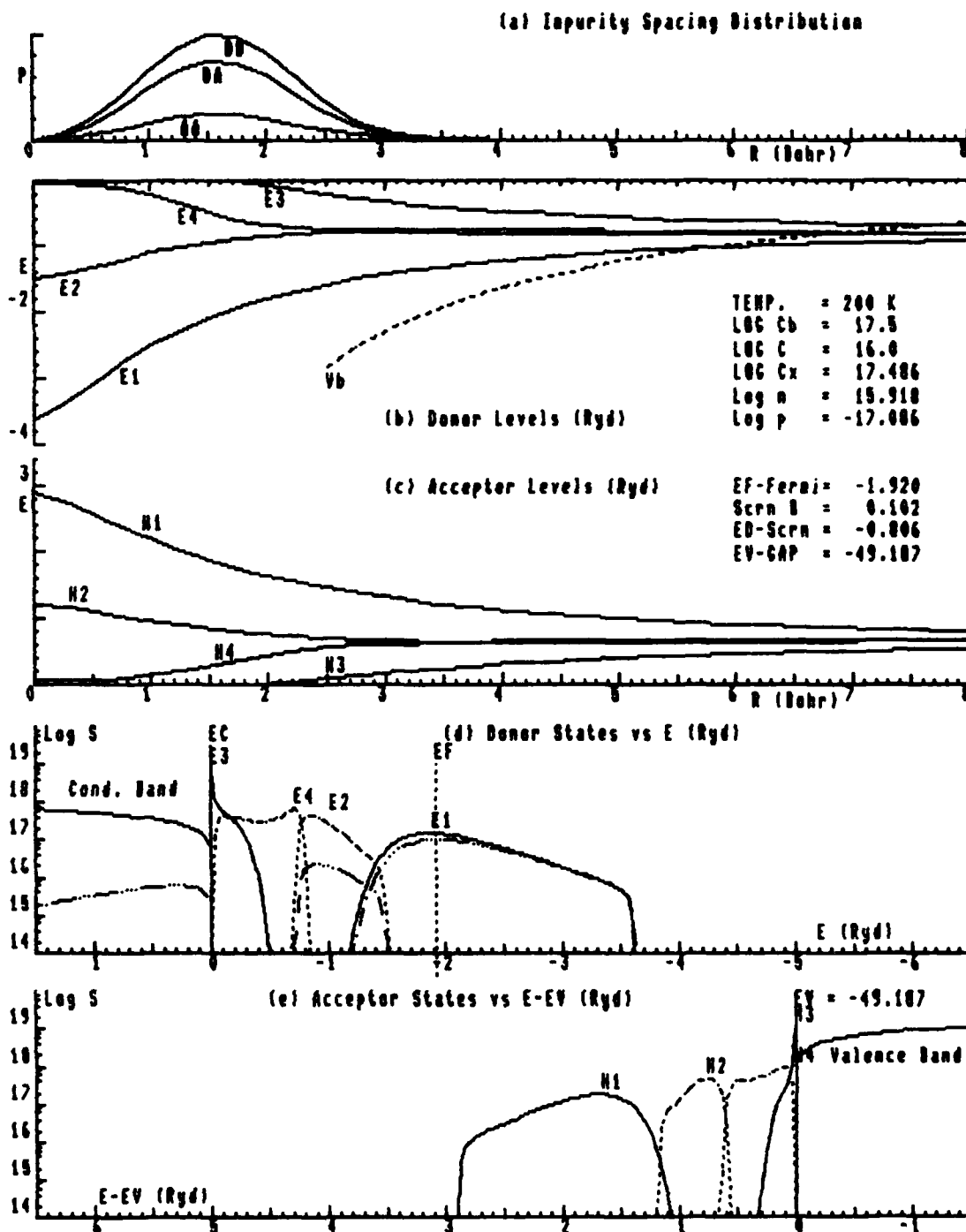


Fig. A 245. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

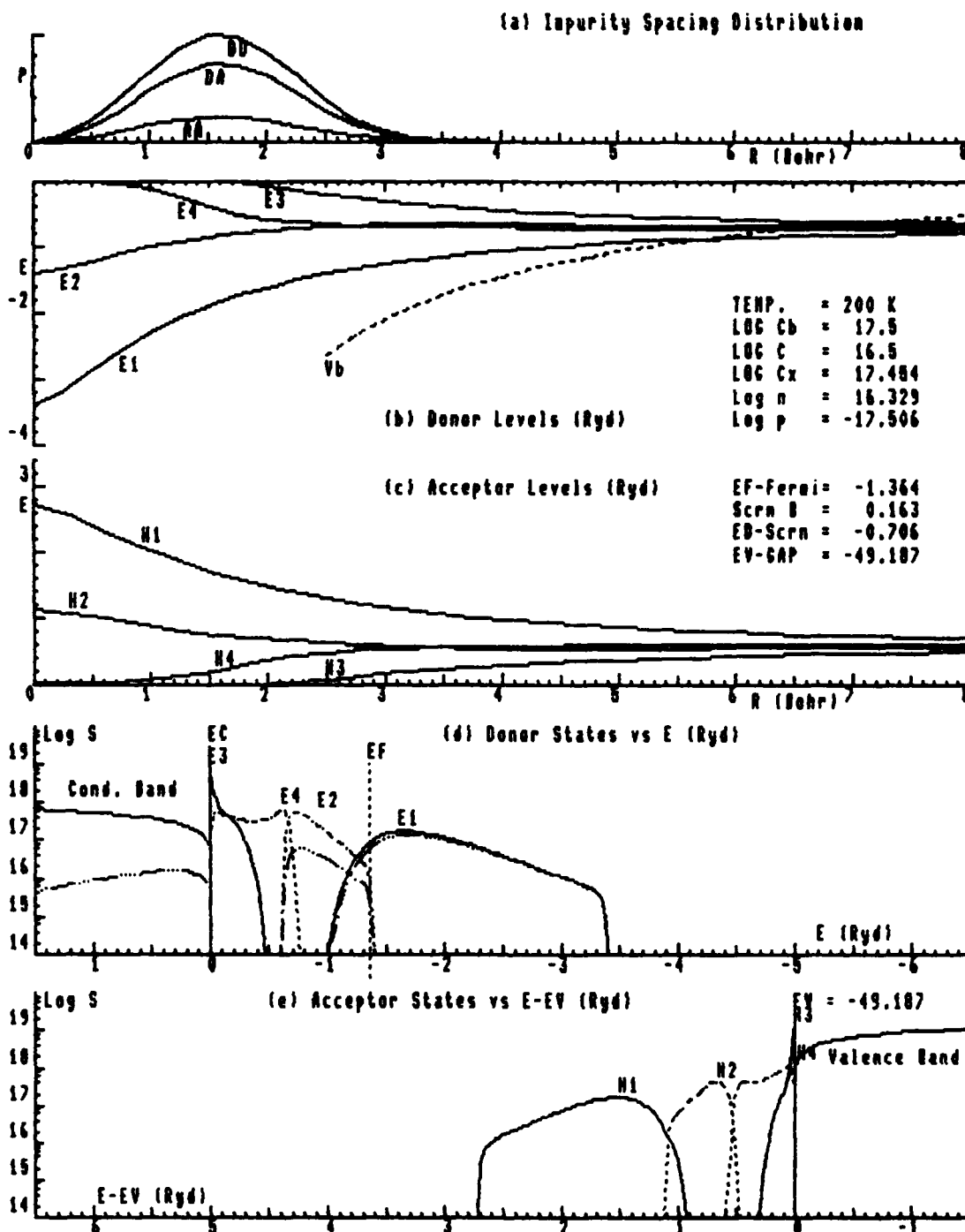


Fig. A 246. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)+, E3; (DA)-, E4 (DA)+ vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)-, H3; (AD)+, H4 (AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

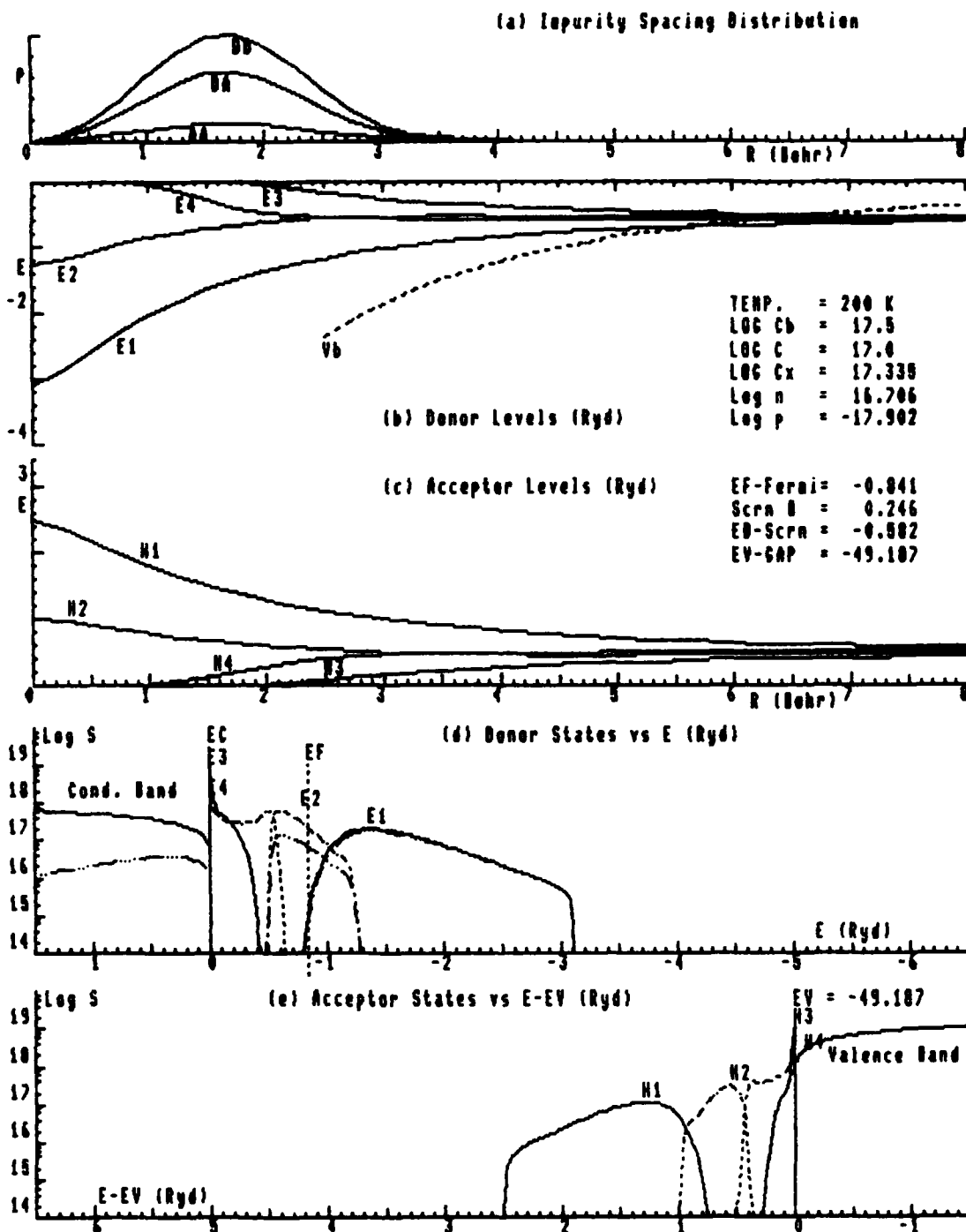


Fig. A 247. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

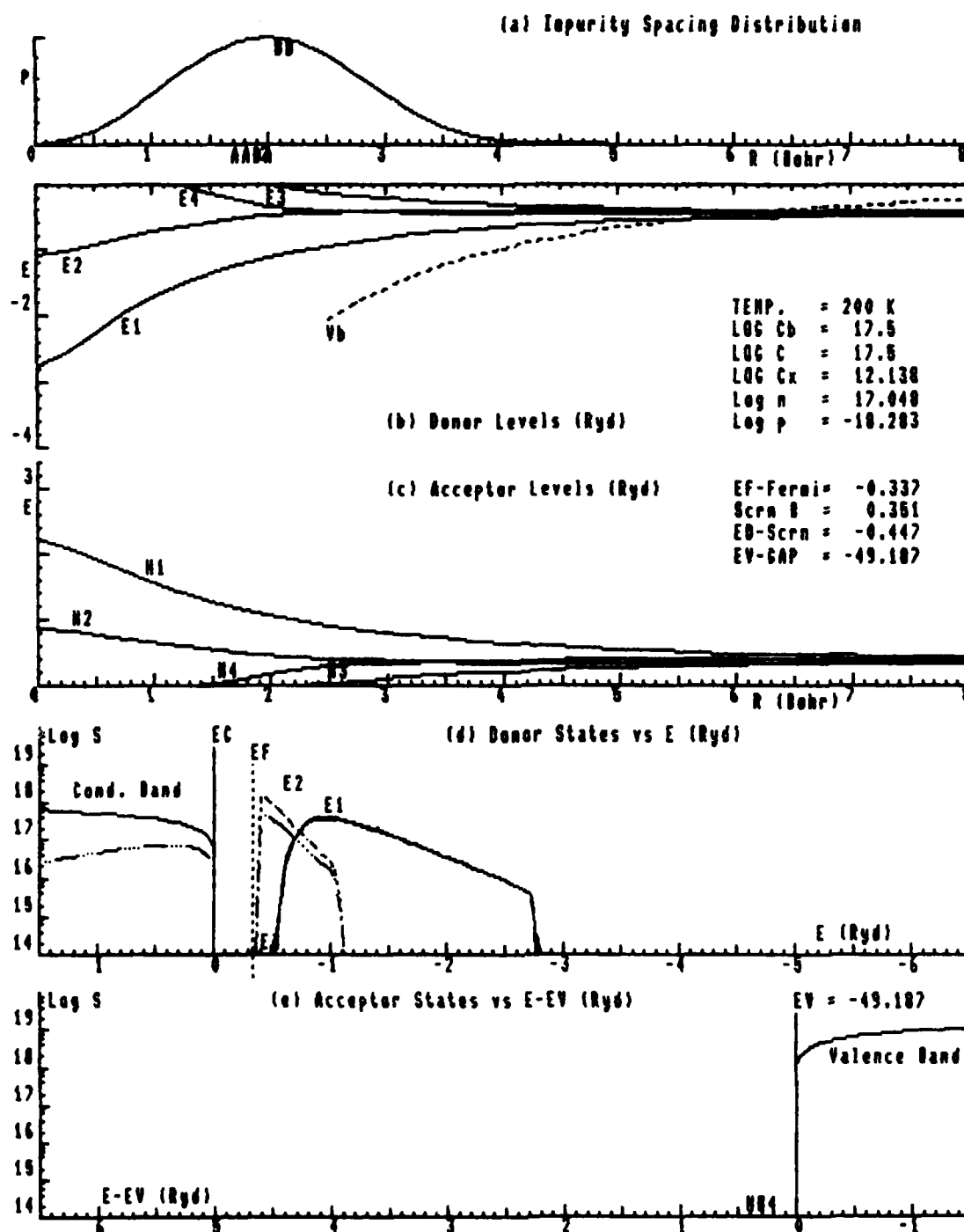


Fig. A 248. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

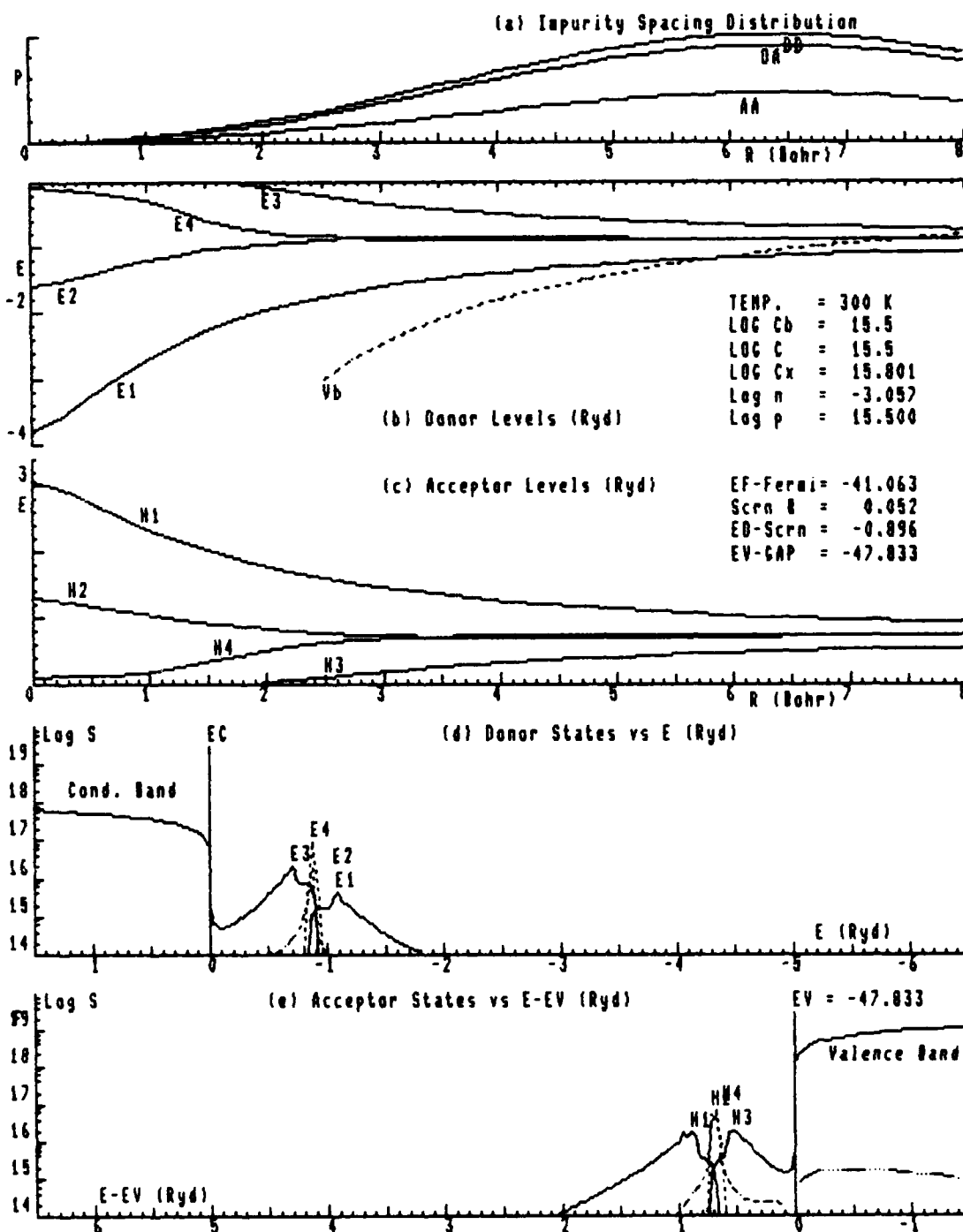


Fig. A 300. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

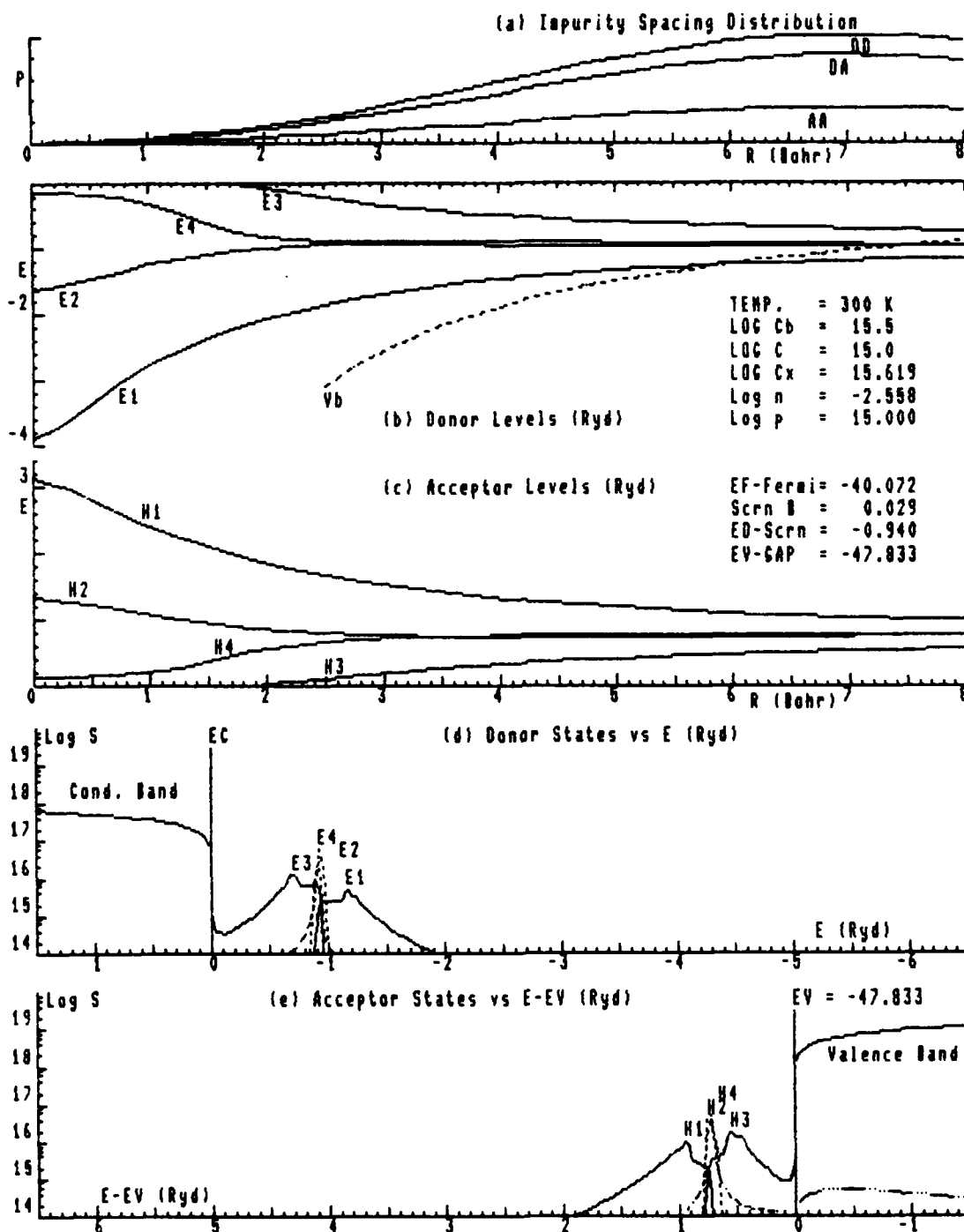


Fig. A 301. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

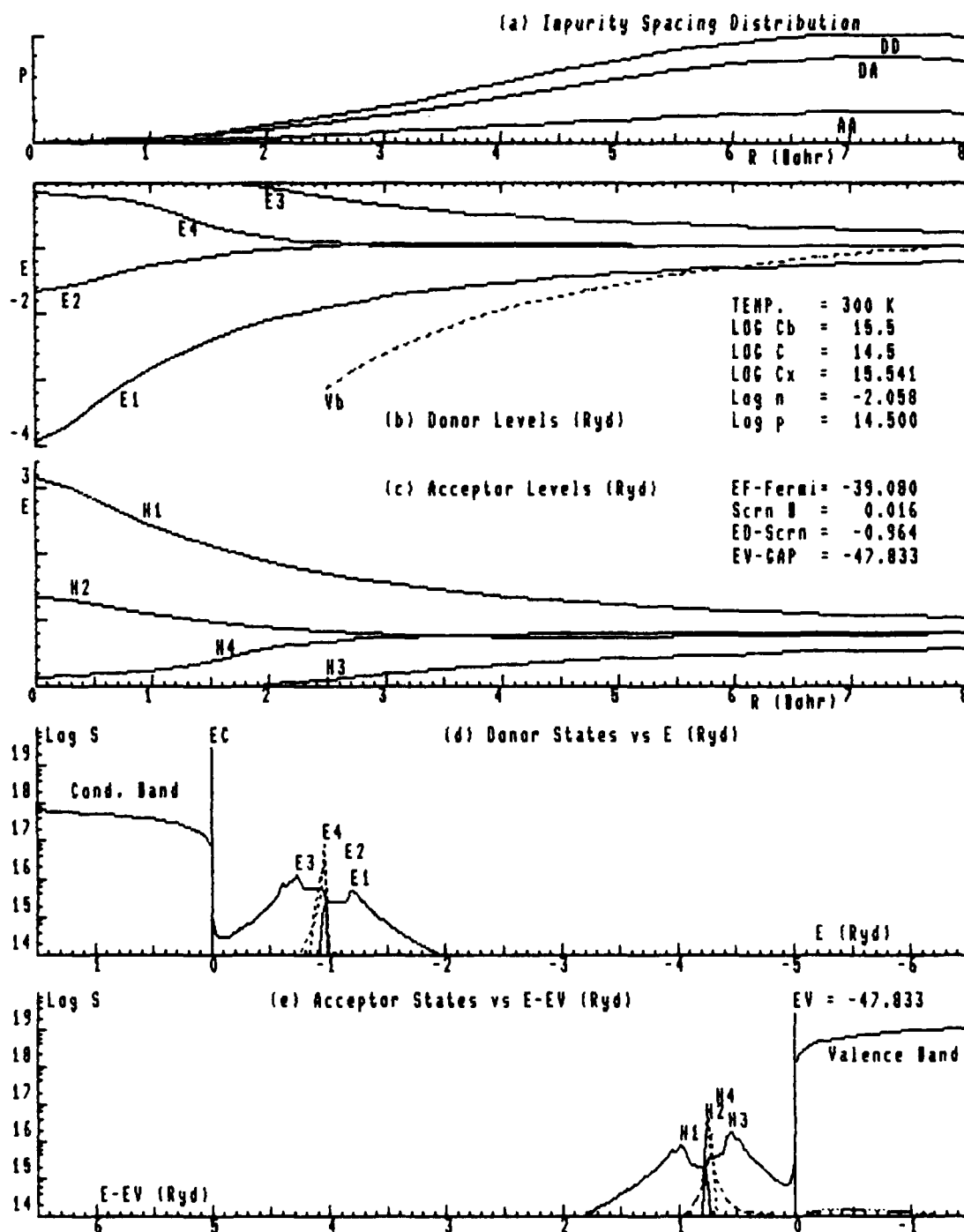


Fig. A 302. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

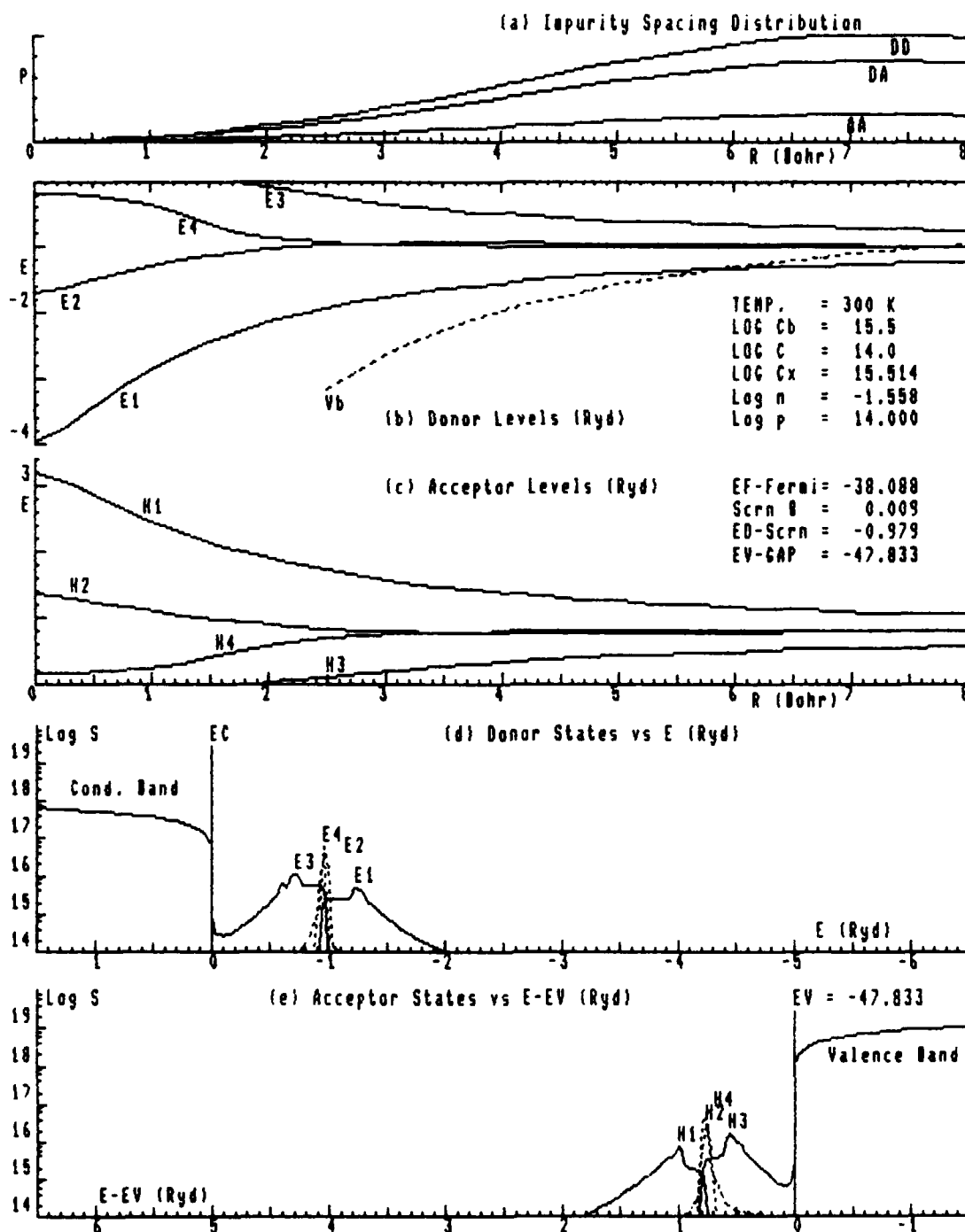


Fig. A 303. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

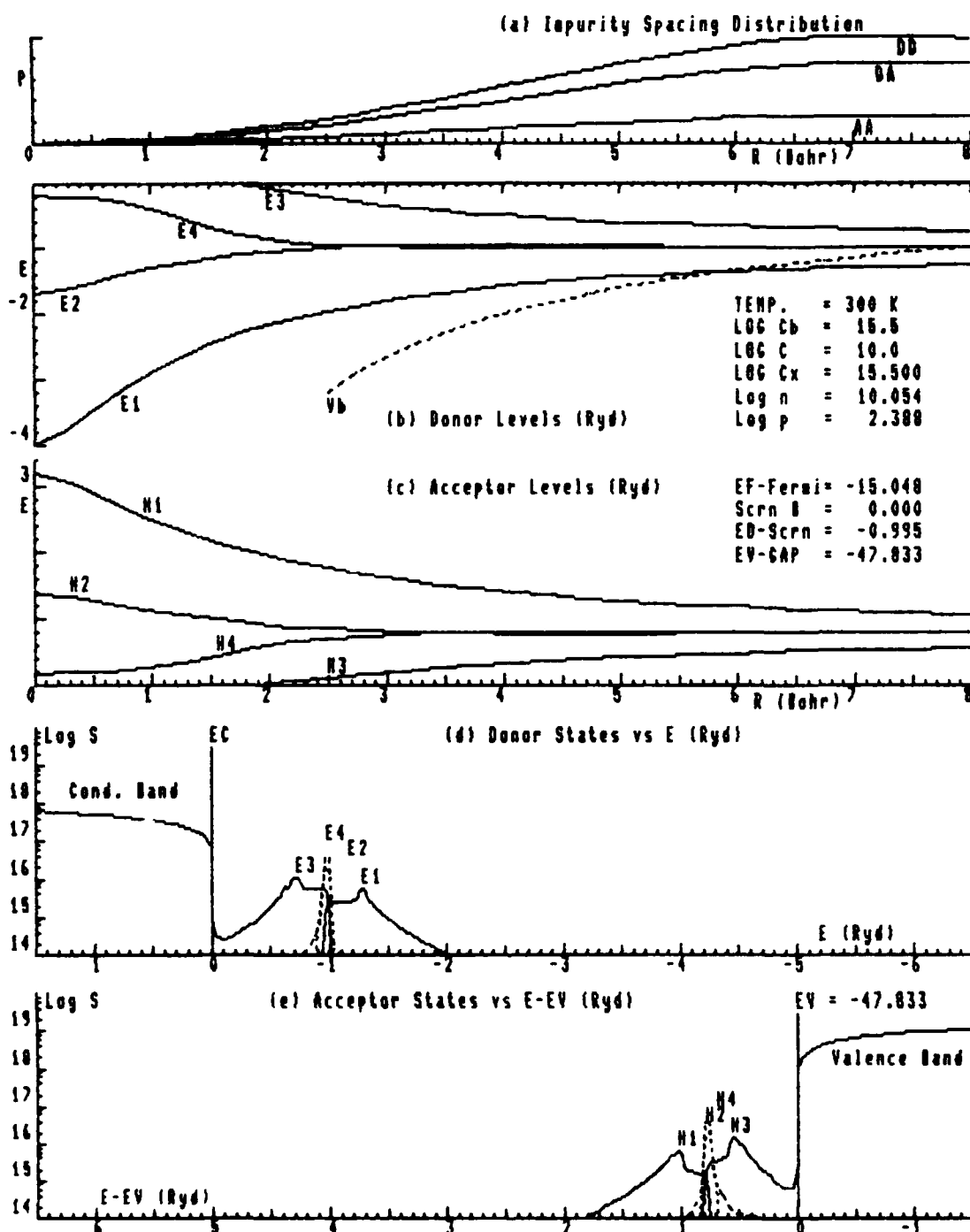


Fig. A 304. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD)-+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

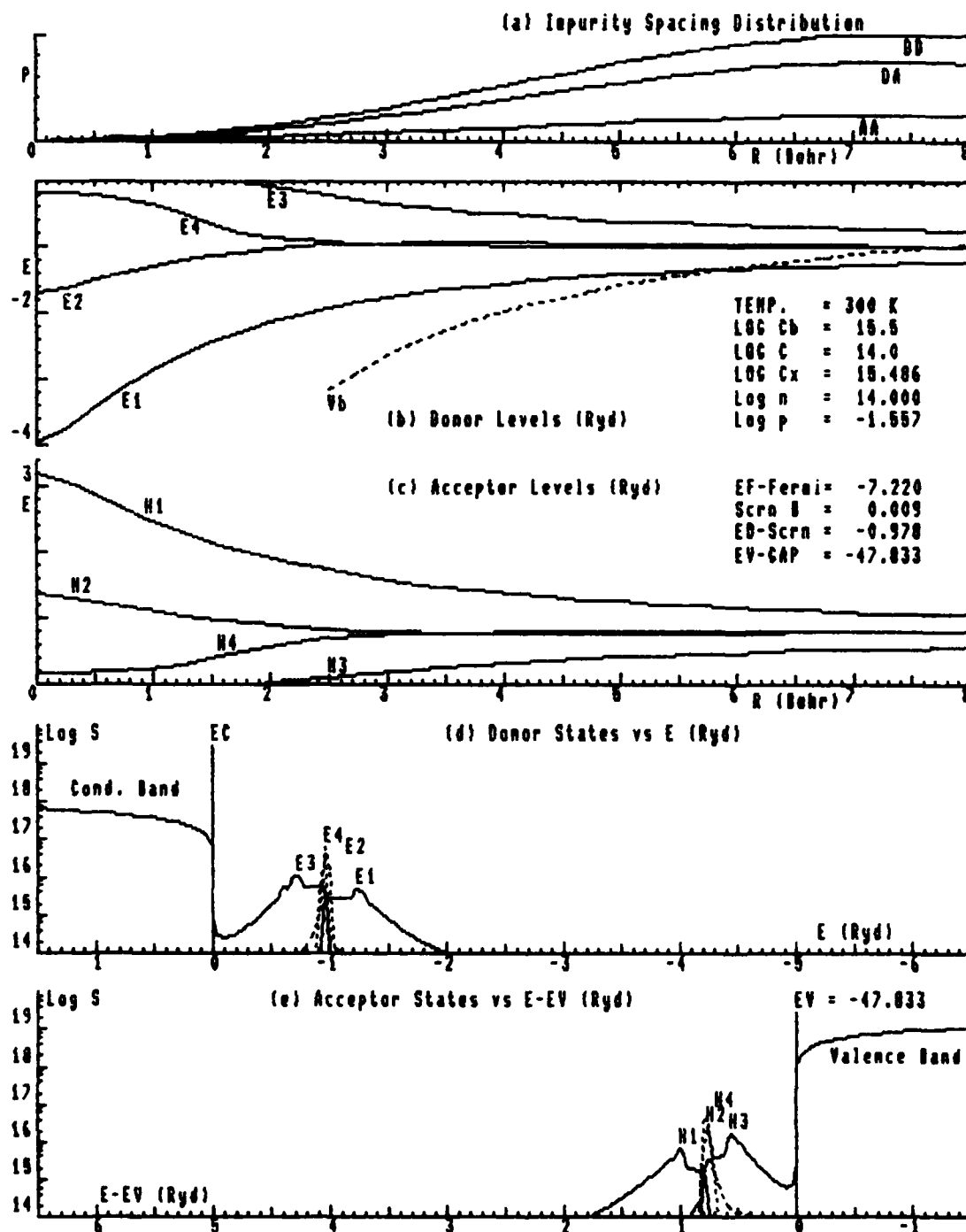


Fig. A 305. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

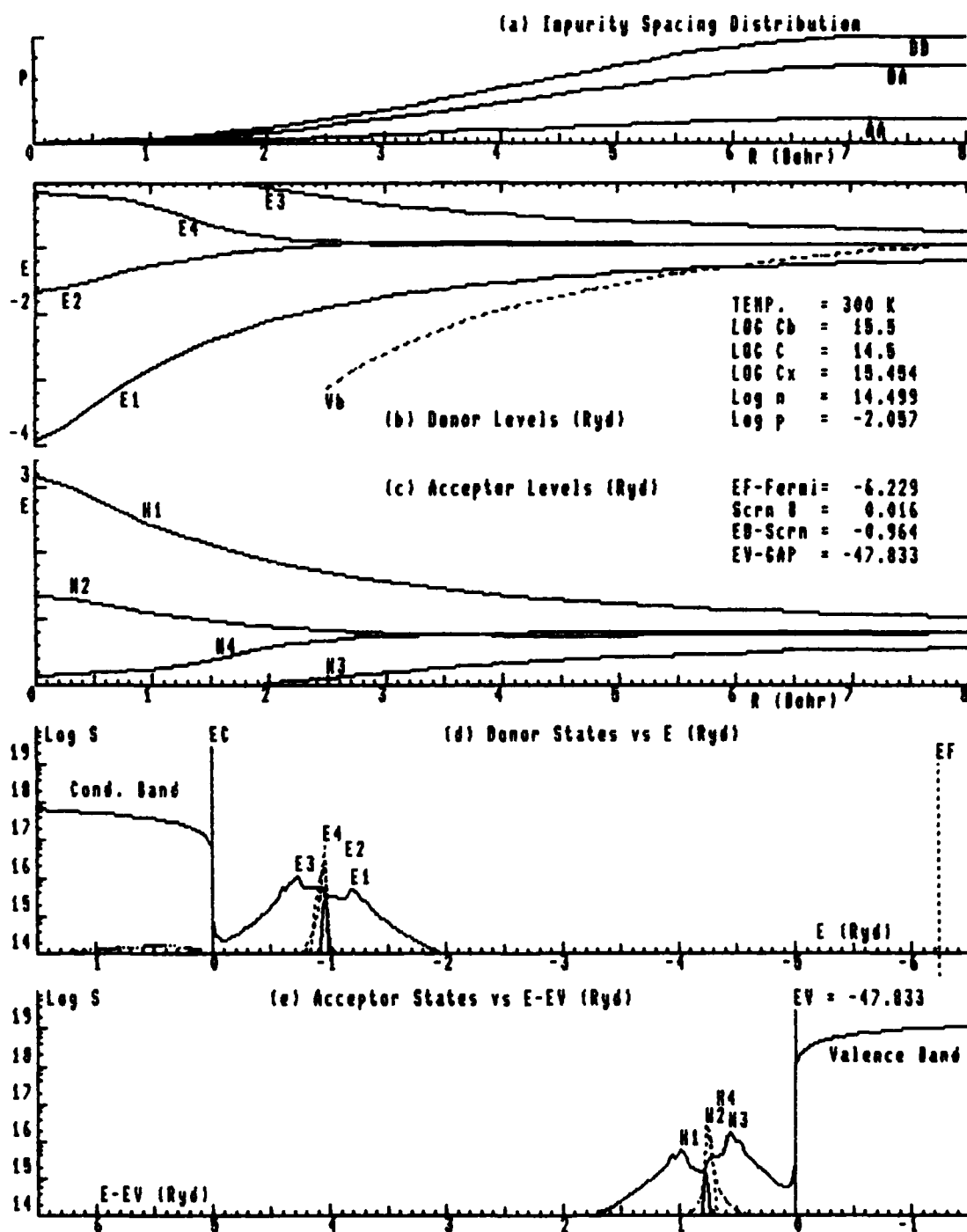


Fig. A 306. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

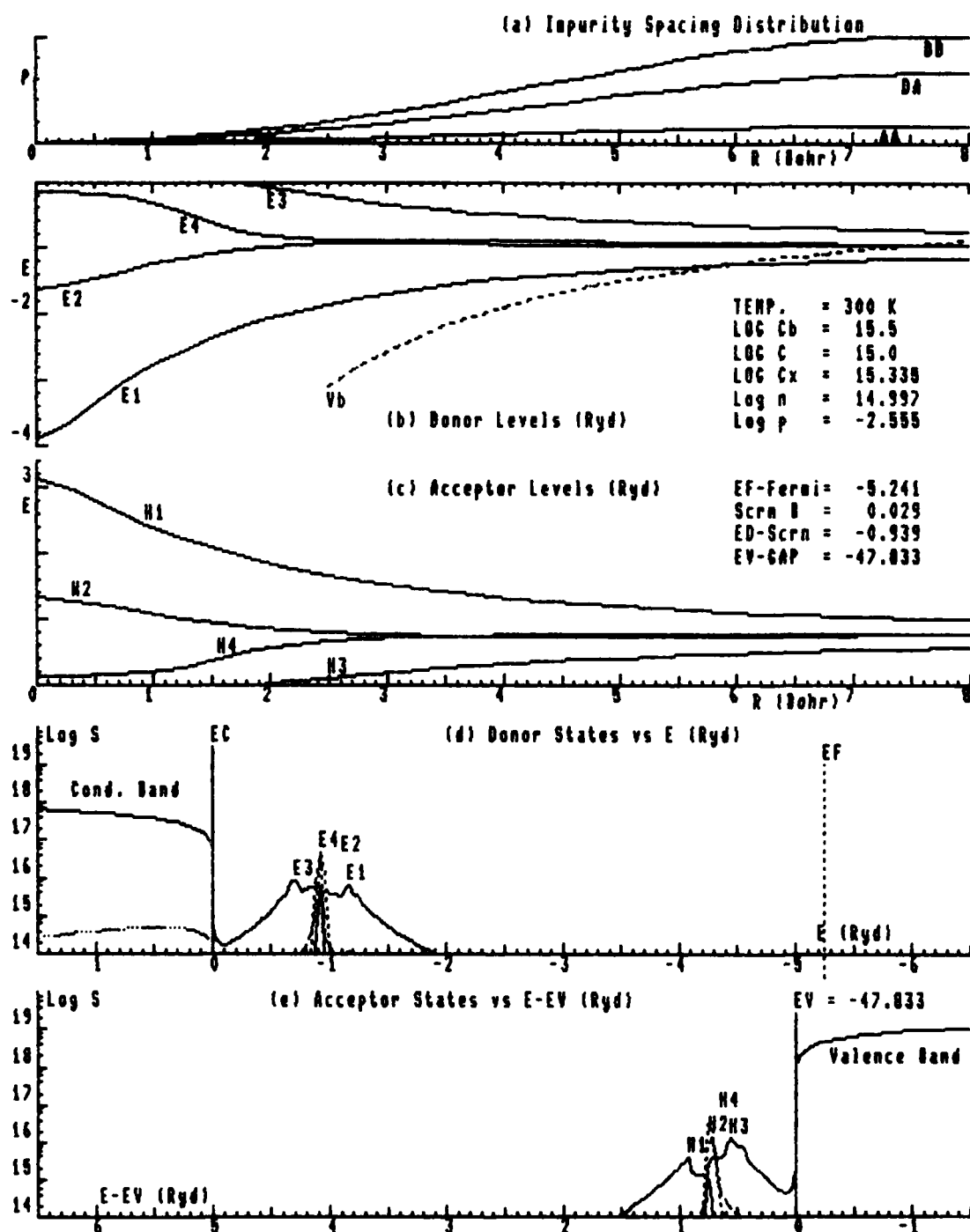


Fig. A 307. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

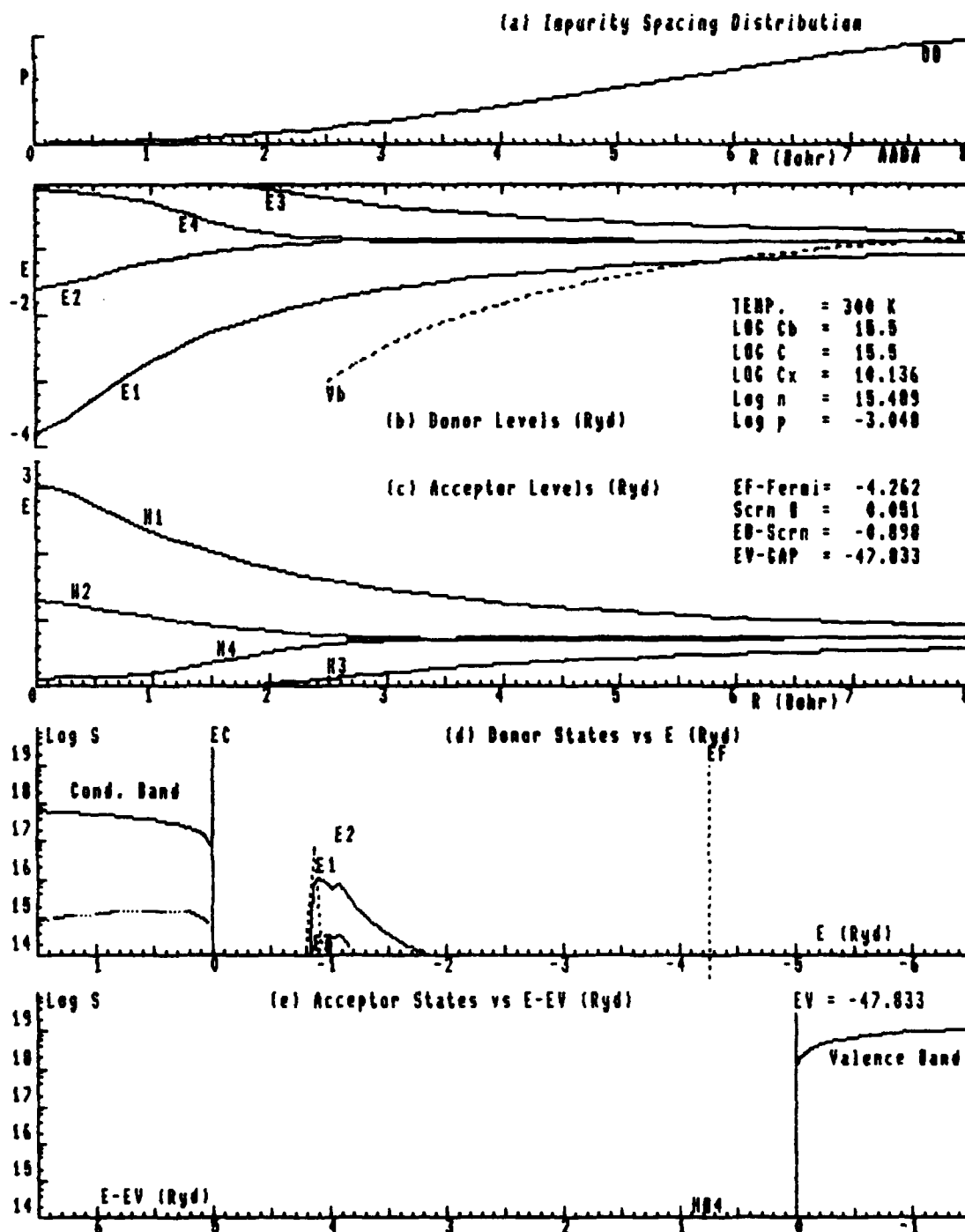


Fig. A 308. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

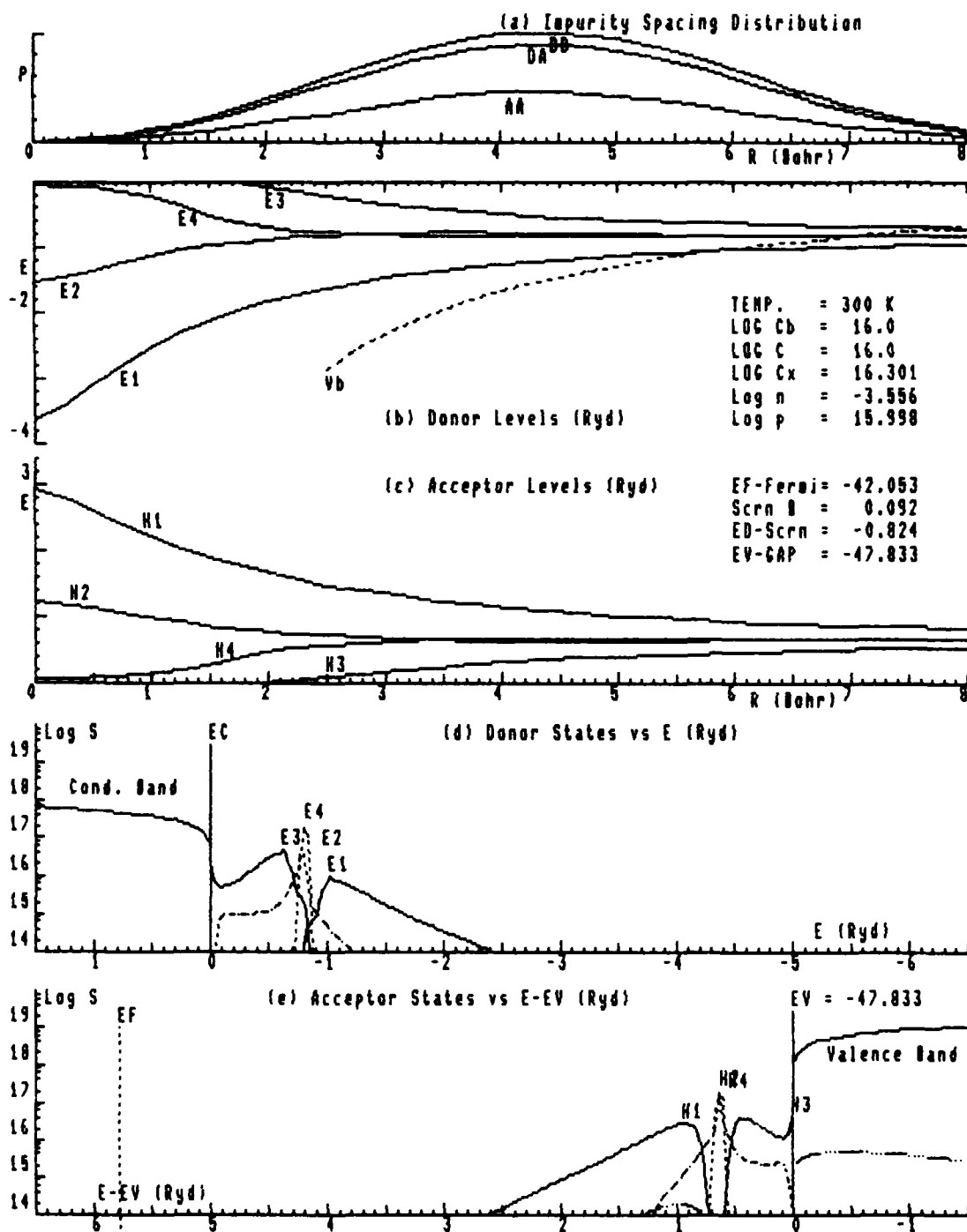


Fig. A 310. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

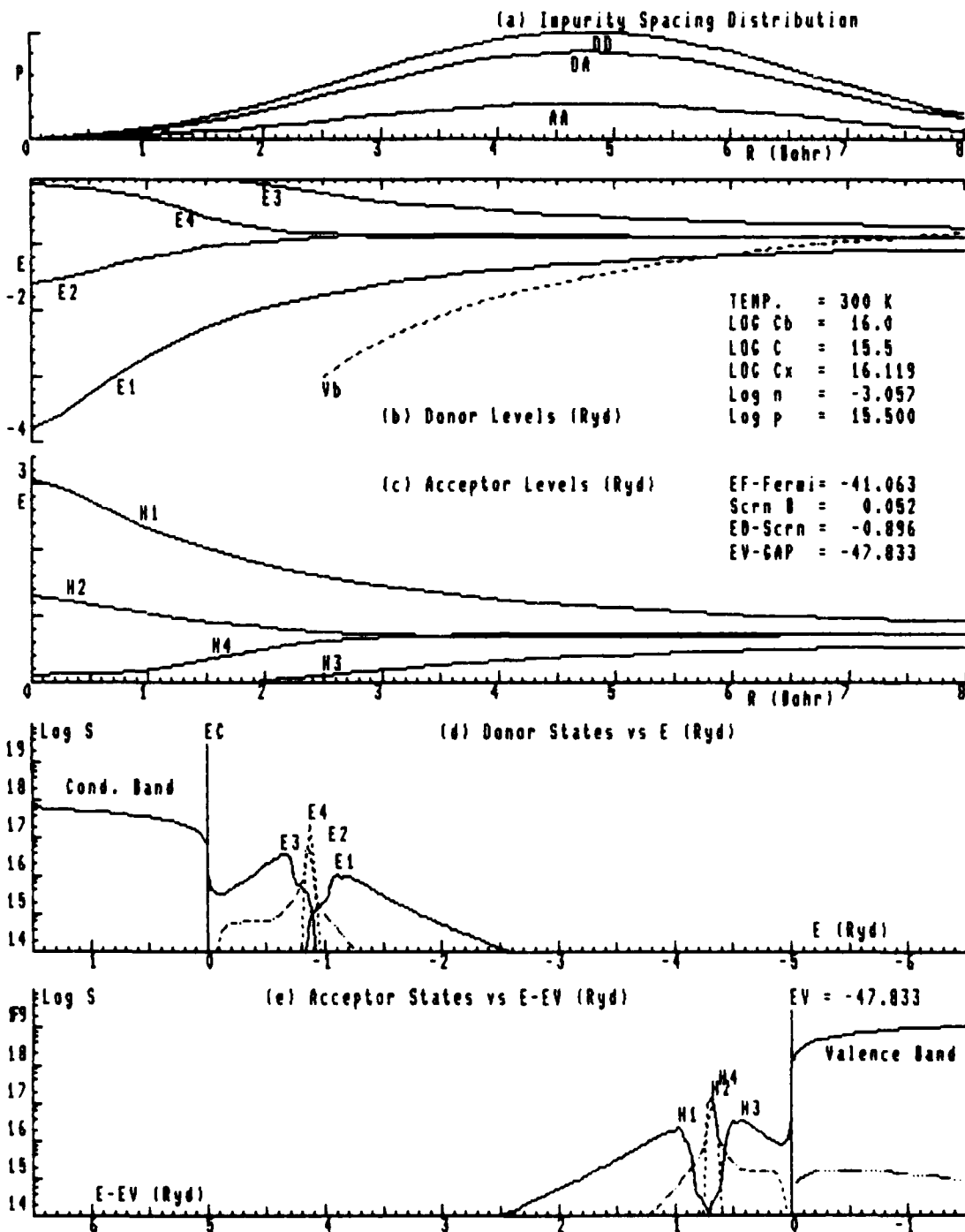


Fig. A 311. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

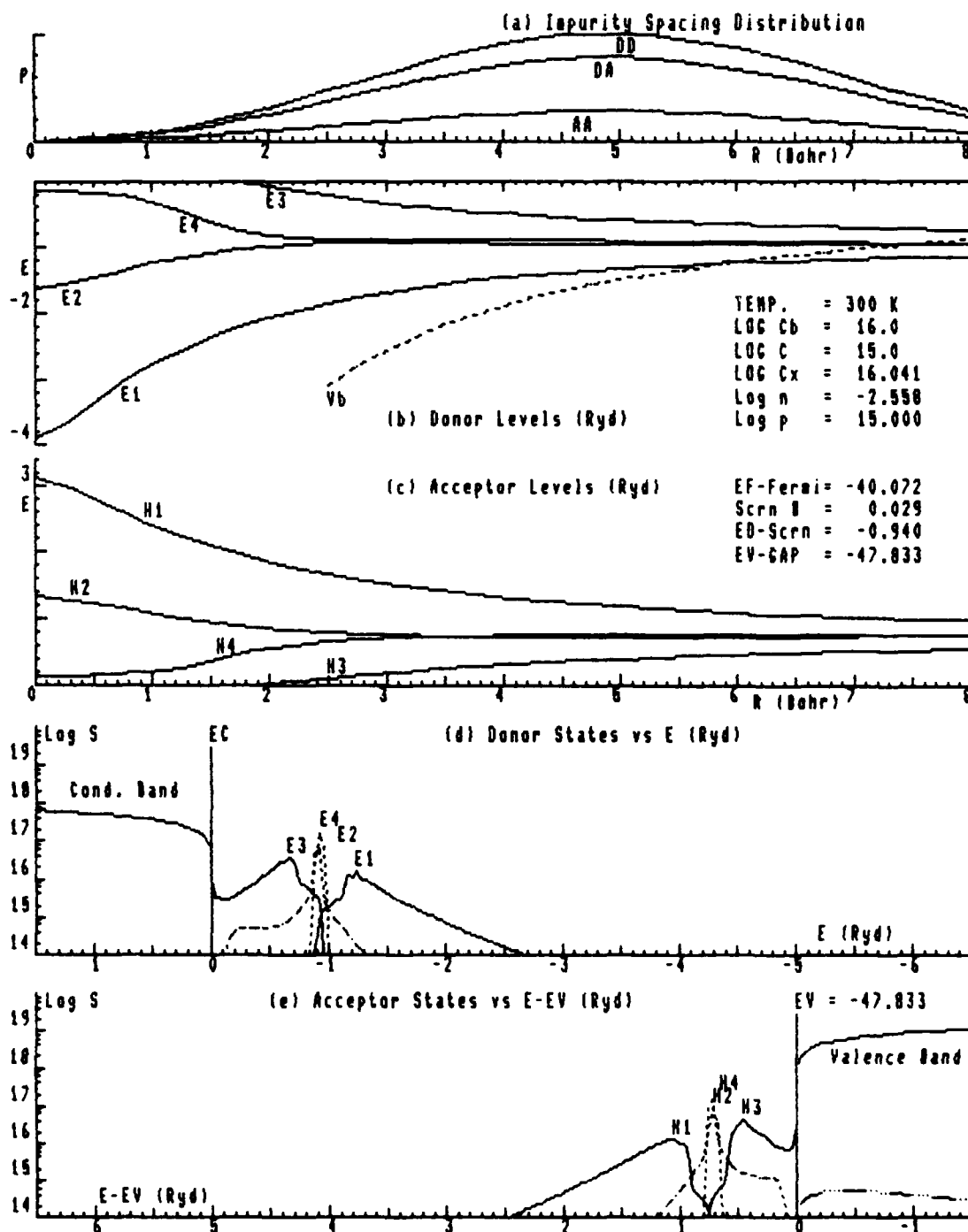


Fig. A 312. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA+)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

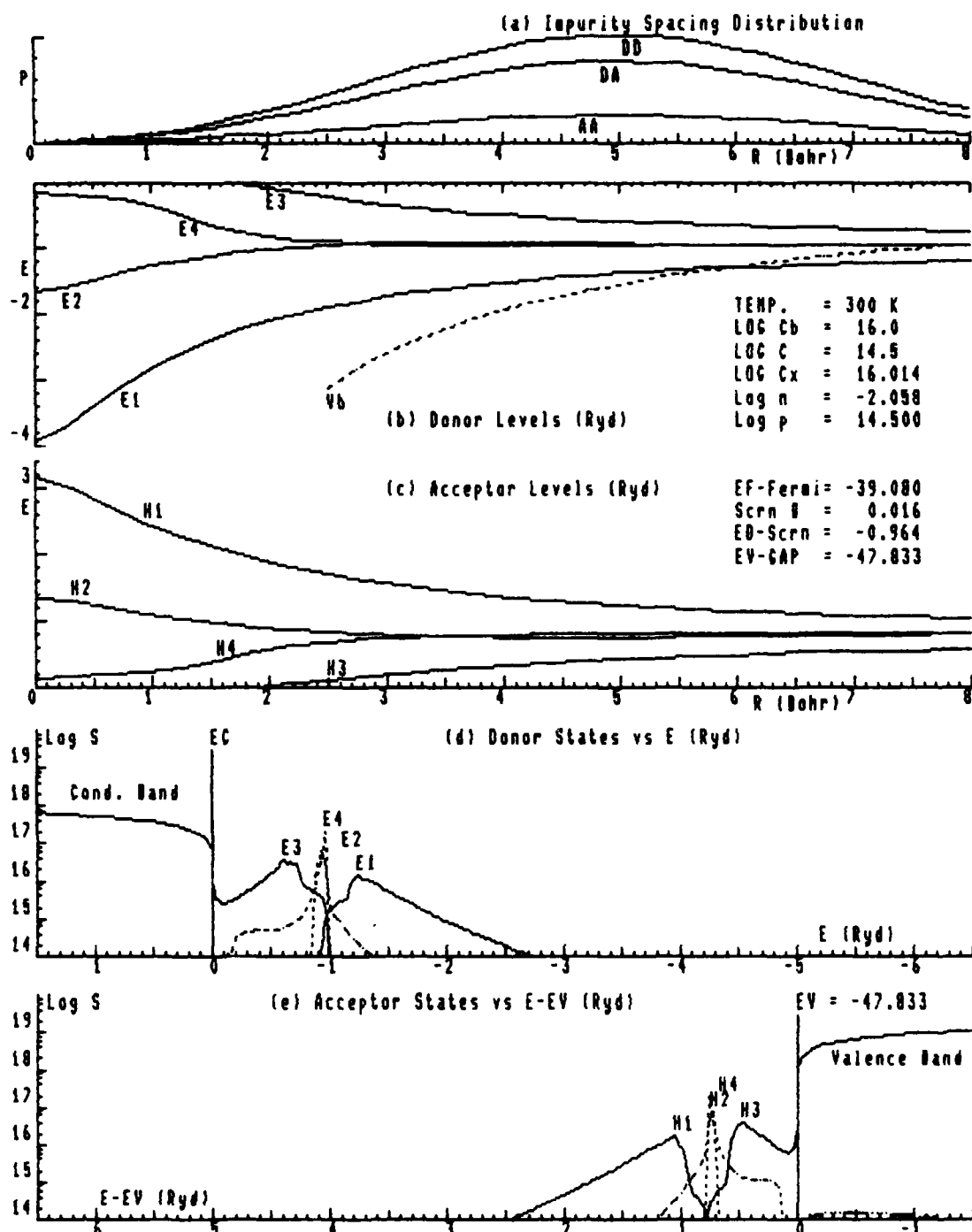


Fig. A 313. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

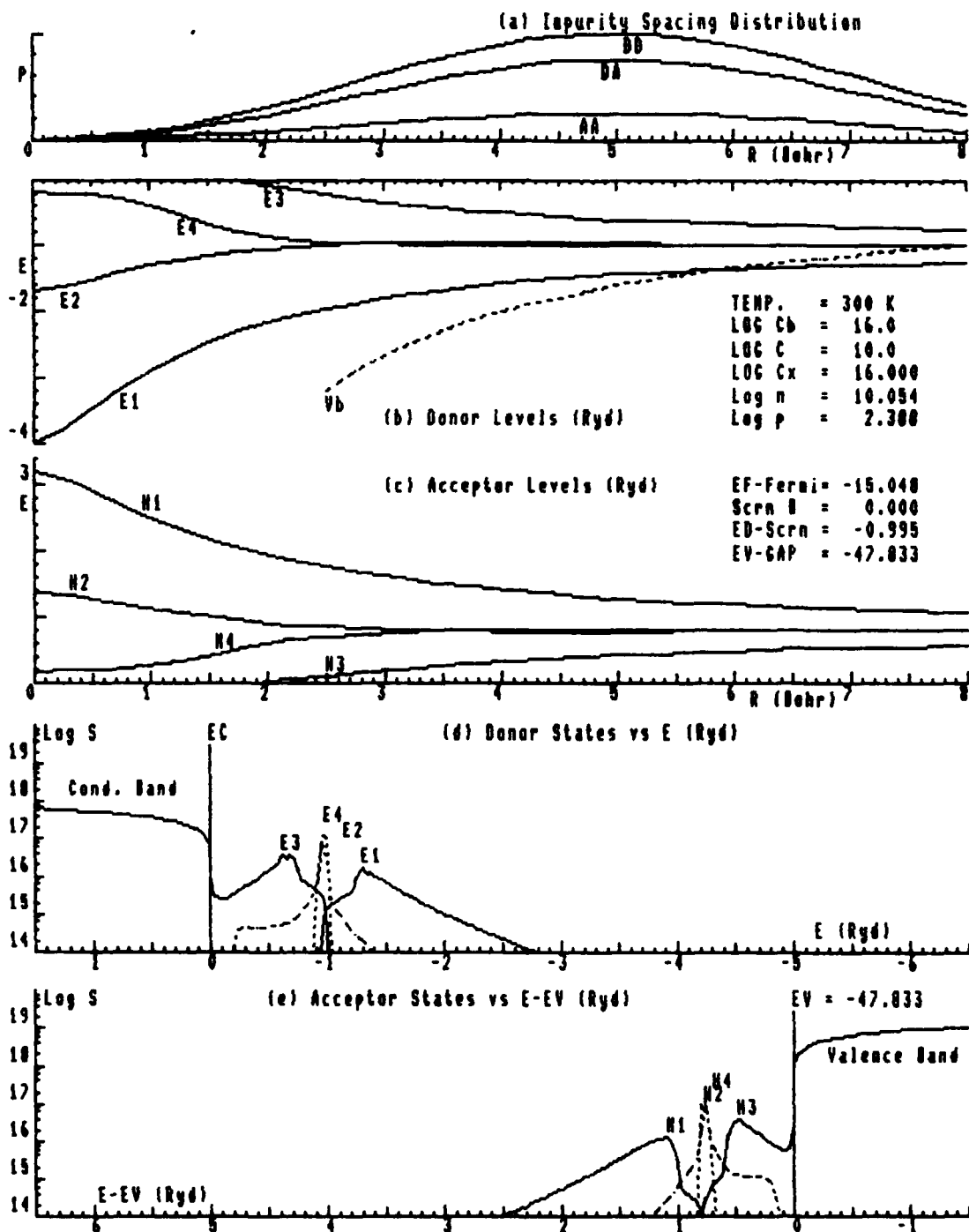


Fig. A 314. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

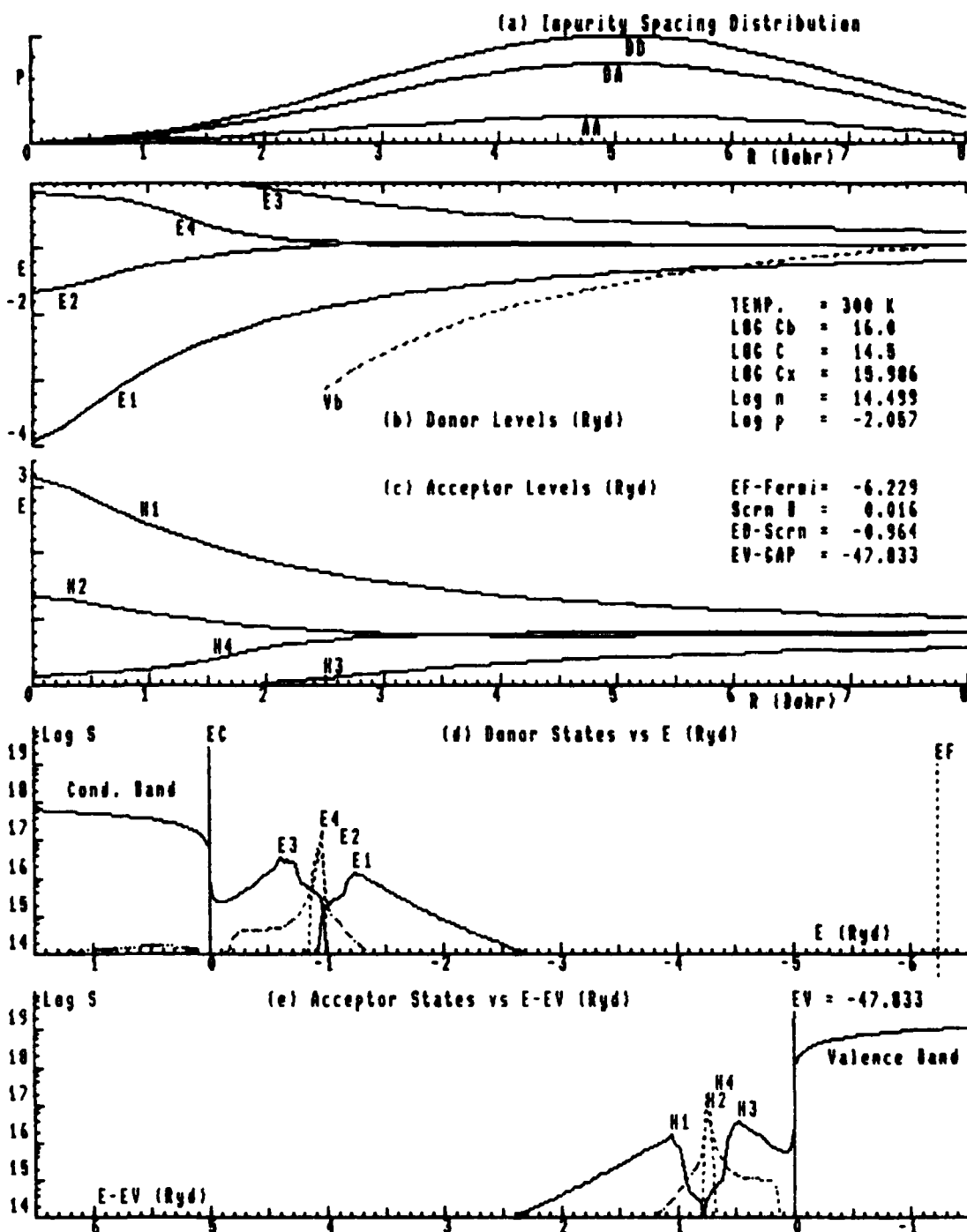


Fig. A 315. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

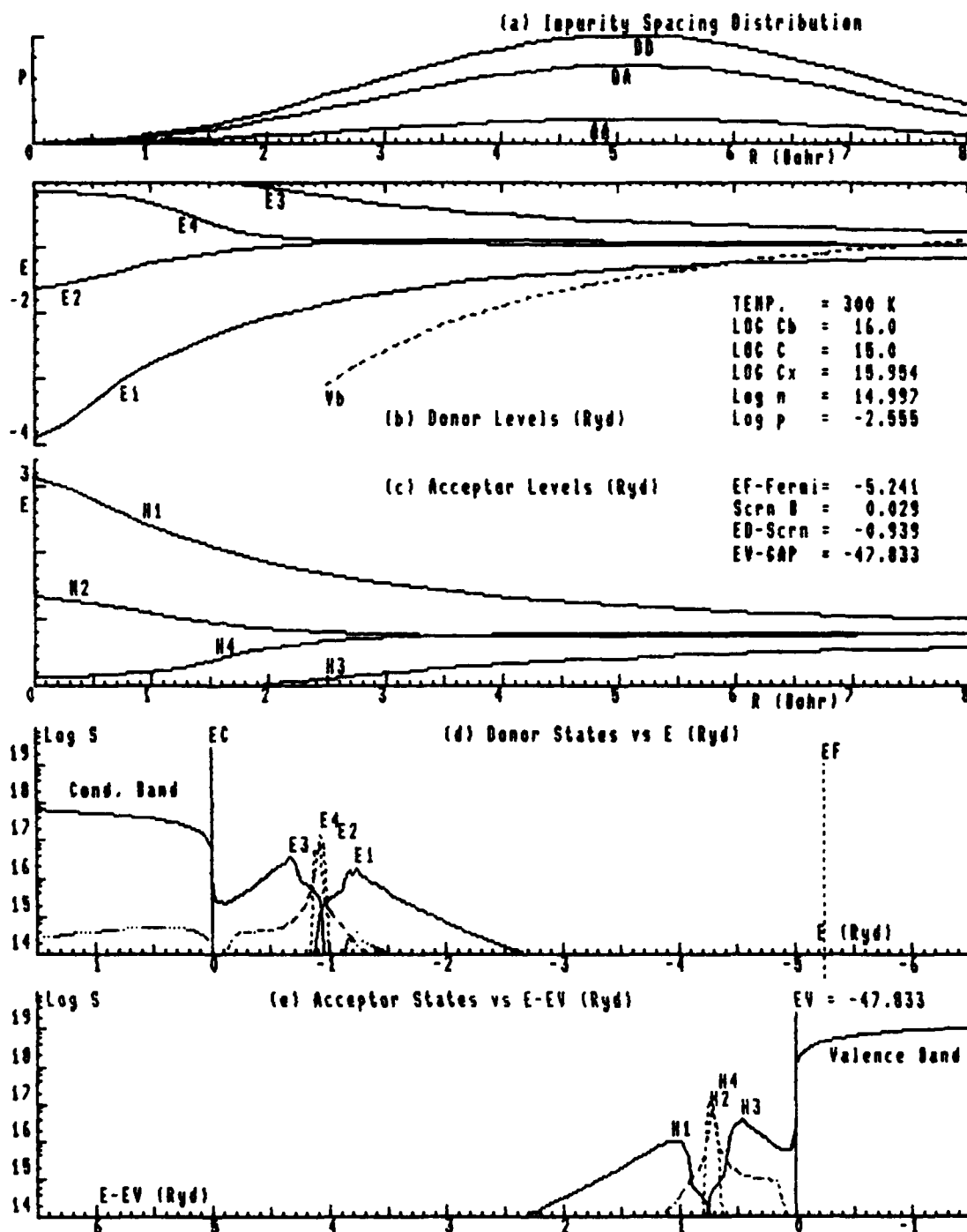


Fig. A 316. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

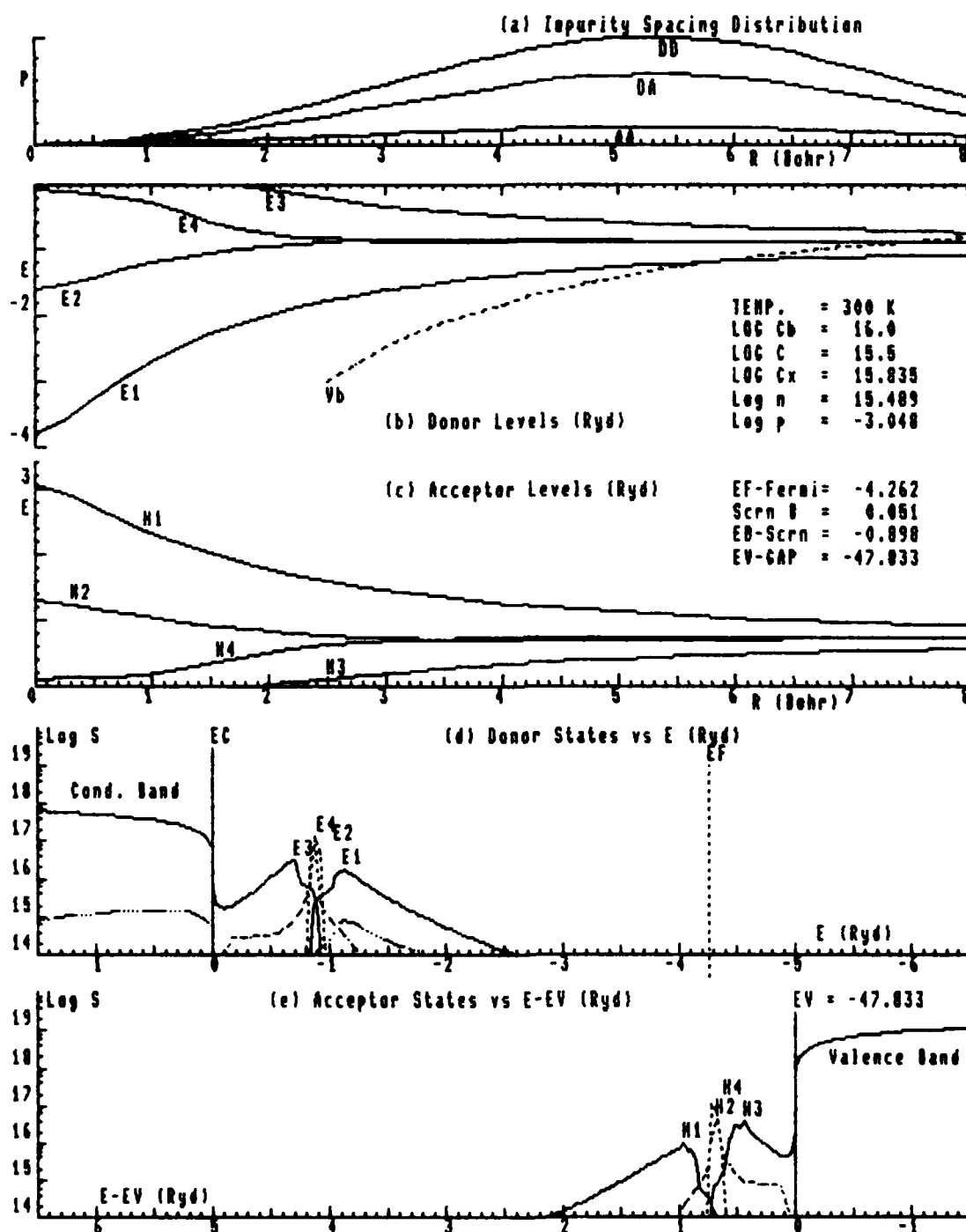


Fig. A 317. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)-+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

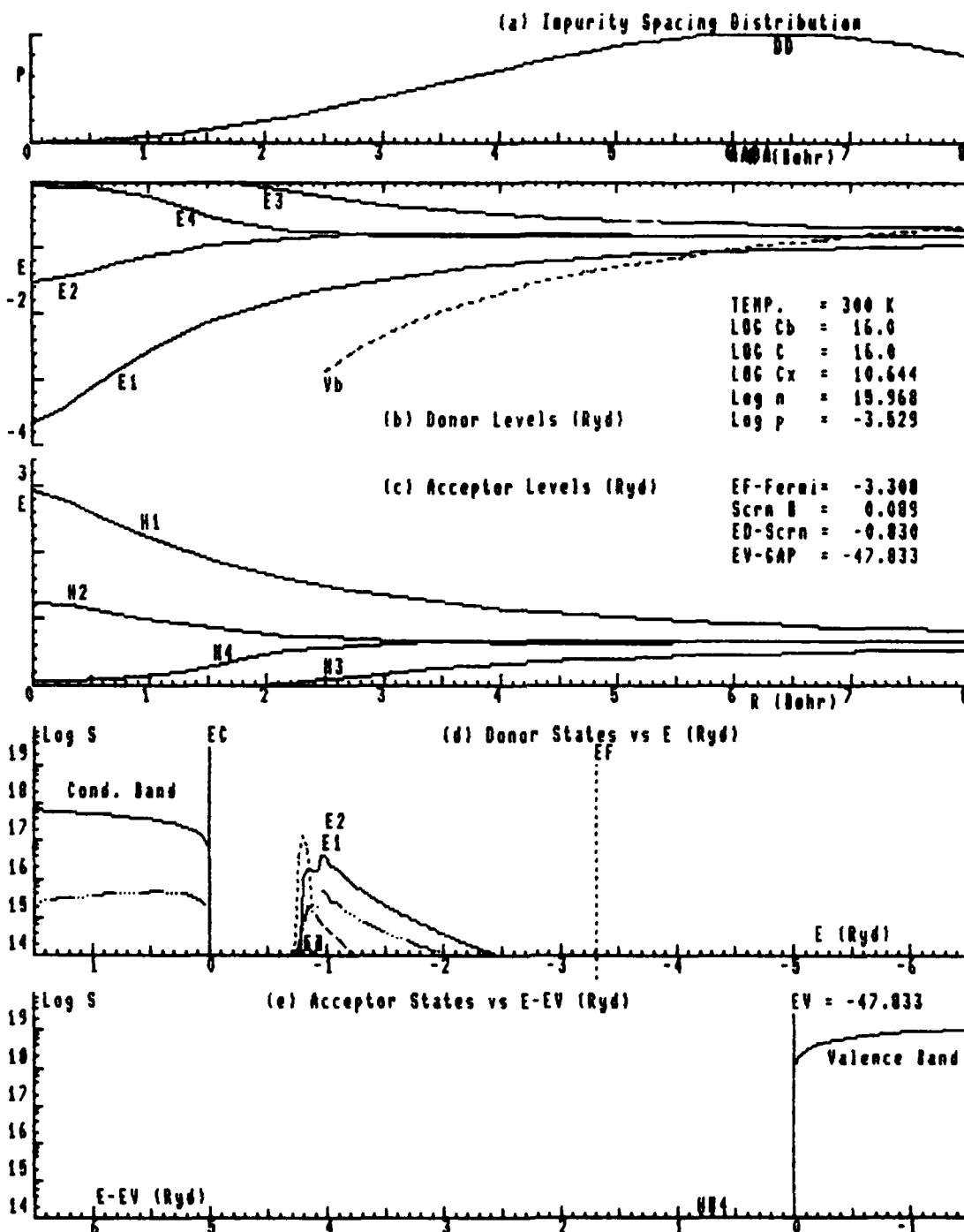


Fig. A 31B. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

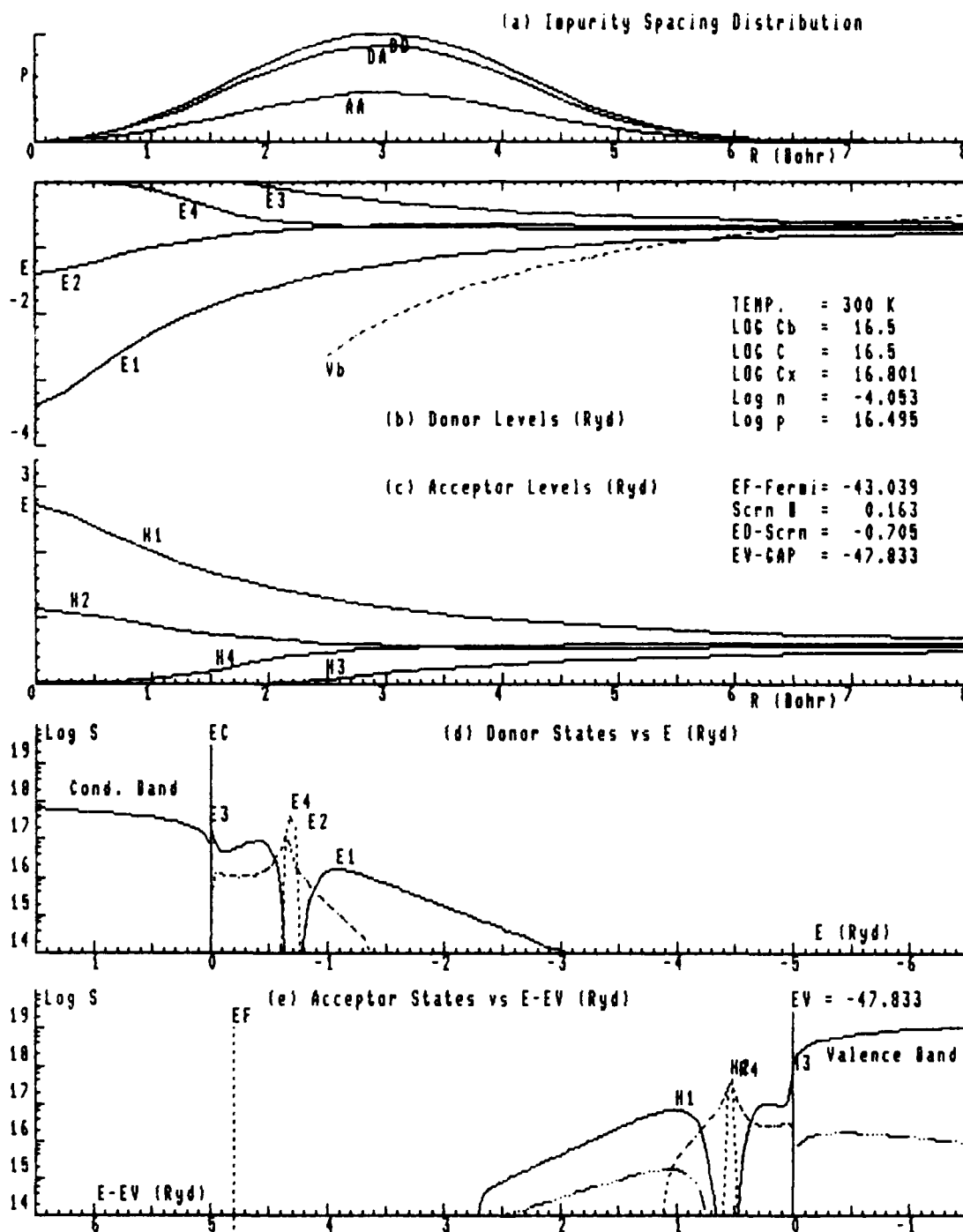


Fig. A 320. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

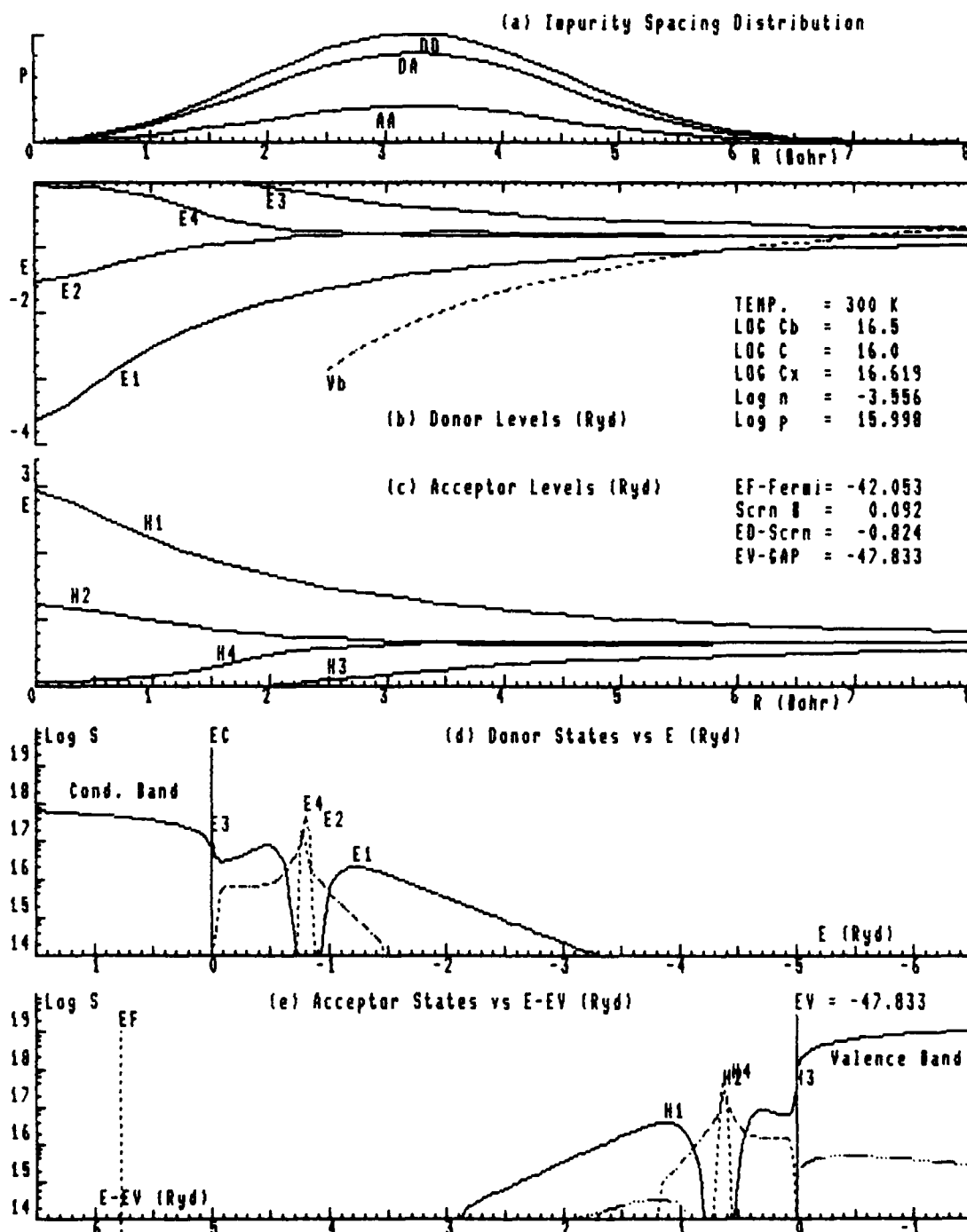


Fig. A 321. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

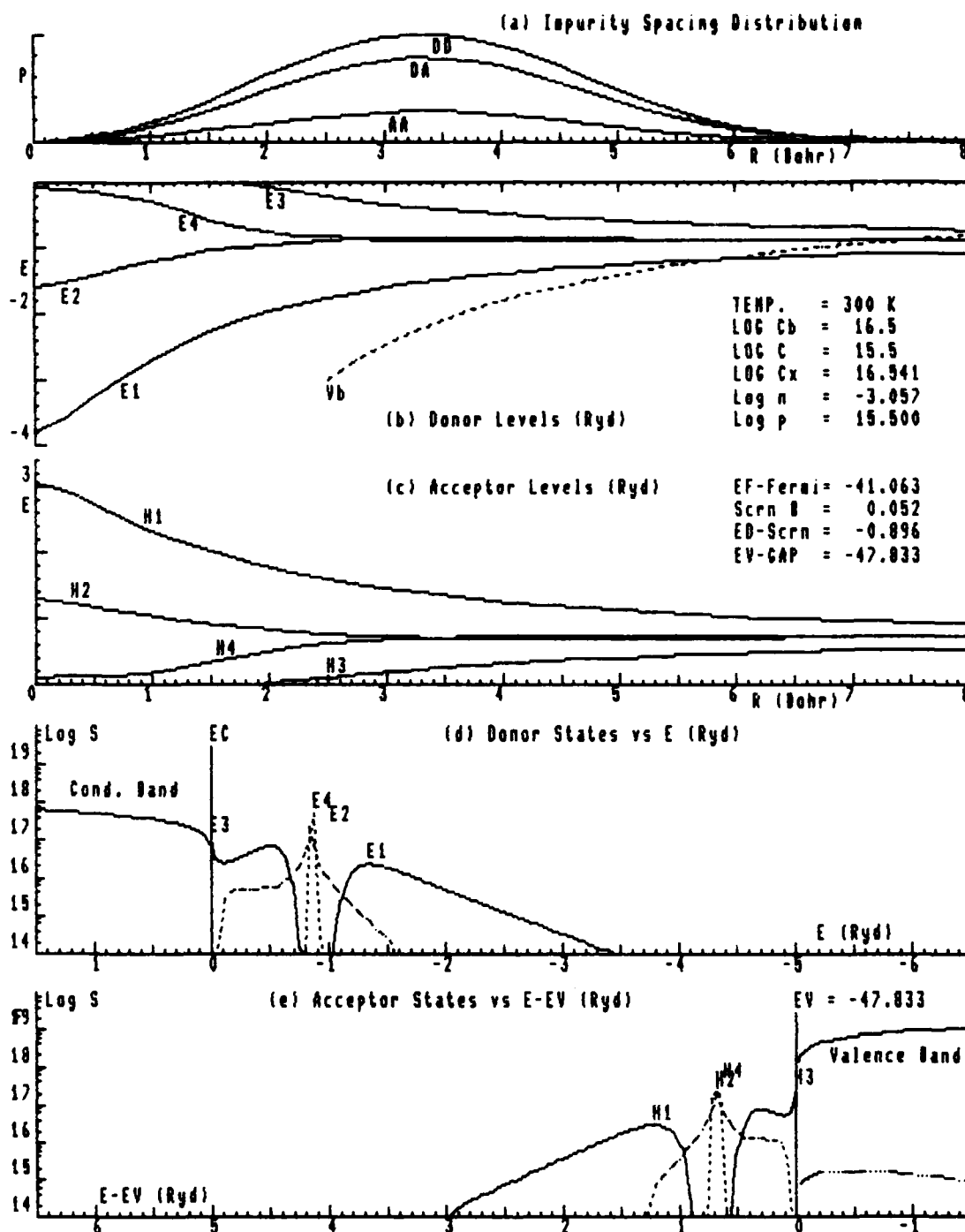


Fig. A 322. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

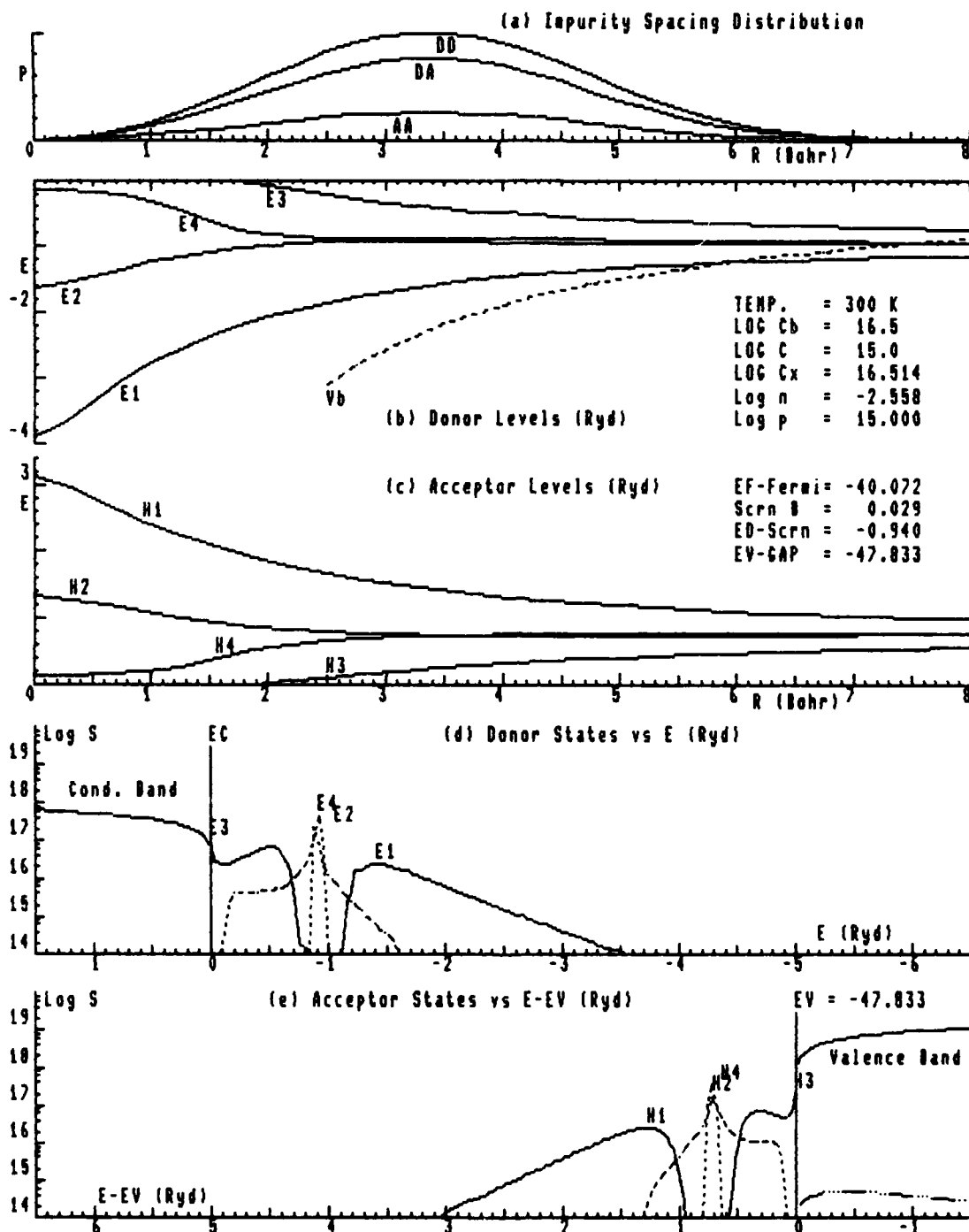


Fig. A 323. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

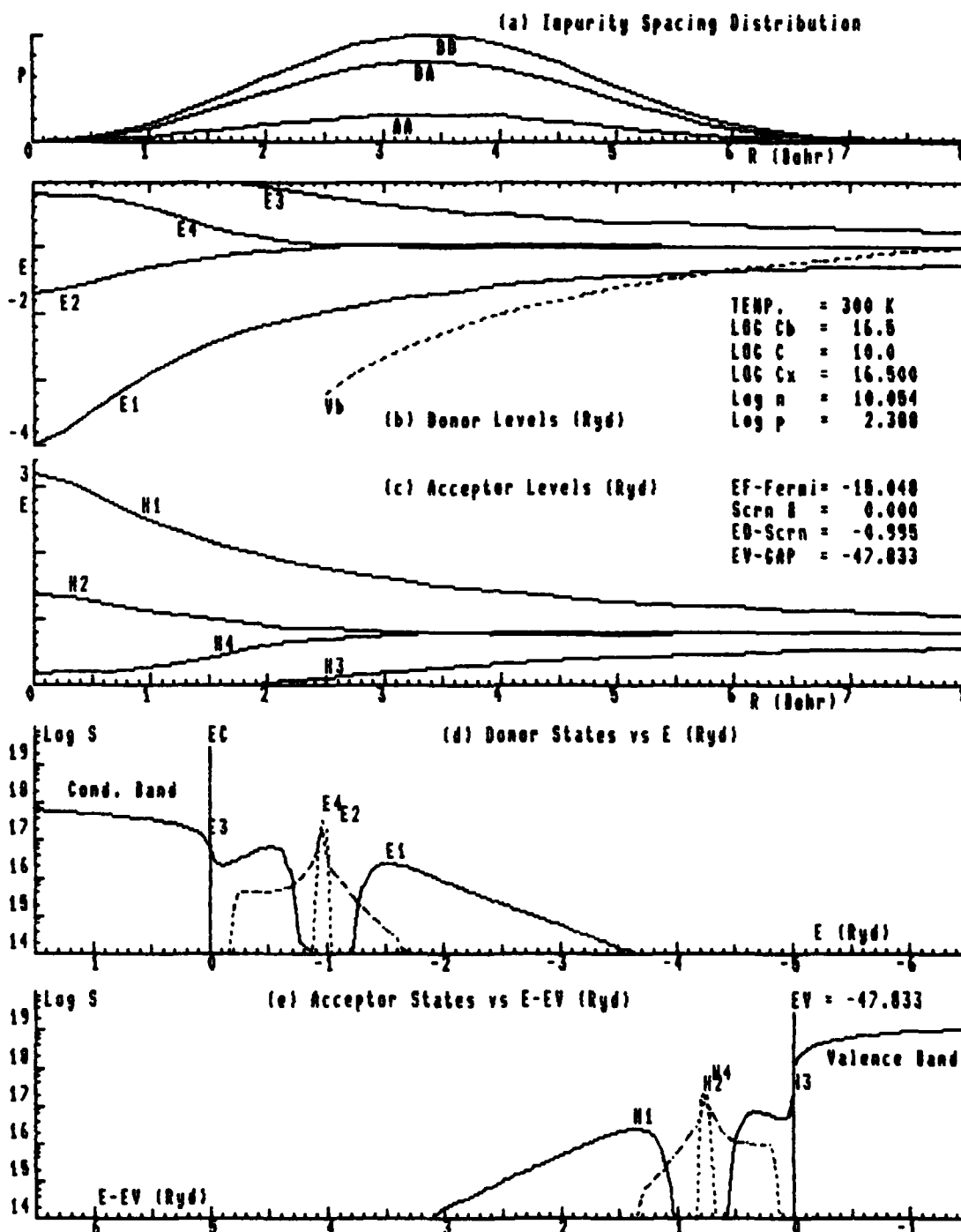


Fig. A 324. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

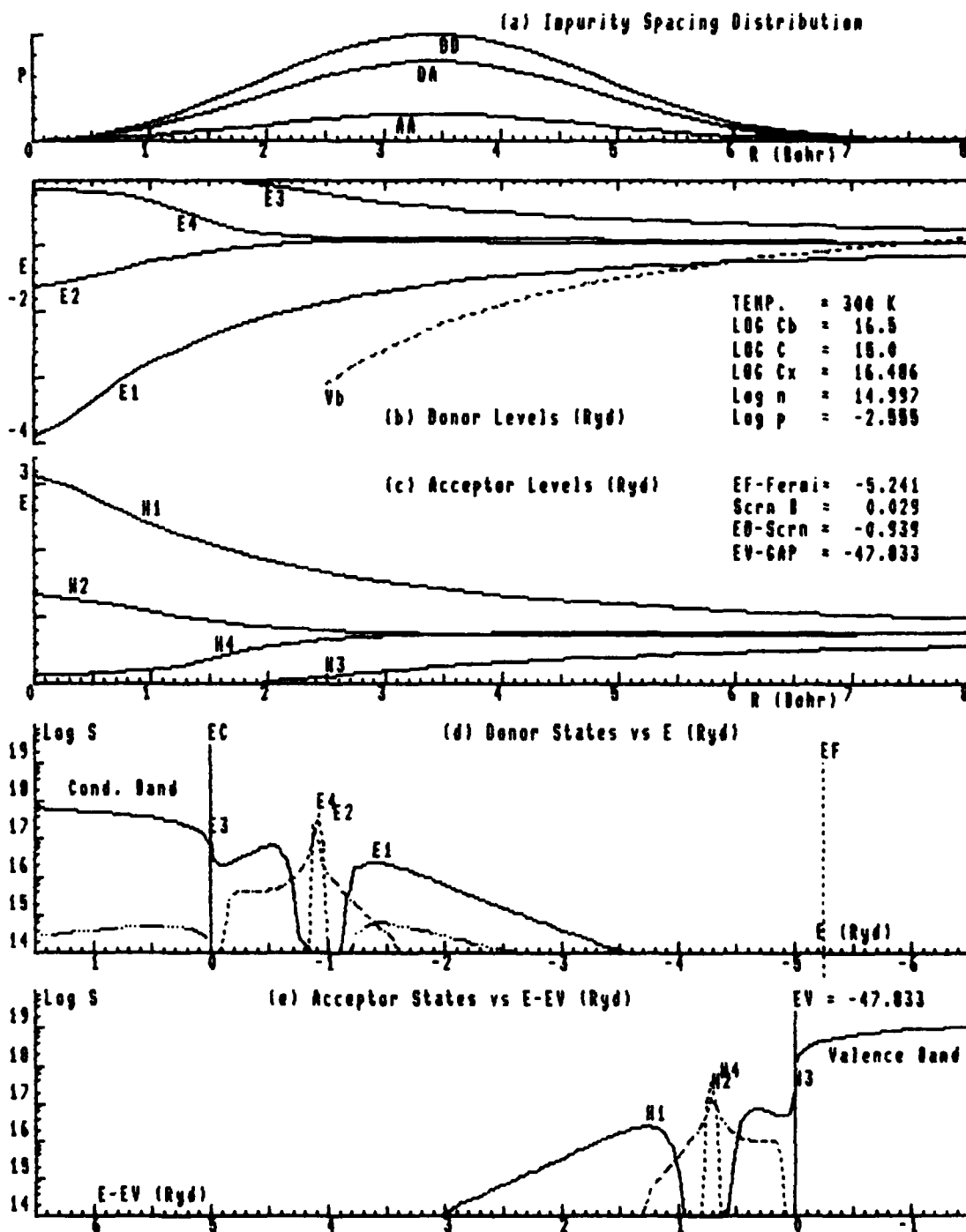


Fig. A 325. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

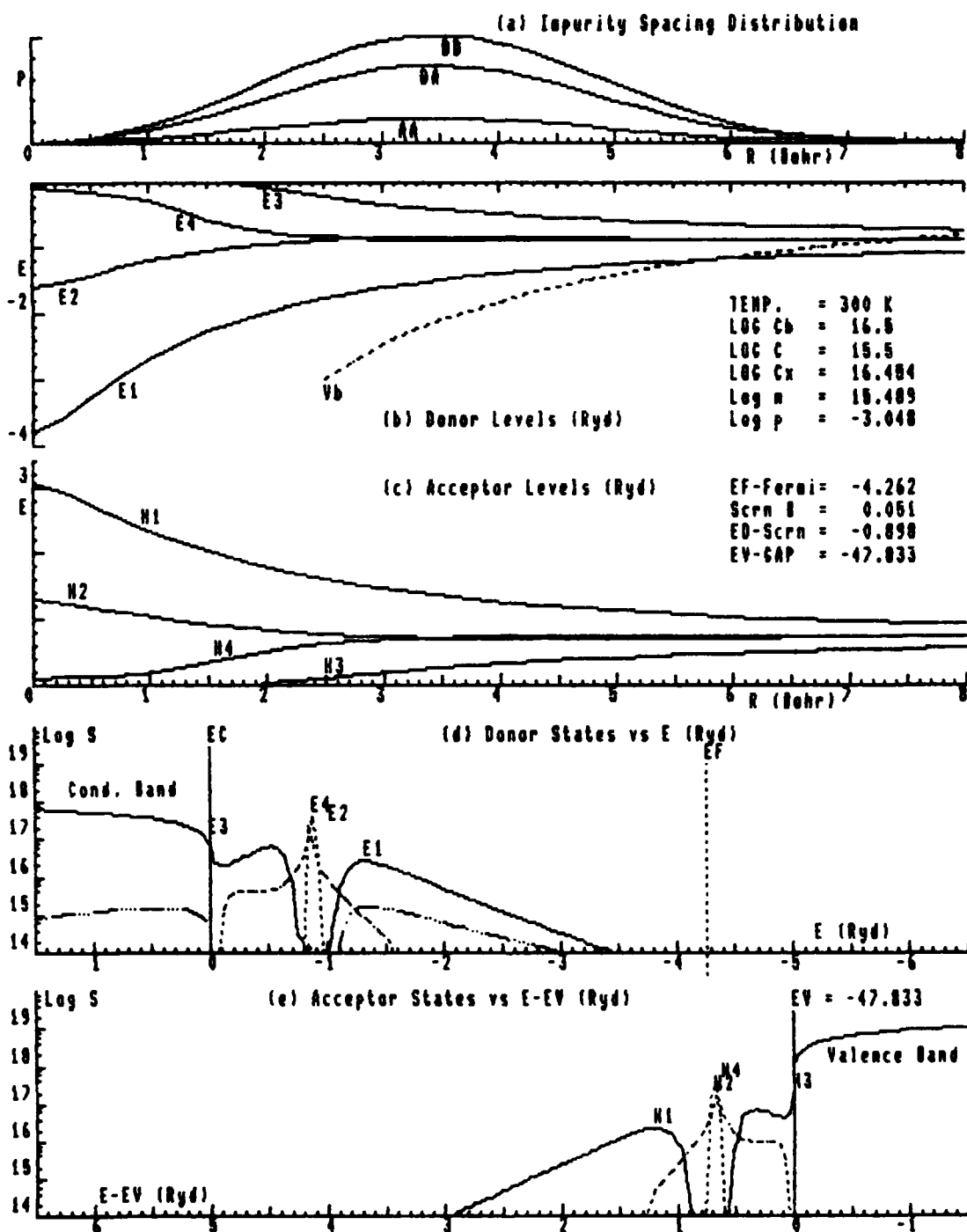


Fig. A 326. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

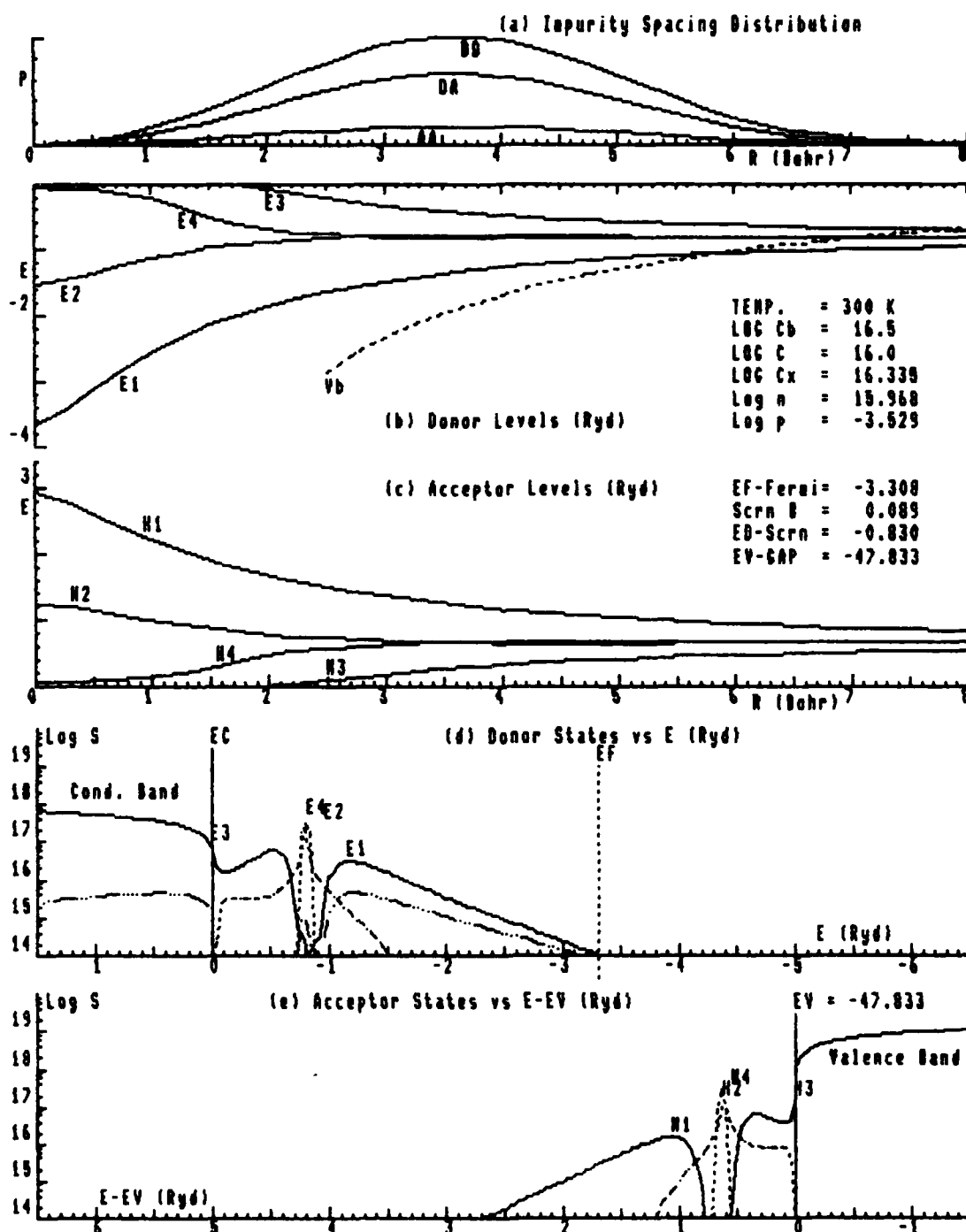


Fig. A 327. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States. H1, H2, H3, & H4 vs E-EV.

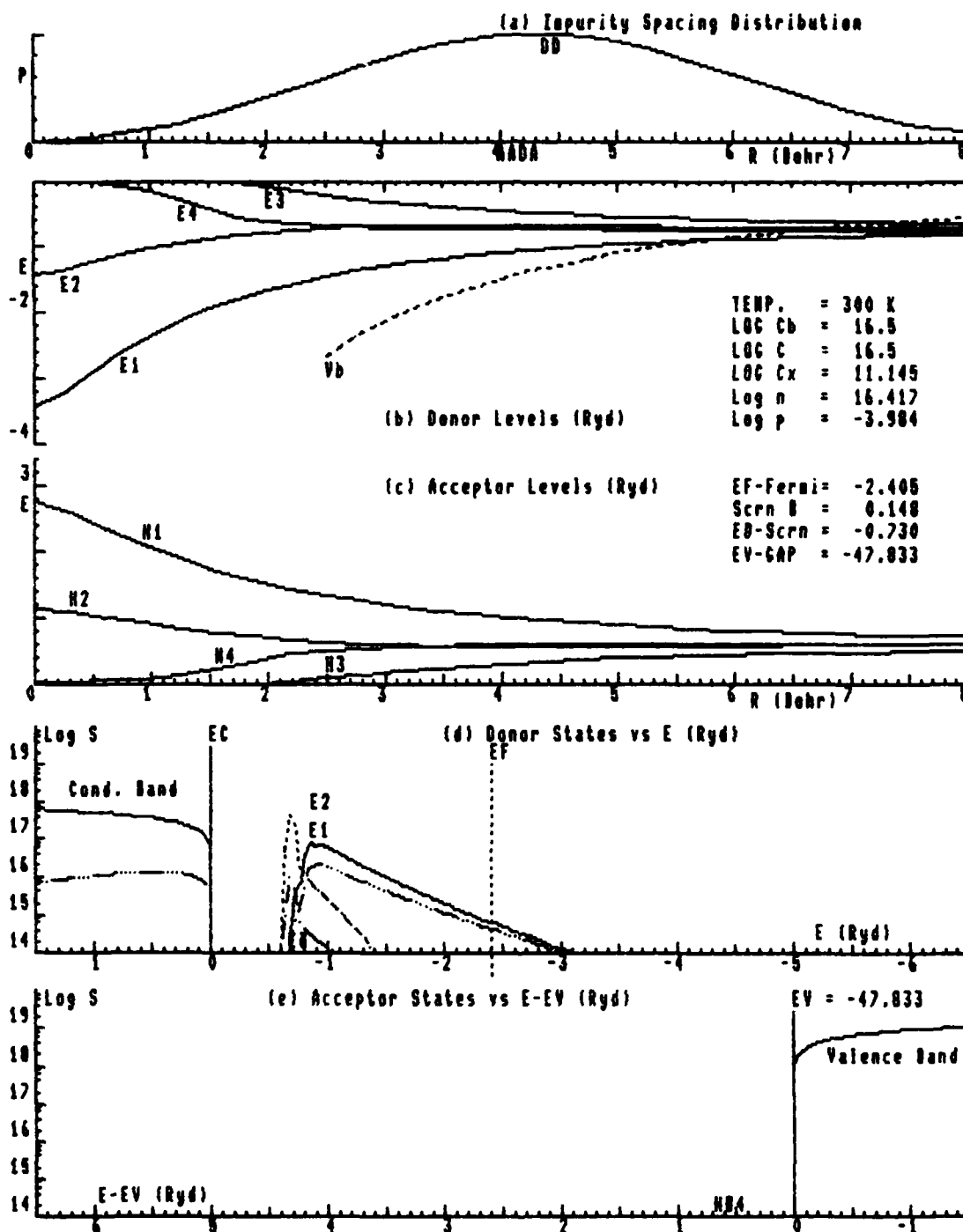


Fig. A 328. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

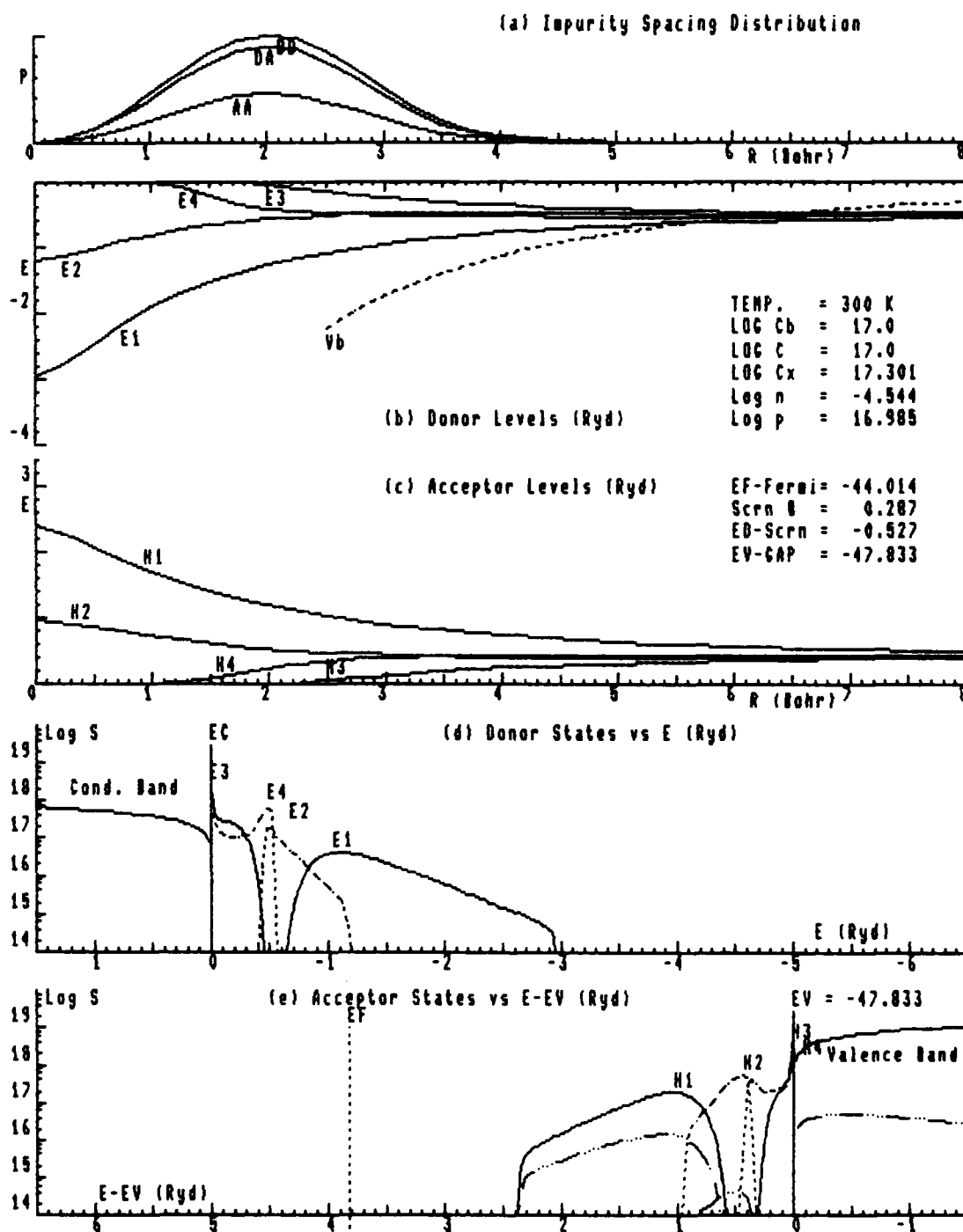


Fig. A 330. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

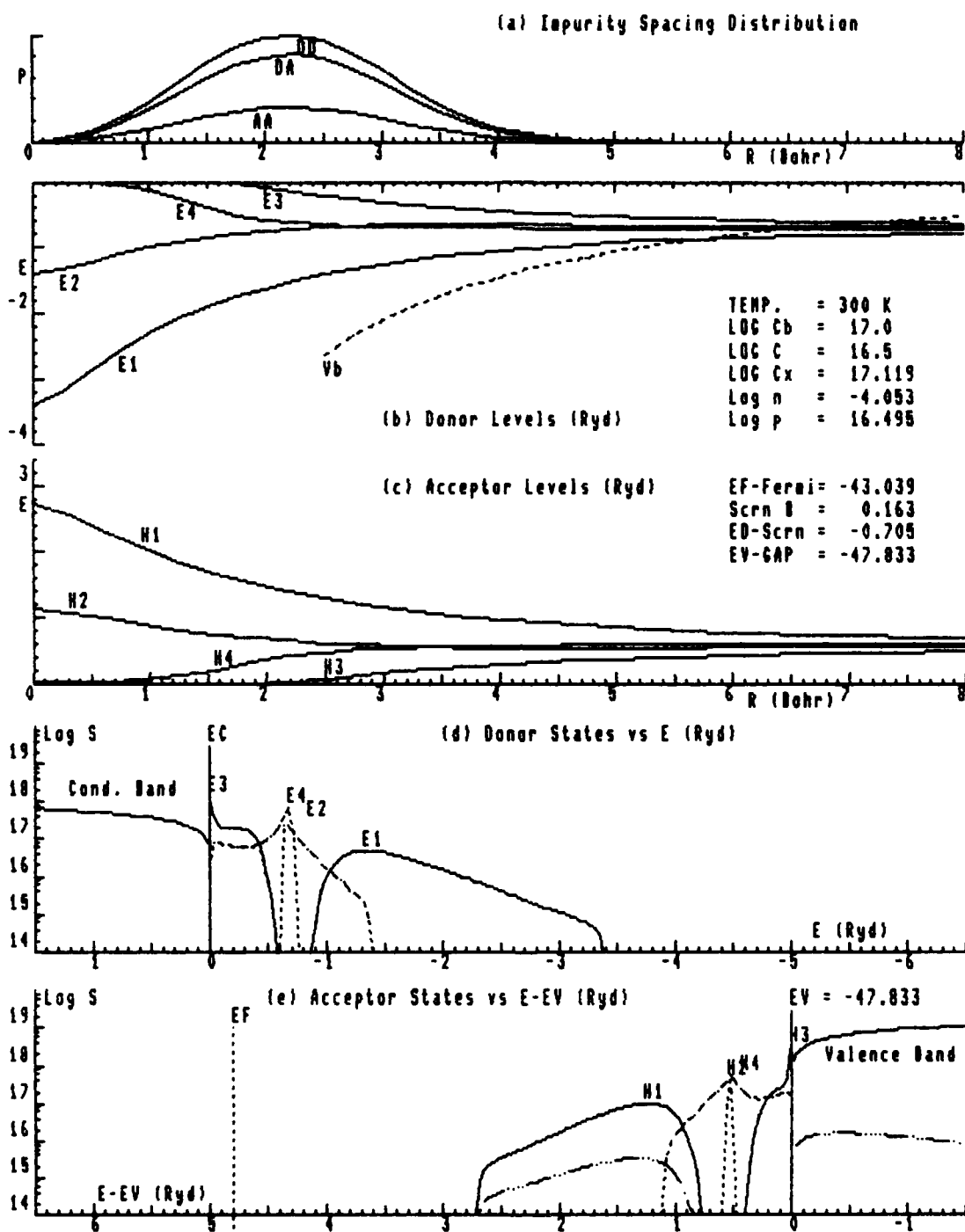


Fig. A 331. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

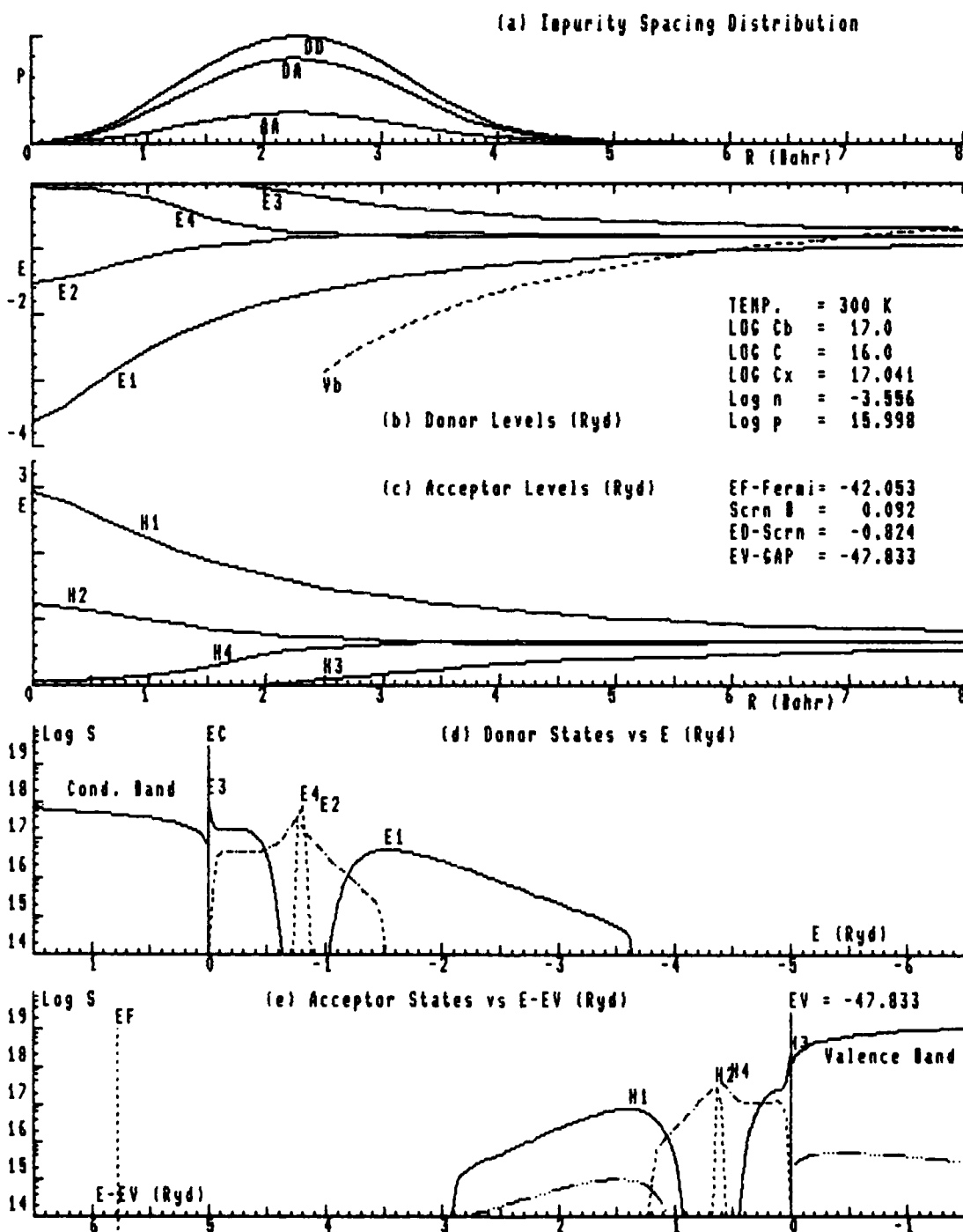


Fig. A 332. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

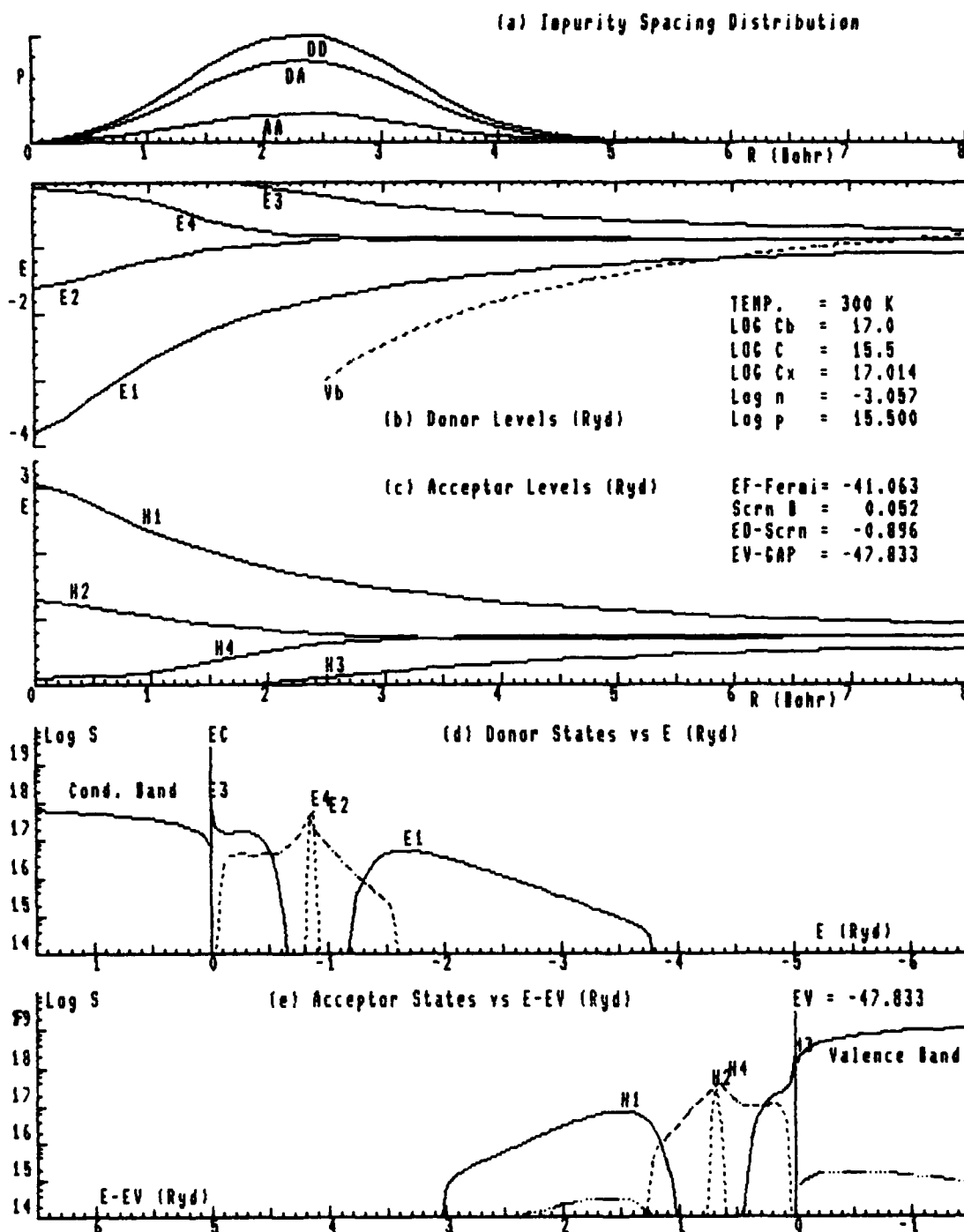


Fig. A 333. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

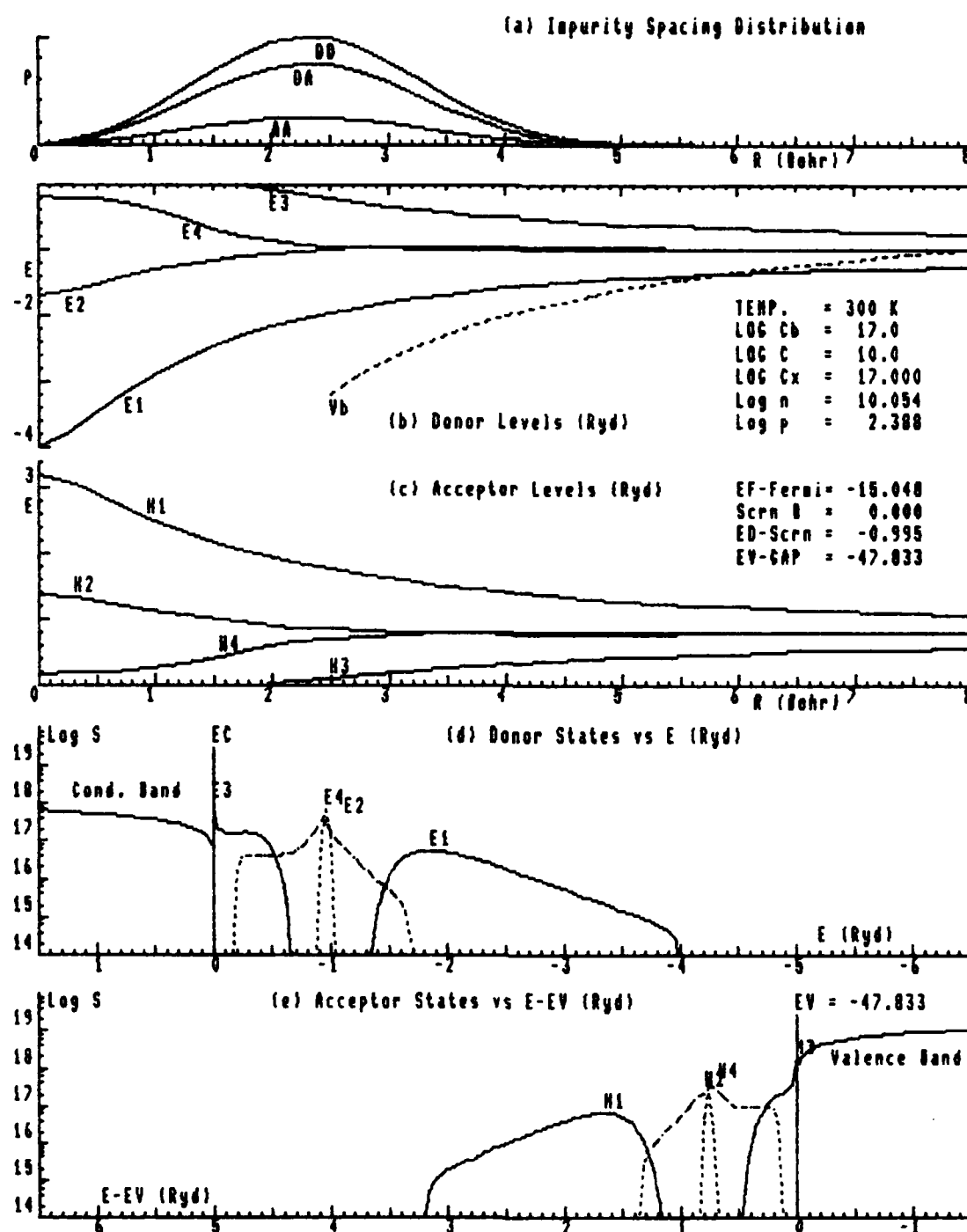


Fig. A 334. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

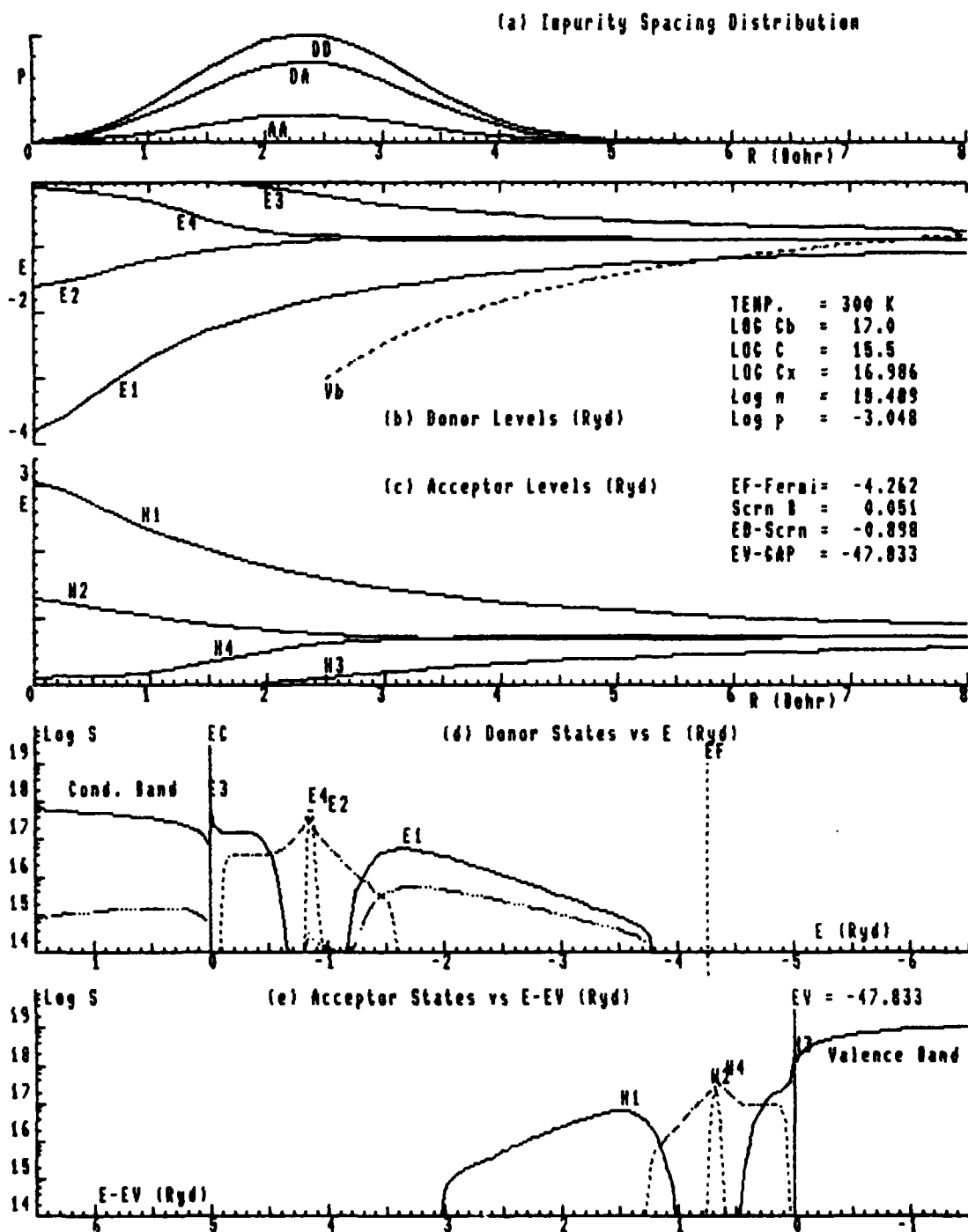


Fig. A 335. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

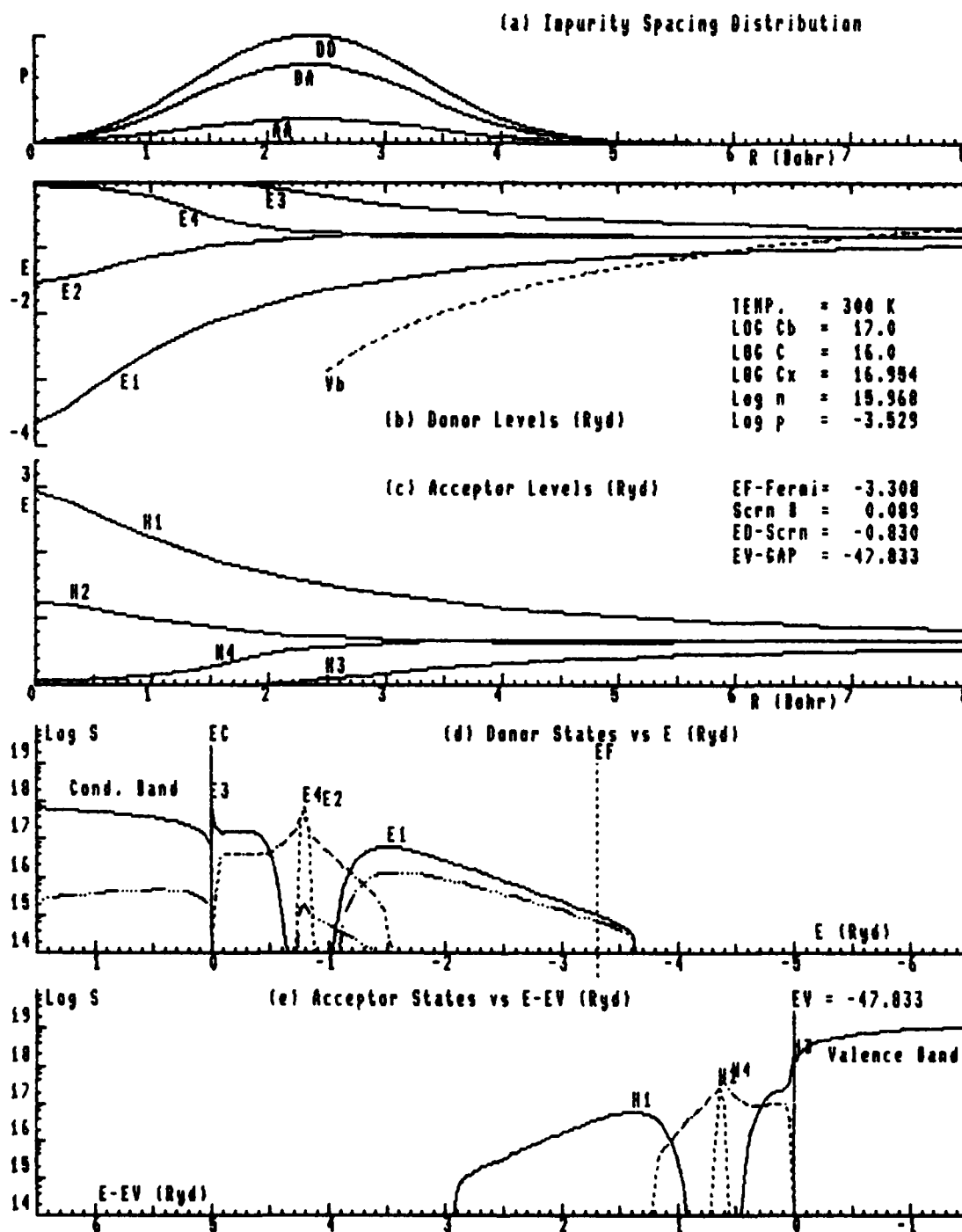


Fig. A 336. (a) Probability, AA + DA + DD, of Pairs vs R
(b) Donor Energy E_1 ; (DD)-, E_2 ; (DD)-, E_3 ; (DA)-, E_4 (DA+)- vs R
(c) Acceptor En. H_1 ; (AA)+, H_2 ; (AA)+, H_3 ; (AD)+, H_4 (AD-)+ vs R
(d) Densities of Donor States, E_1 , E_2 , E_3 , & E_4 , vs E
(e) Densities of Acceptor States, H_1 , H_2 , H_3 , & H_4 vs E-EV.

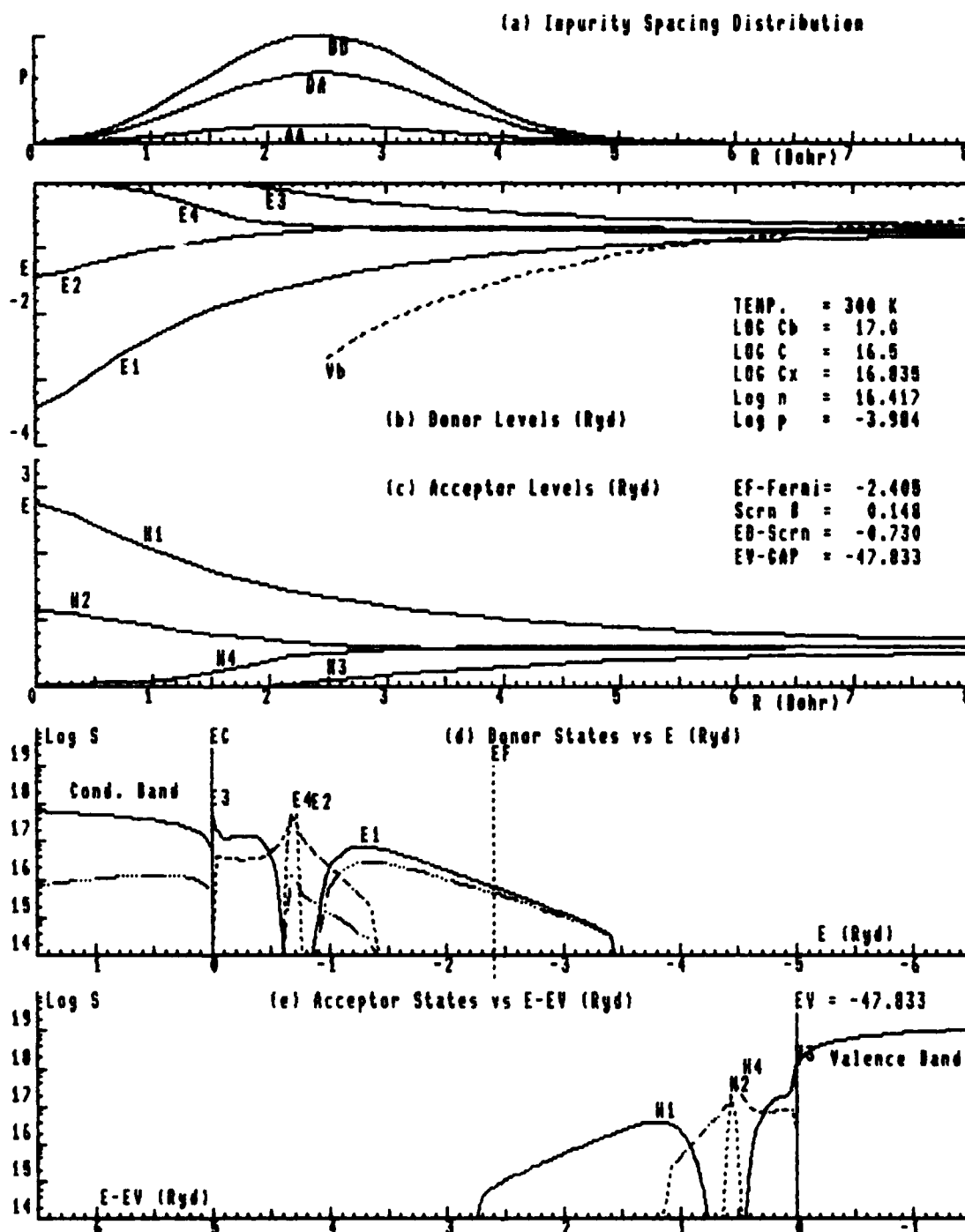


Fig. A 337. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

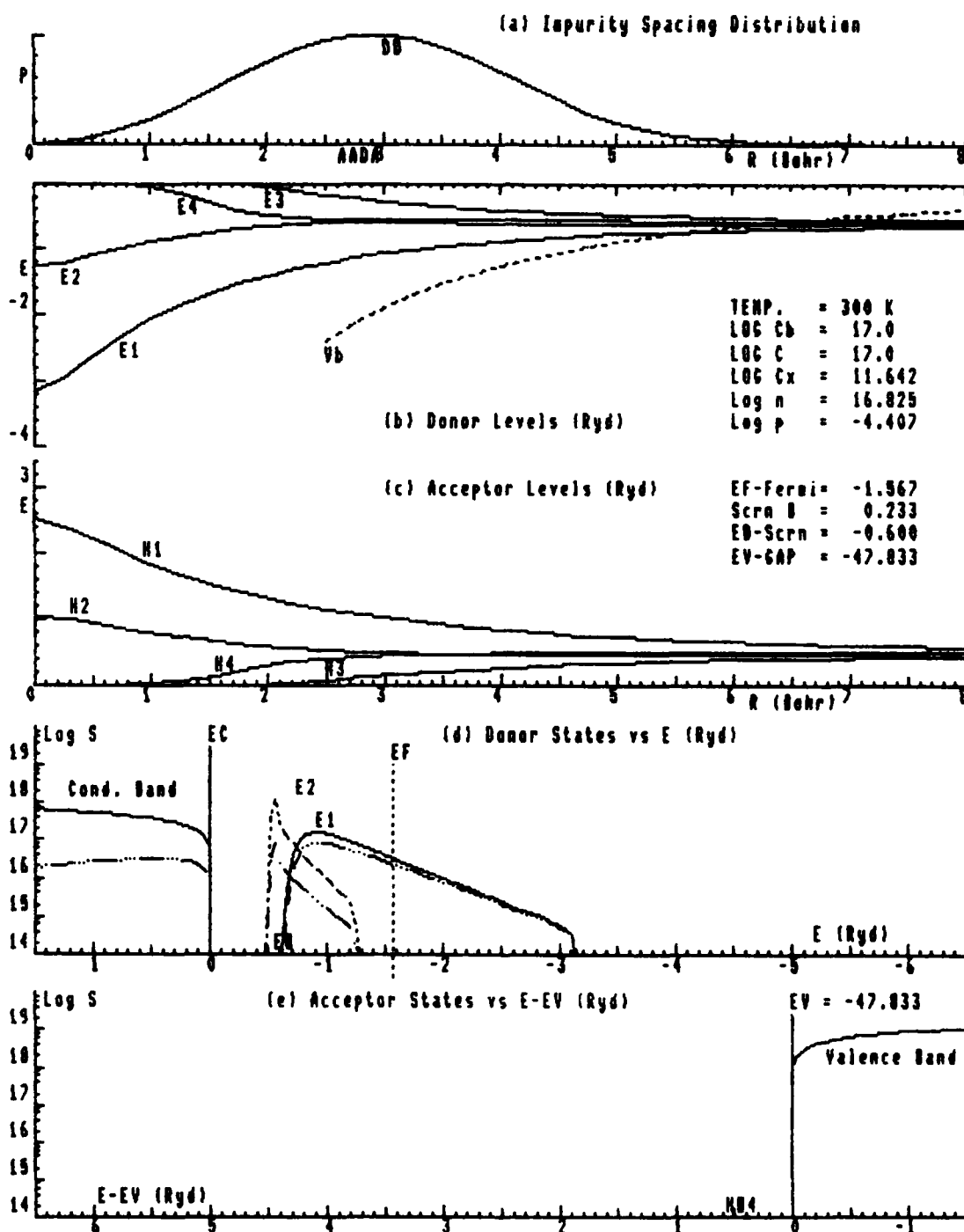


Fig. A 338. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

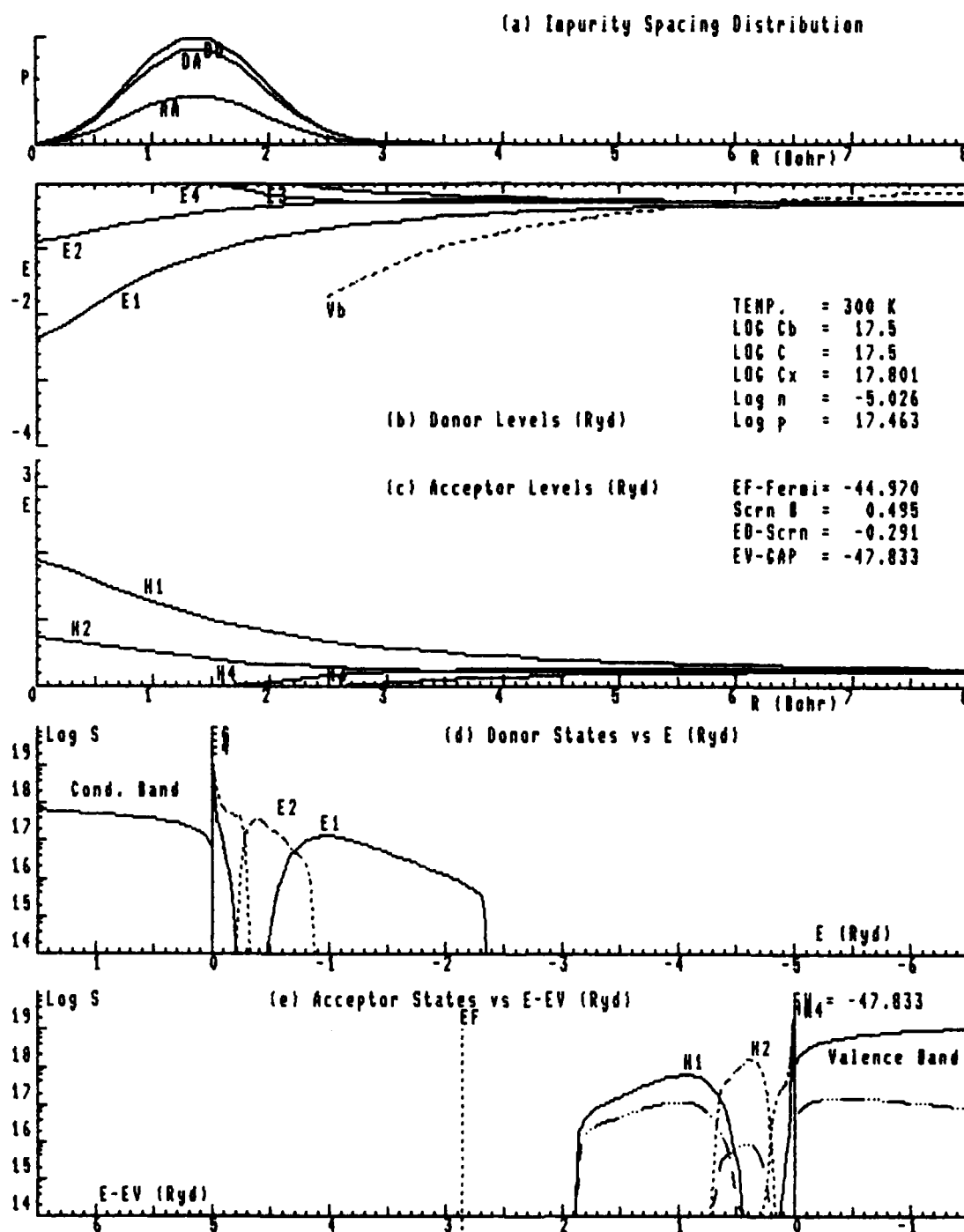


Fig. A 340. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA+)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

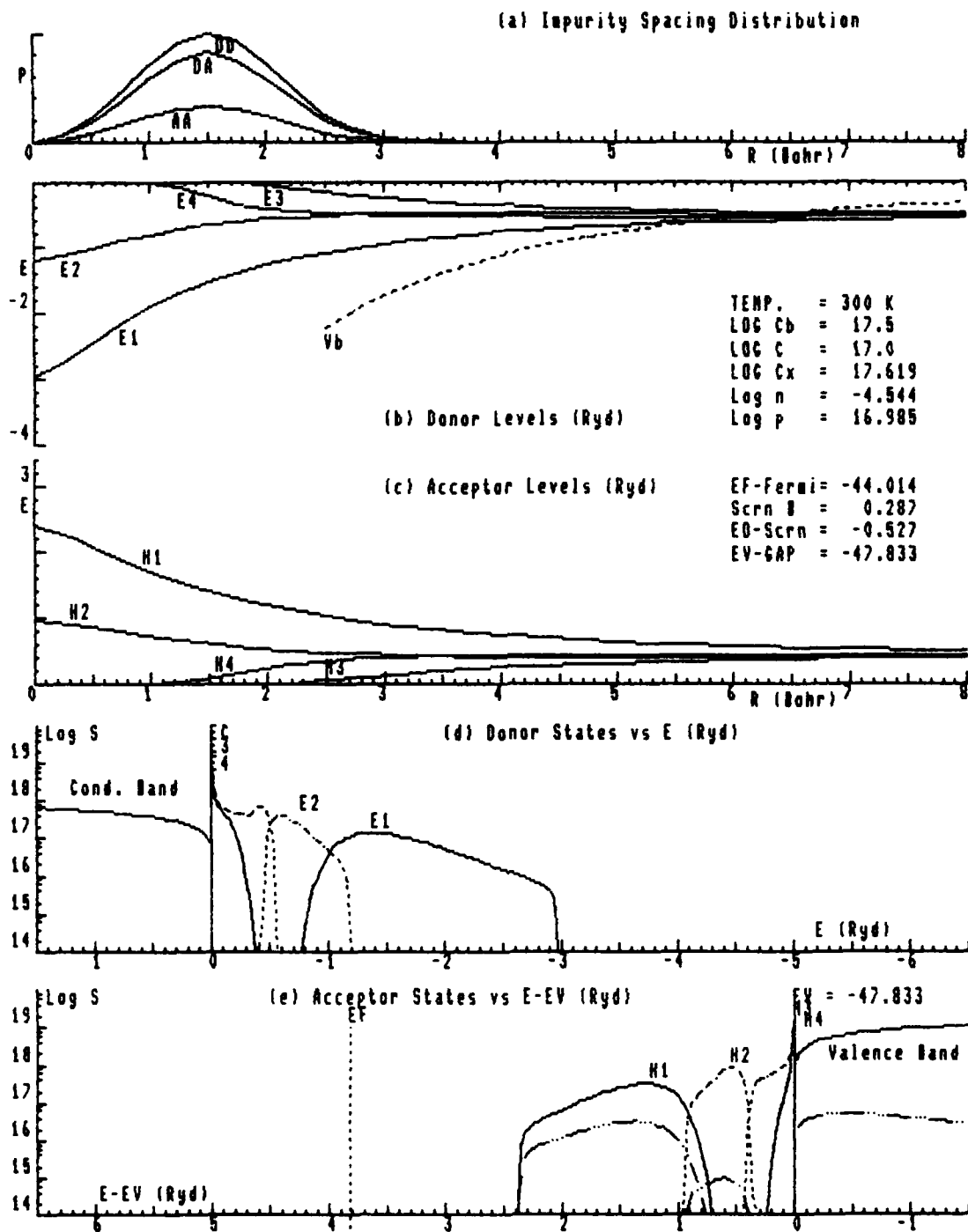


Fig. A 341. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

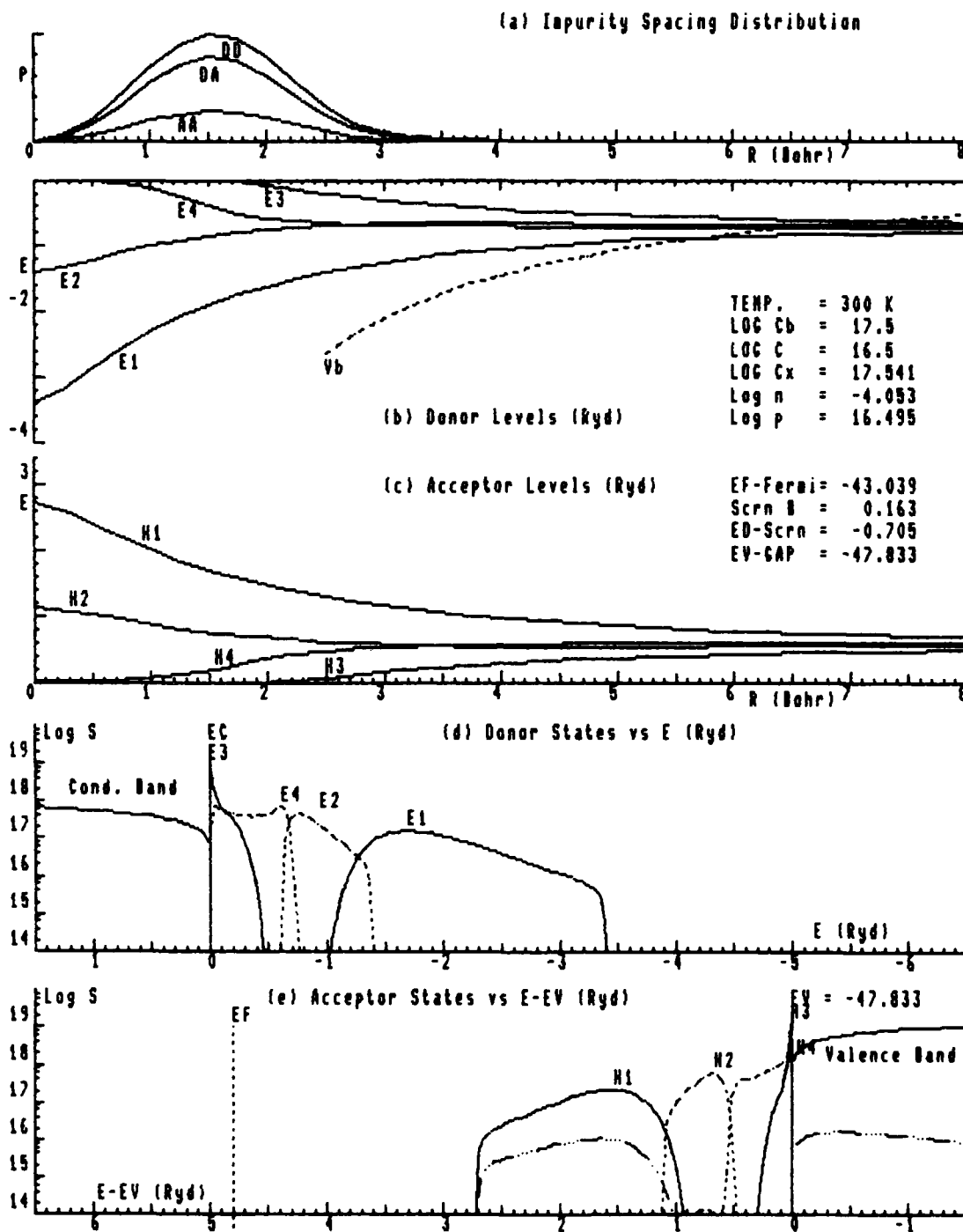


Fig. A 342. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

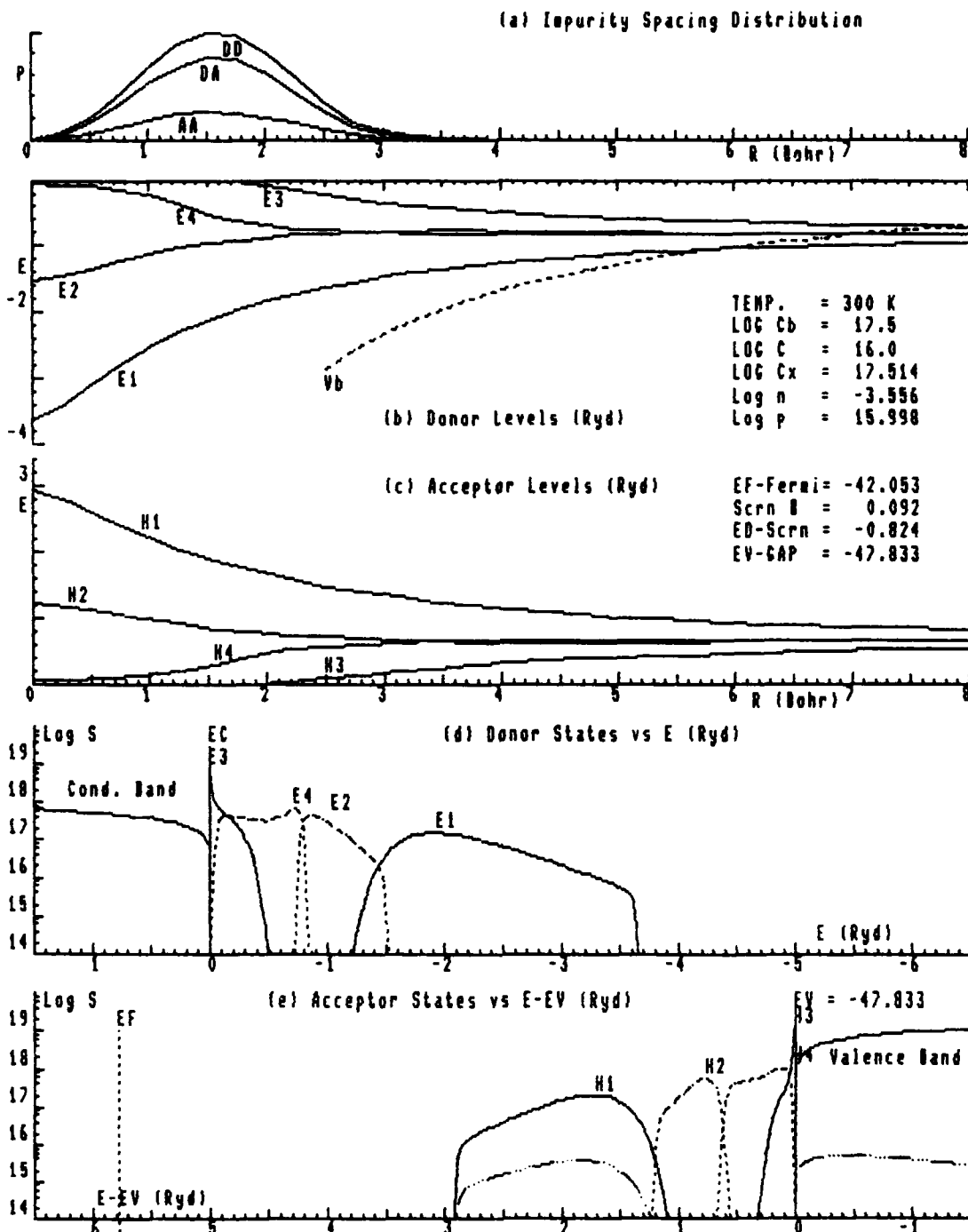


Fig. A 343. (a) Probability, AA + DA + DD, of Pairs (vs R)
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

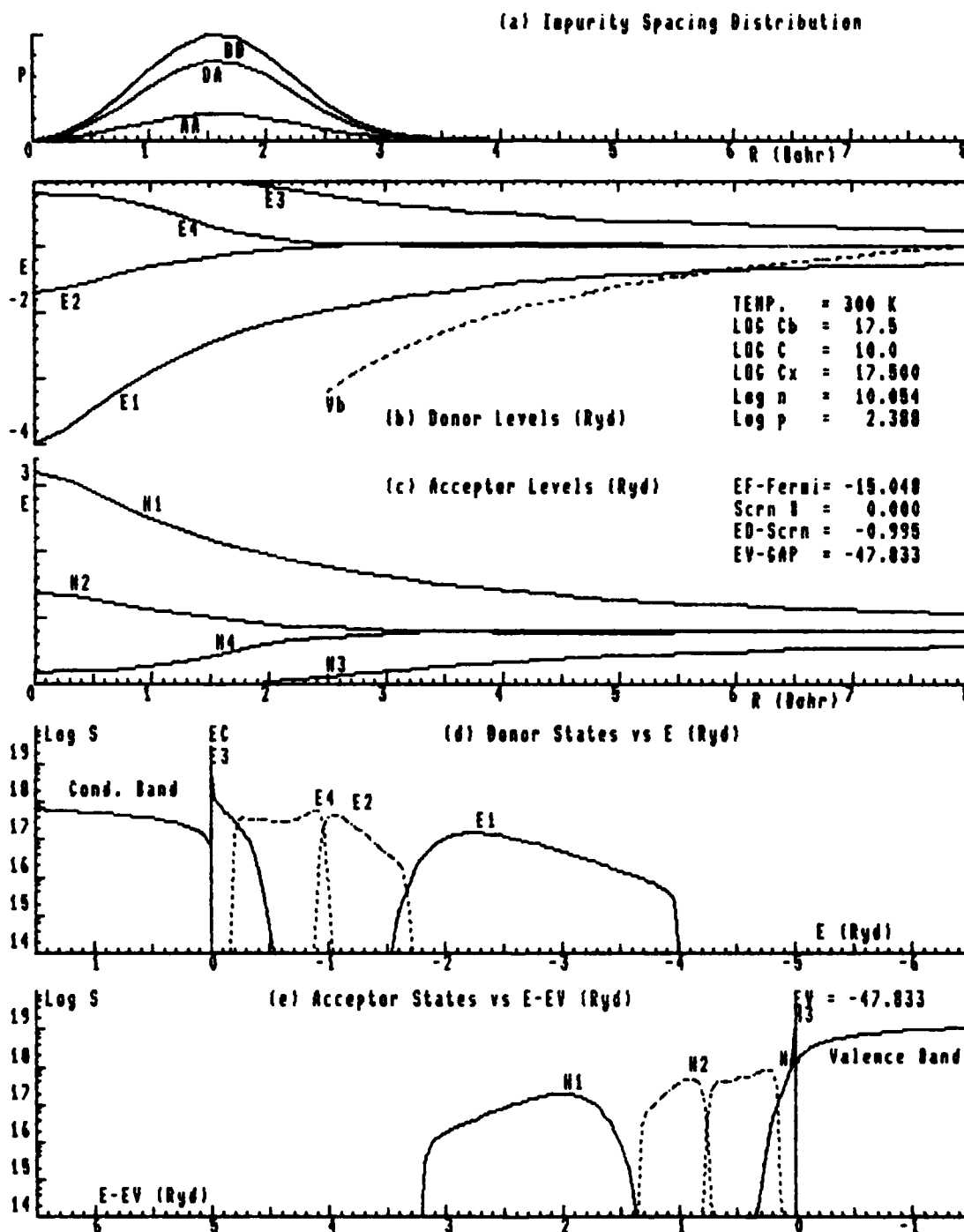


Fig. A 344. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

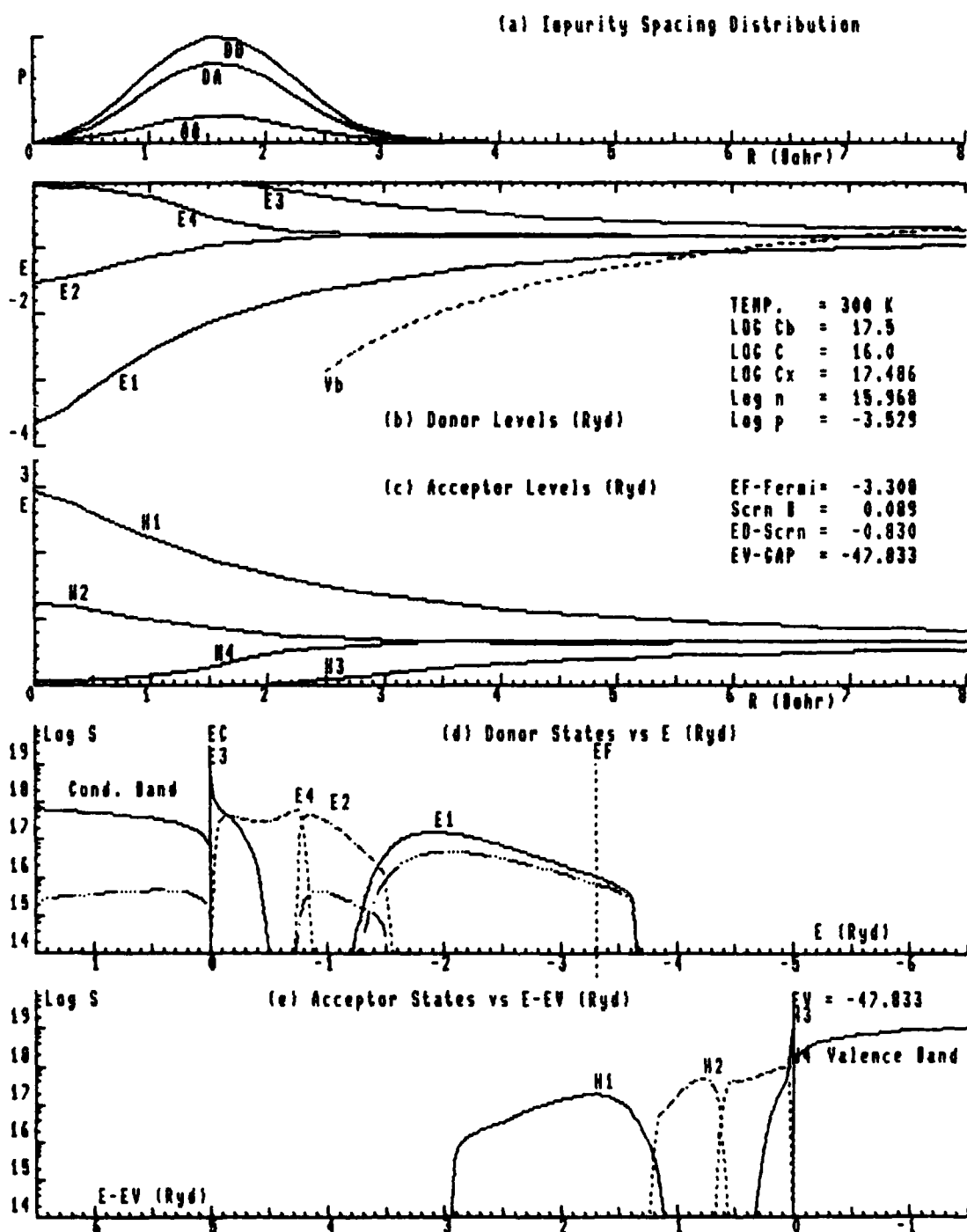


Fig. A 345. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

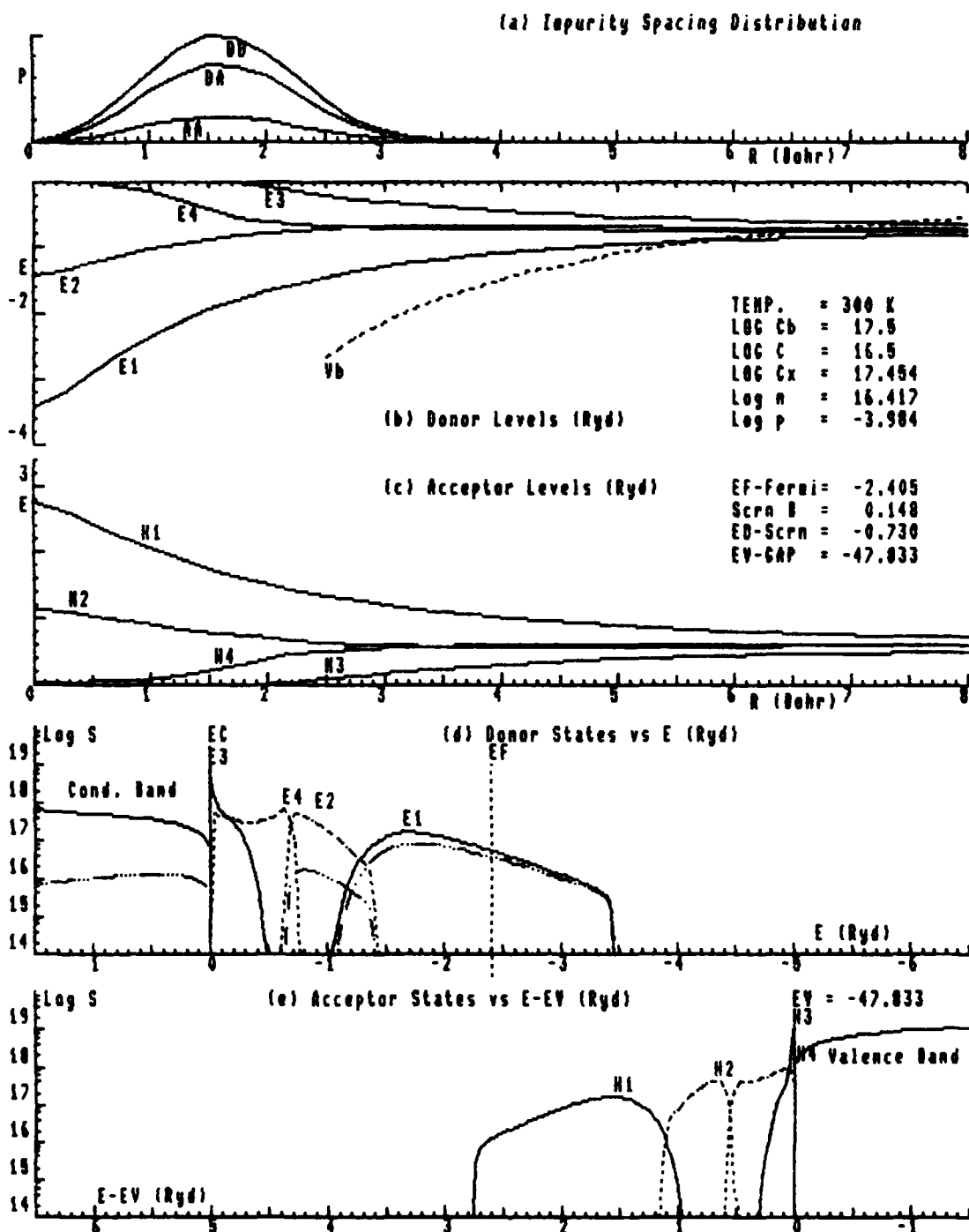


Fig. A 346. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

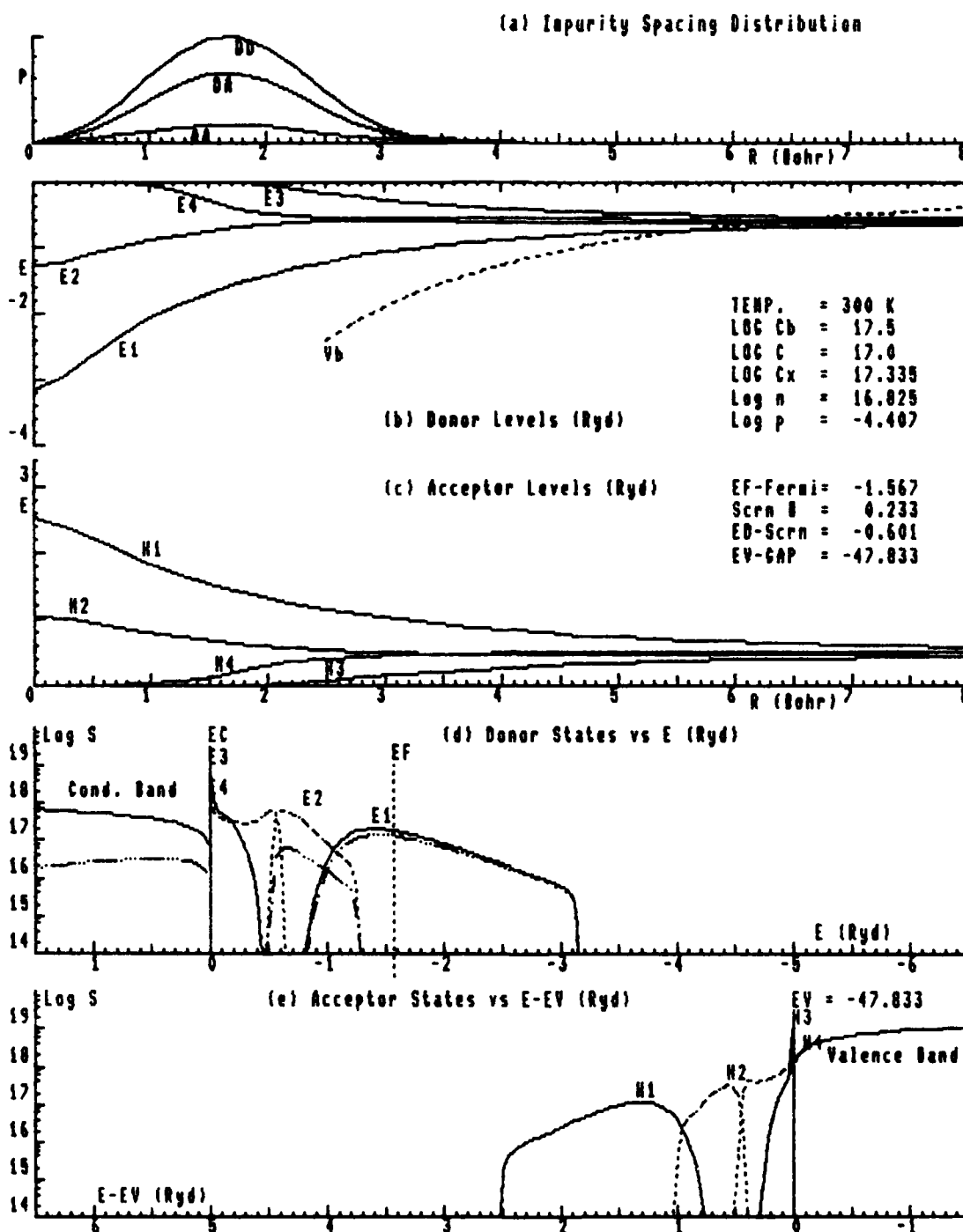


Fig. A 347. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

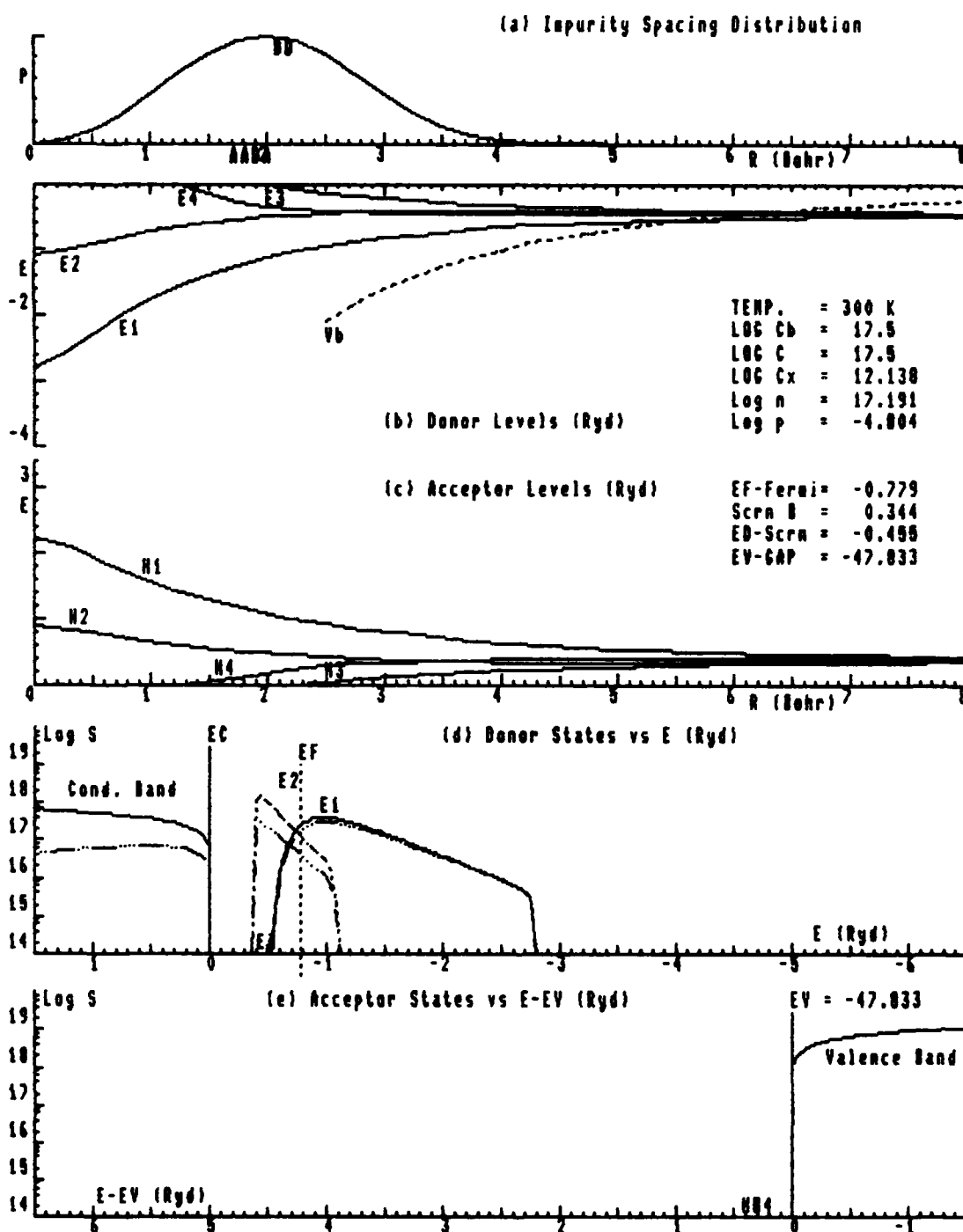


Fig. A 34B. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States. H1, H2, H3, & H4 vs E-EV.

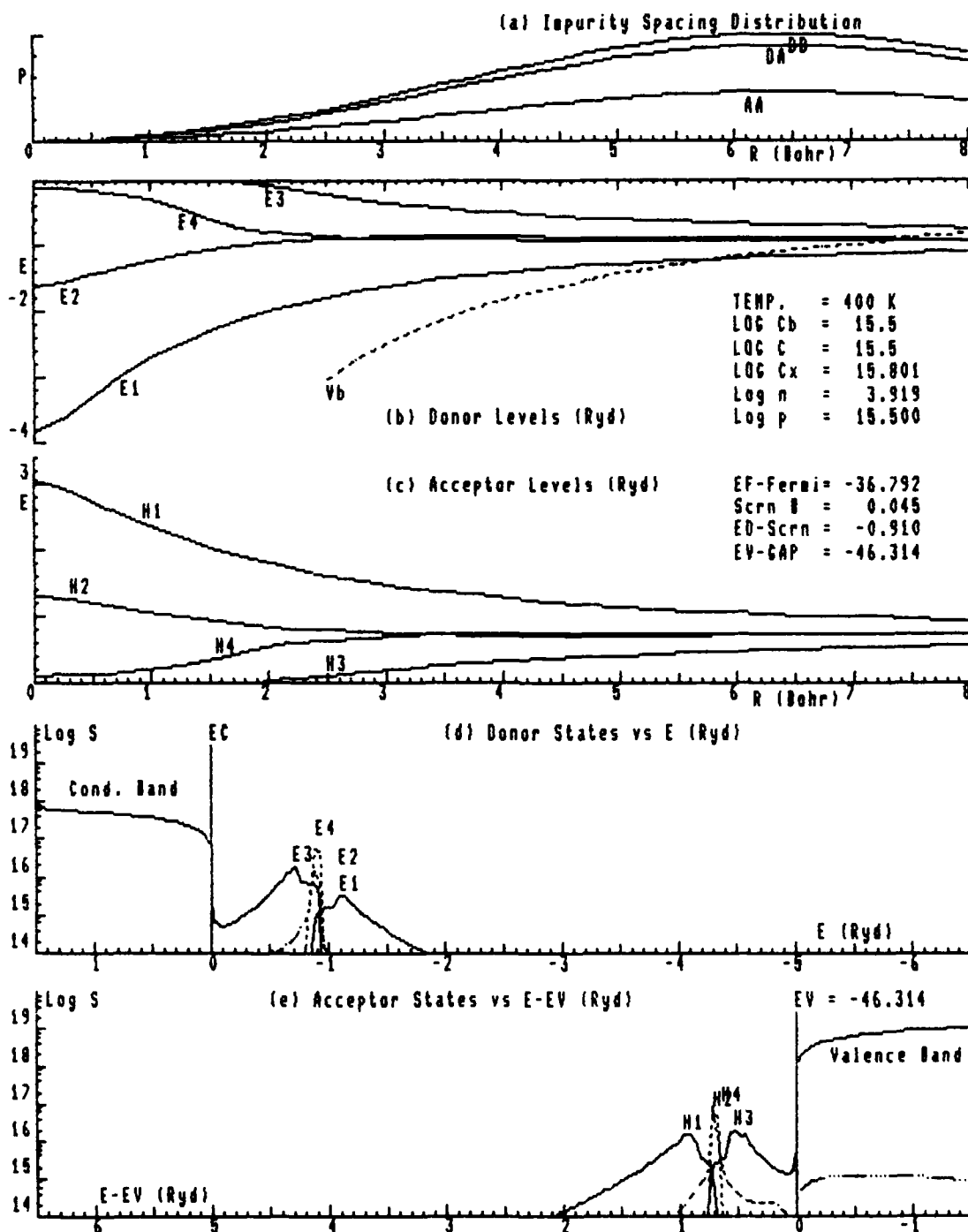


Fig. A 400. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

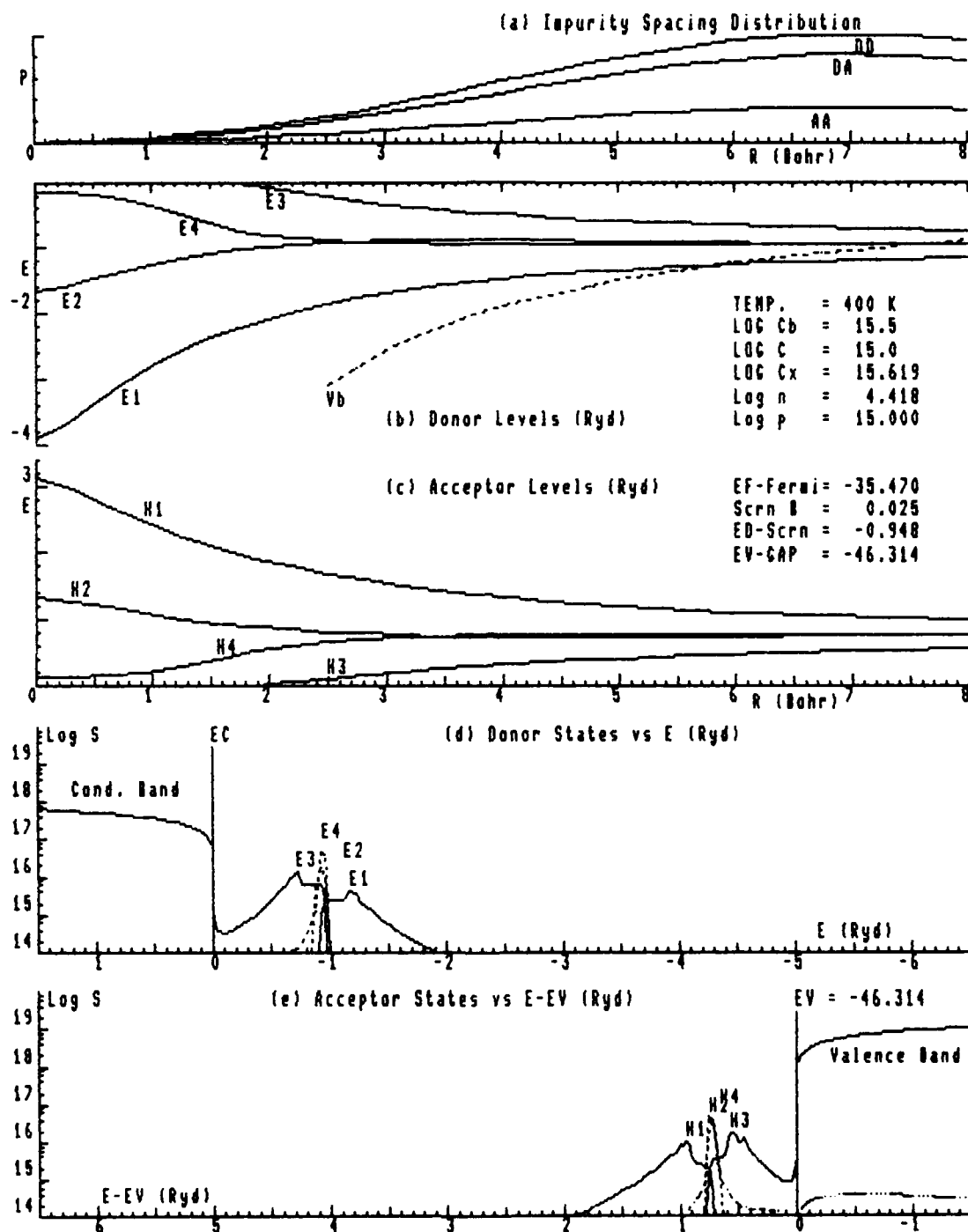


Fig. A 401. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

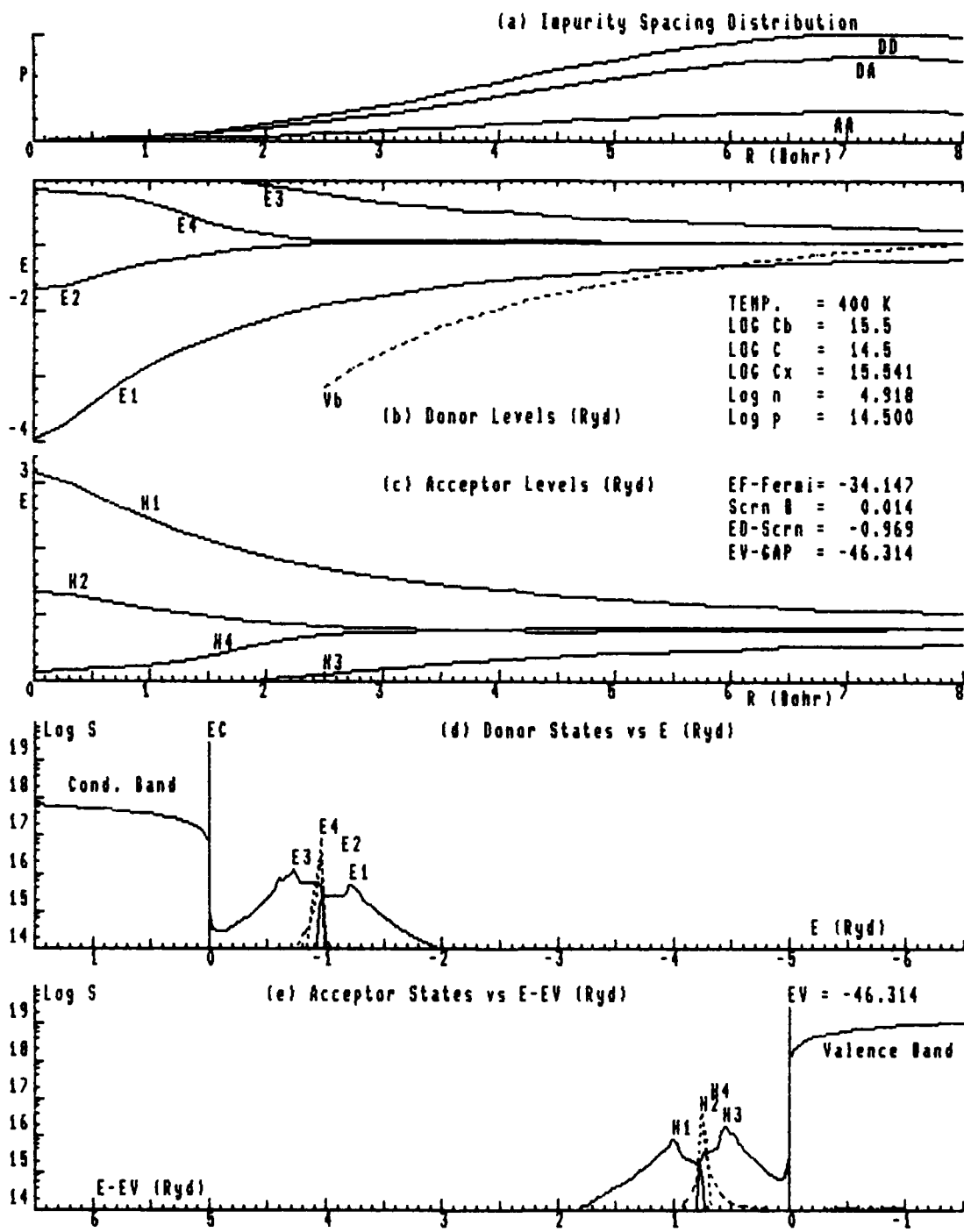


Fig. A 402. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

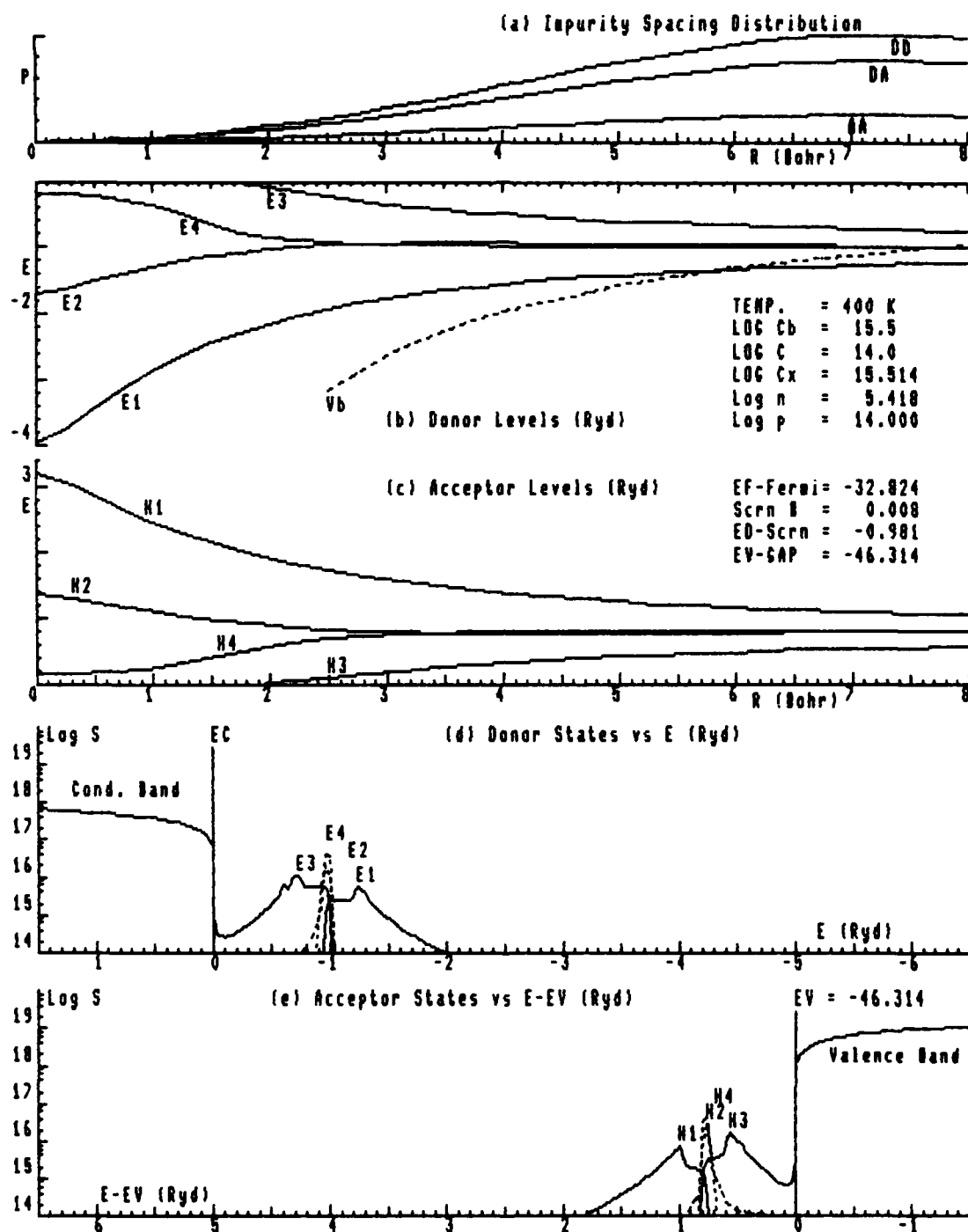


Fig. A 403. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

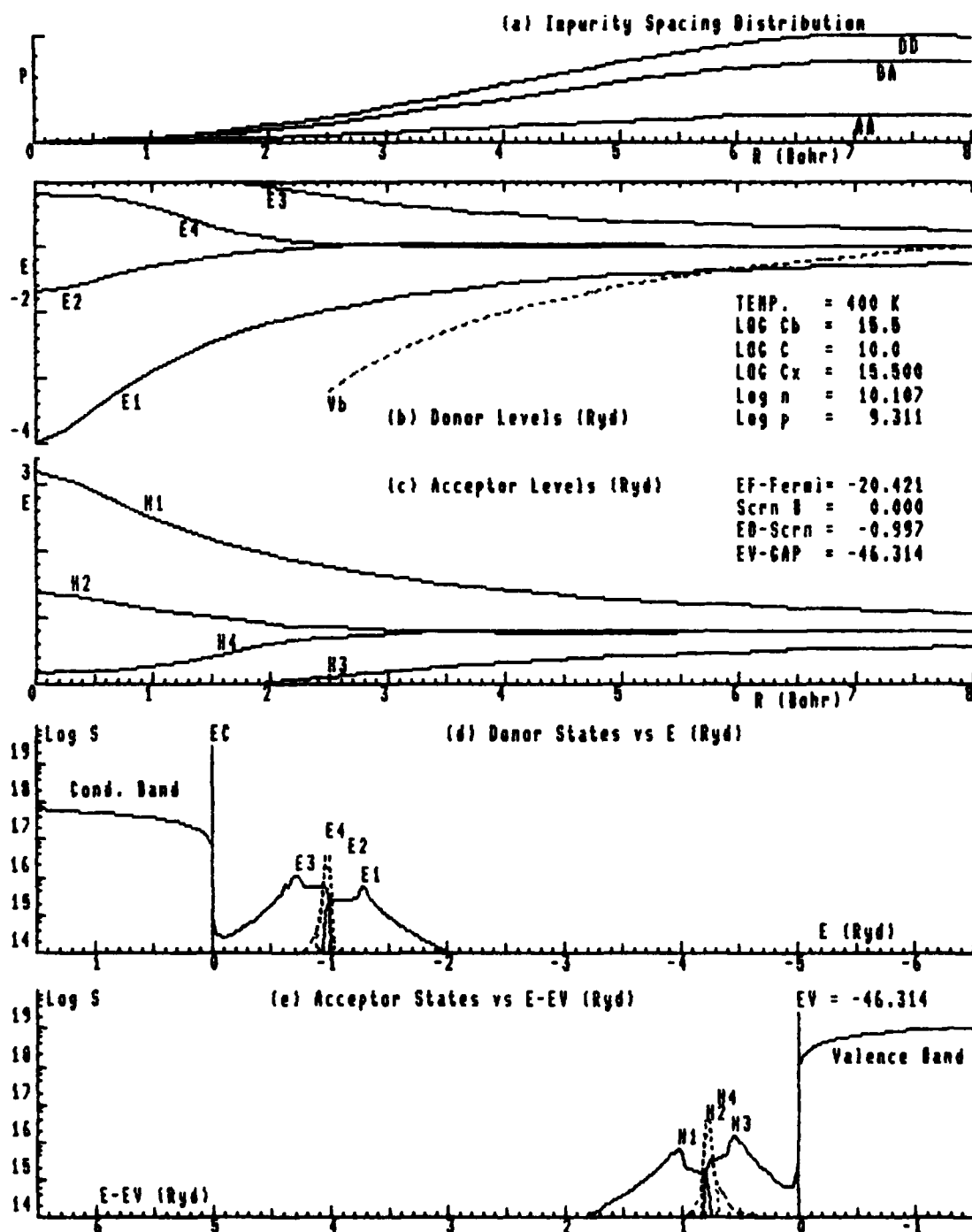


Fig. A 404. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

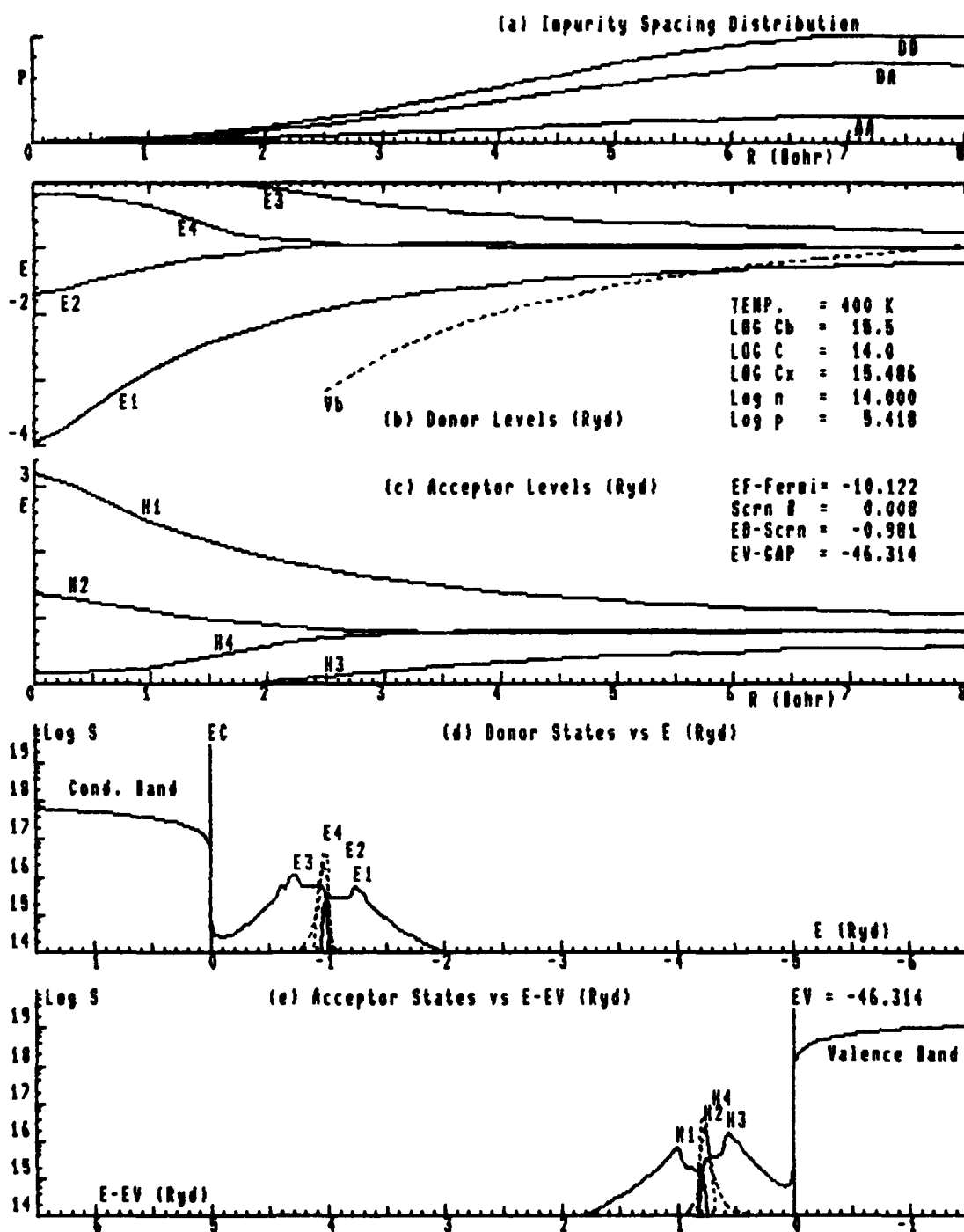


Fig. A 405. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

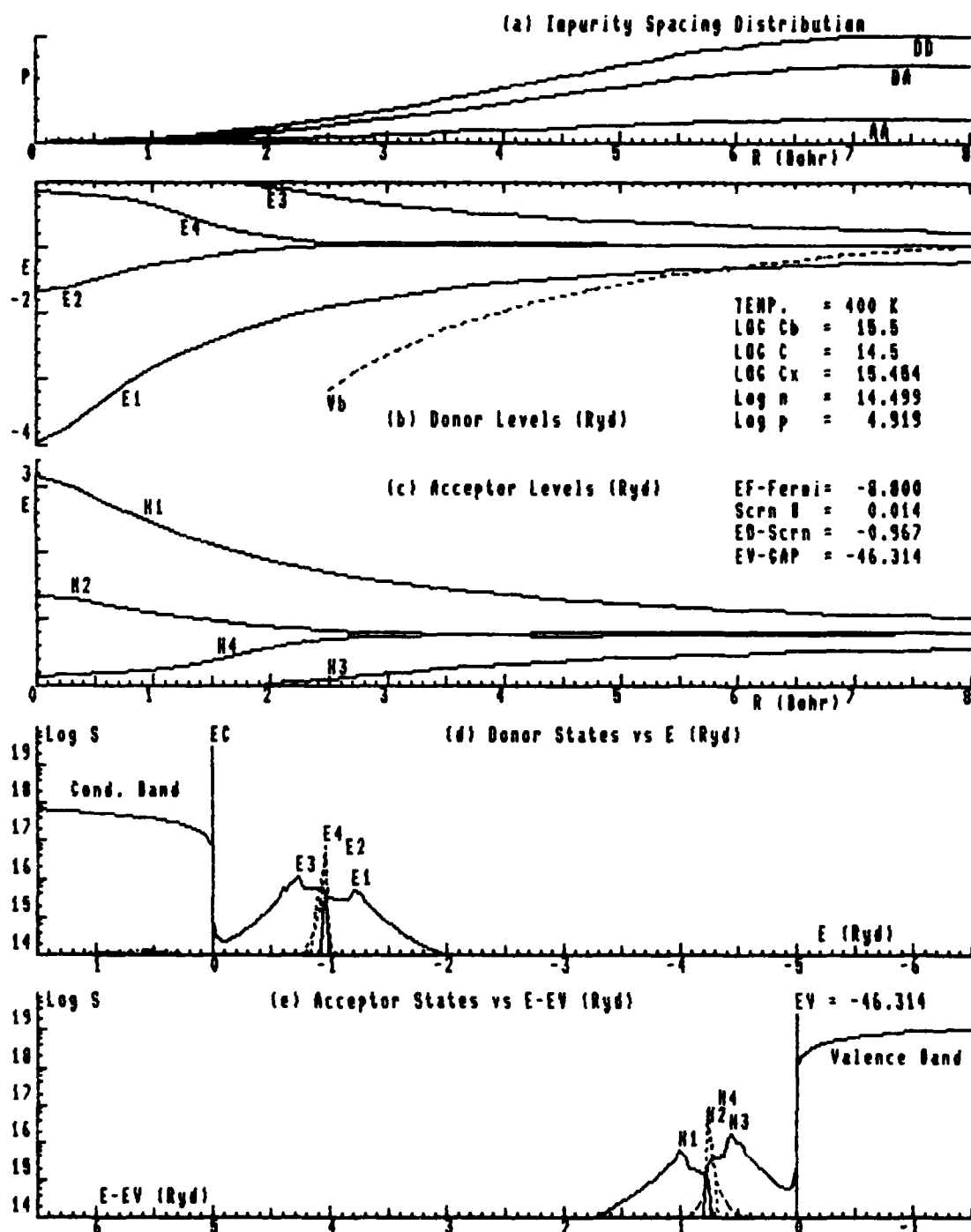


Fig. A 406. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

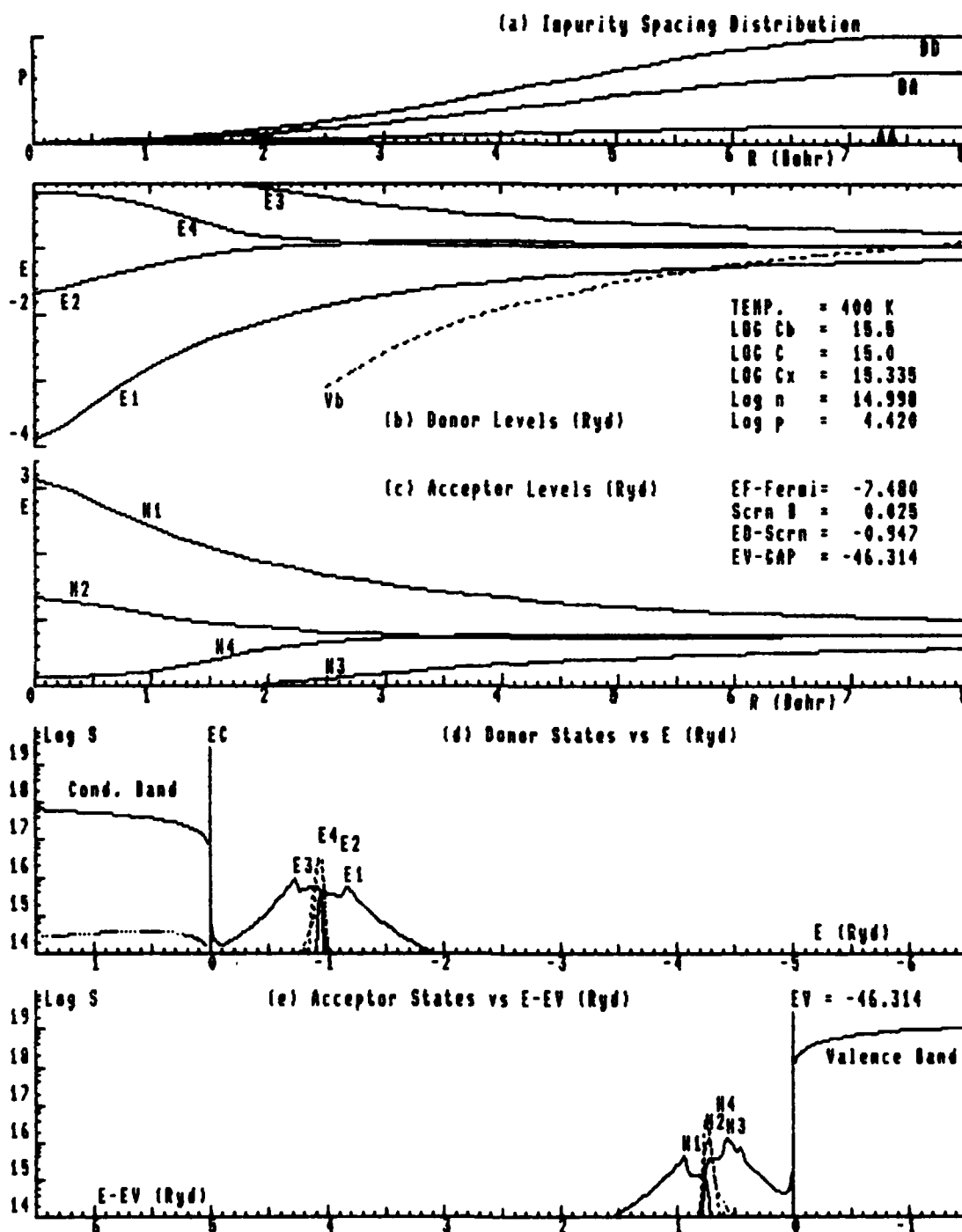


Fig. A 407. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

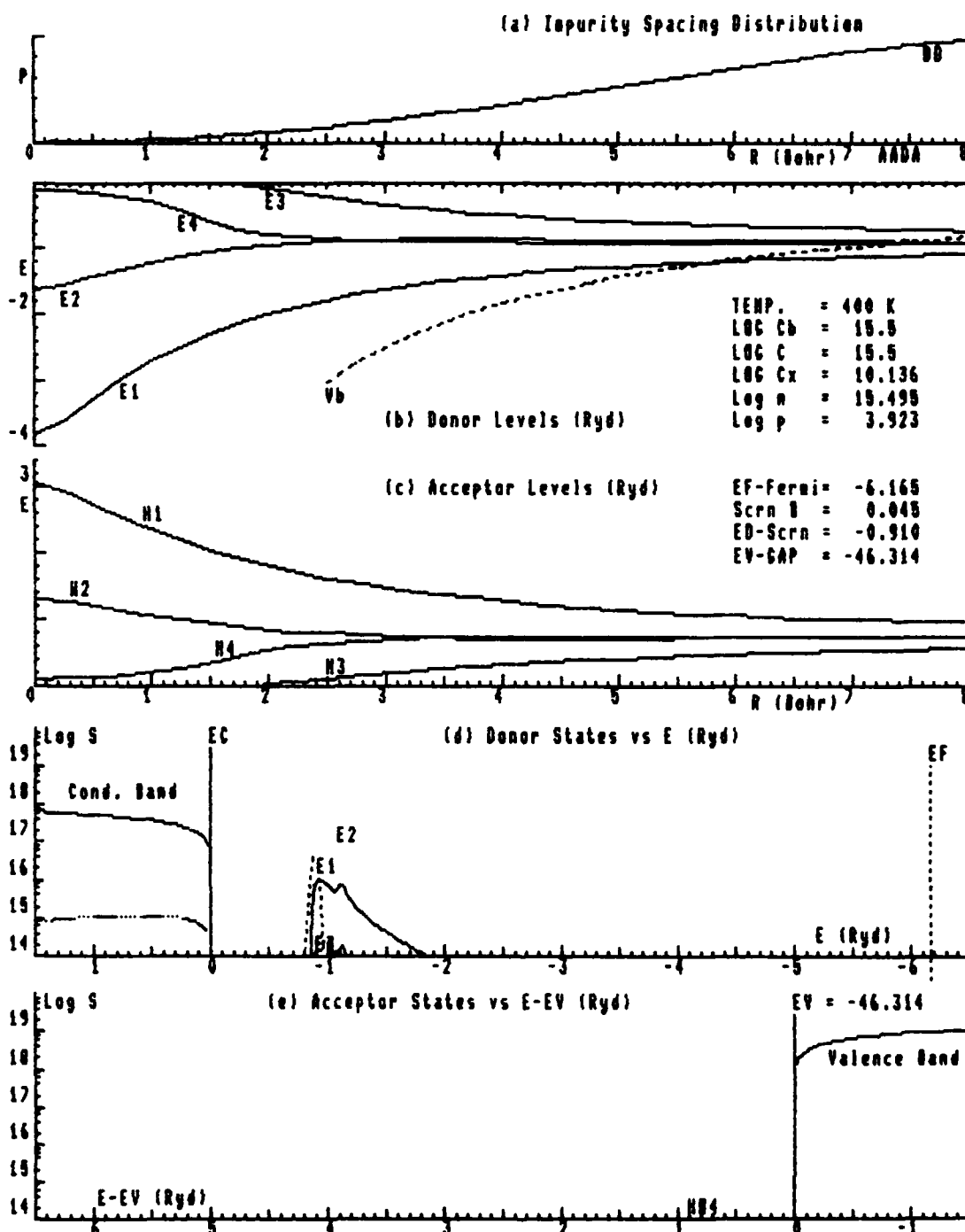


Fig. A 408. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

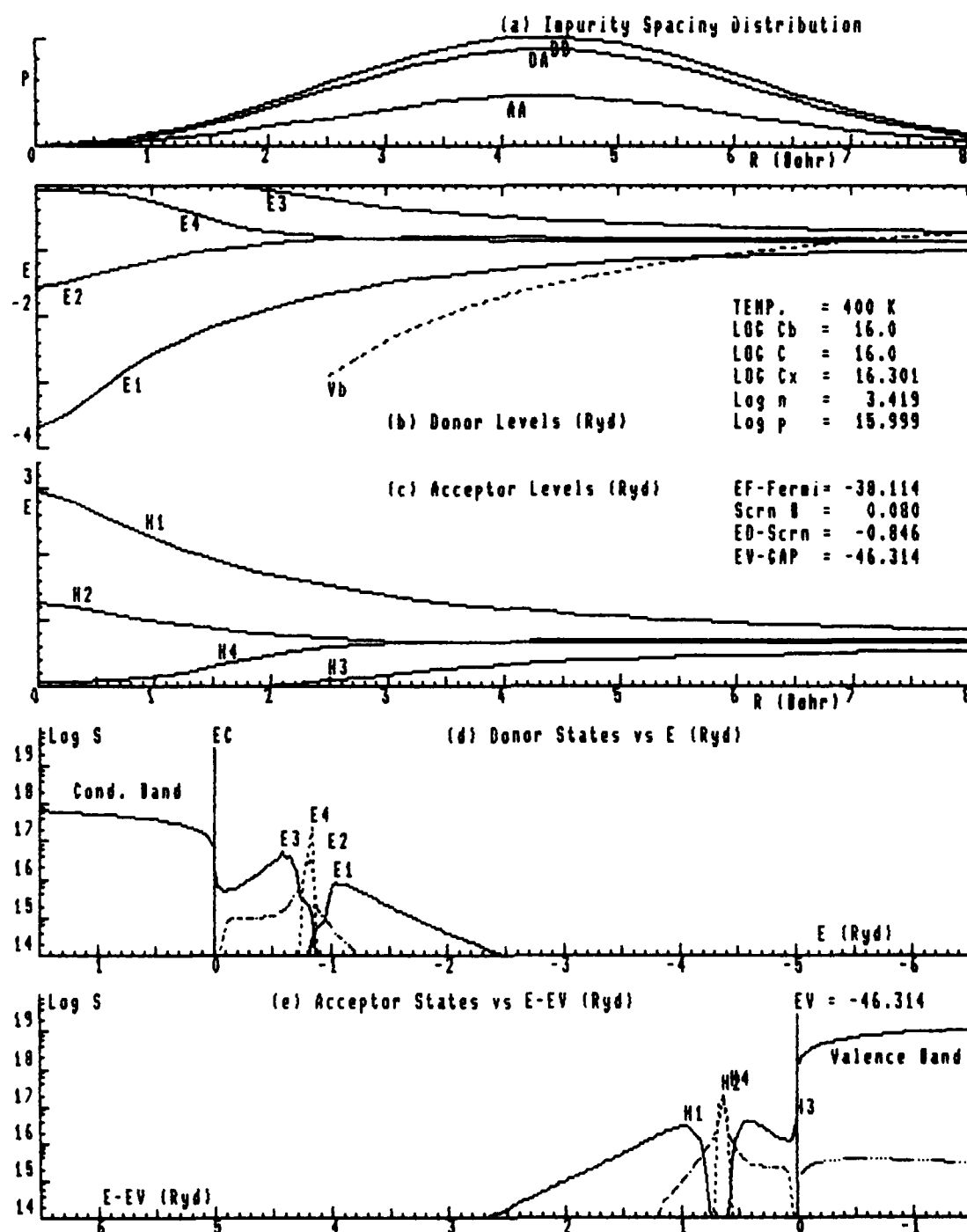


Fig. A 410. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

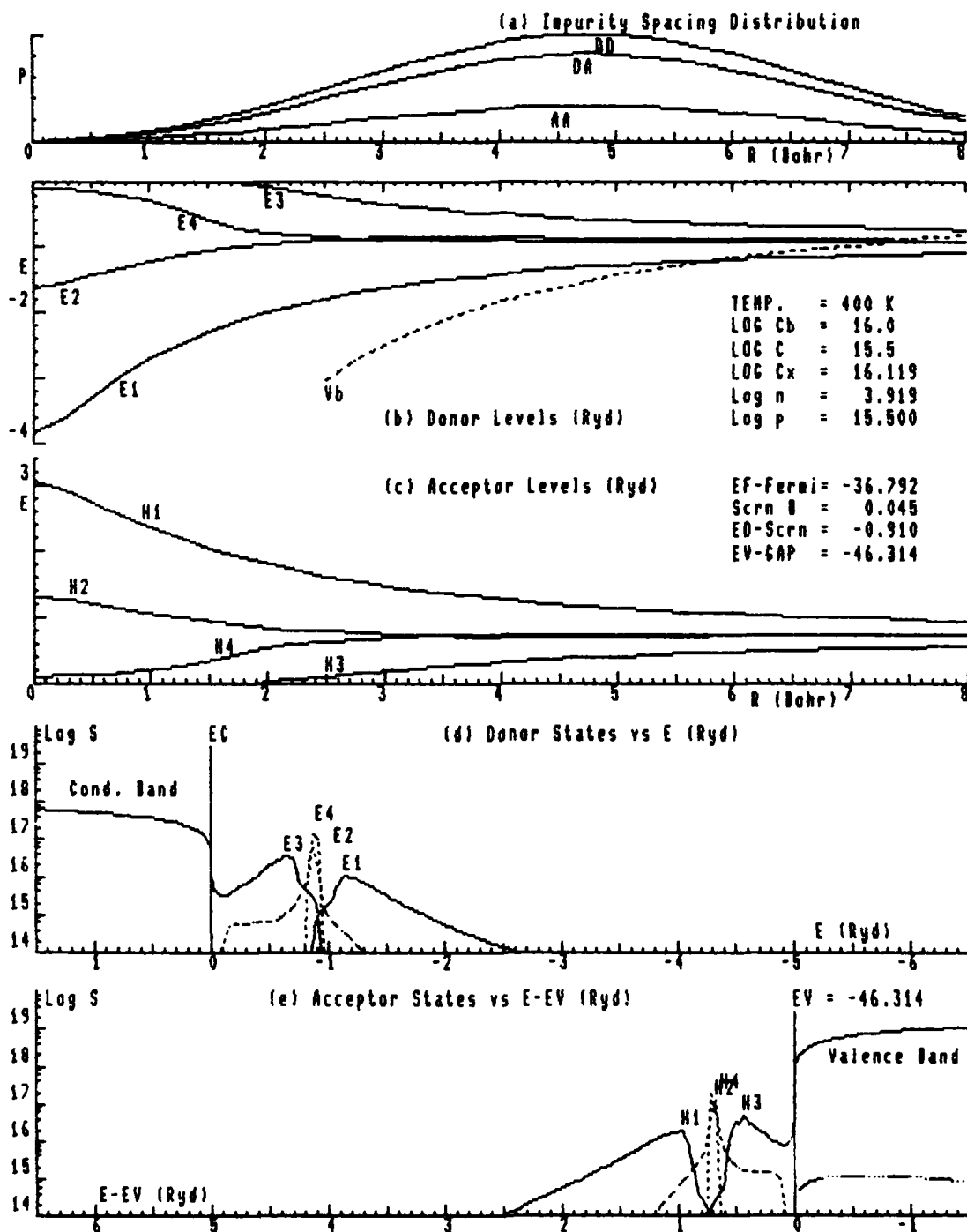


Fig. A 411. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

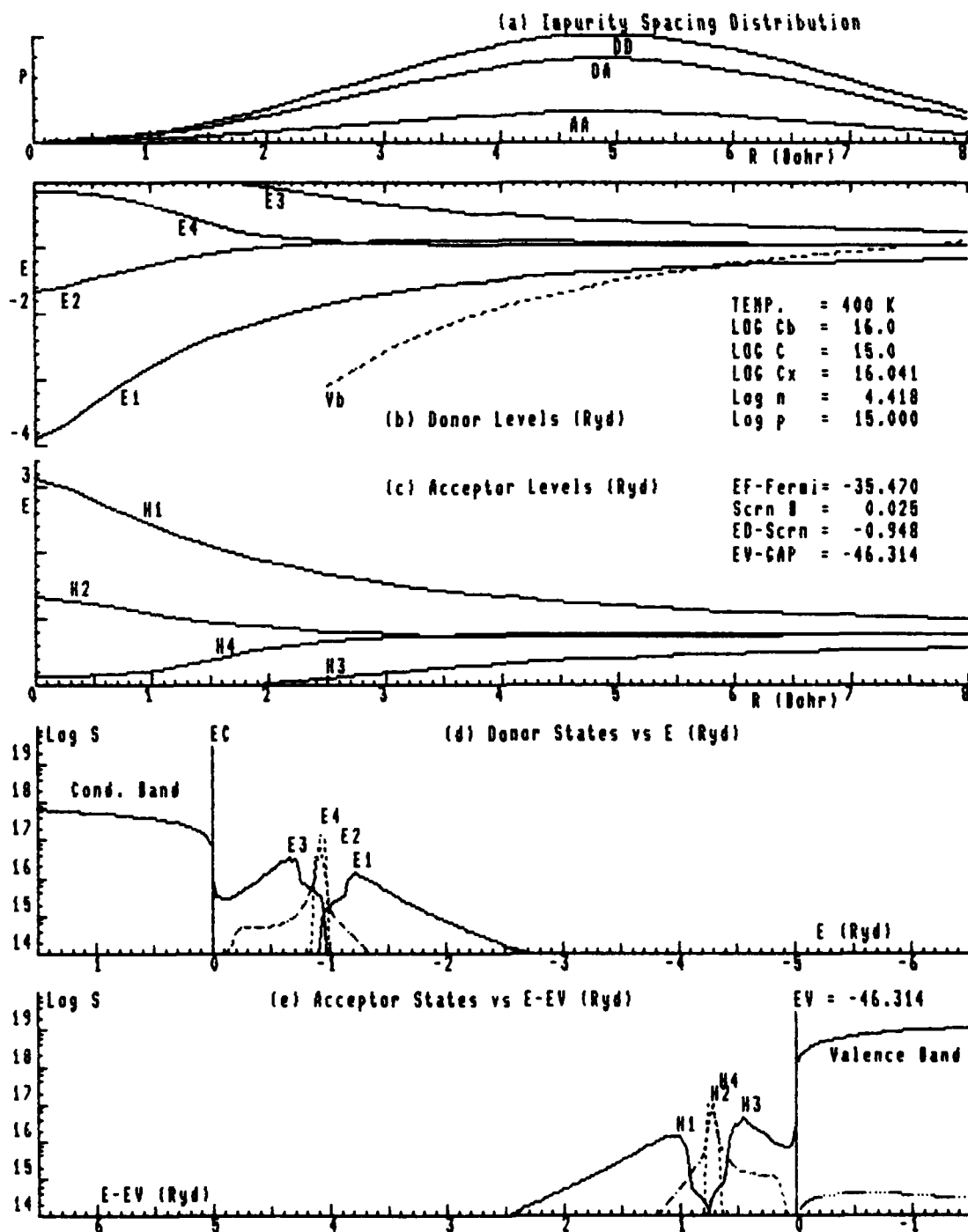


Fig. A 412. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA+)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

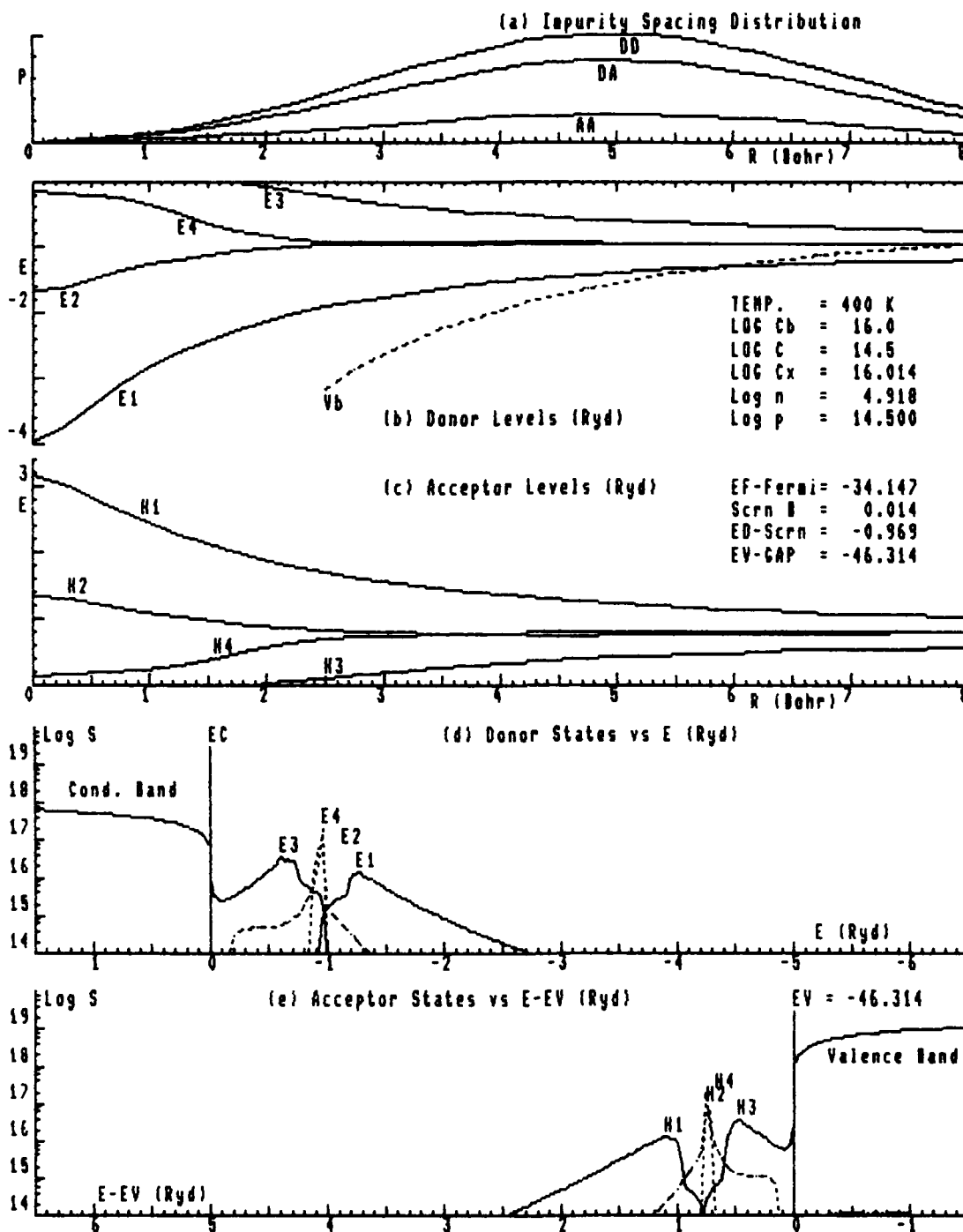


Fig. A 413. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

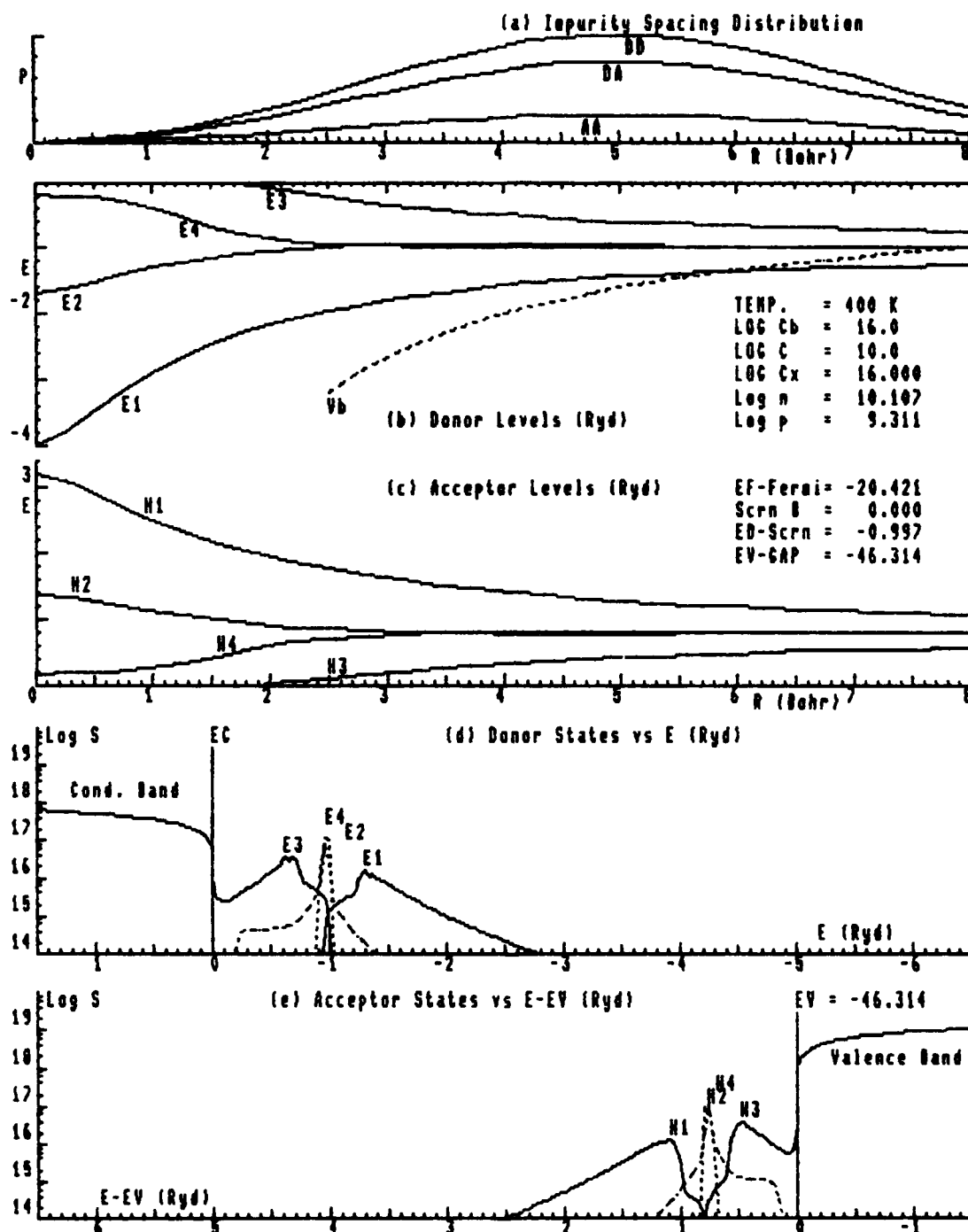


Fig. A 414. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

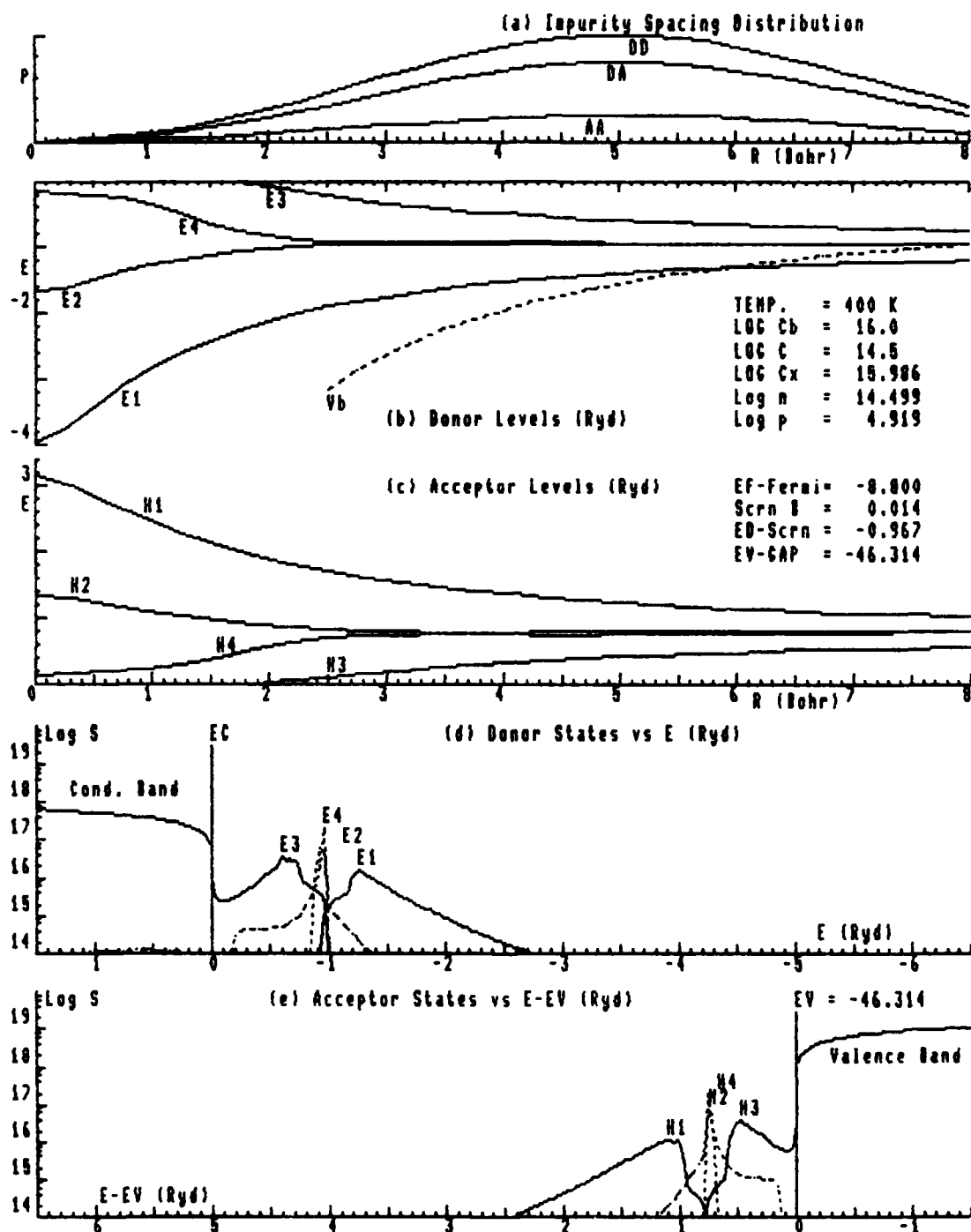


Fig. A 415. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

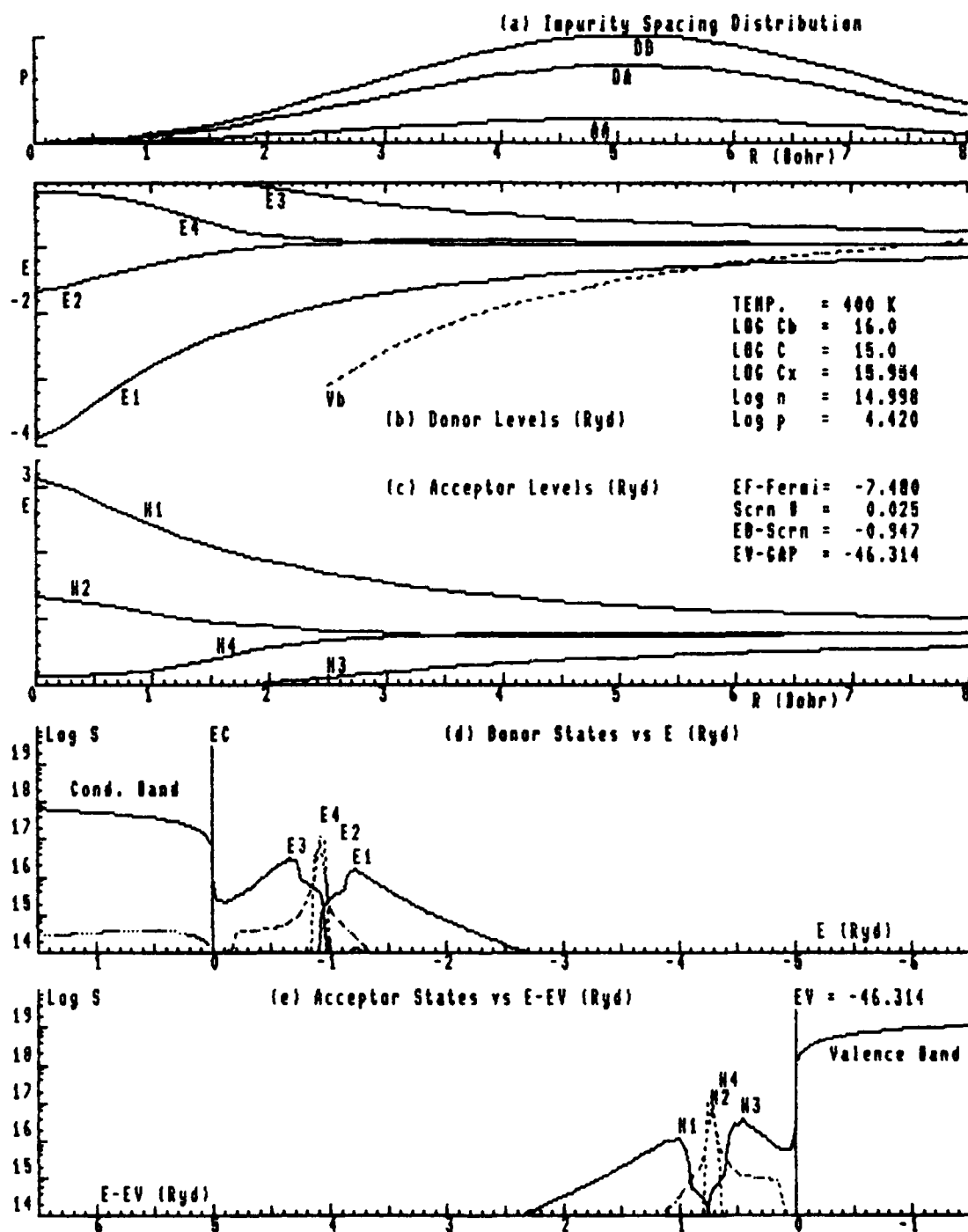


Fig. A 416. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

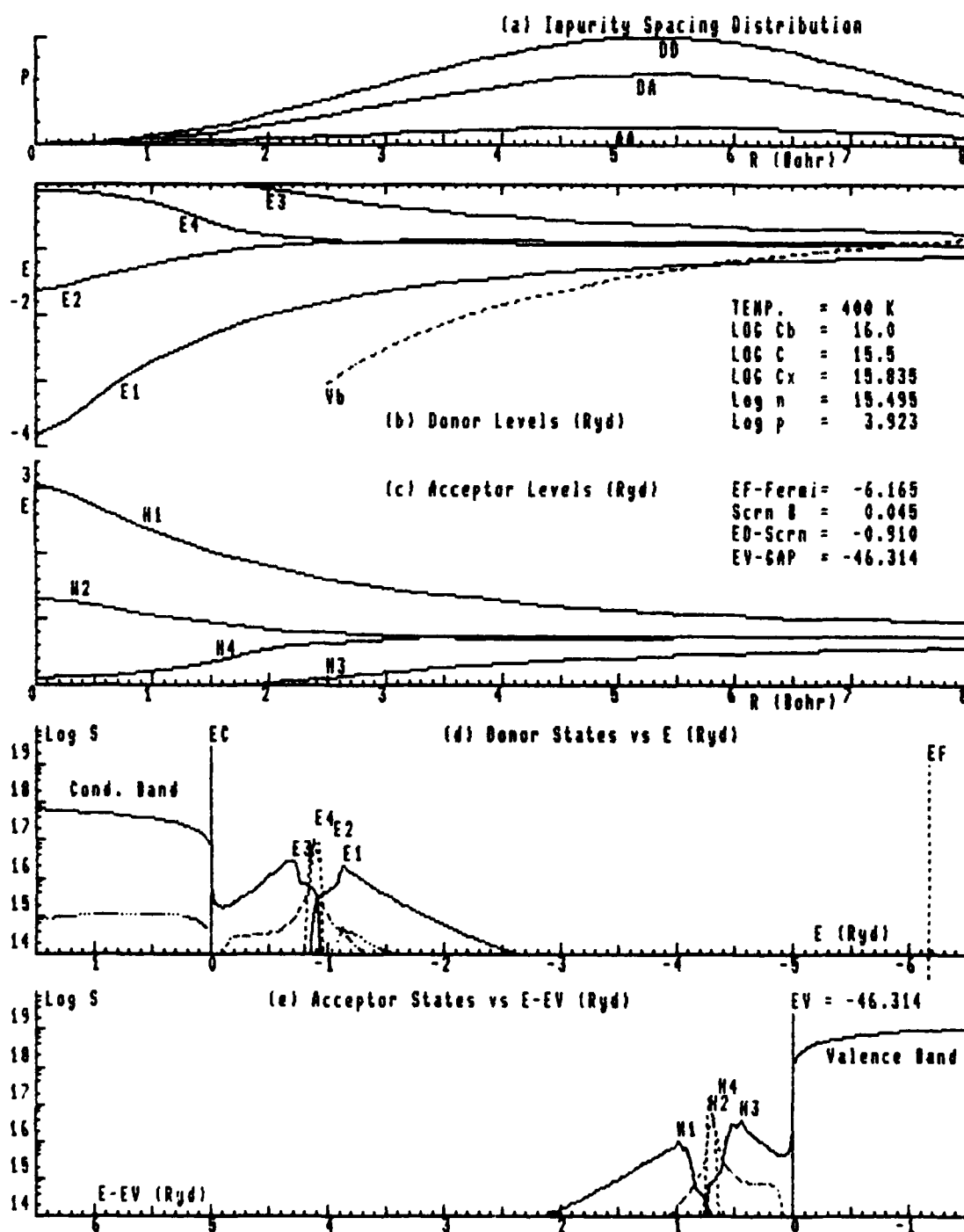


Fig. A 417. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

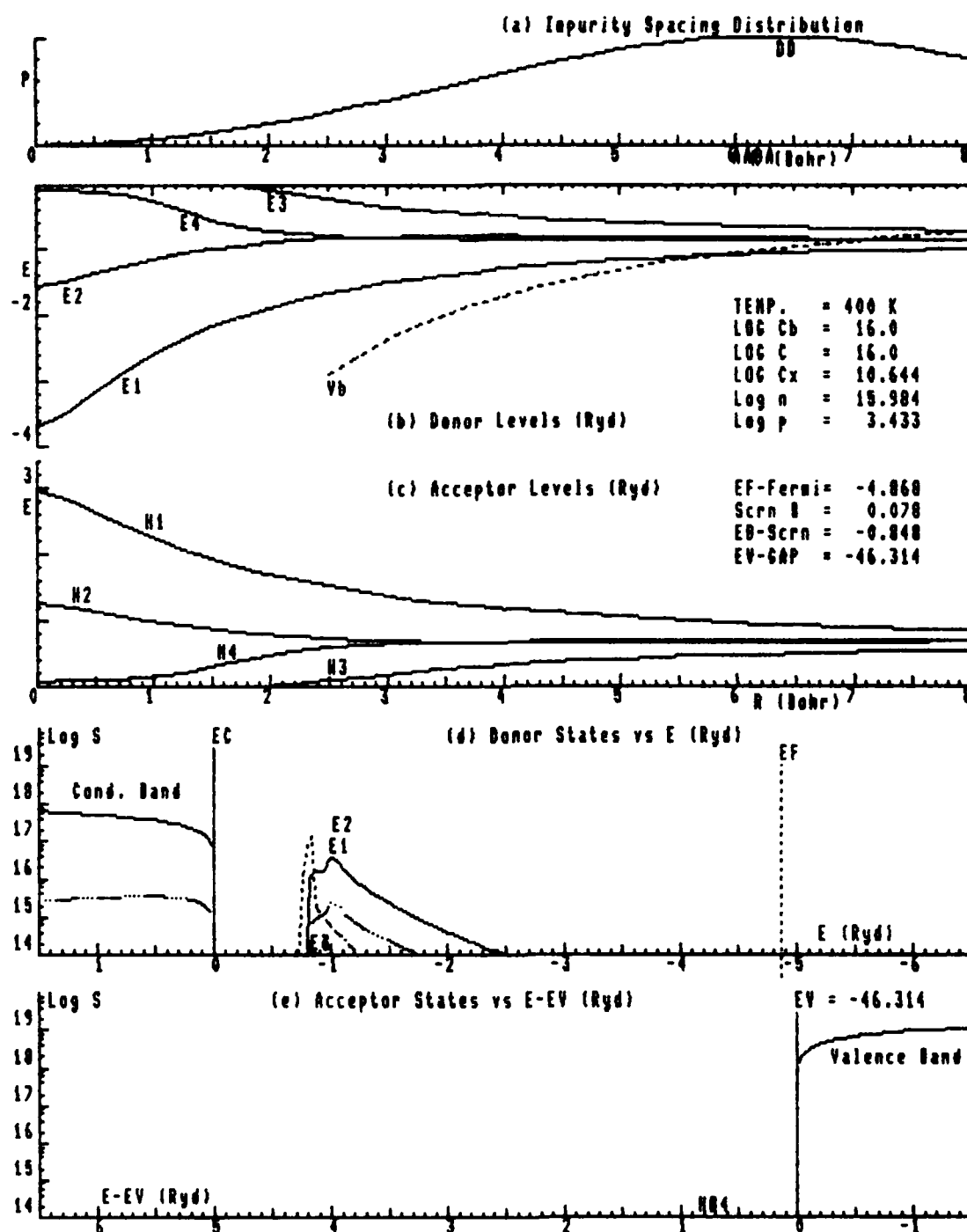


Fig. A 41B. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

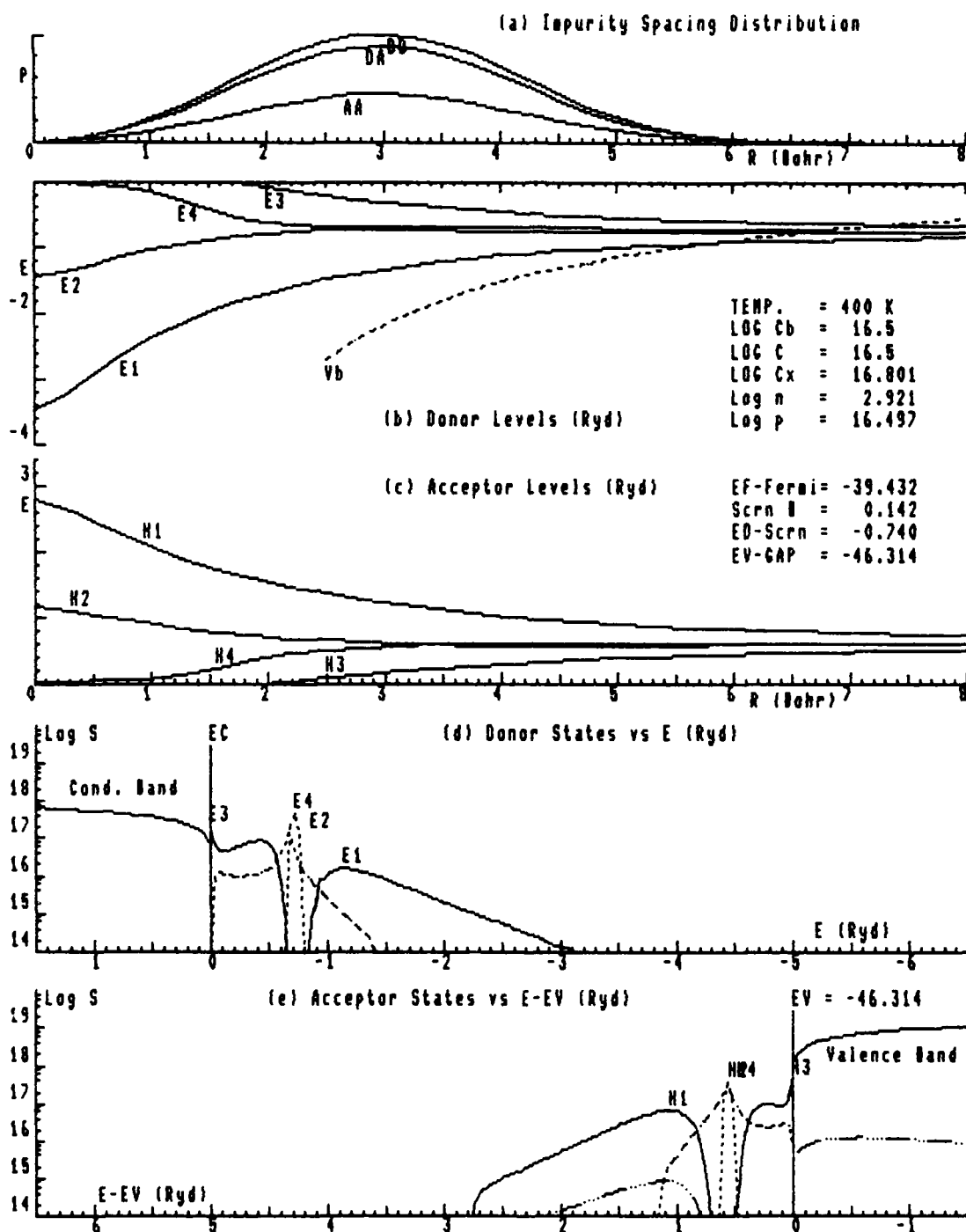


Fig. A 420. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

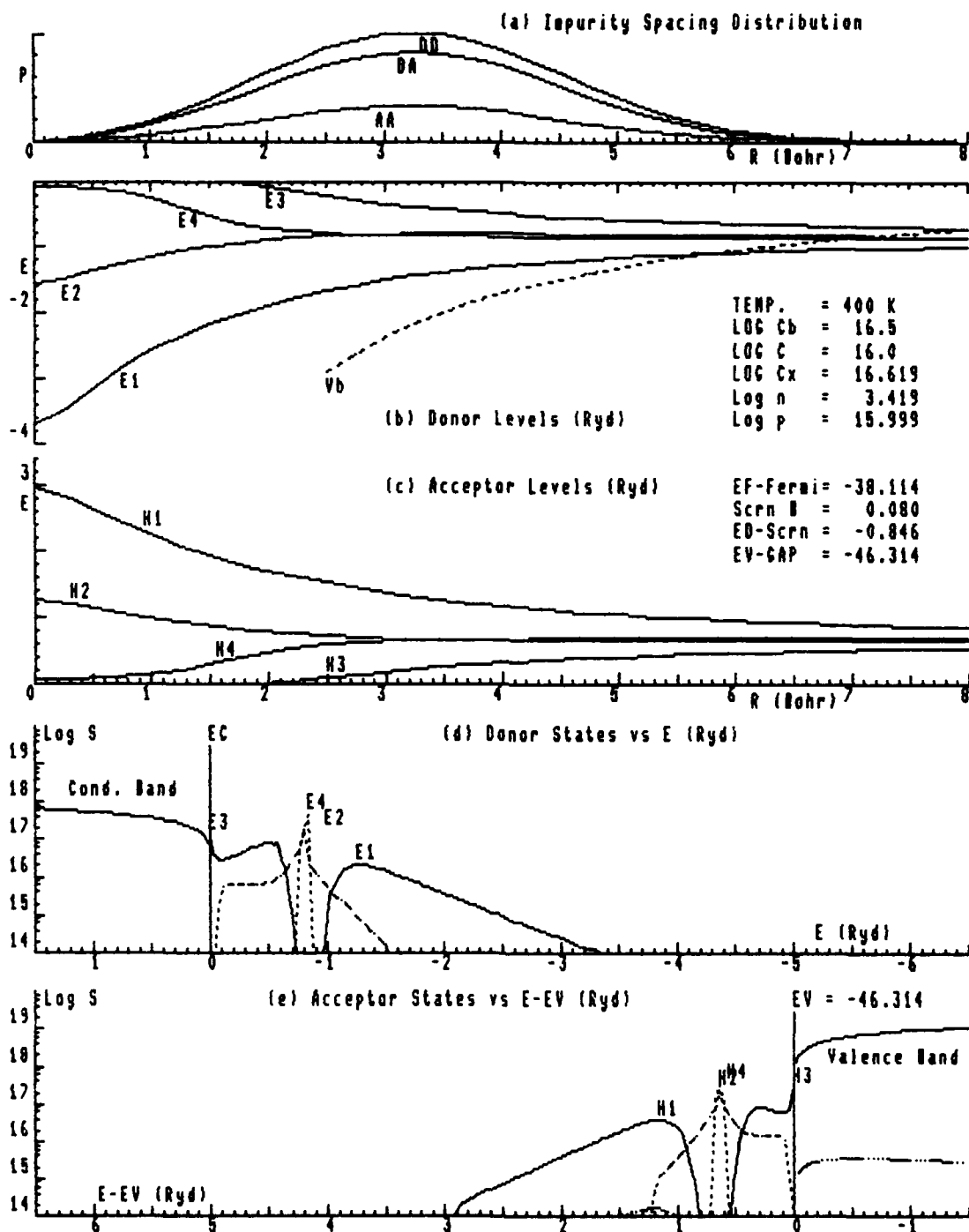


Fig. A 421. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

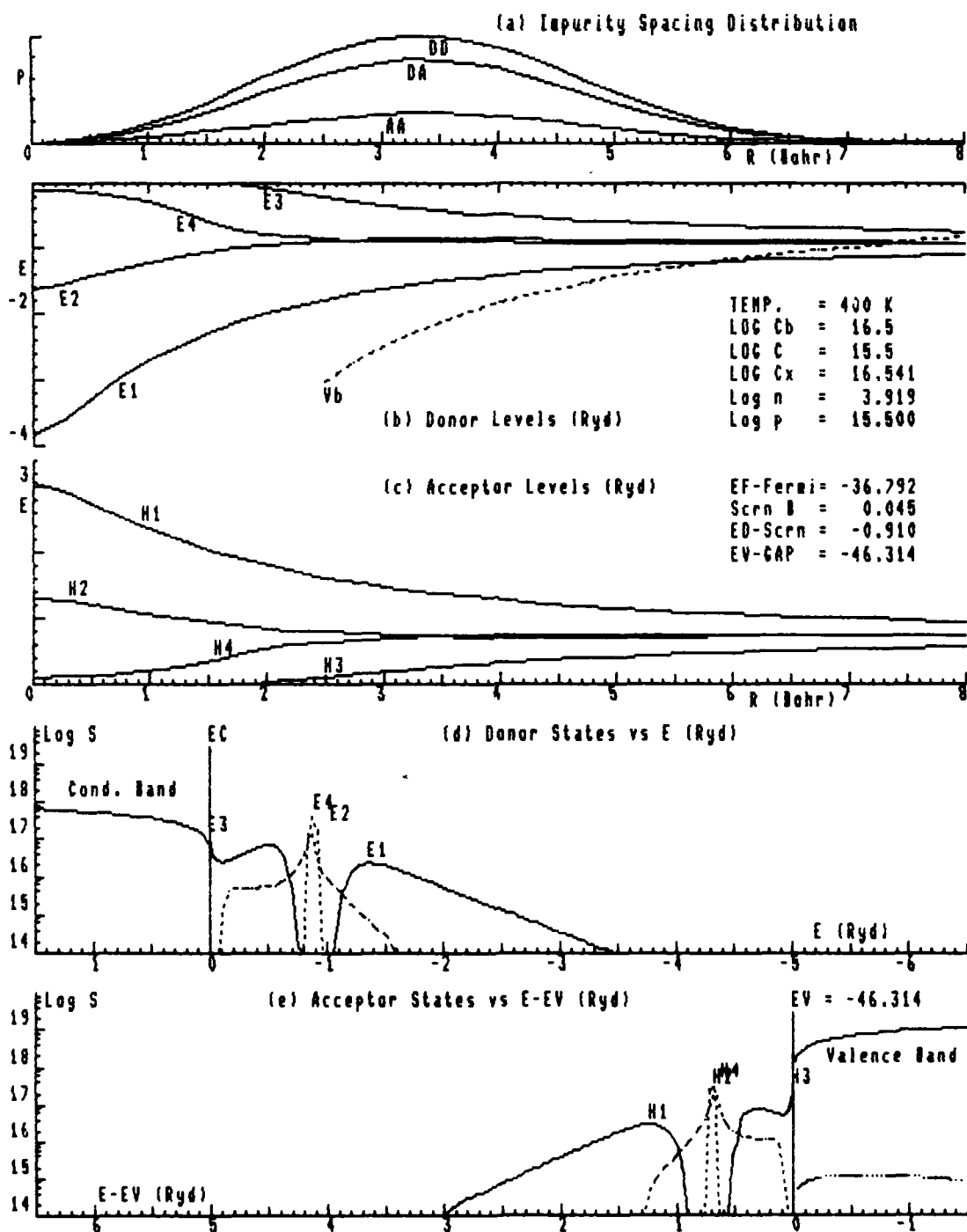


Fig. A 422. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

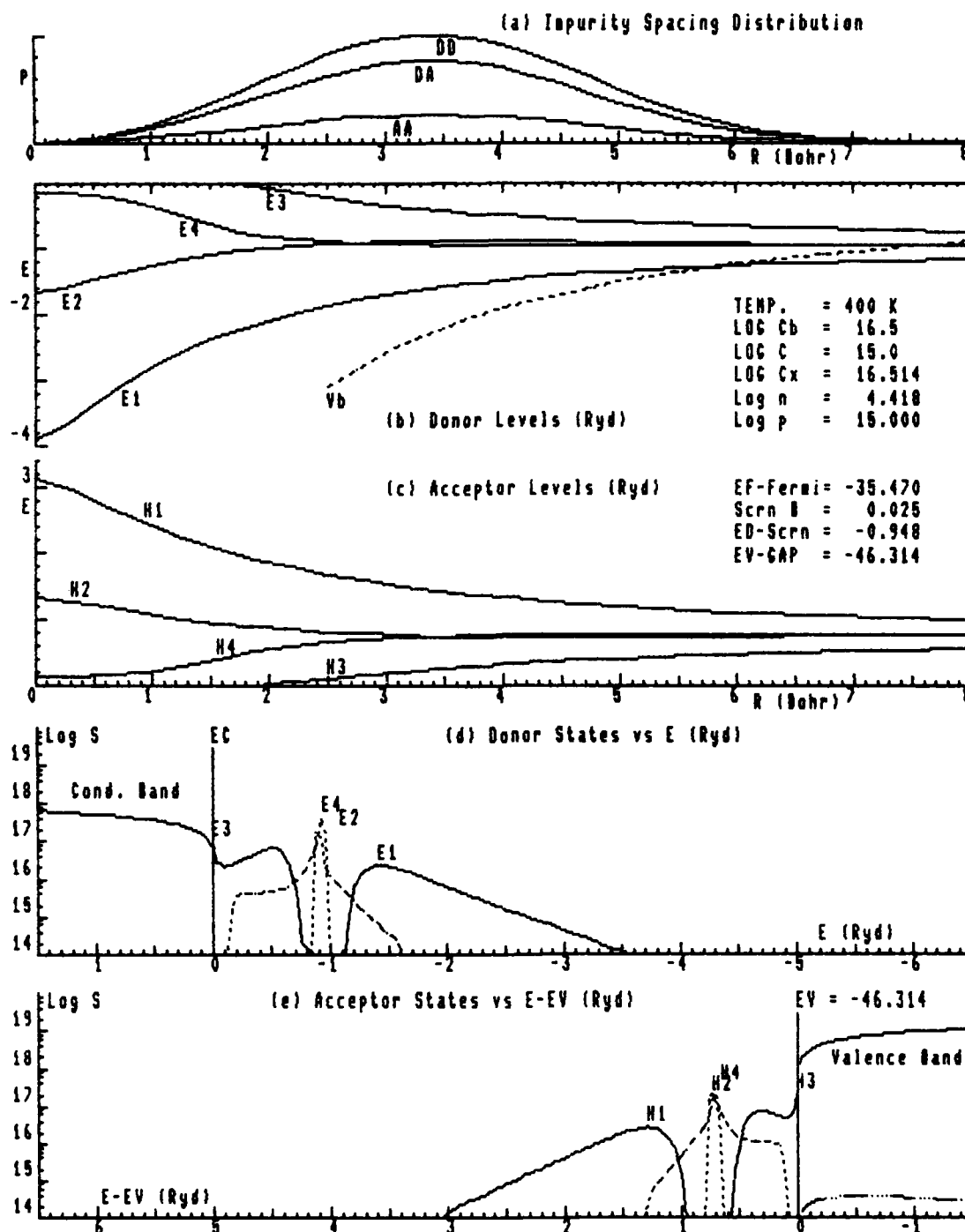


Fig. A 423. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

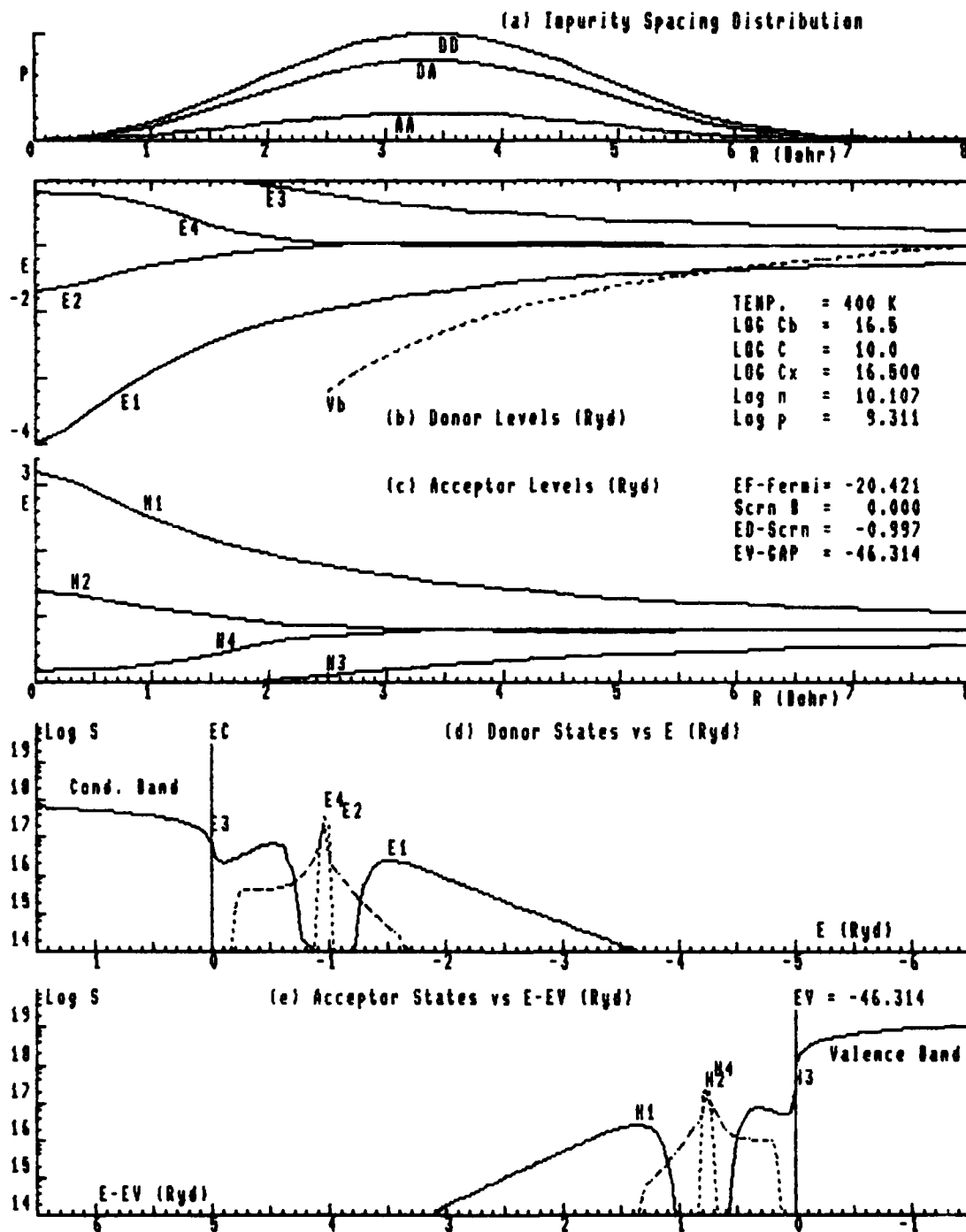


Fig. A 424. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

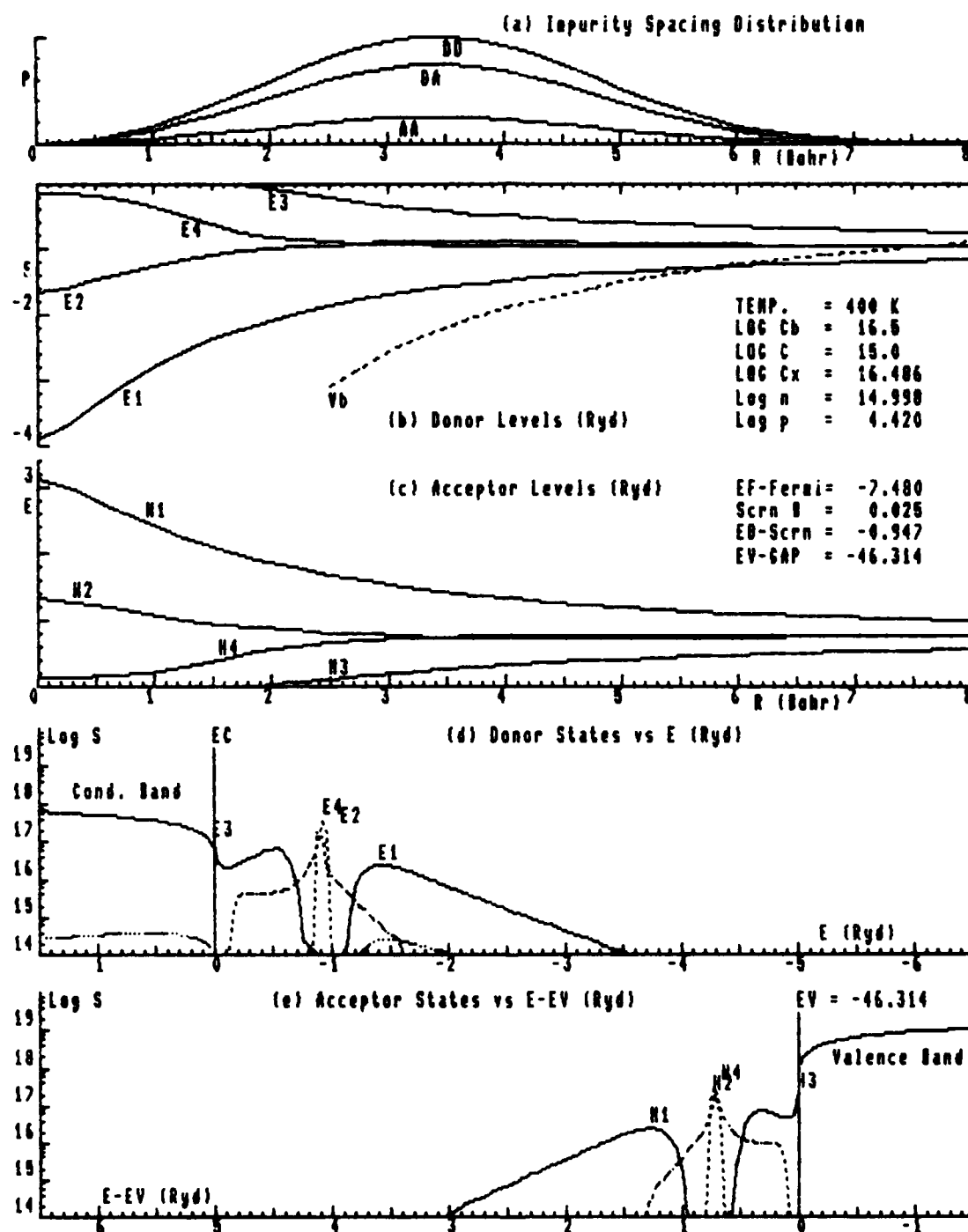


Fig. A 425. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)-+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

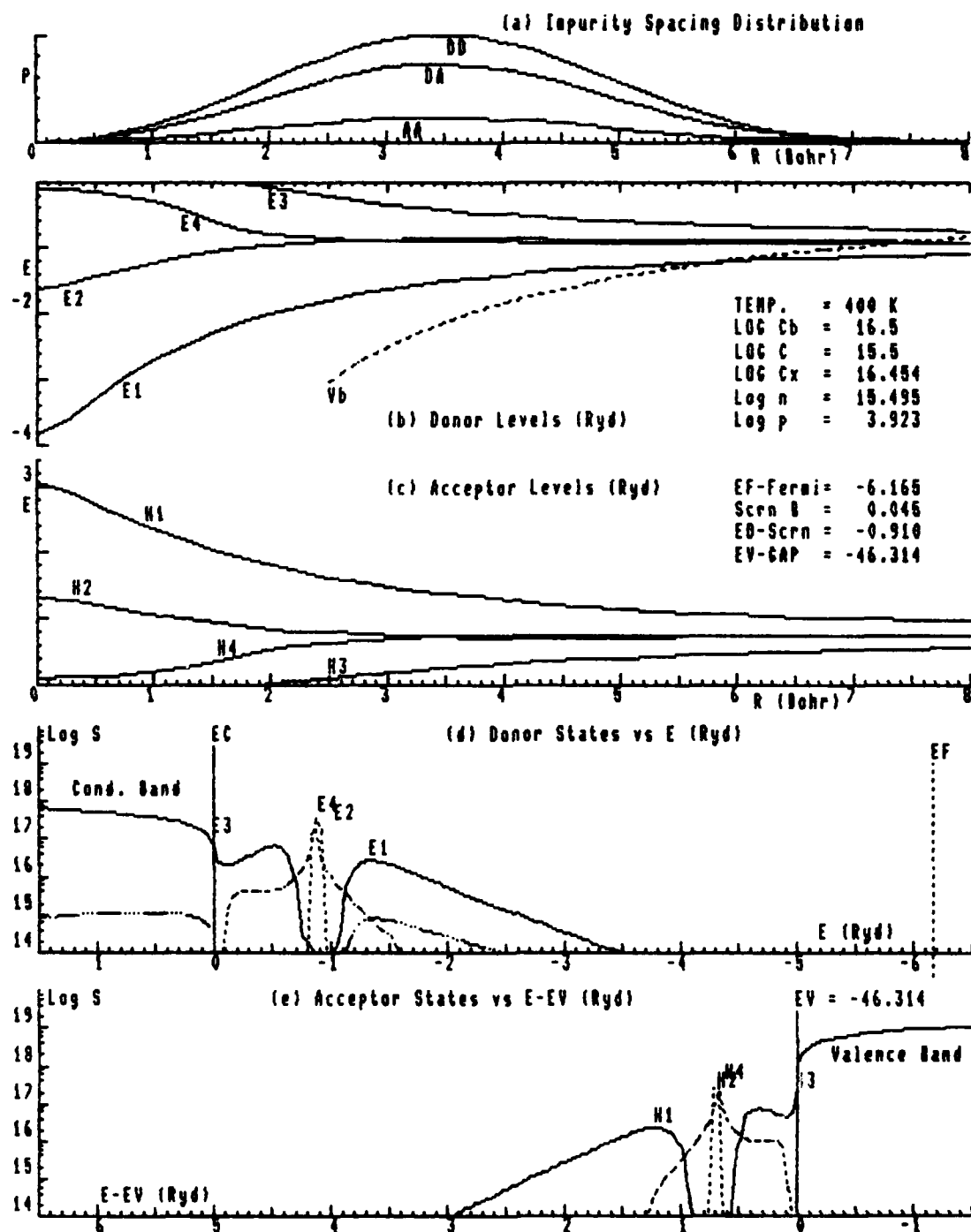


Fig. A 426. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

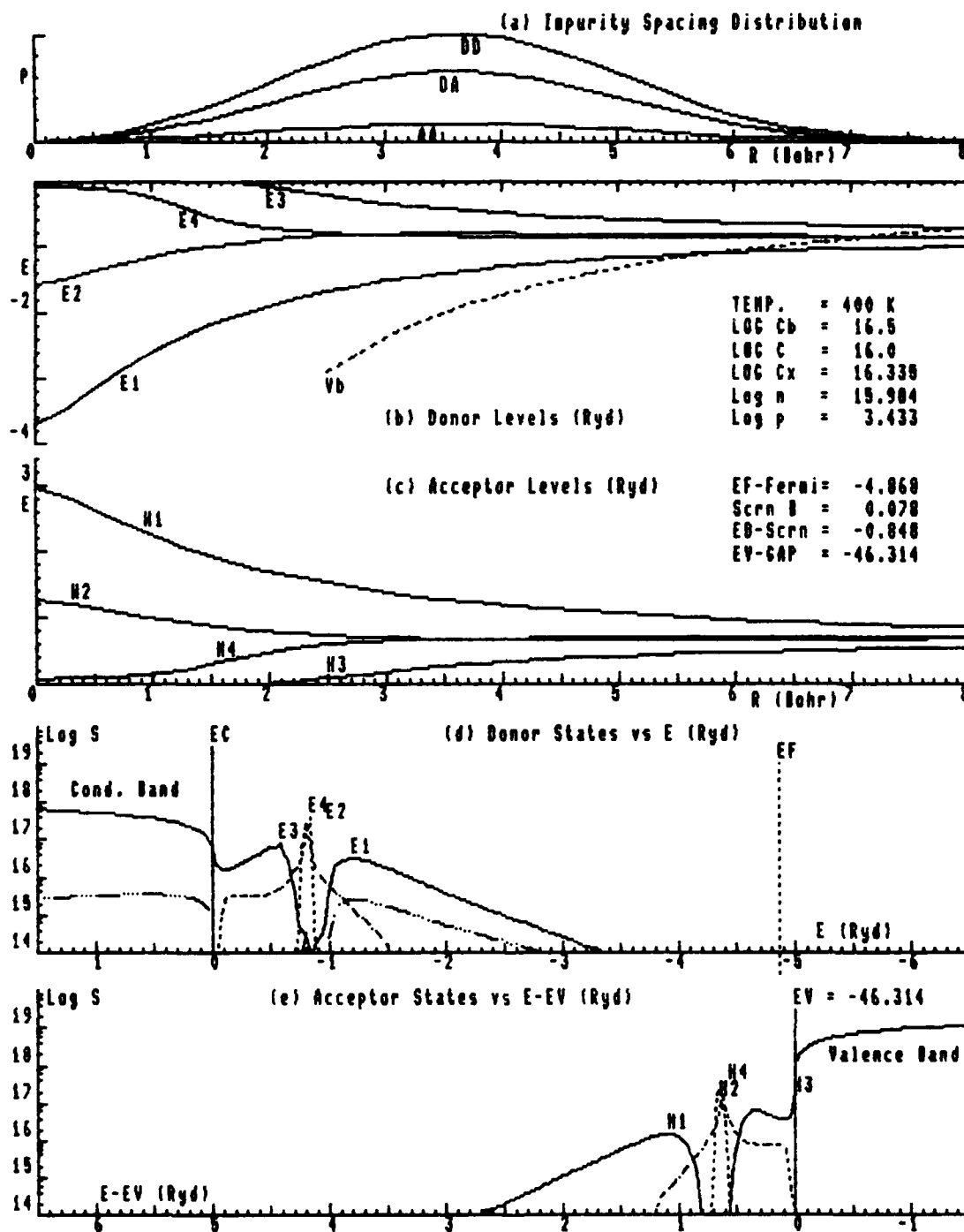


Fig. A 427. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

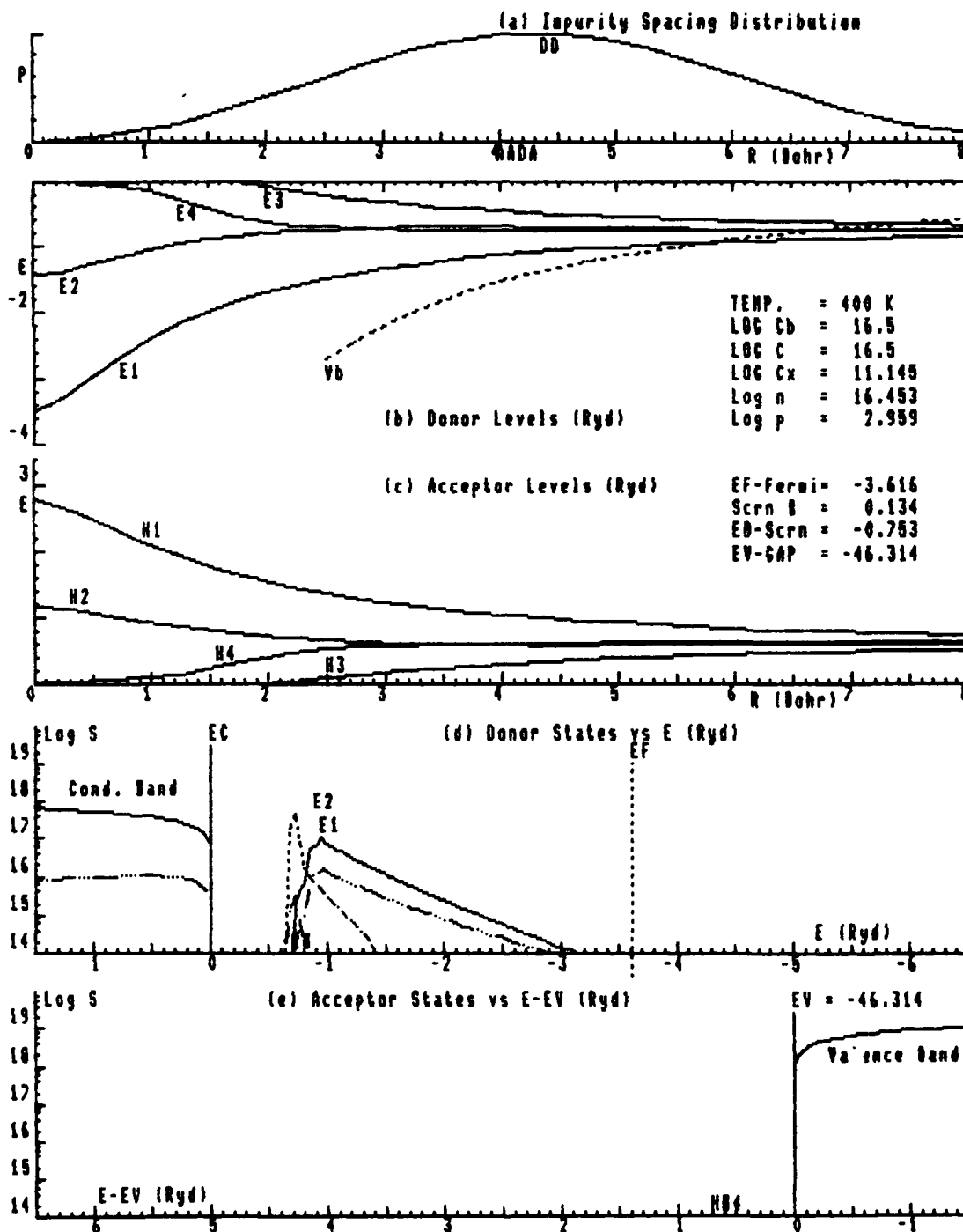


Fig. A 428. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

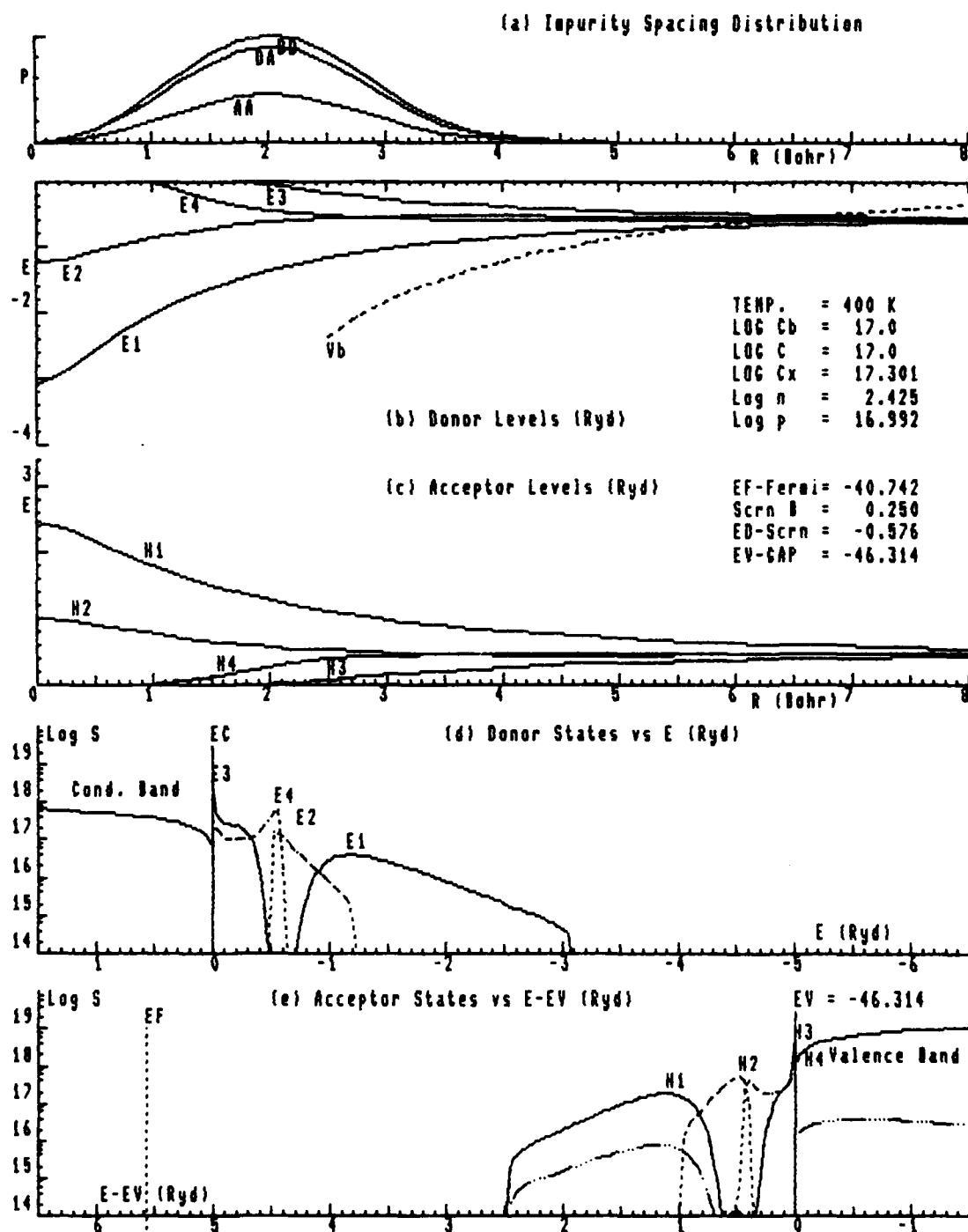


Fig. A 430. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

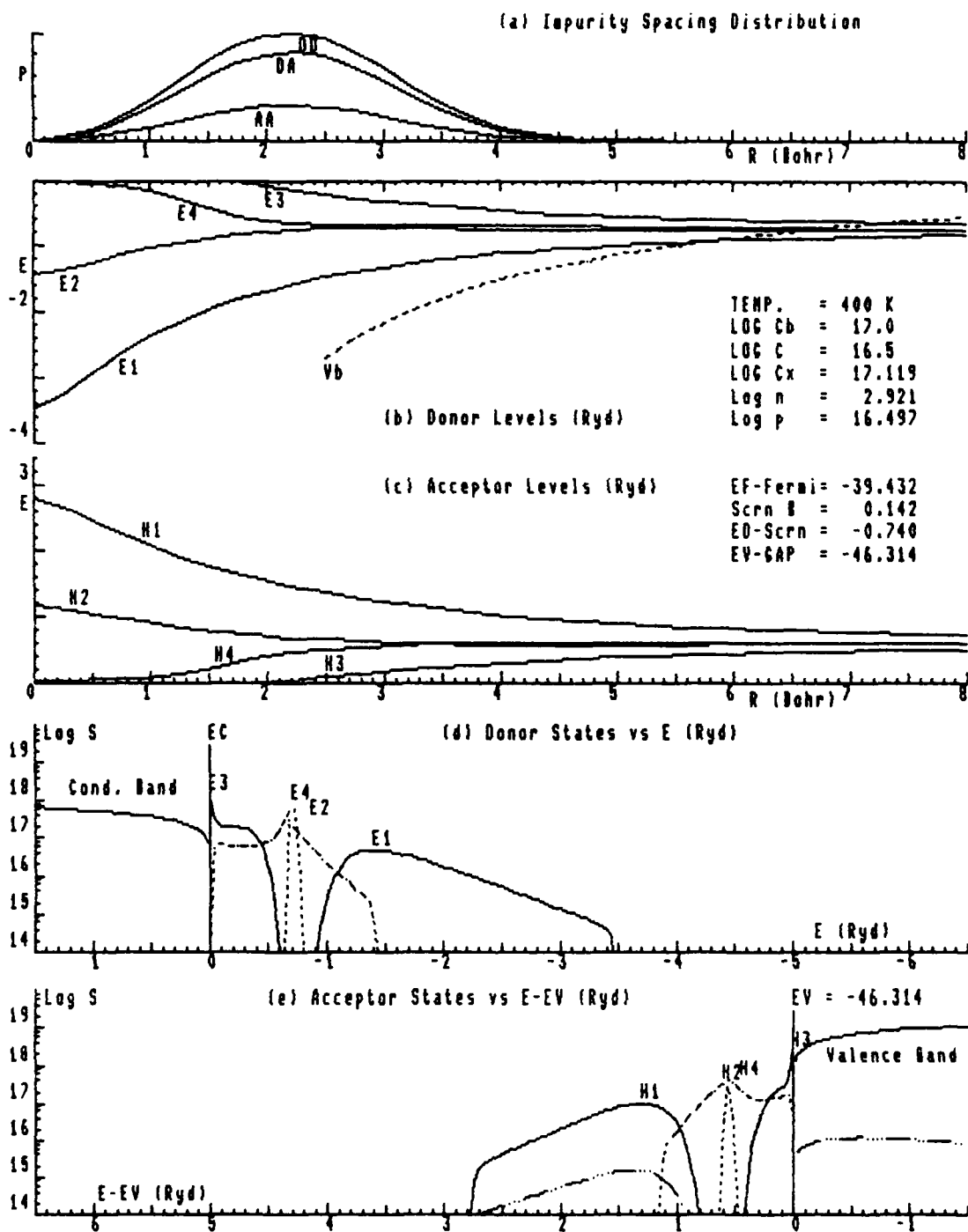


Fig. A 431. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

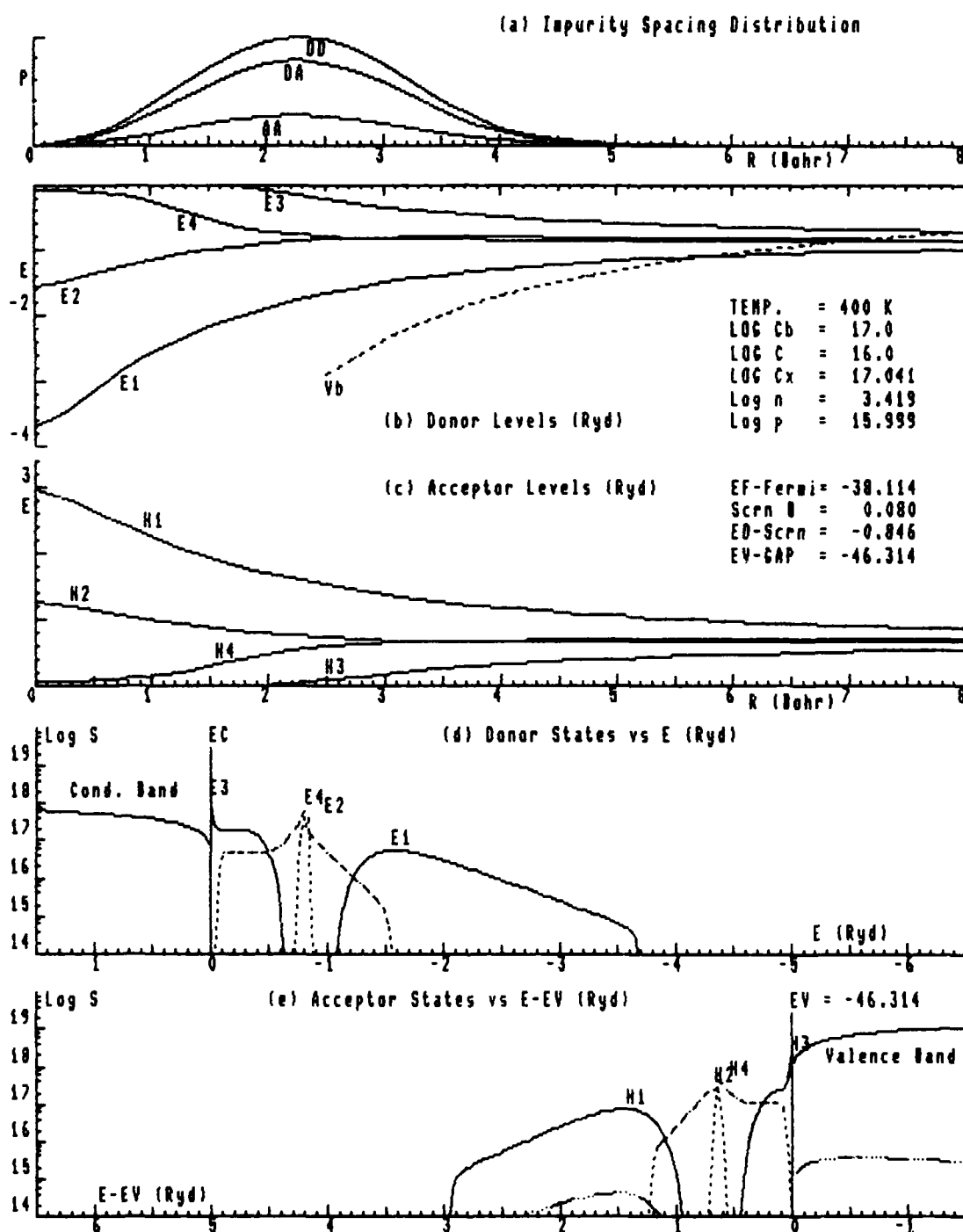


Fig. A 432. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

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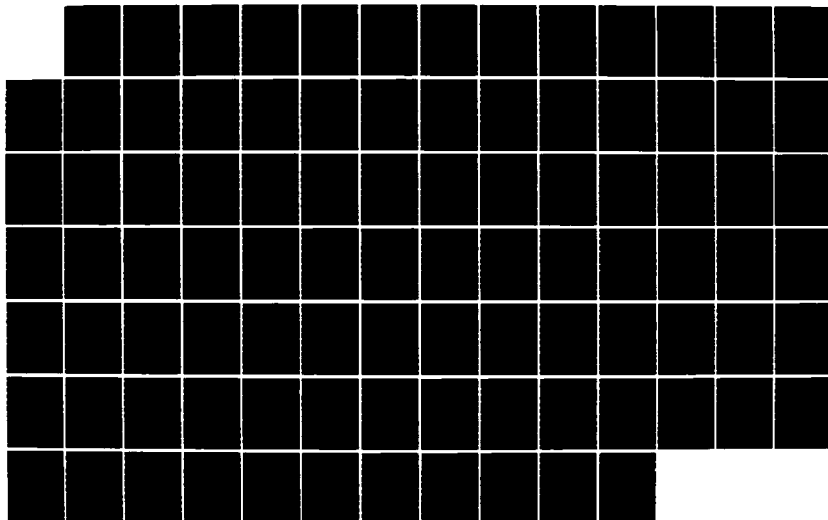
ANALYSIS OF IMPURITY BAND FORMATION AND RELATED EFFECTS
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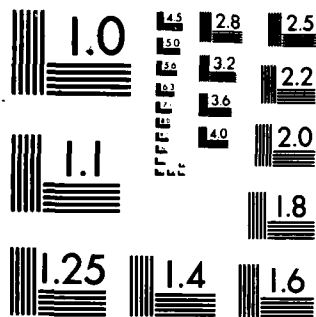
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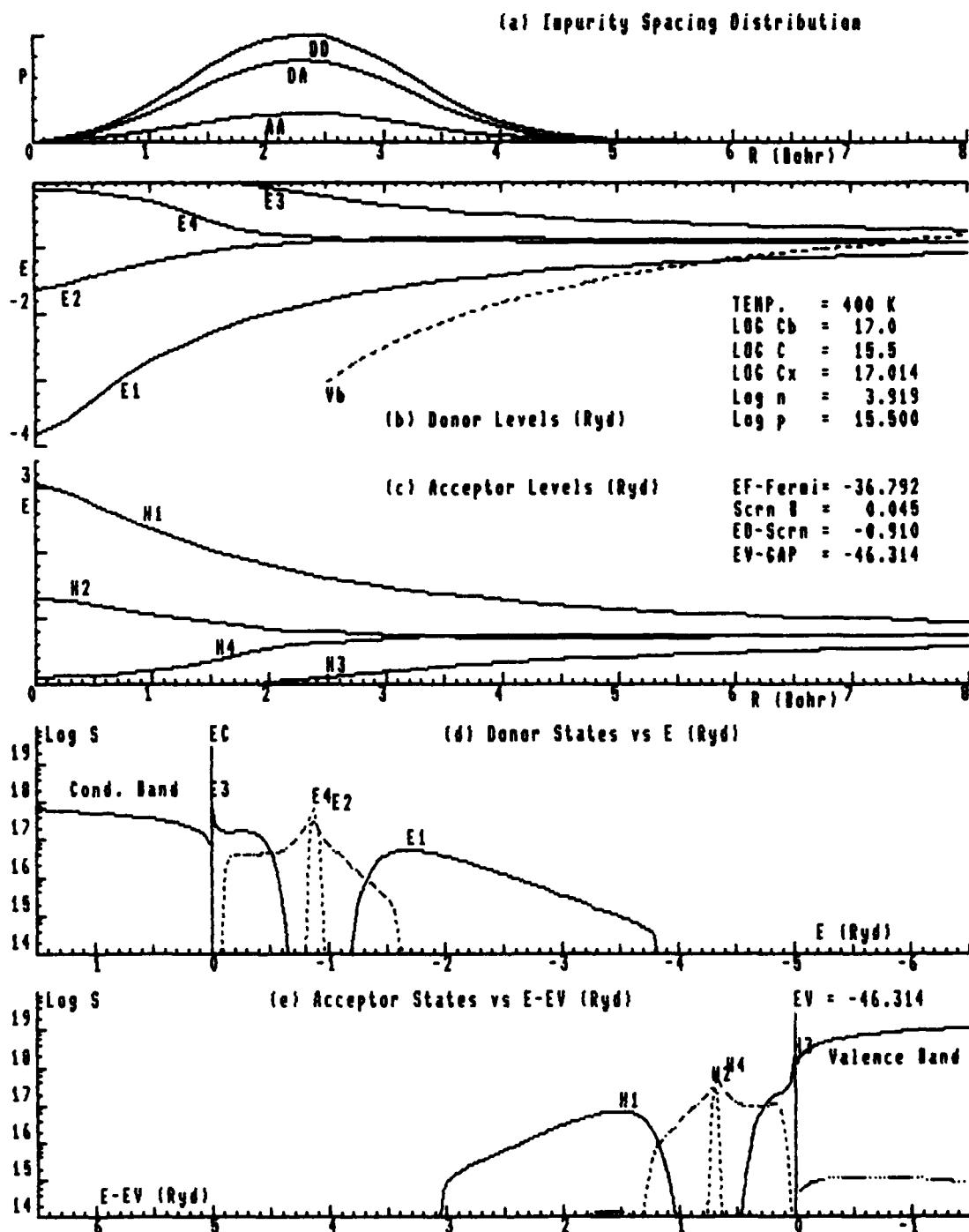


Fig. A 433. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD+)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

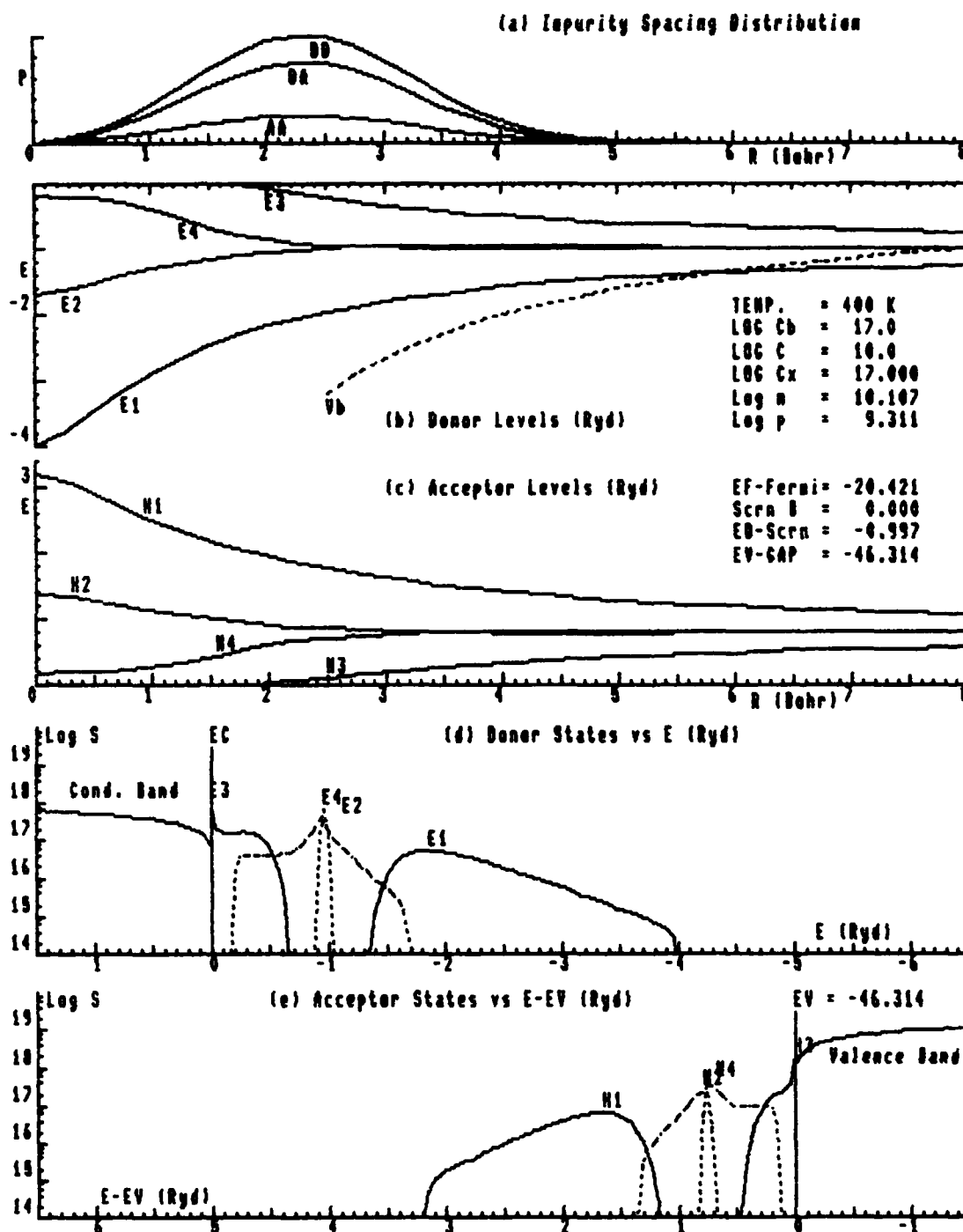


Fig. A 434. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

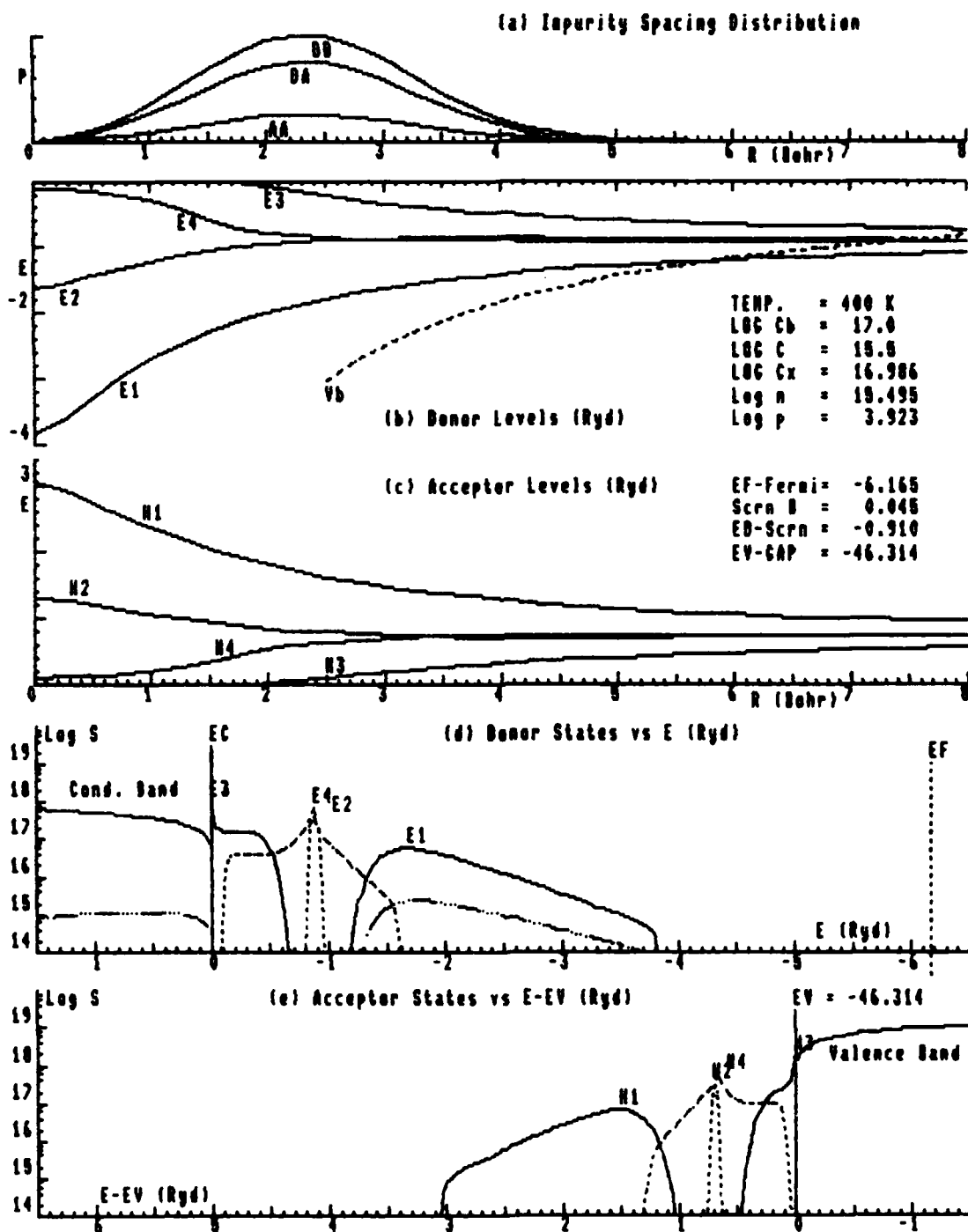


Fig. A 435. (a) Probability, $AA + DA + DD$, of Pairs vs R
 (b) Donor Energy $E1; (DD)^-, E2; (DD)^-, E3; (DA)^-, E4(DA)^+$ vs R
 (c) Acceptor En. $H1; (AA)^+, H2; (AA)^+, H3; (AD)^+, H4(AD)^+$ vs R
 (d) Densities of Donor States, $E1, E2, E3, \& E4$, vs E
 (e) Densities of Acceptor States, $H1, H2, H3, \& H4$ vs $E-EV$.

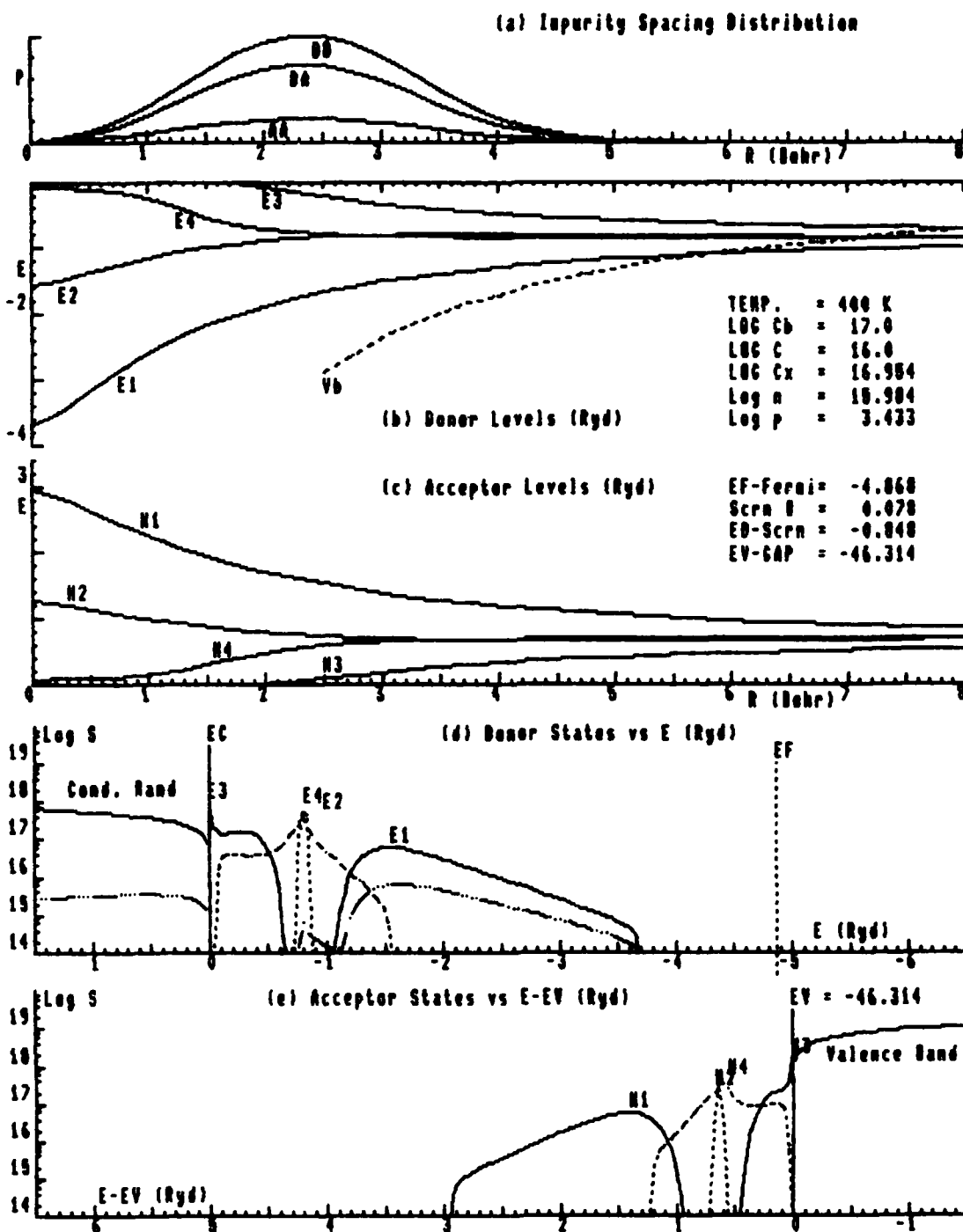


Fig. A 436. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

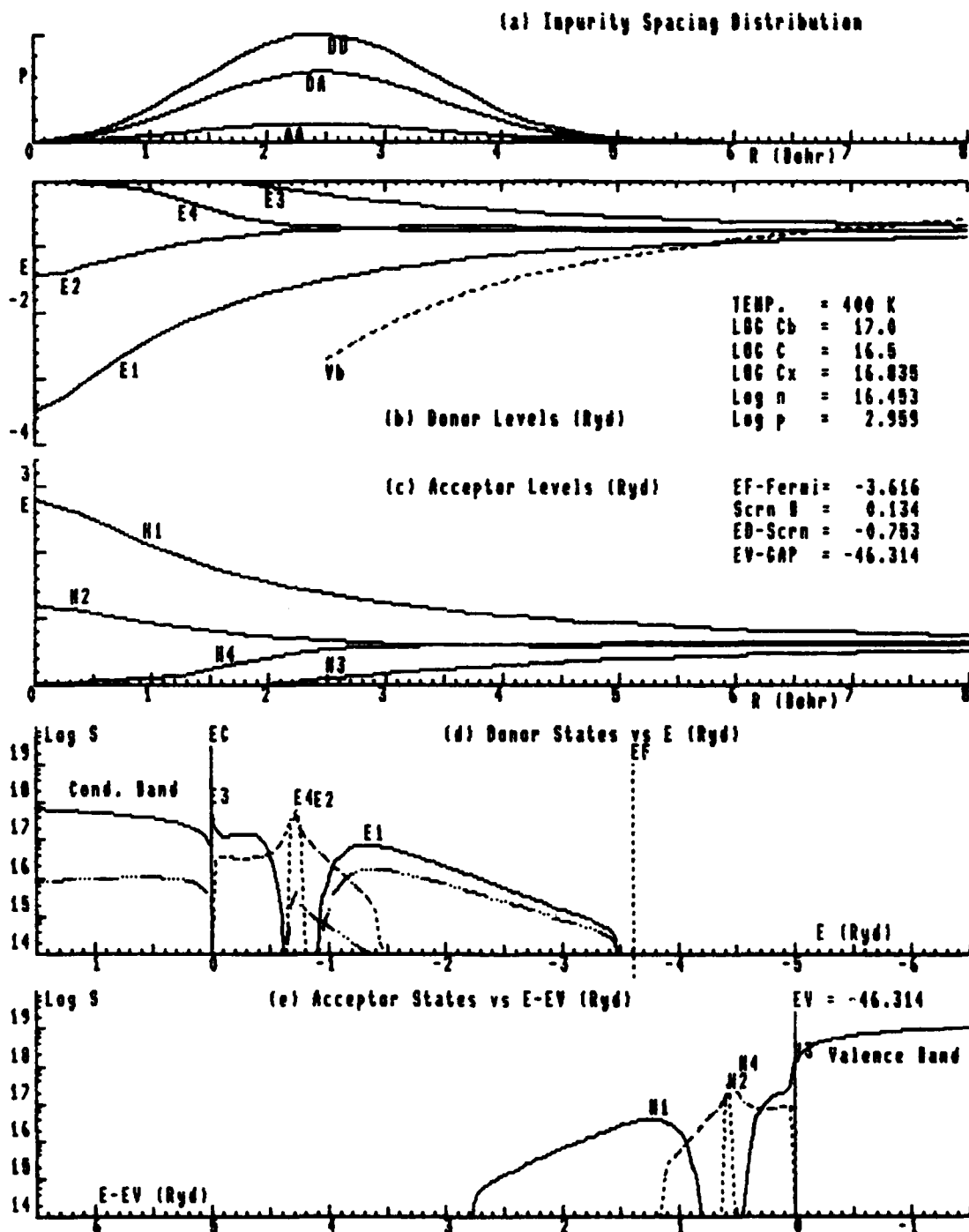


Fig. A 437. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

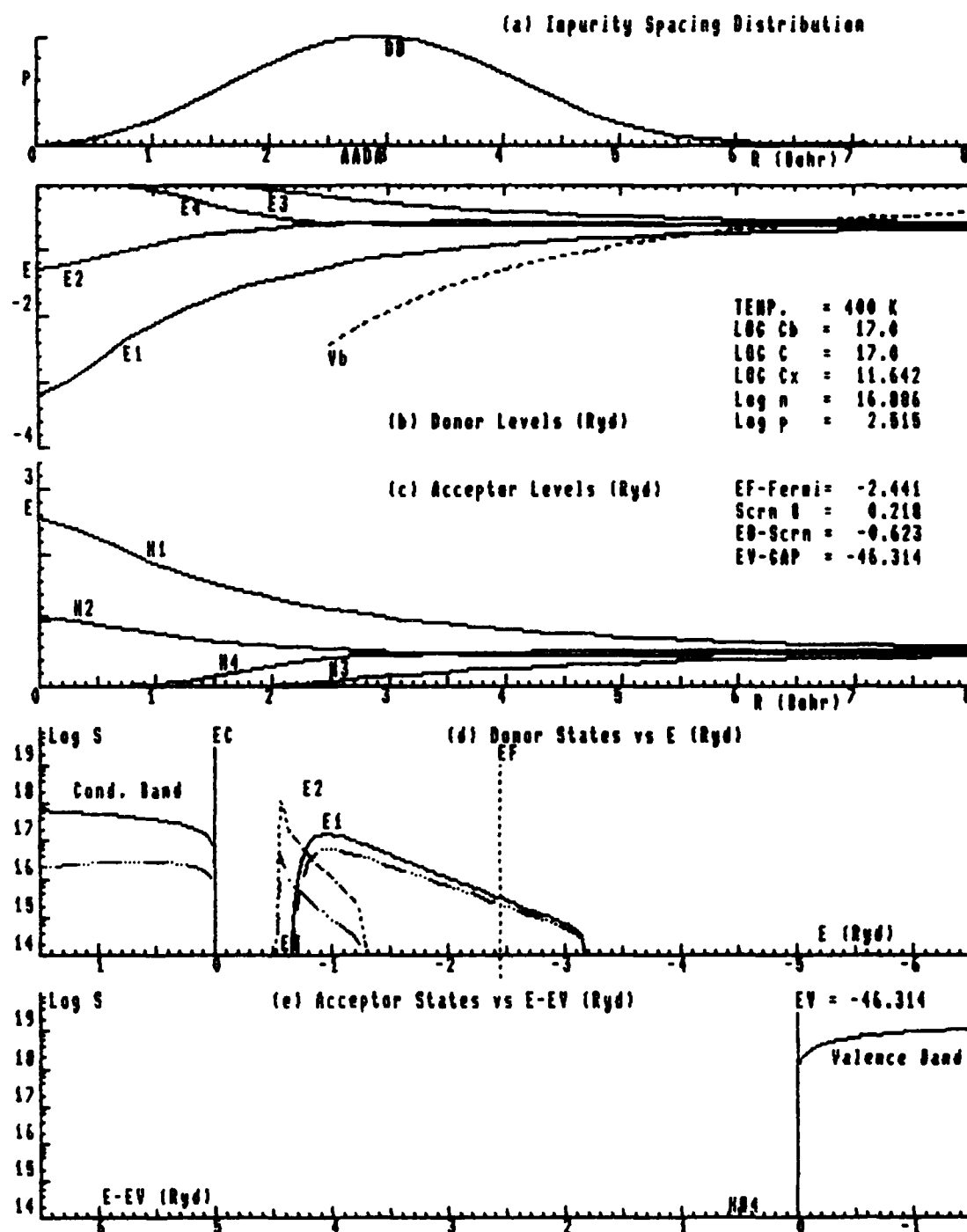


Fig. A 438. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA+)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

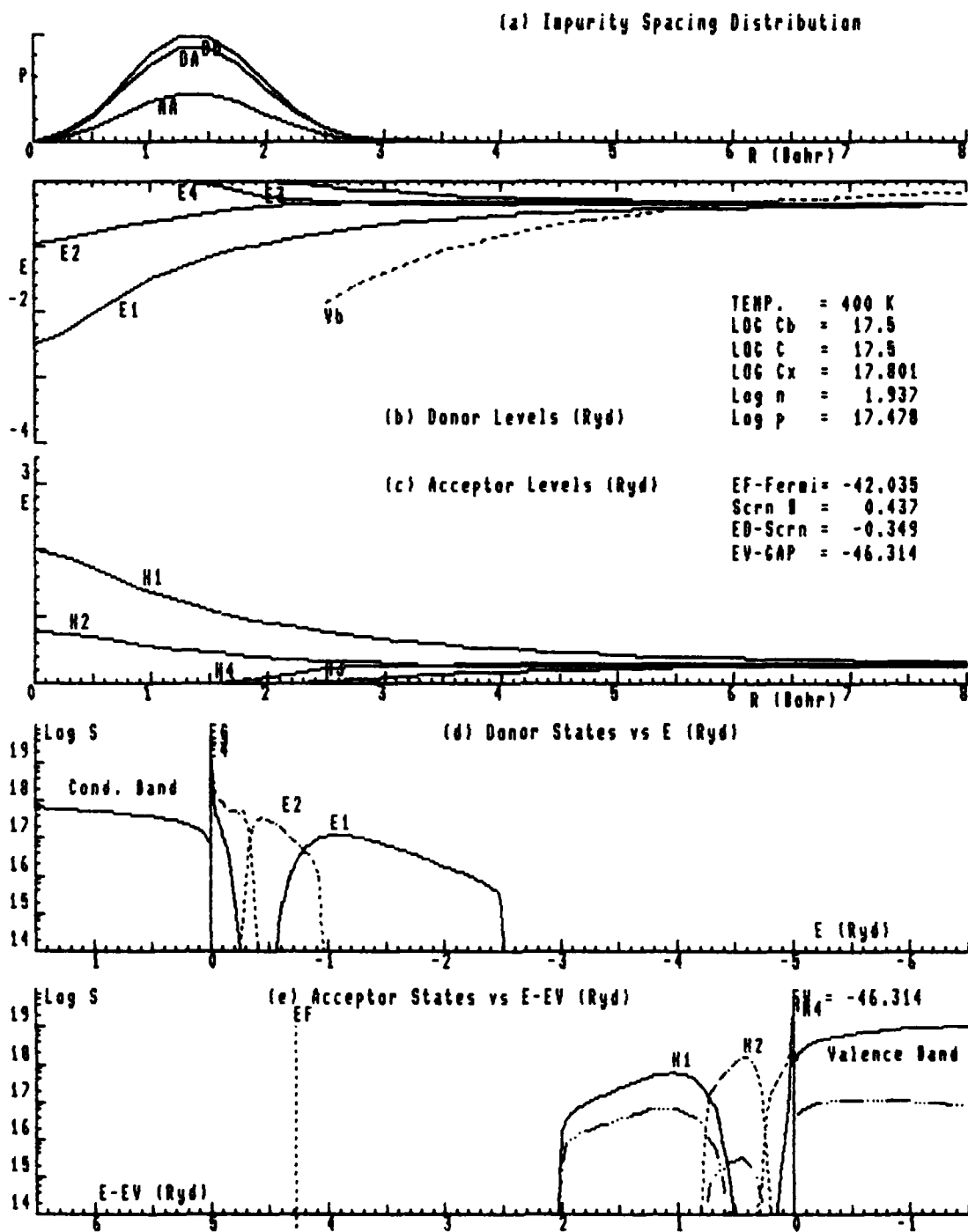


Fig. A 440. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

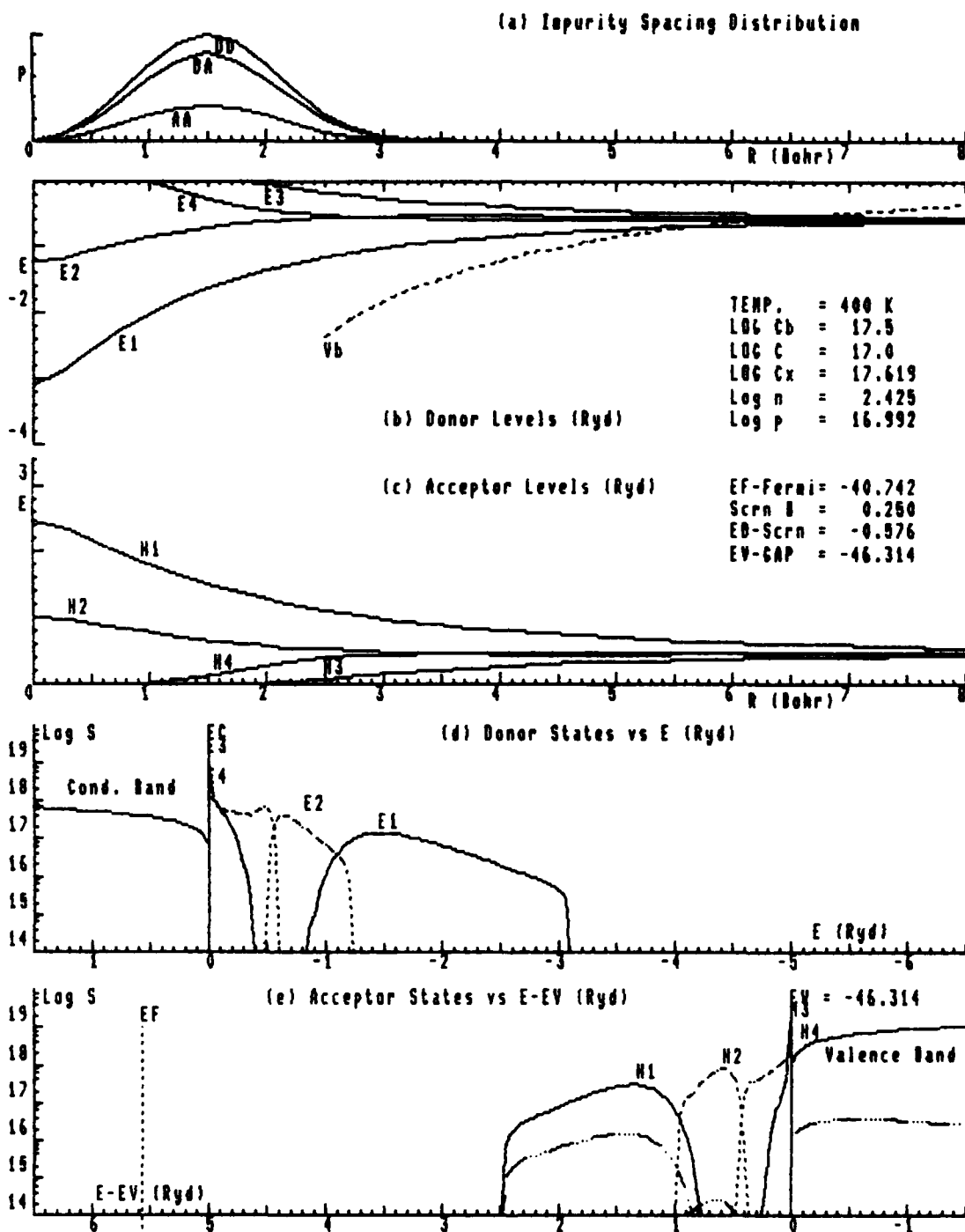


Fig. A 441. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

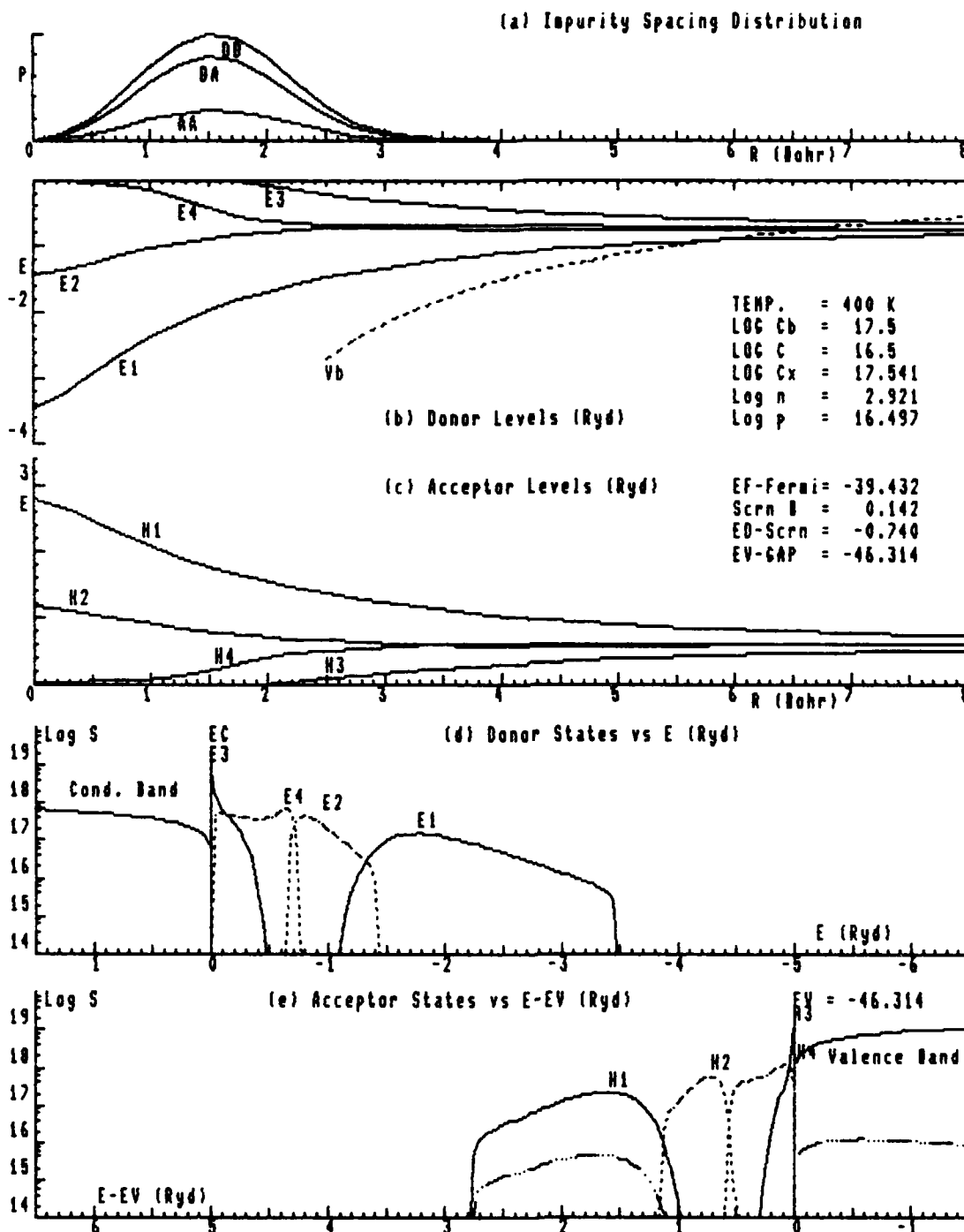


Fig. A 442. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA+)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

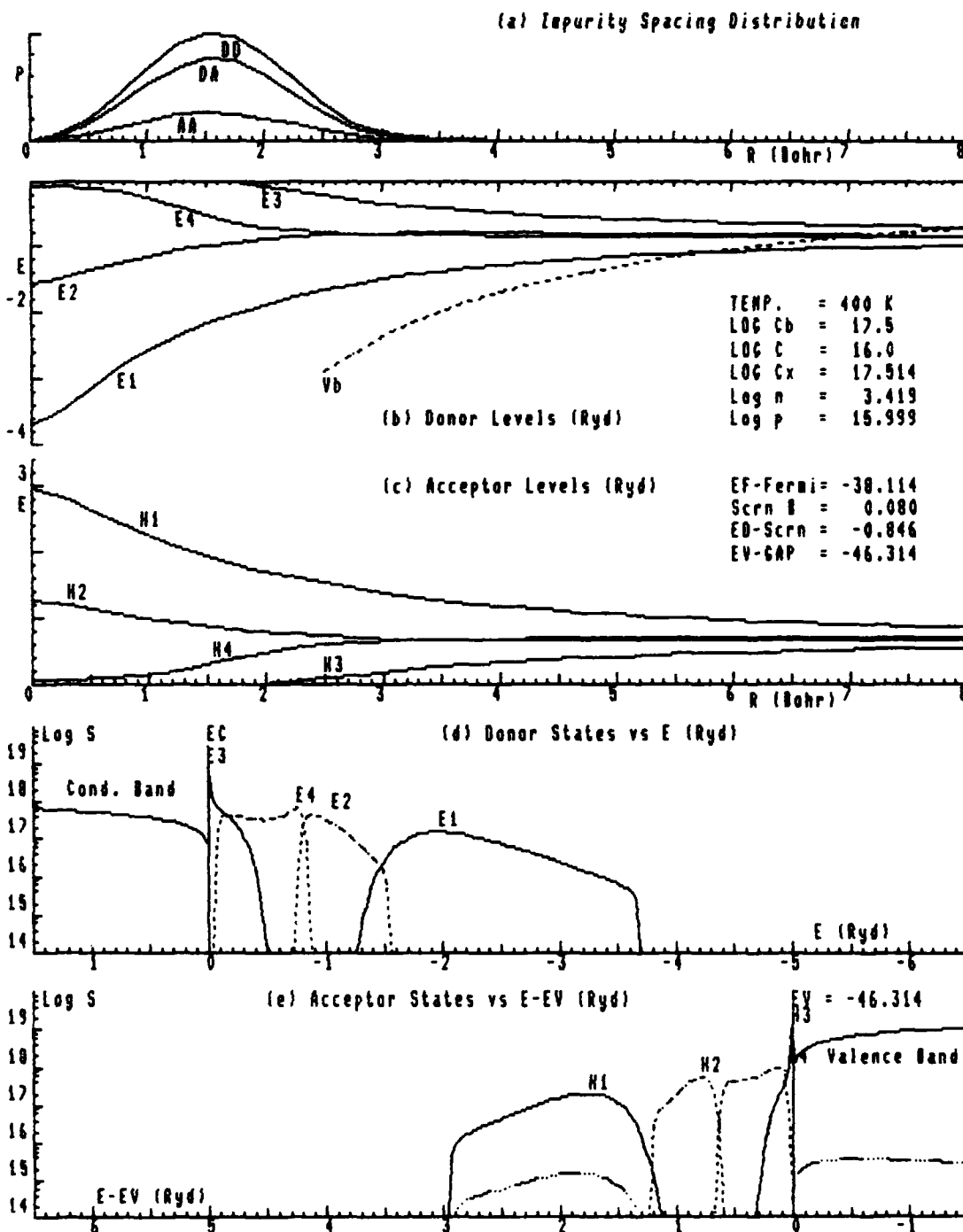


Fig. A 443. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD+)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

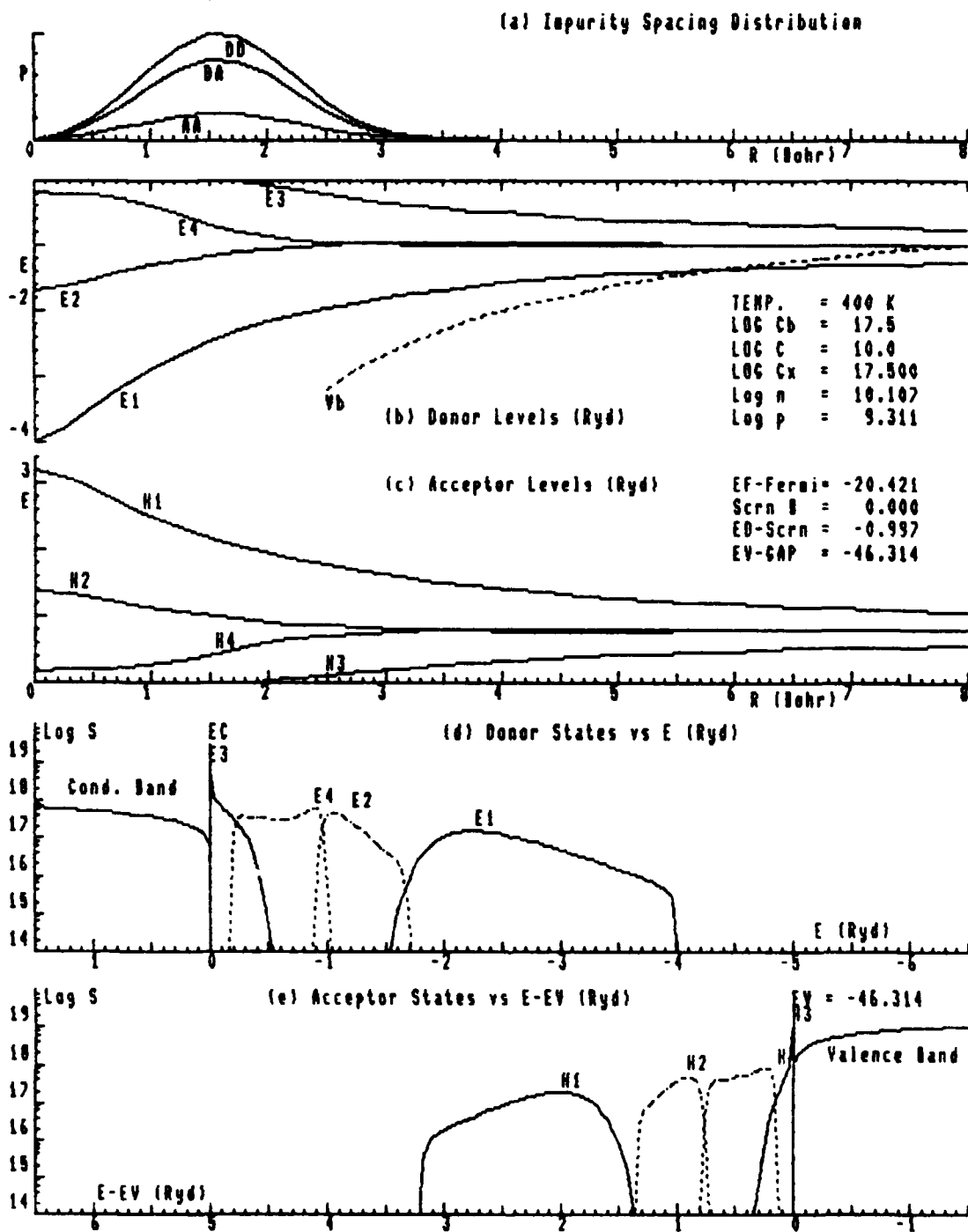


Fig. A 444. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

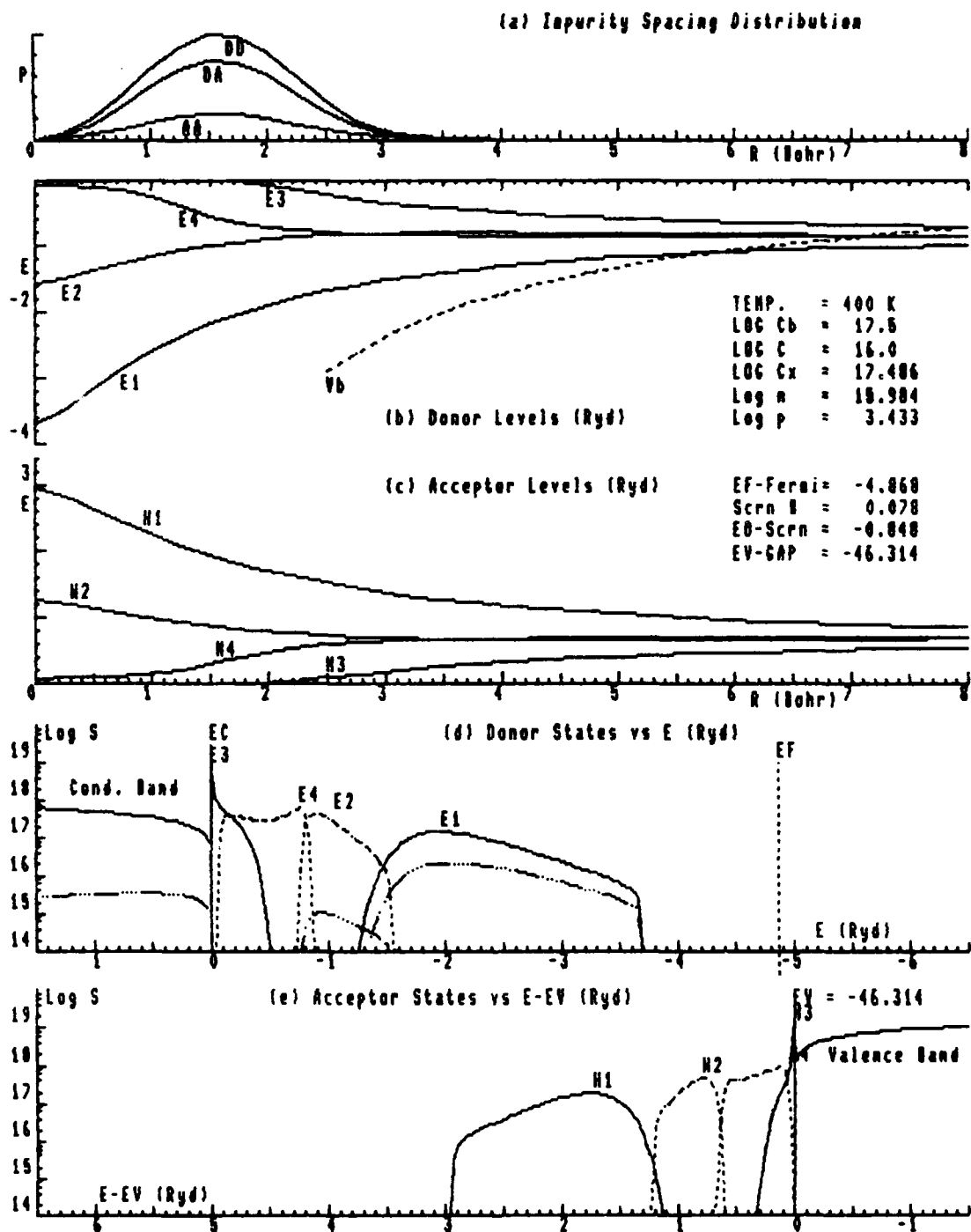


Fig. A 445. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

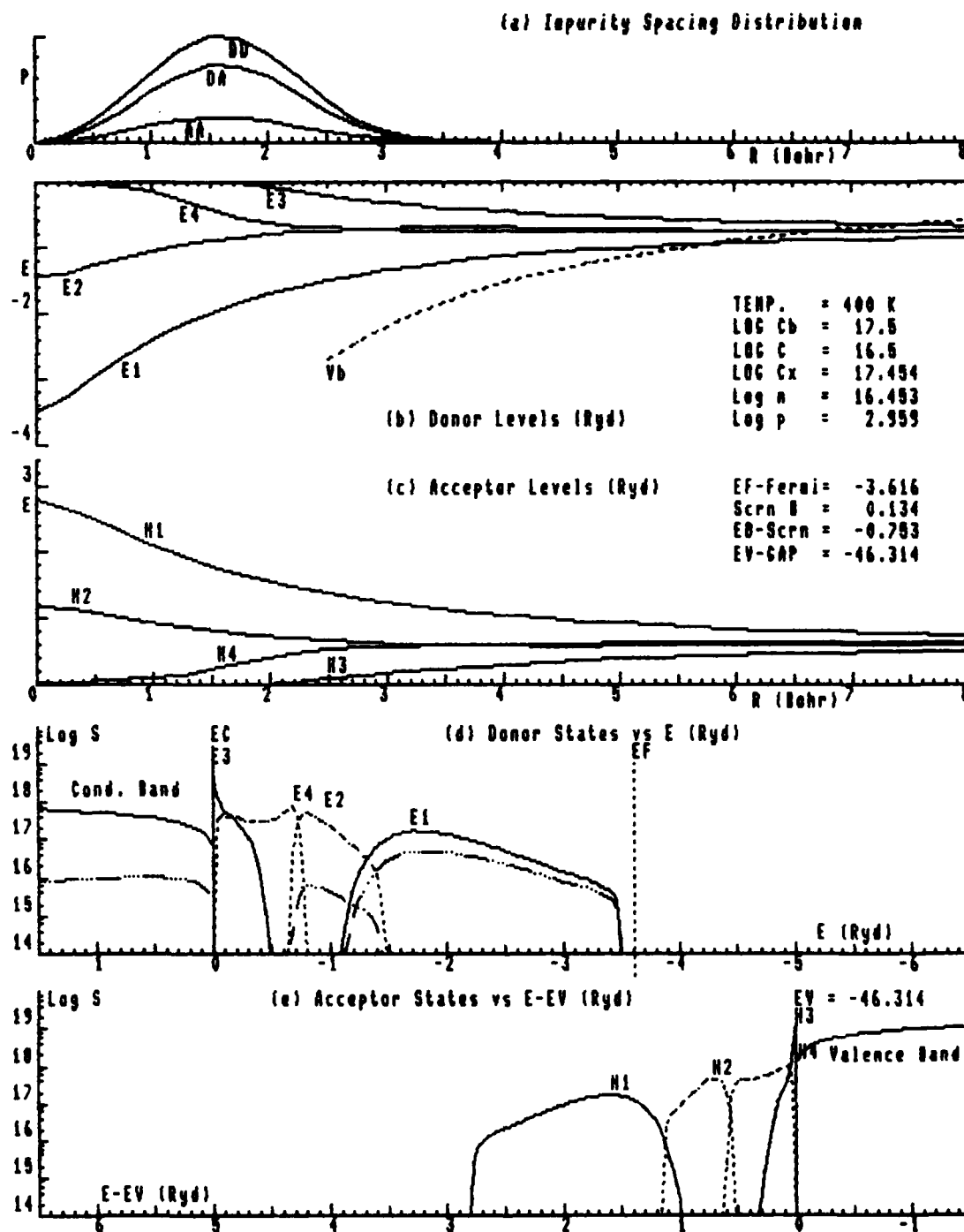


Fig. A 446. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

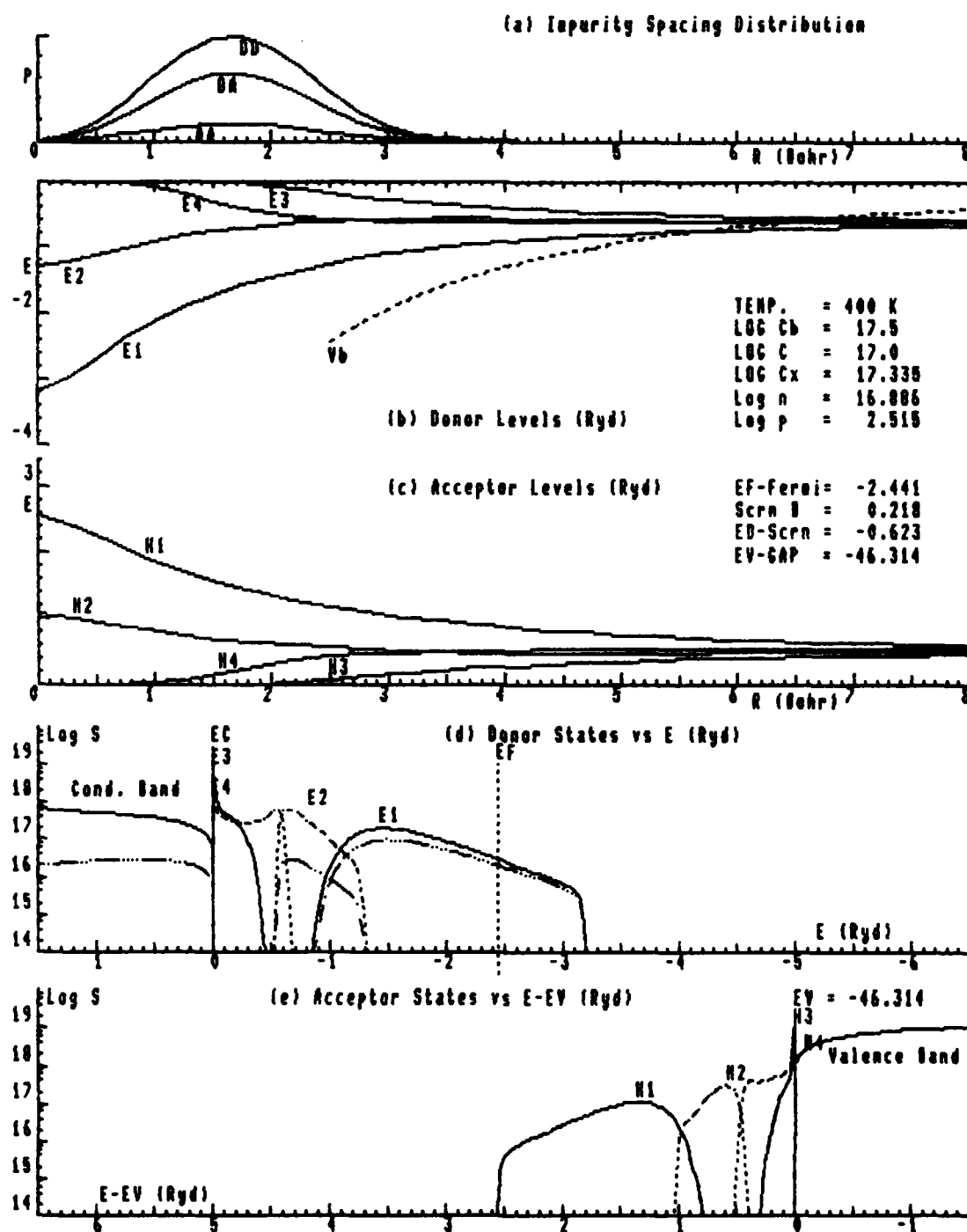


Fig. A 447. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

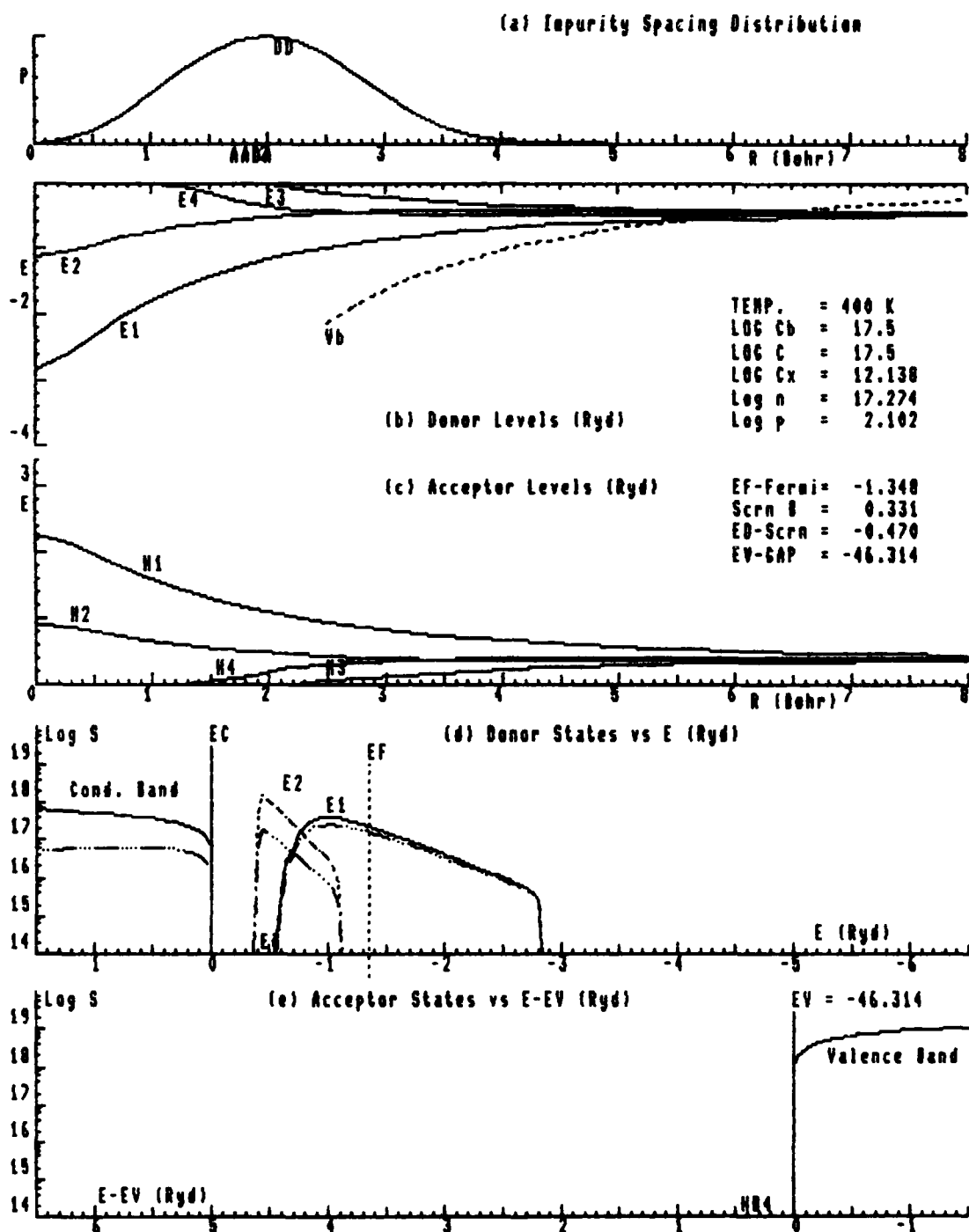


Fig. A 448. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

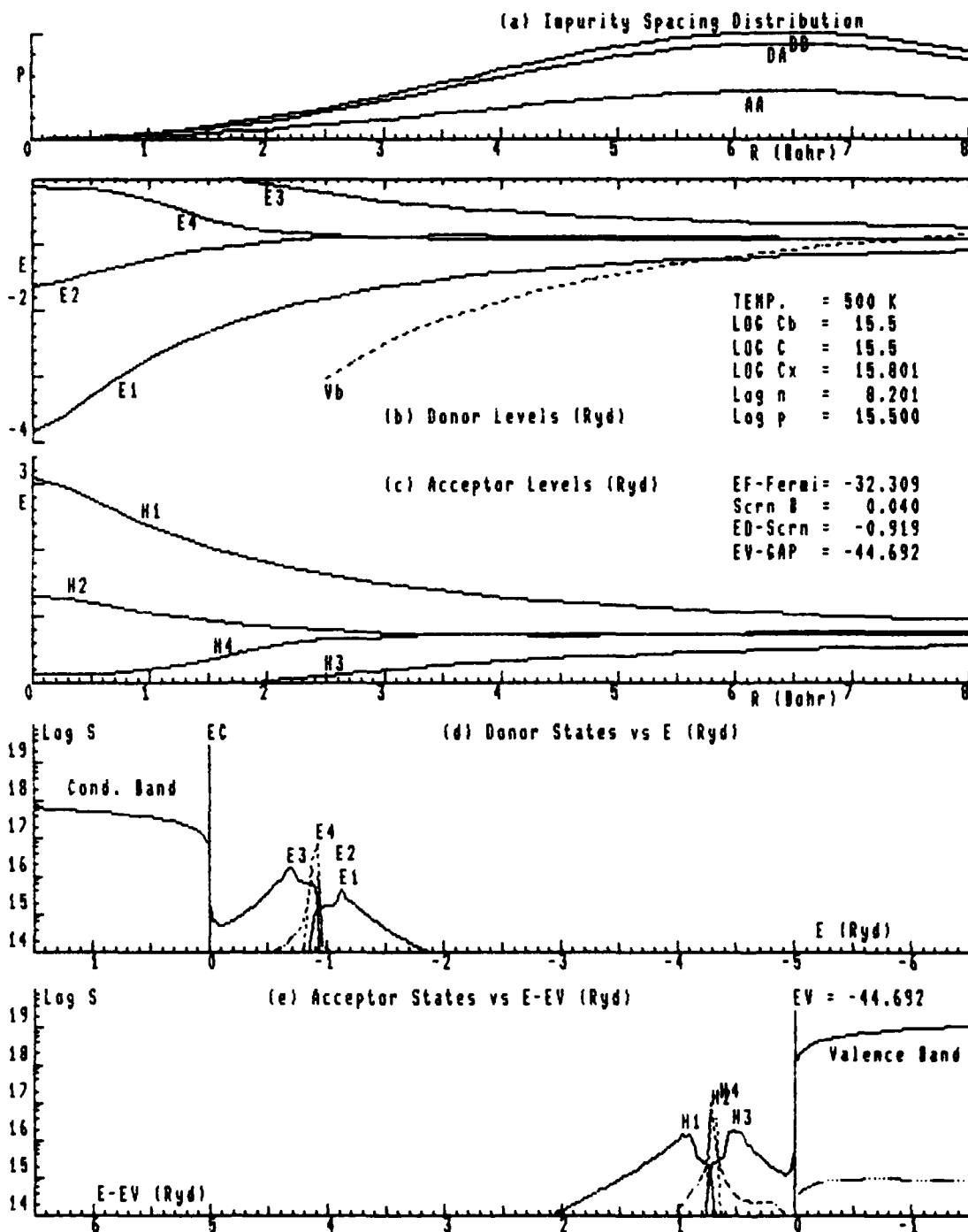


Fig. A 500. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

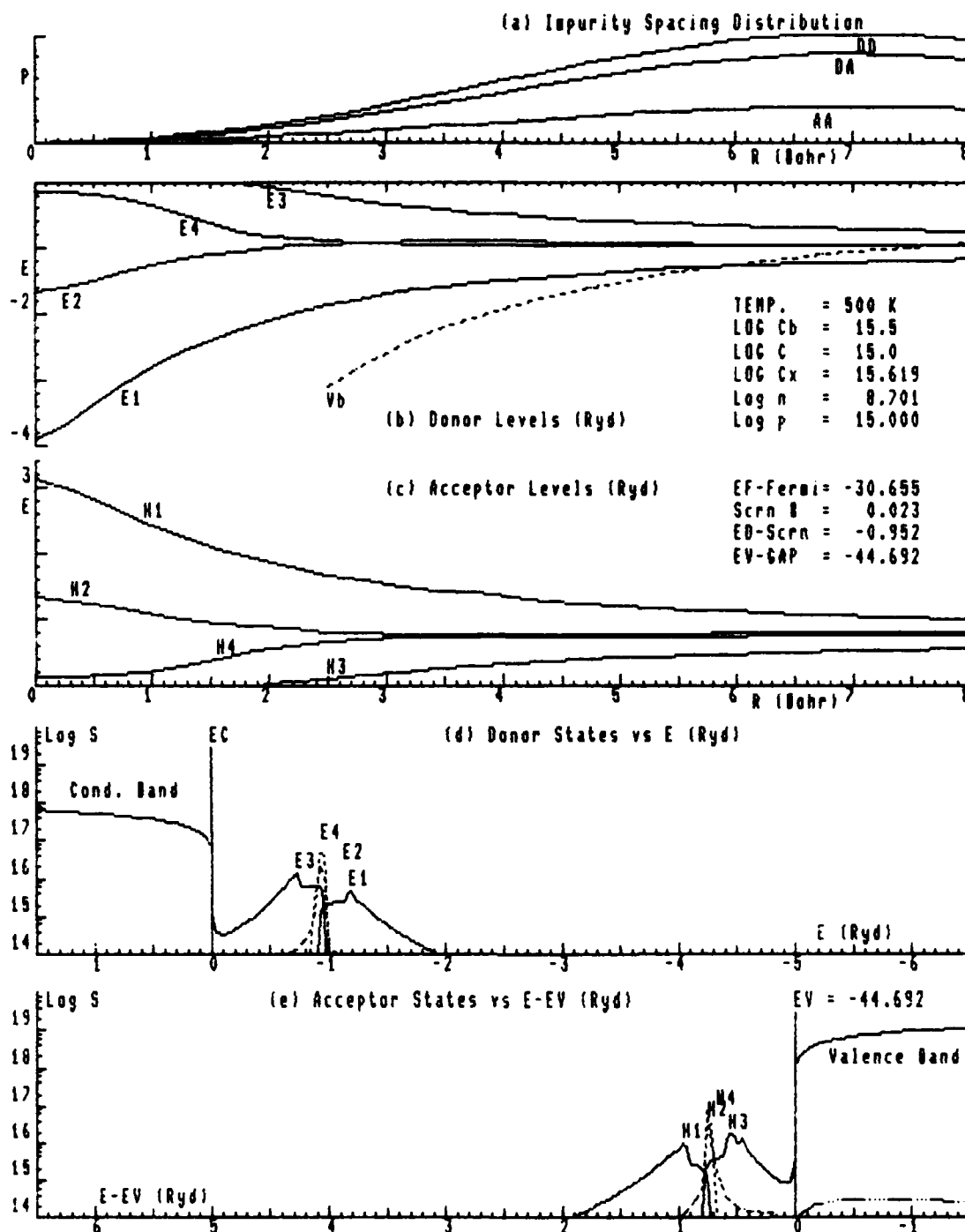


Fig. A 501. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

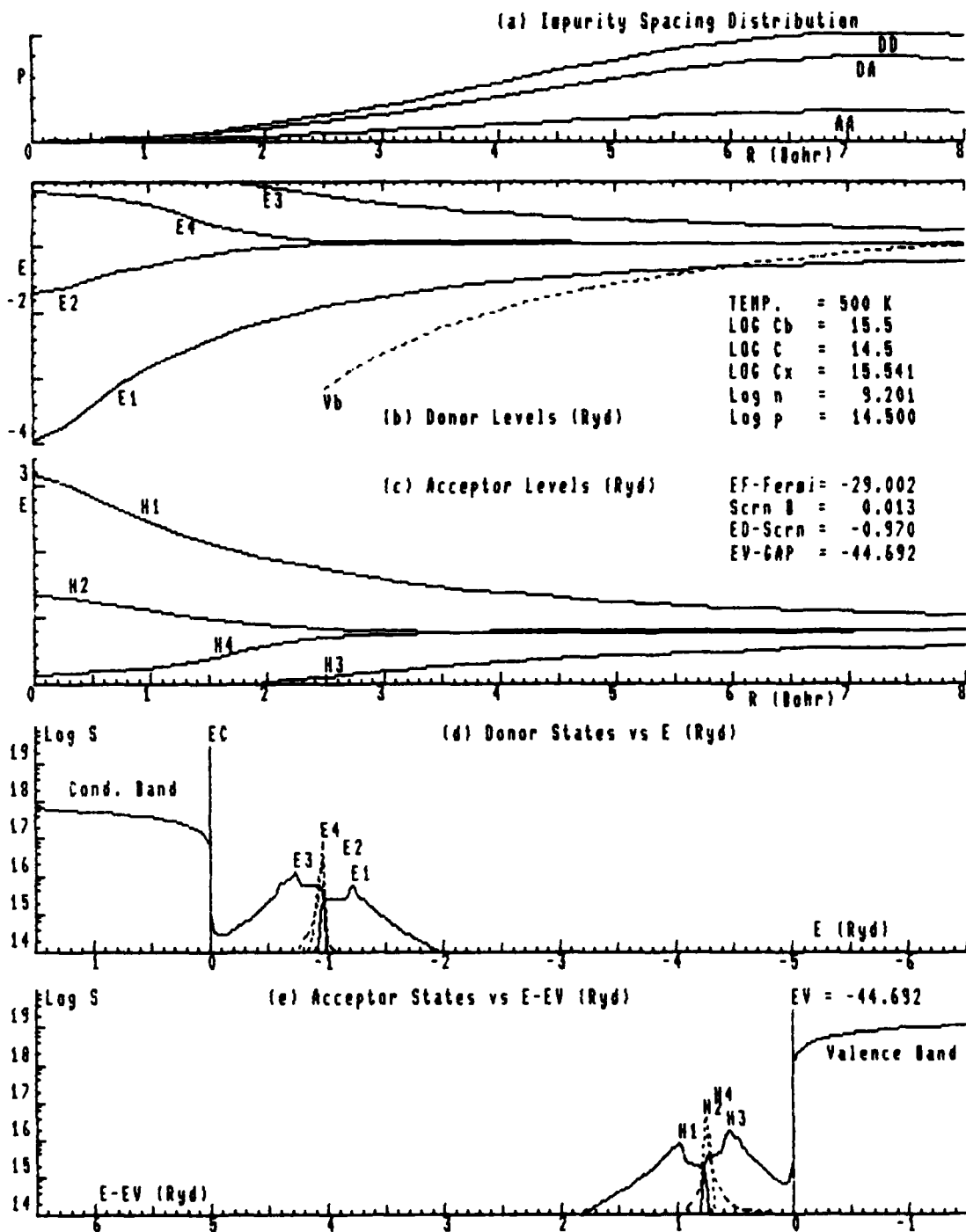


Fig. A 502. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

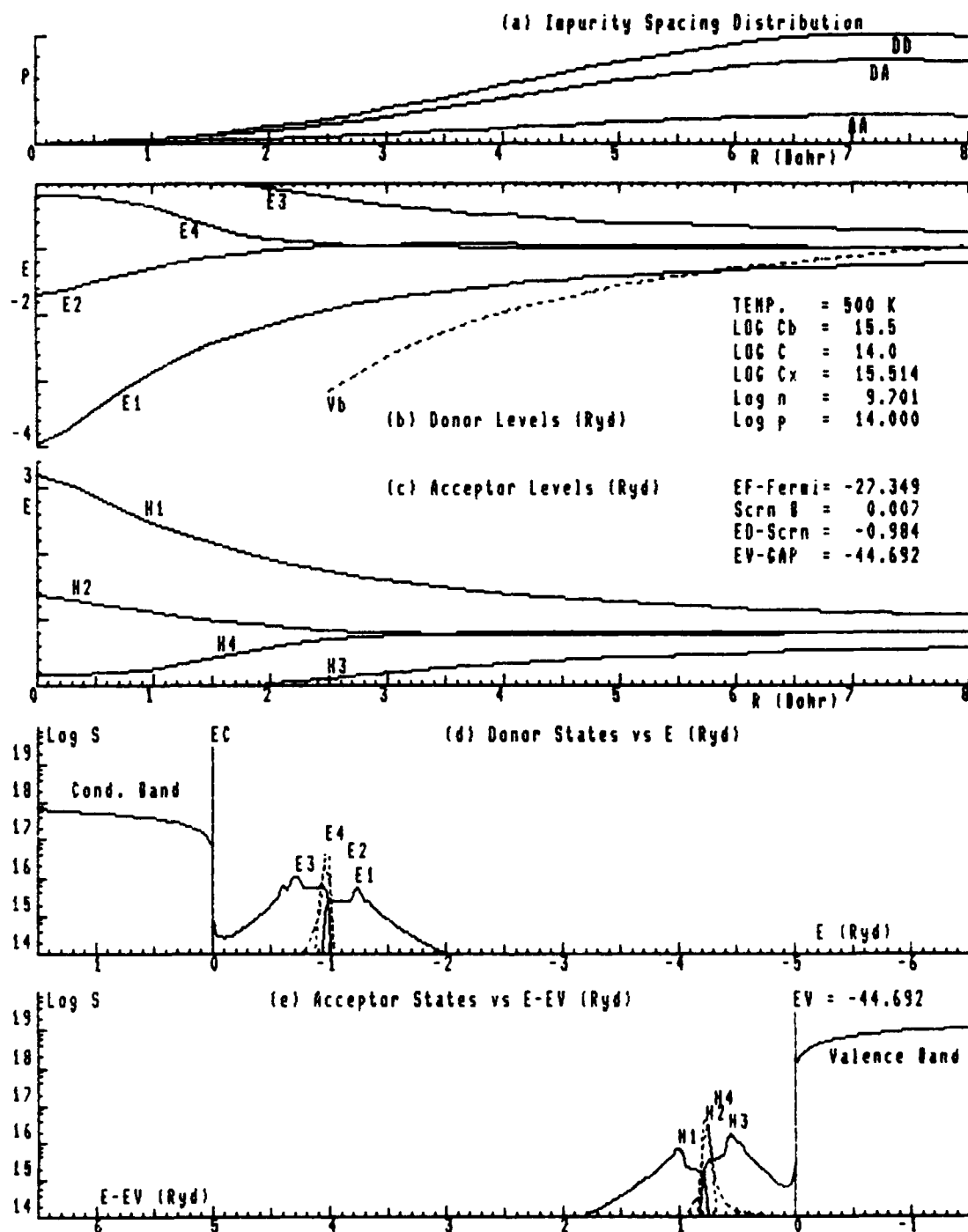


Fig. A 503. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

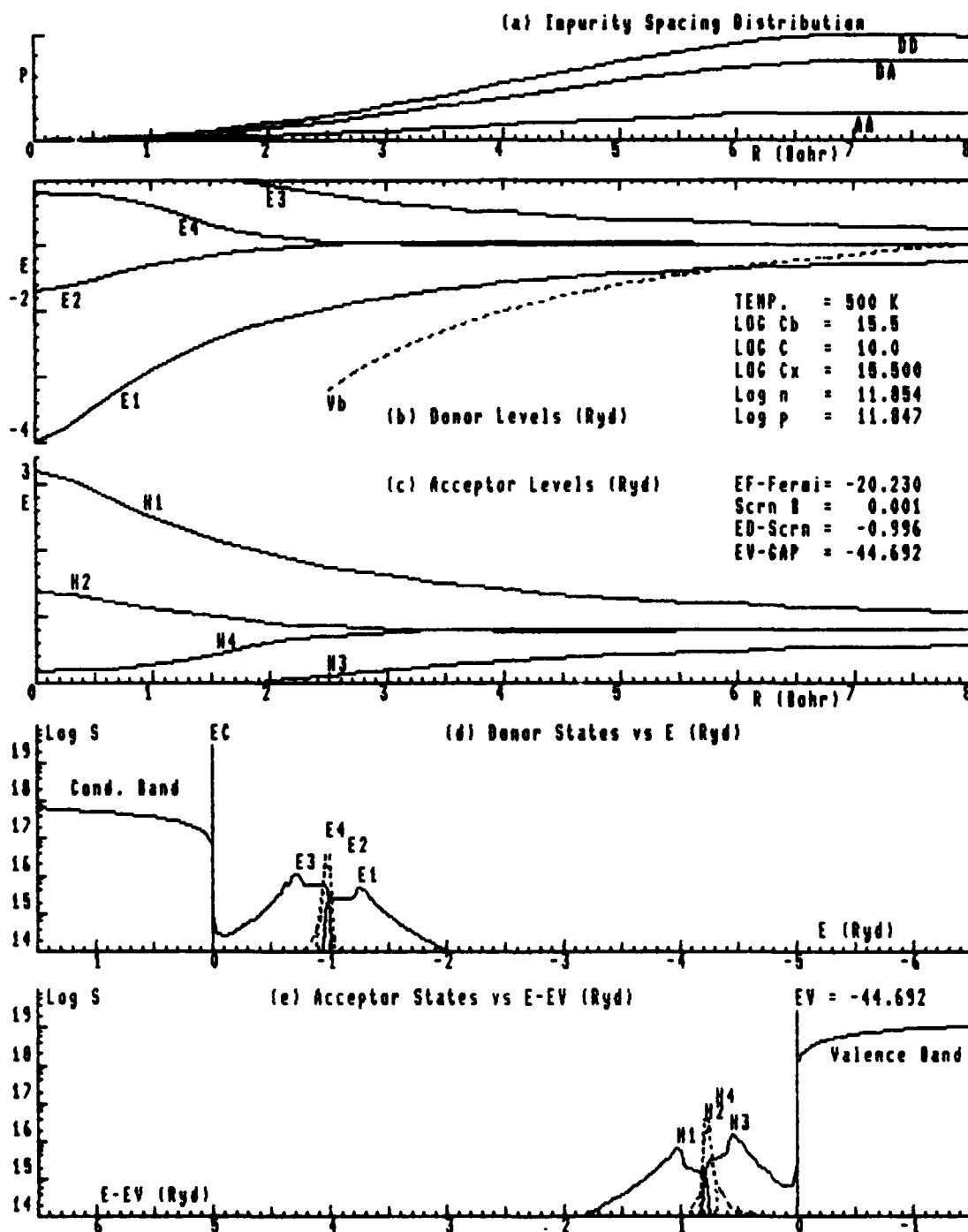


Fig. A 504. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

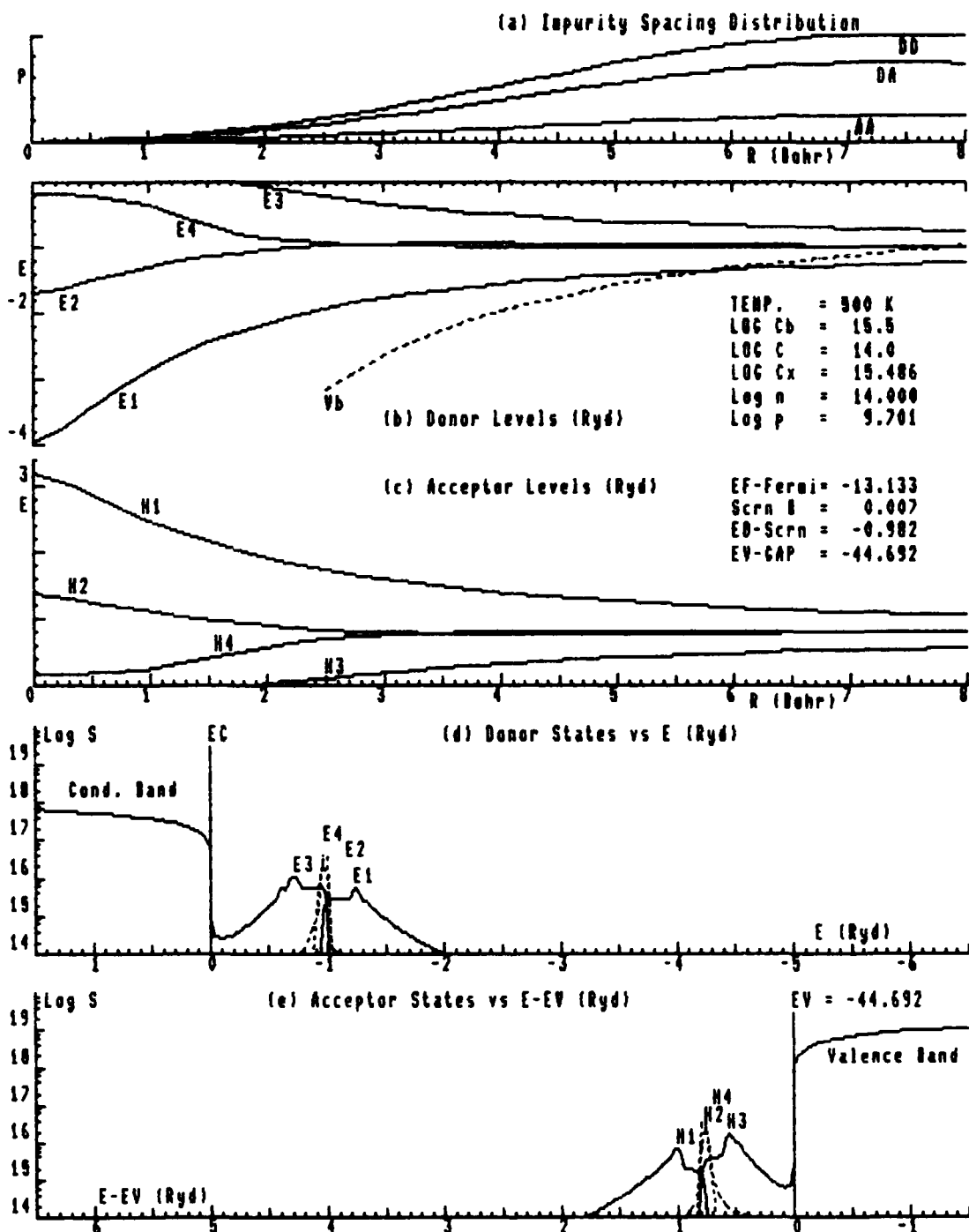


Fig. A 505. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

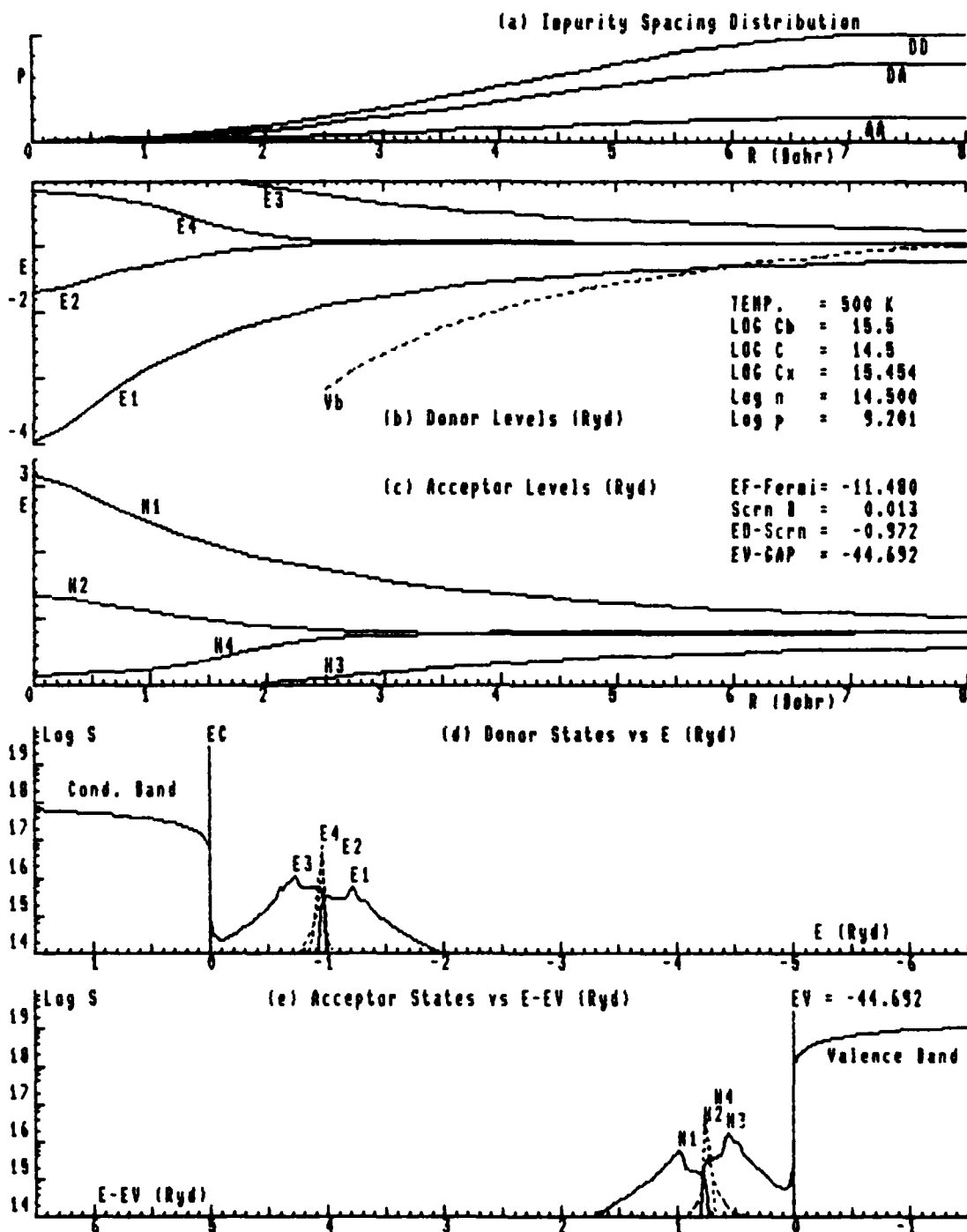


Fig. A 506. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

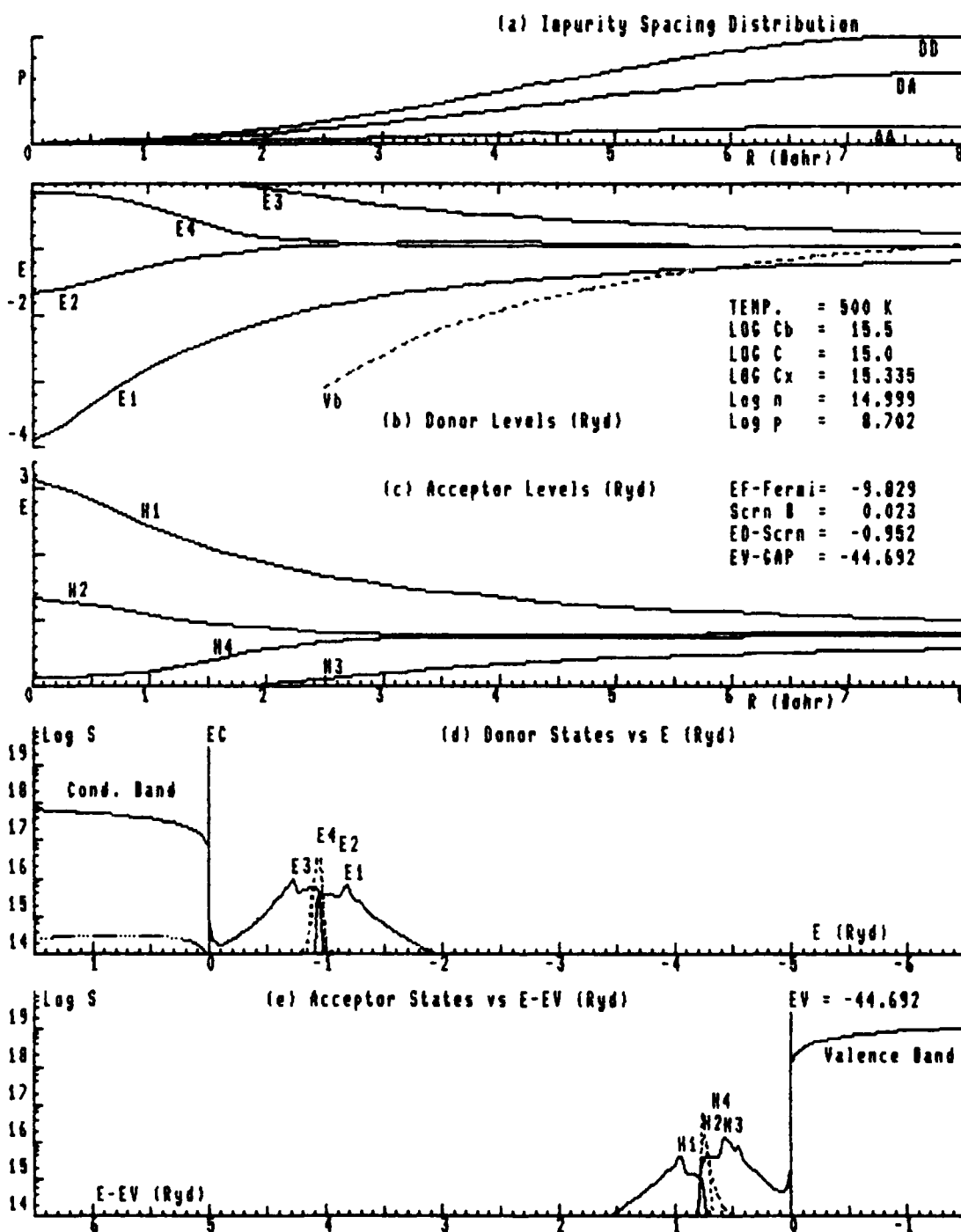


Fig. A 507. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

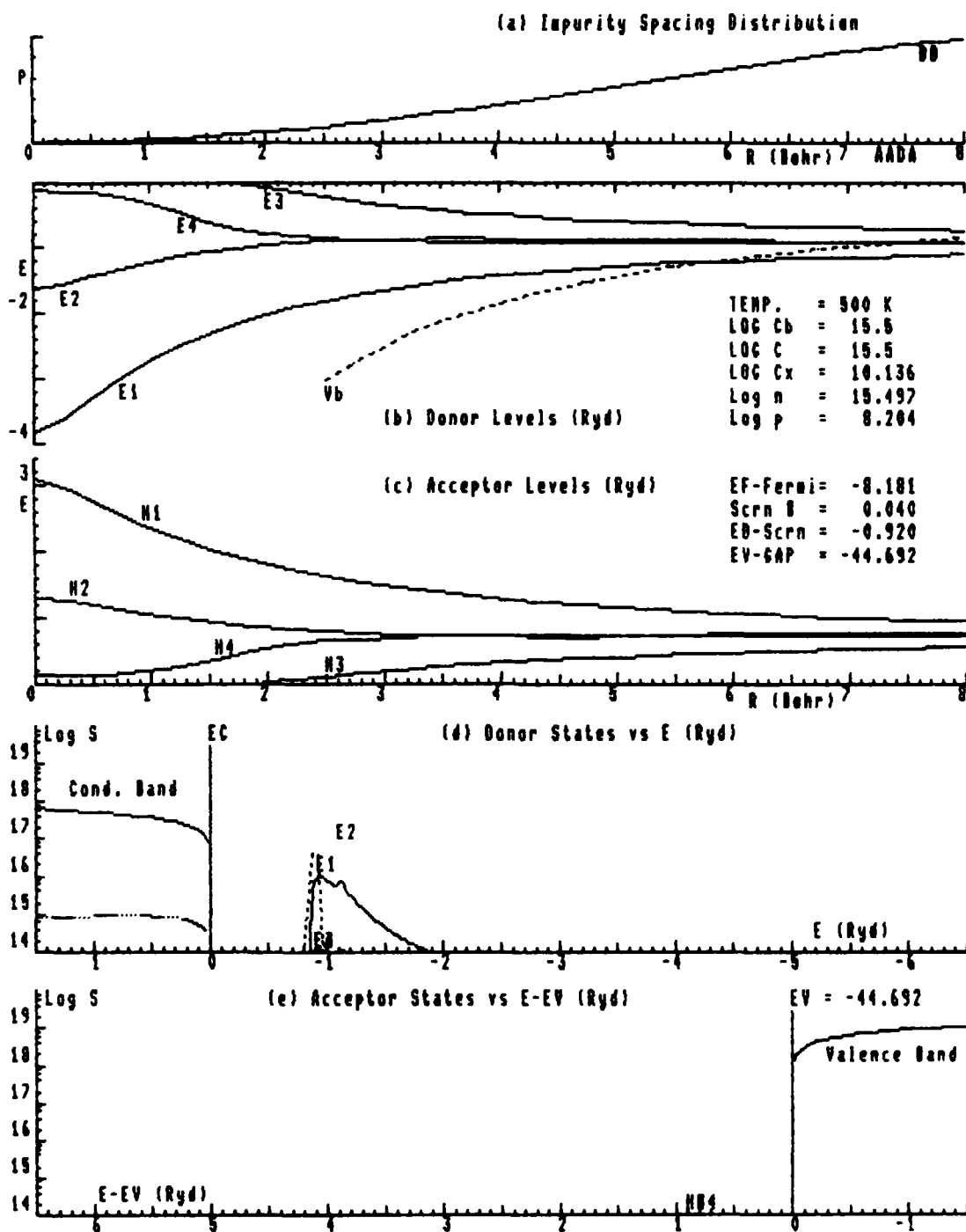


Fig. A 50B. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

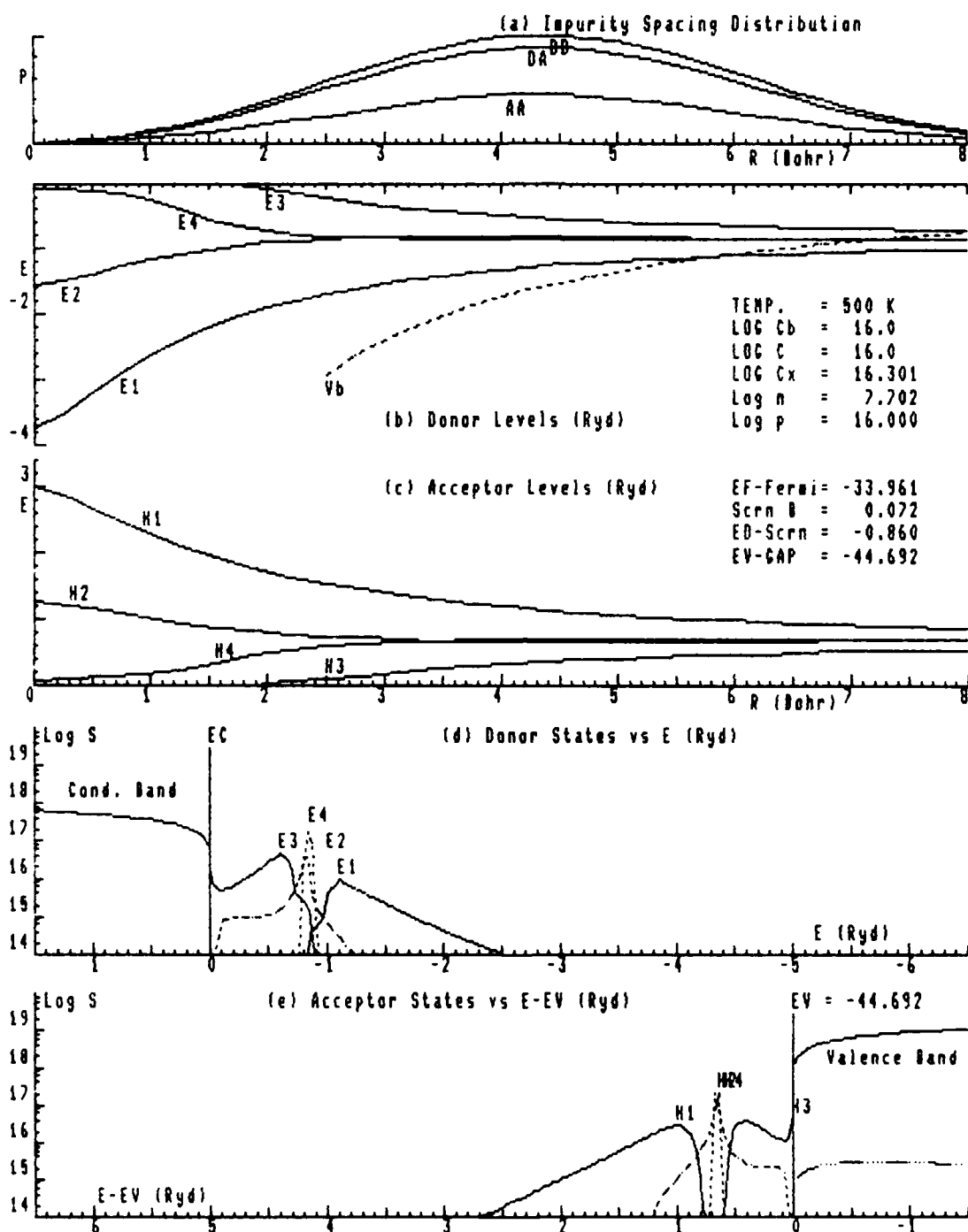


Fig. A 510. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

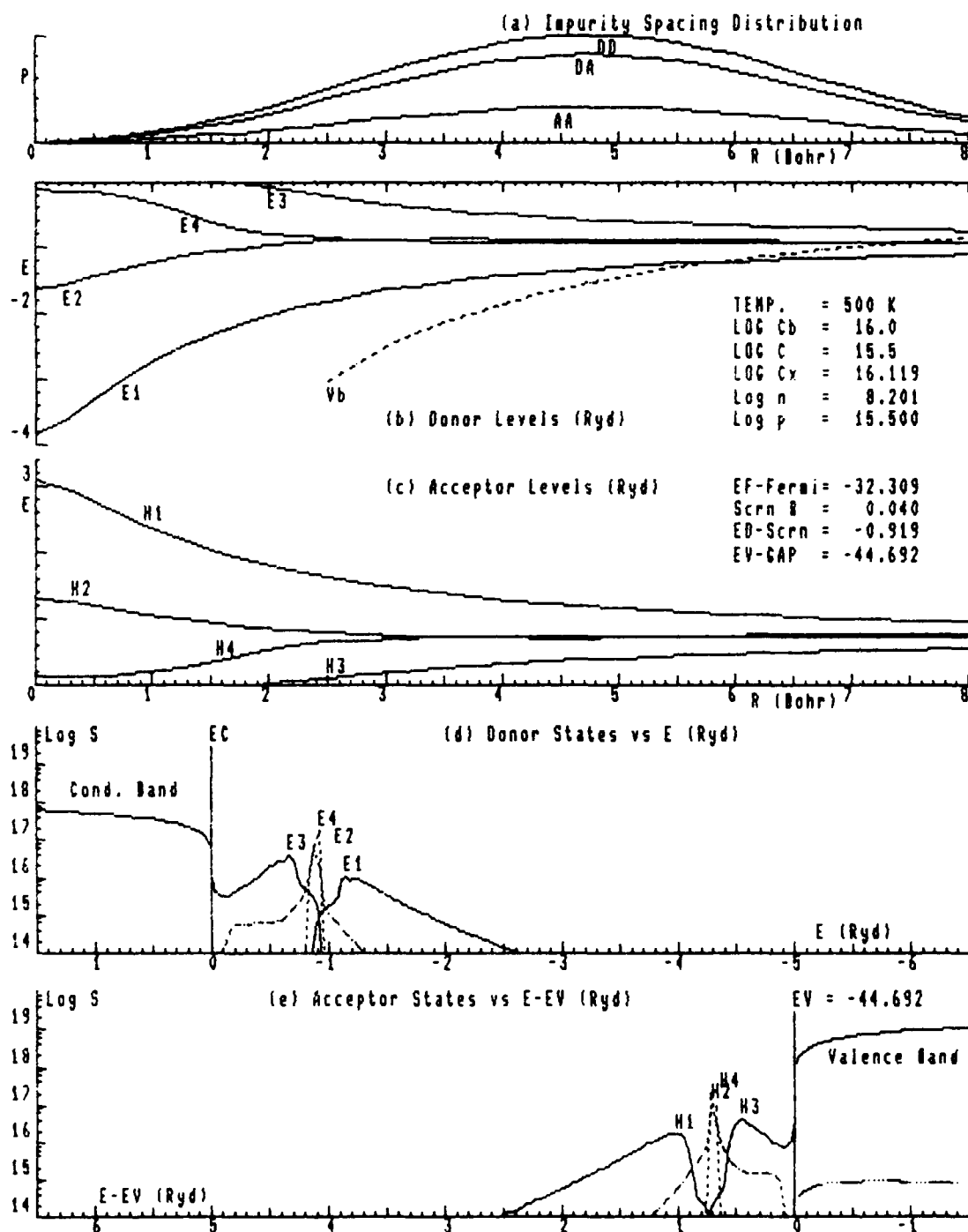


Fig. A 511. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

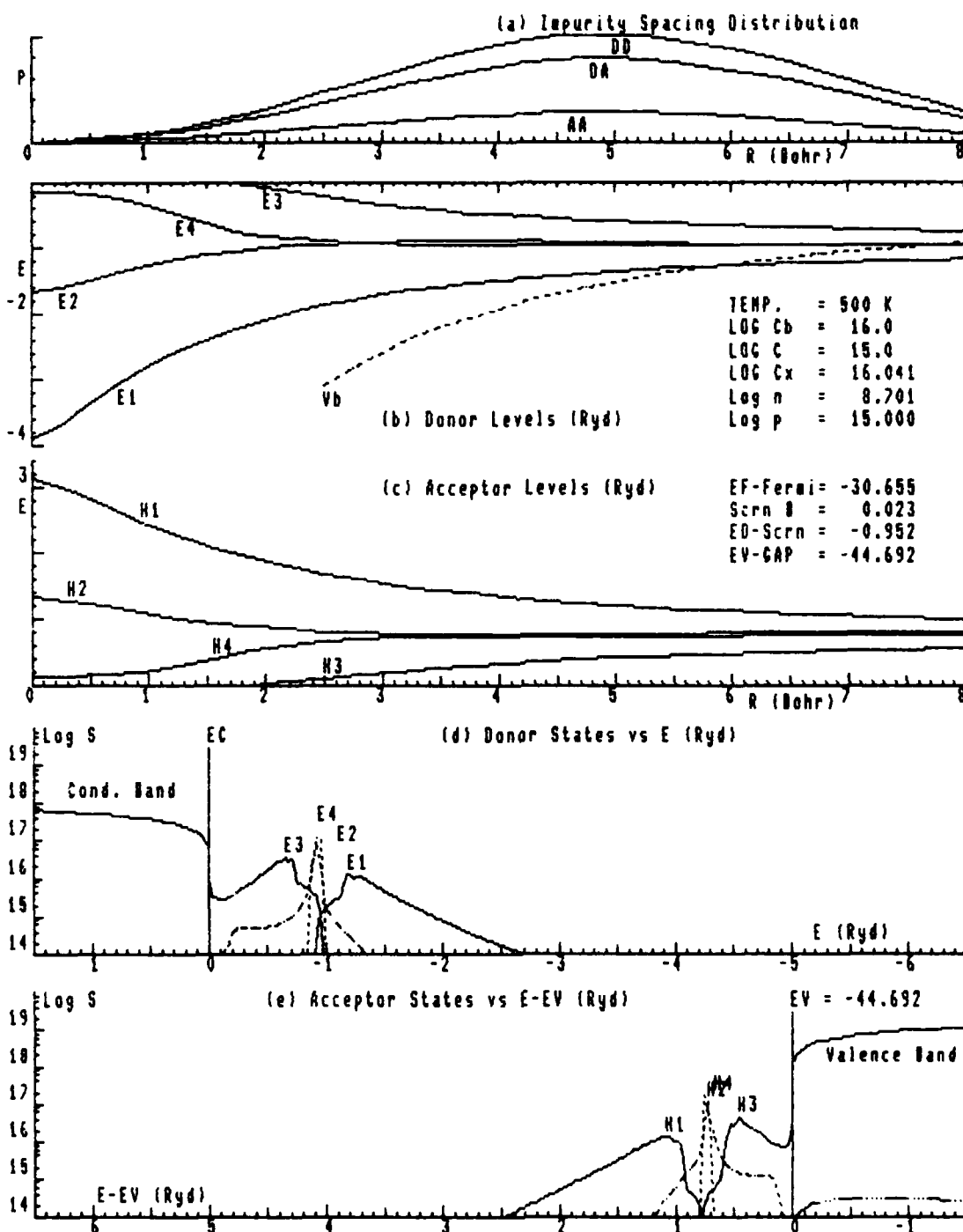


Fig. A 512. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

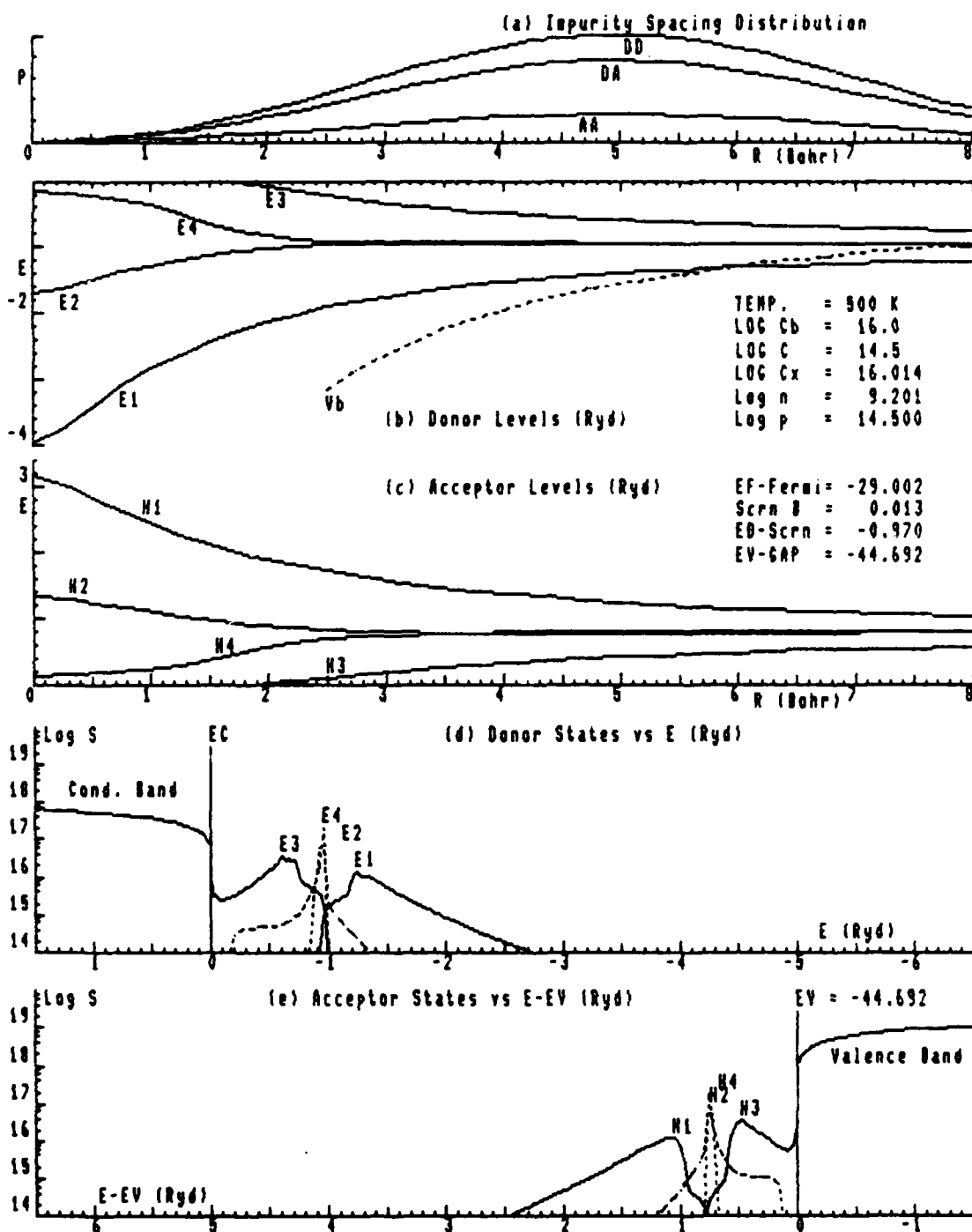


Fig. A 513. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

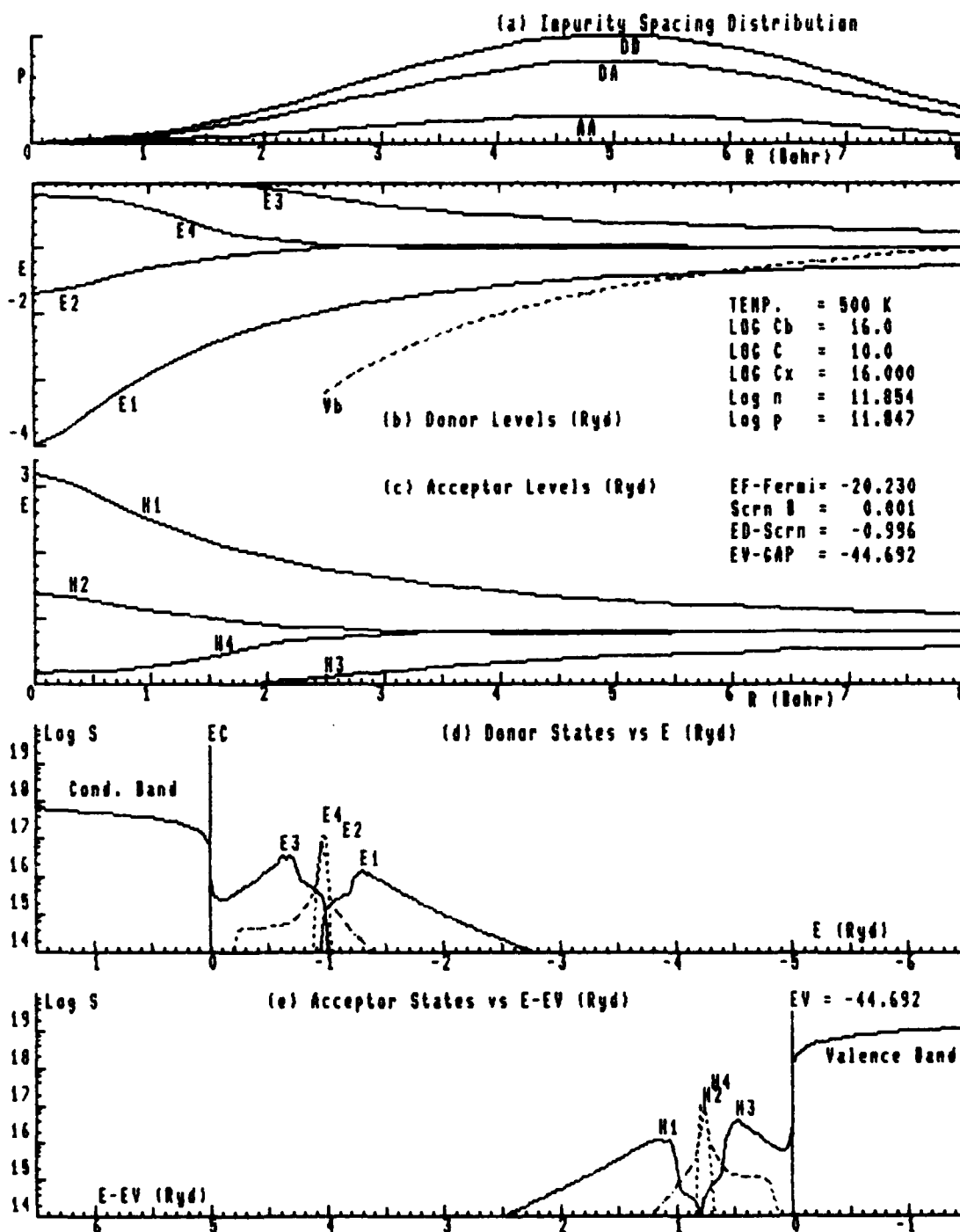


Fig. A B14. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

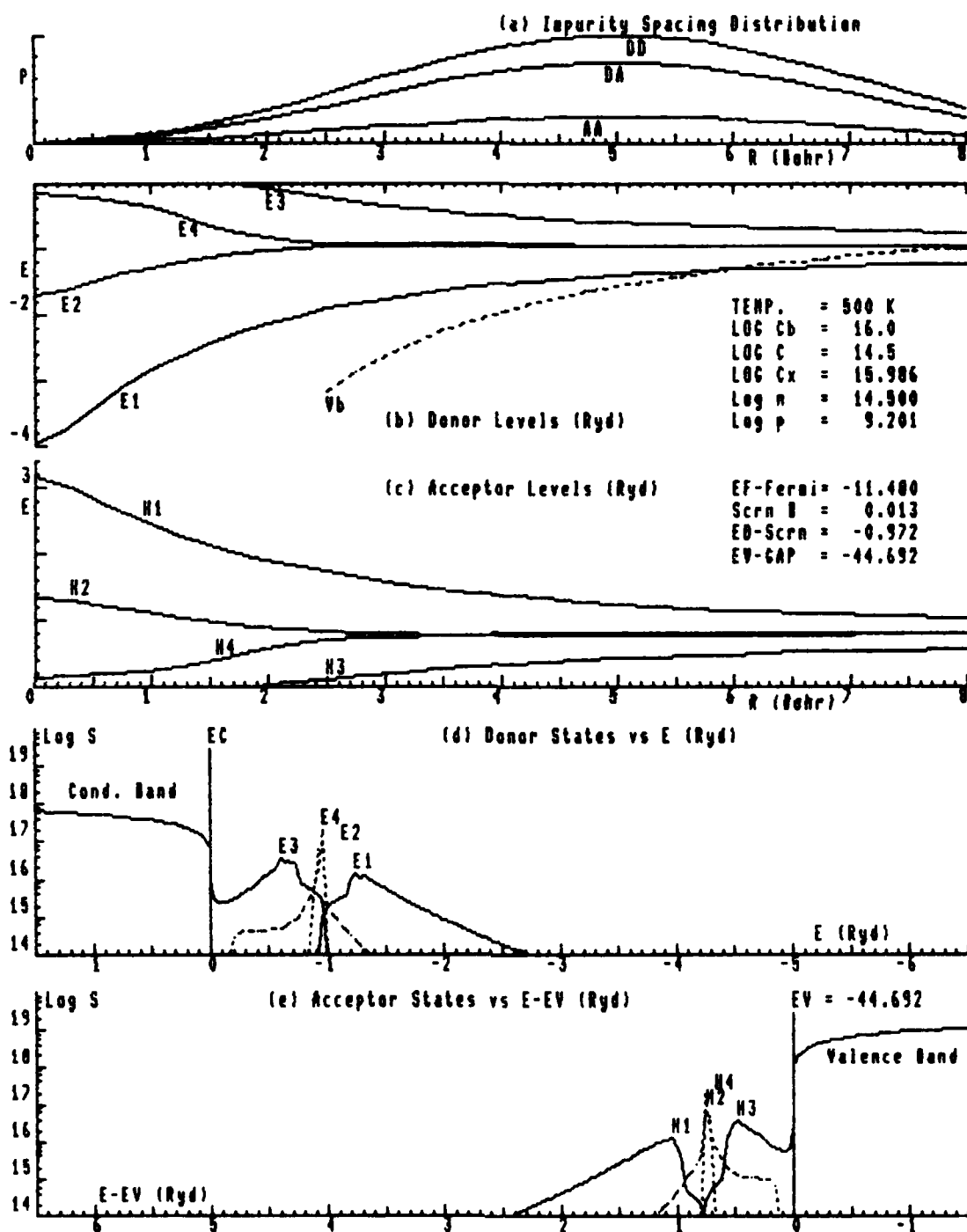


Fig. A 515. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

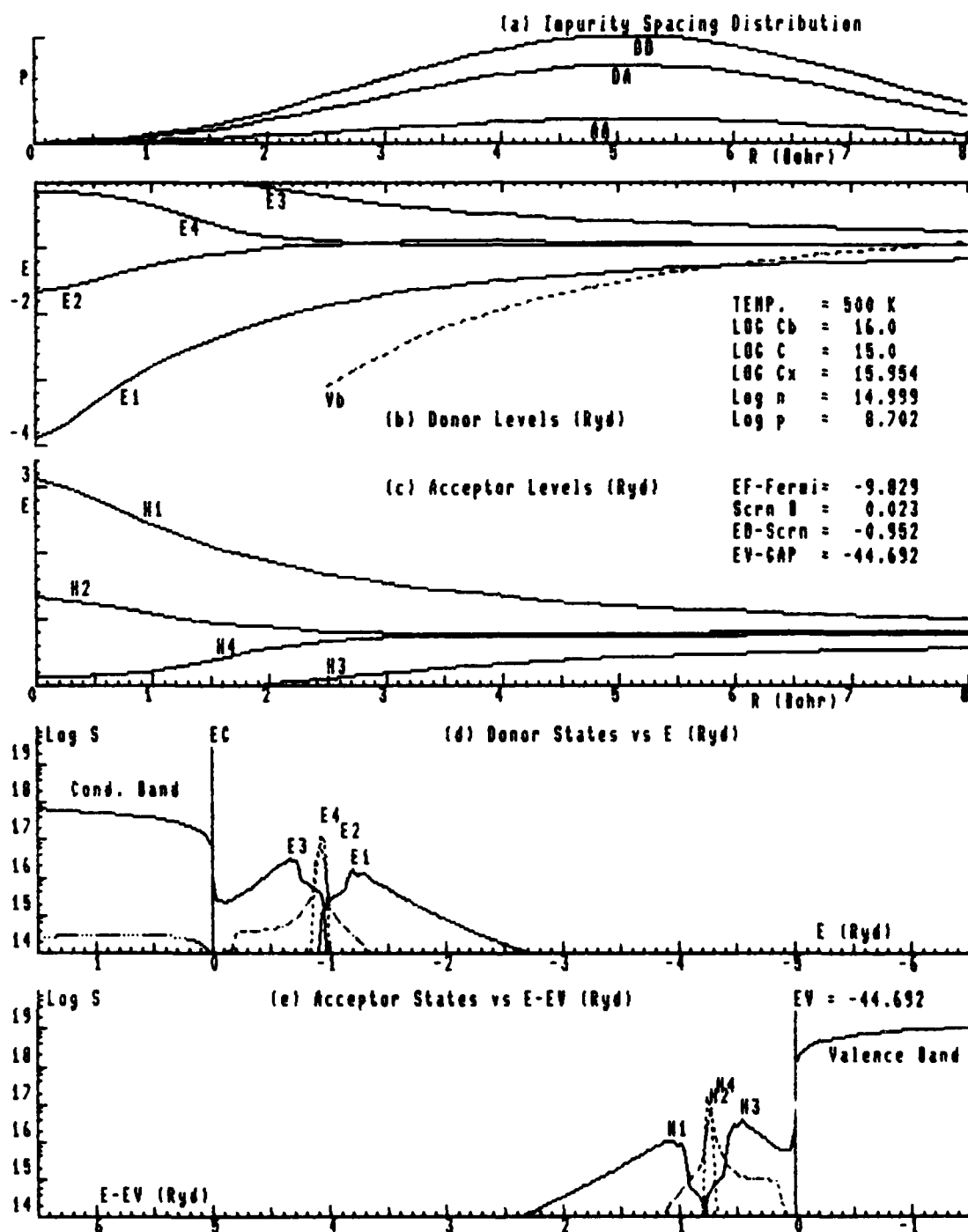


Fig. A 516. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

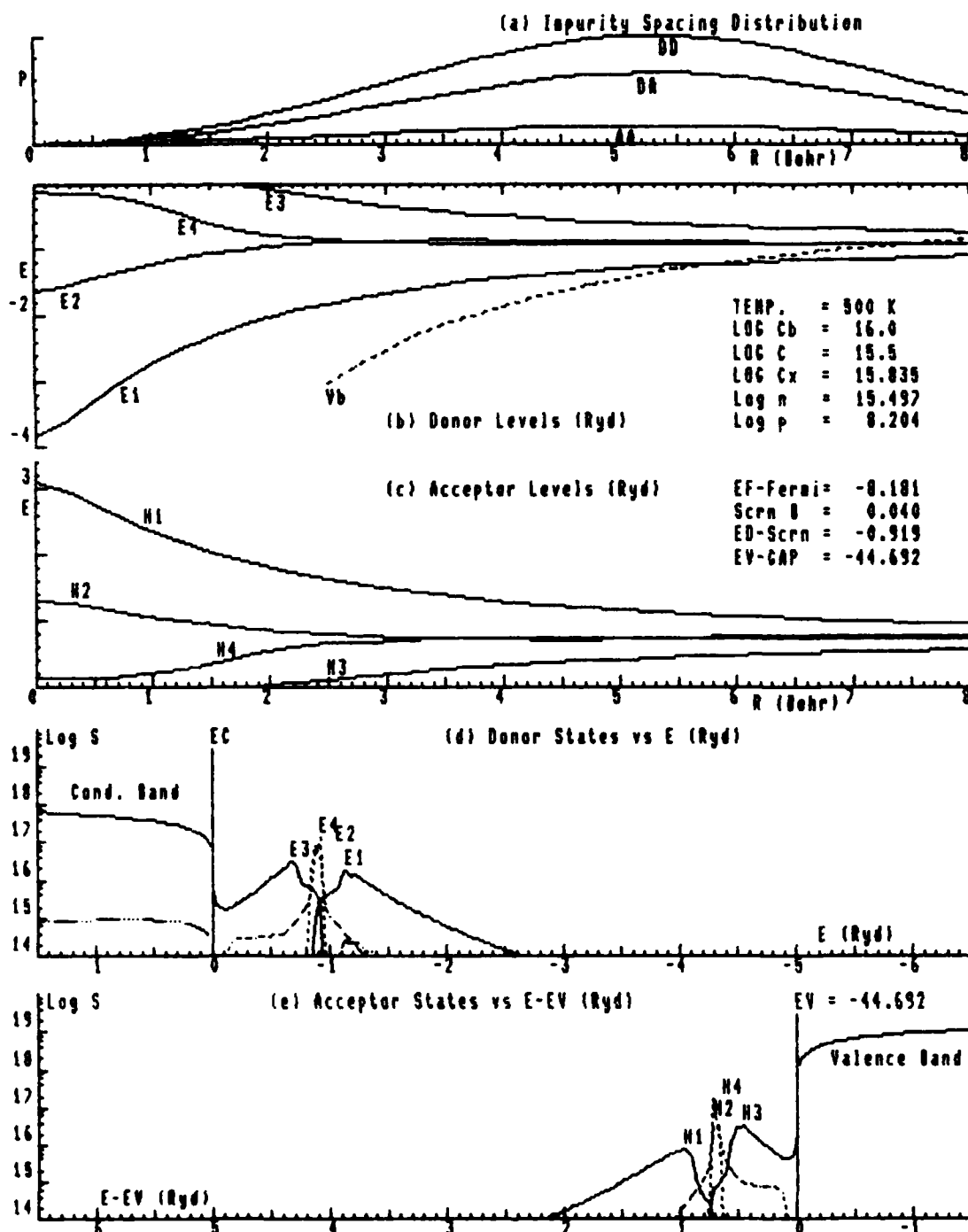


Fig. A 517. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

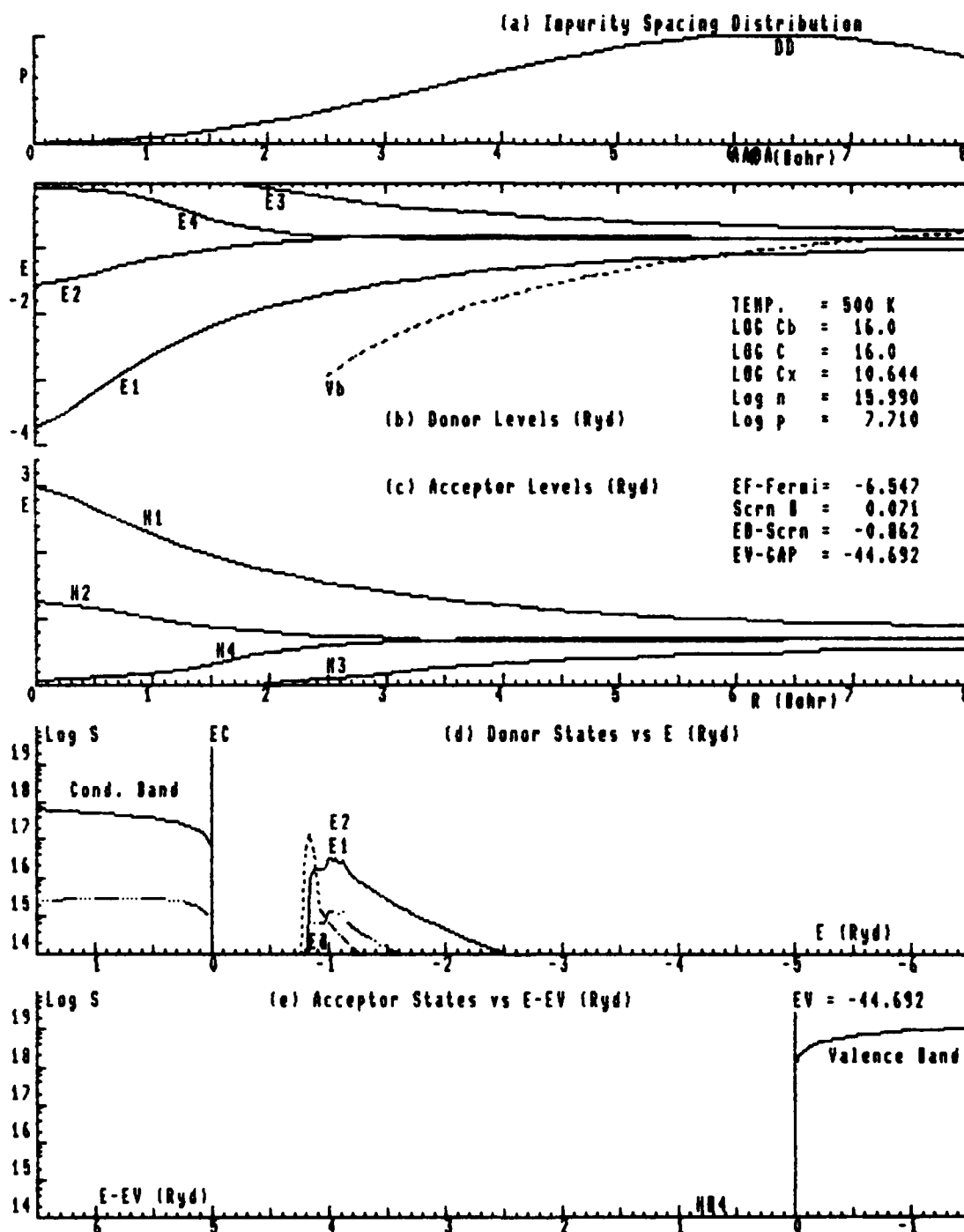


Fig. A 51B. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

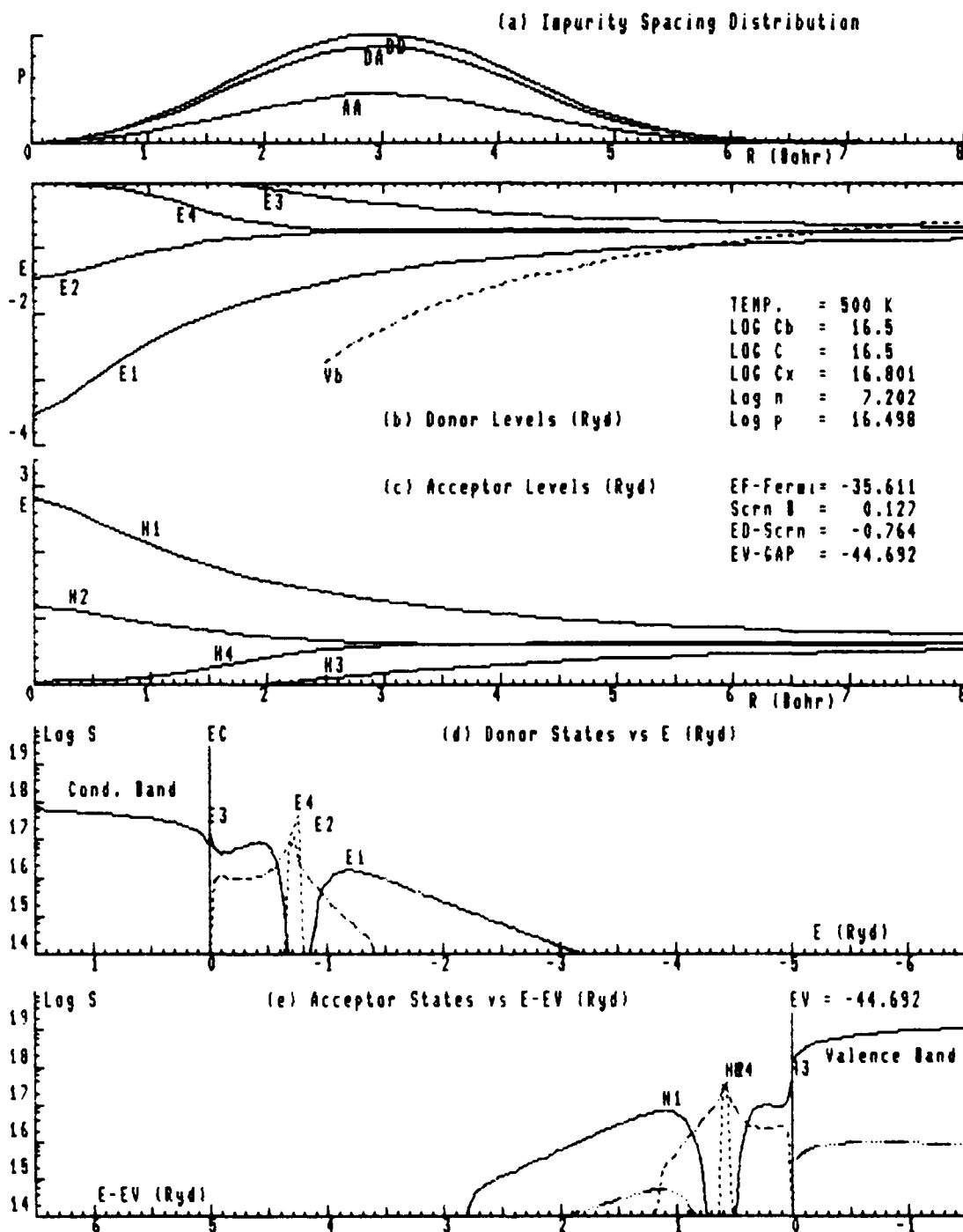


Fig. A 520. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

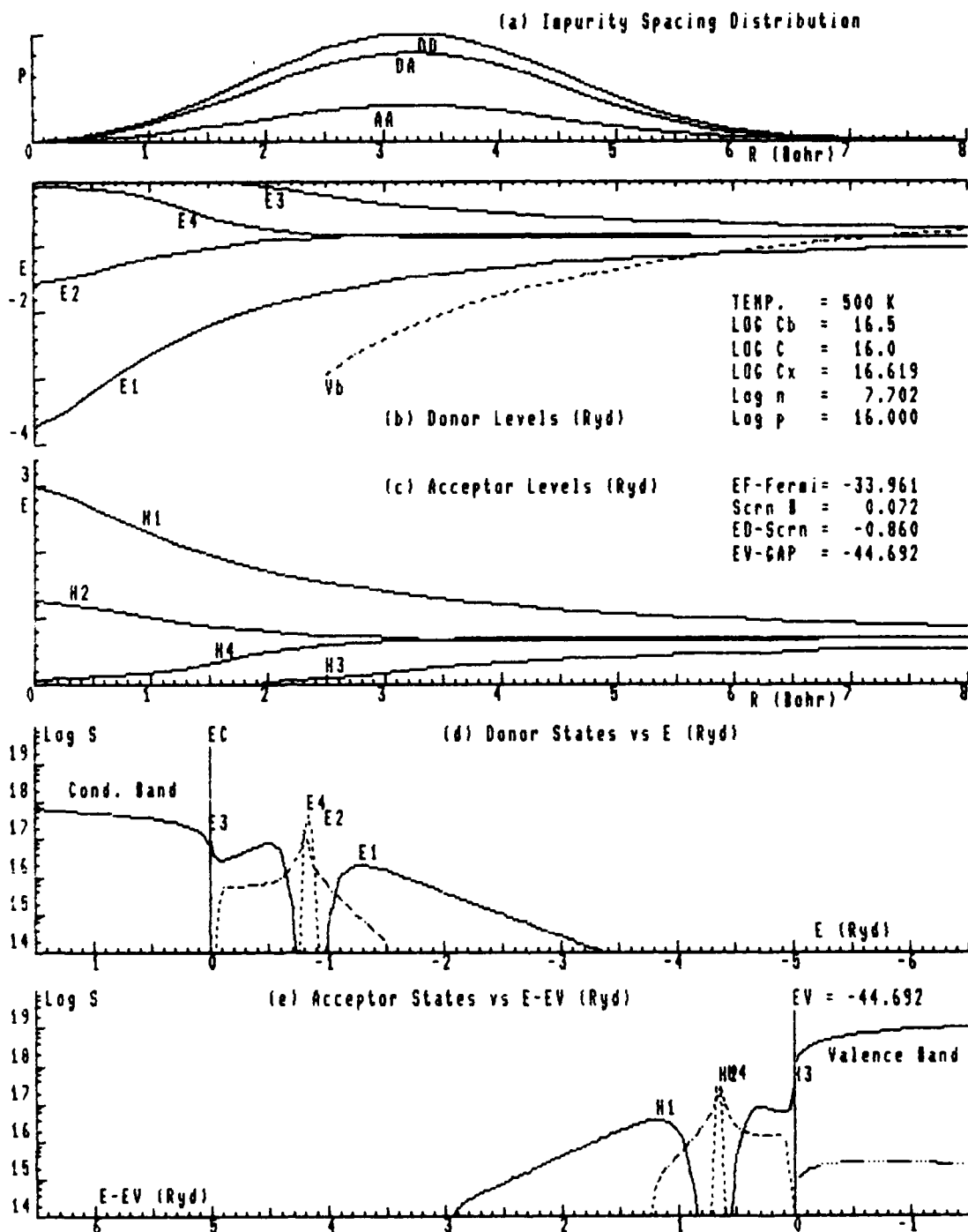


Fig. A 521. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

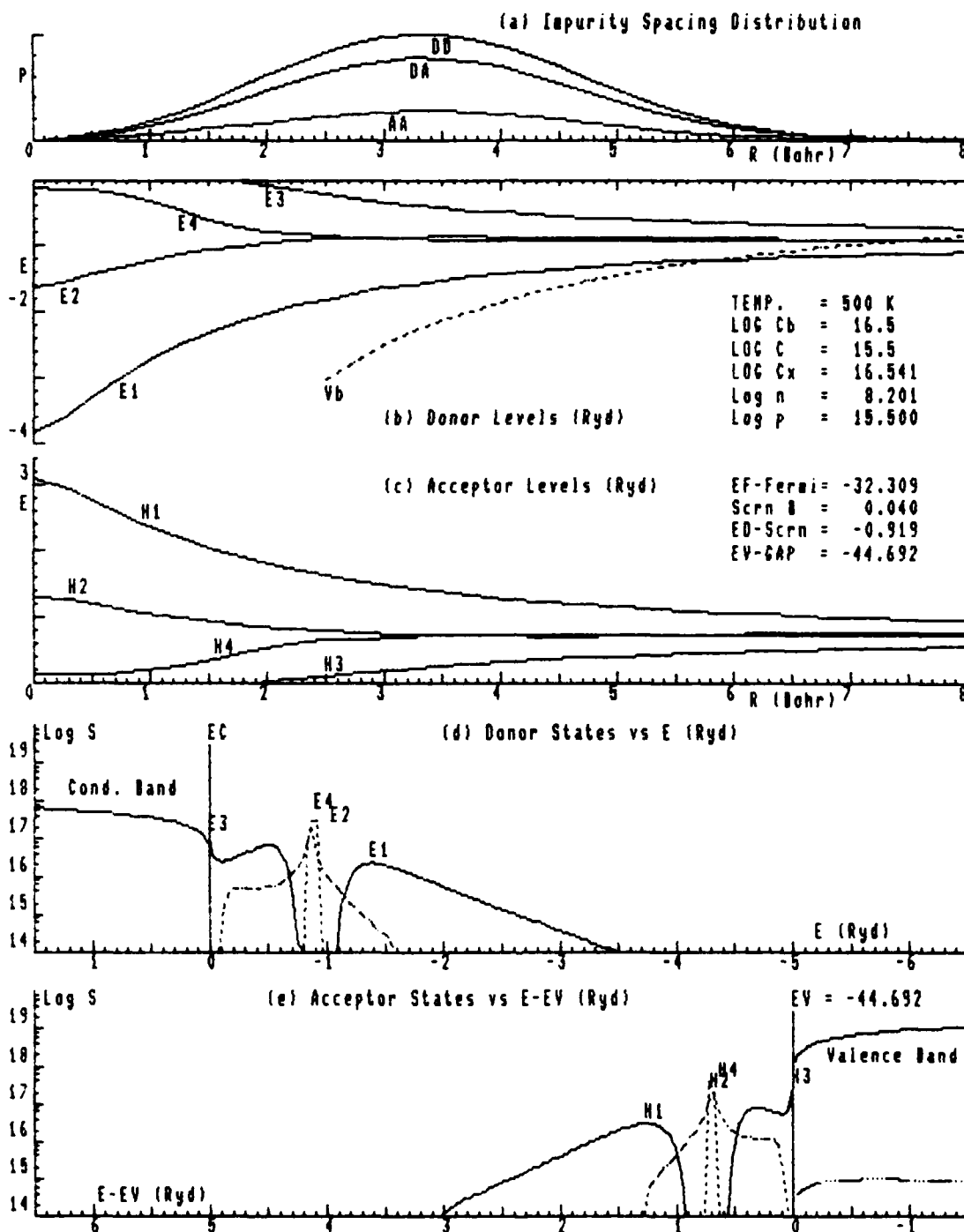


Fig. A 522. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

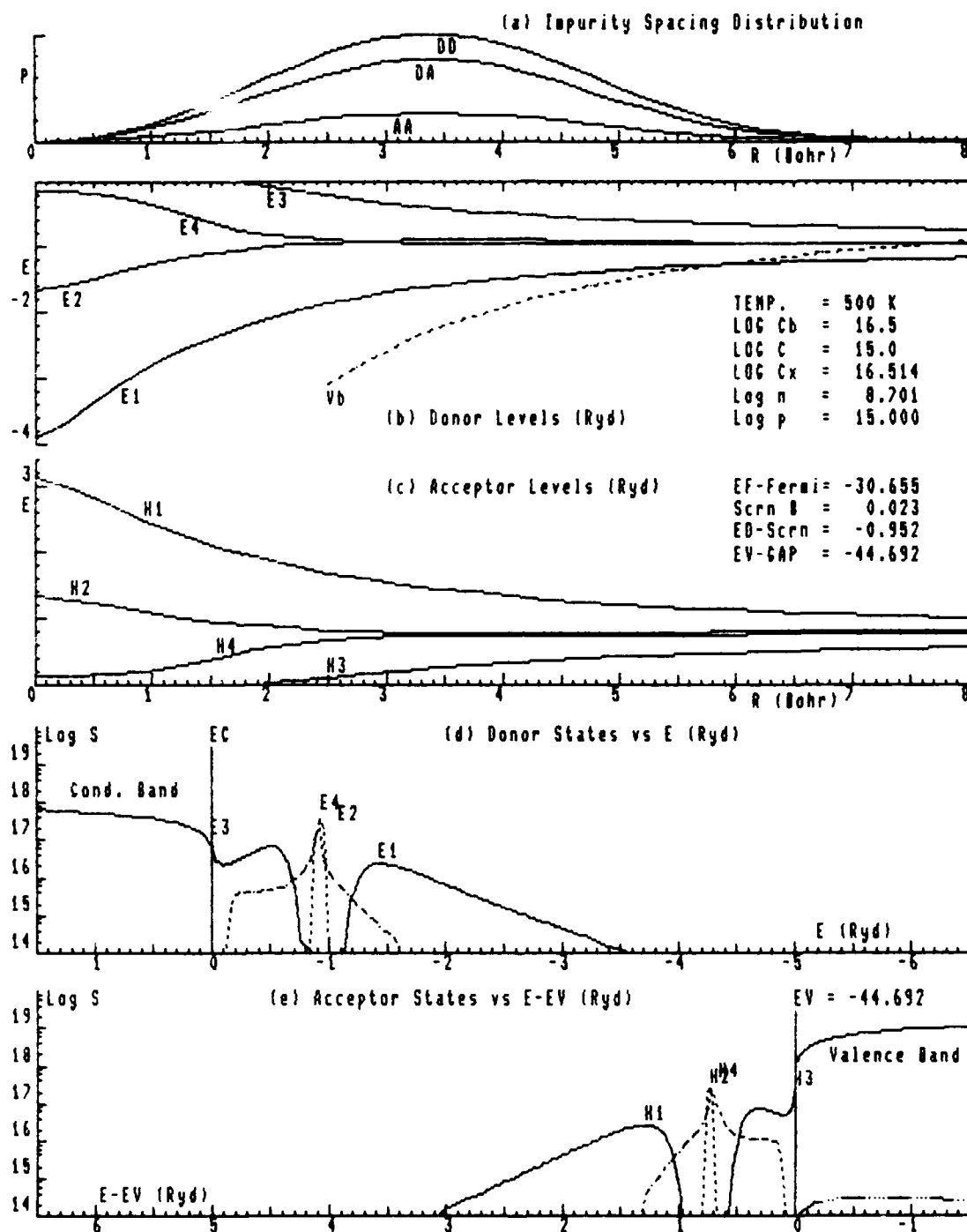


Fig. A 523. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

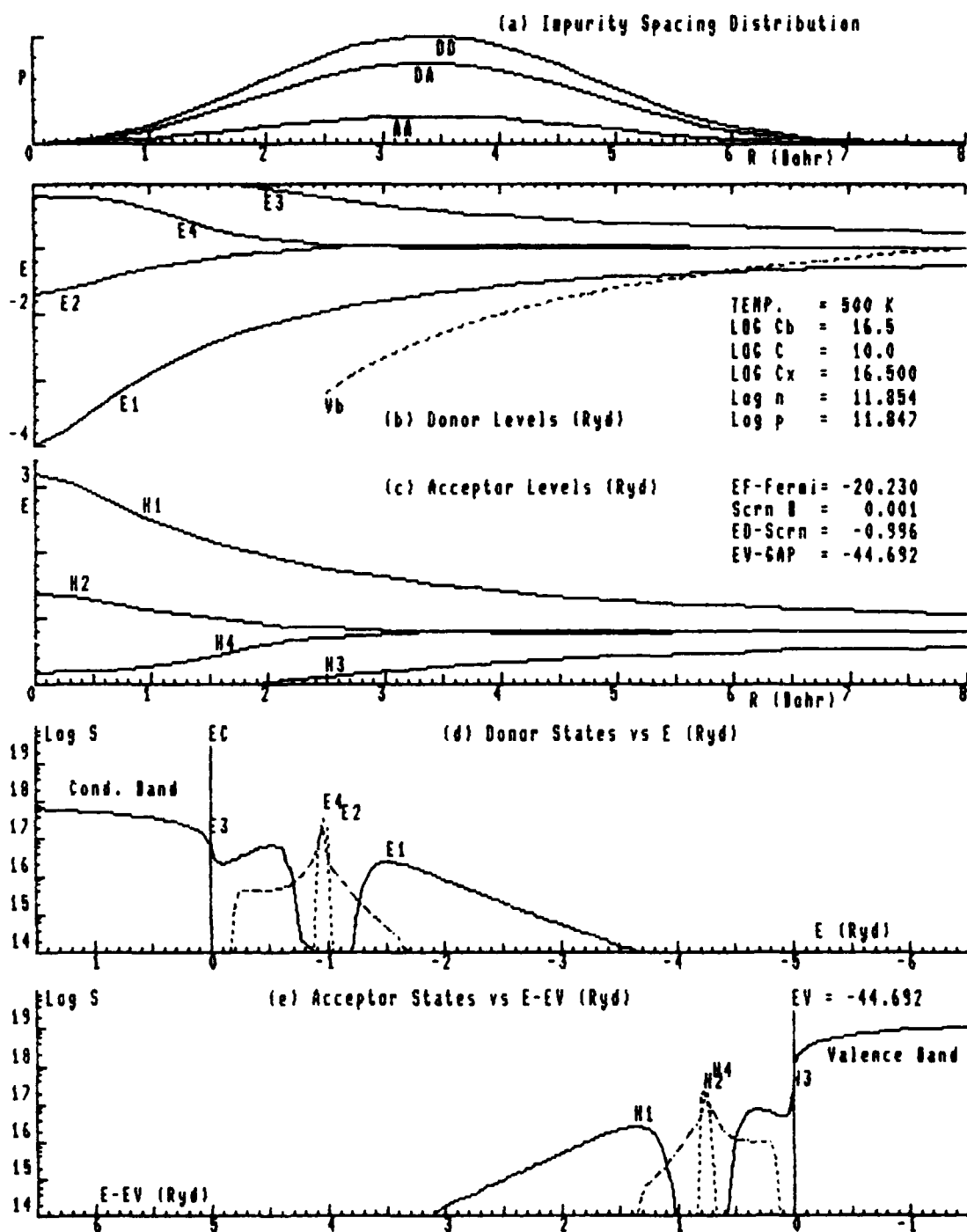


Fig. A 524. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

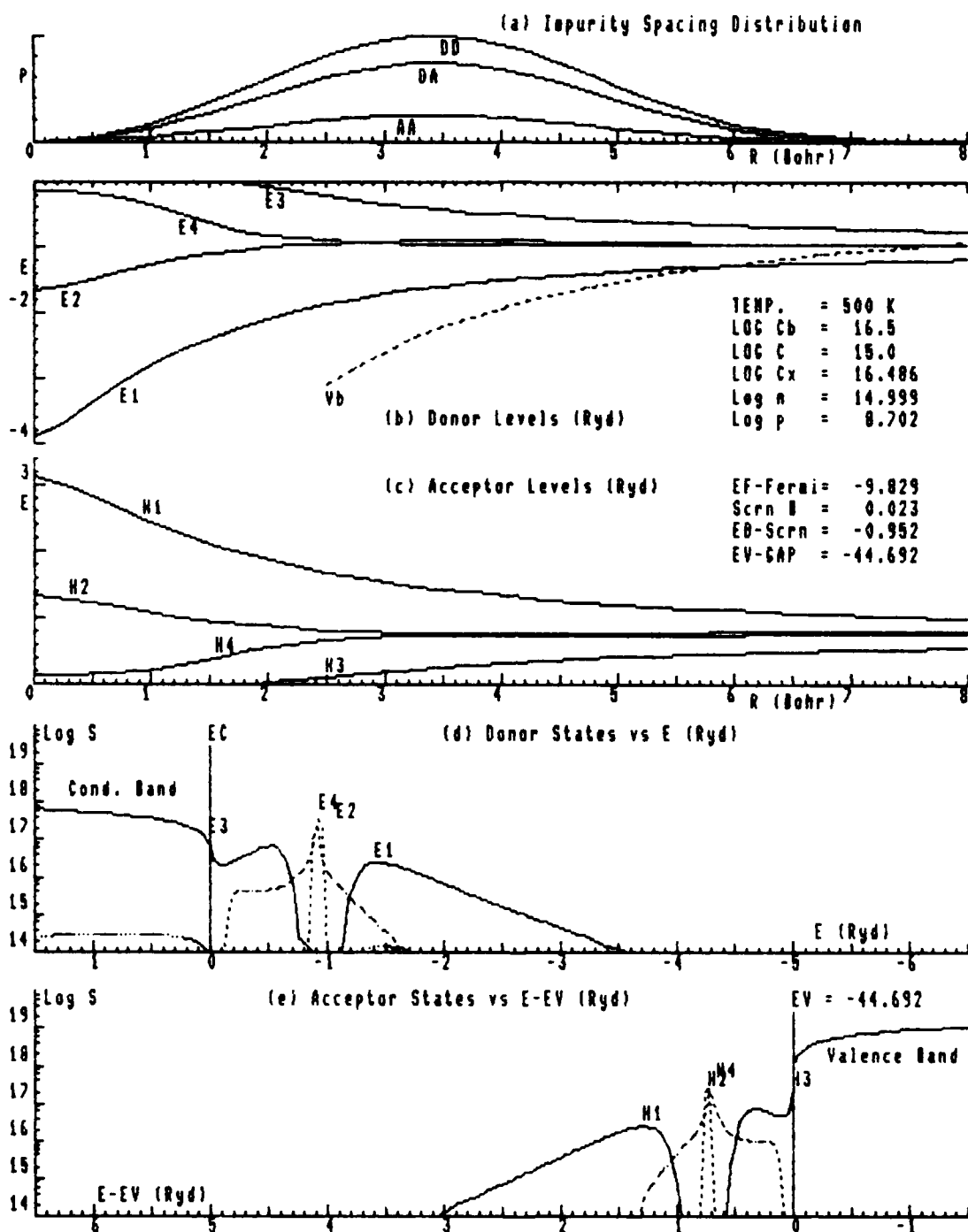


Fig. A 525. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

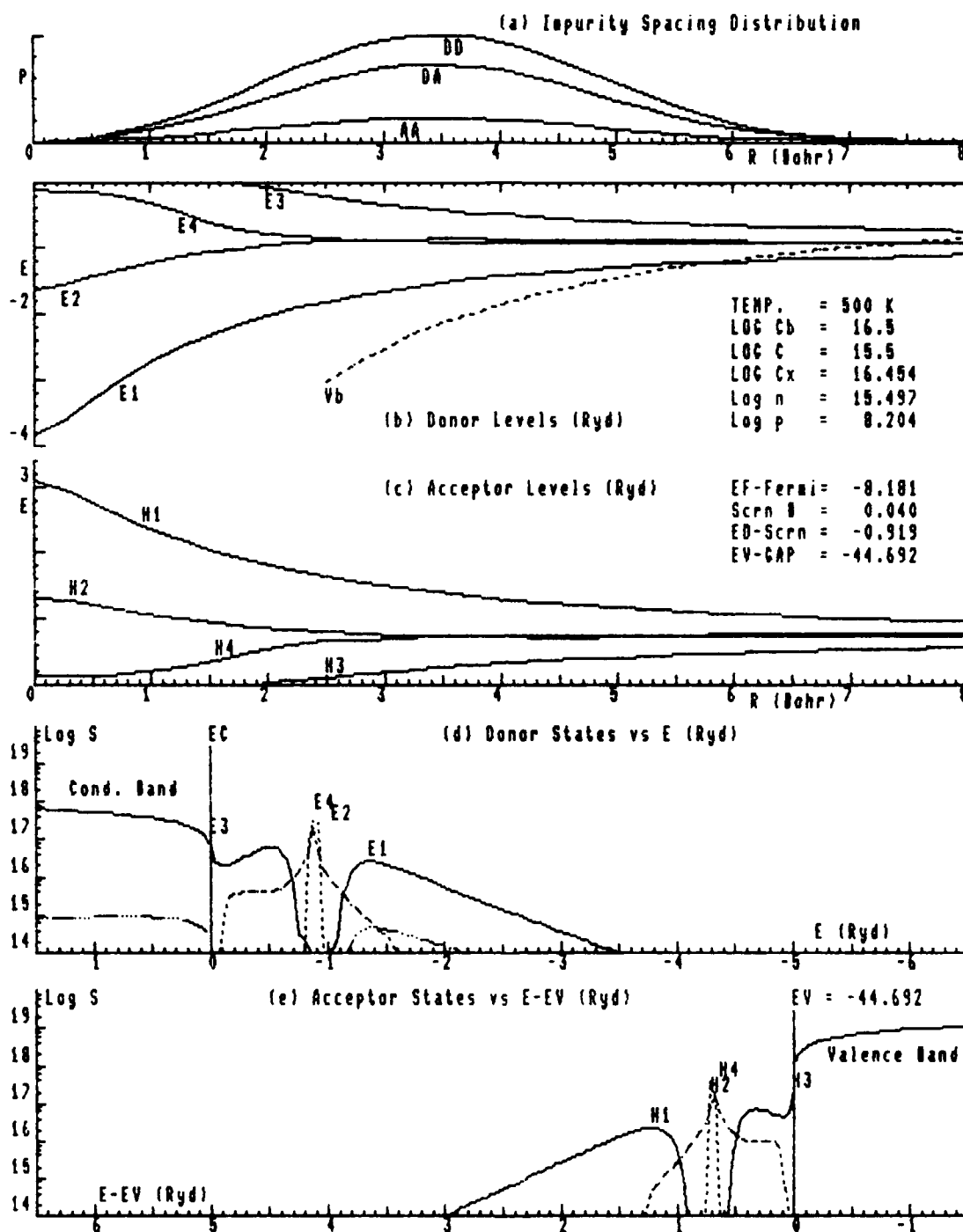


Fig. A 526. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

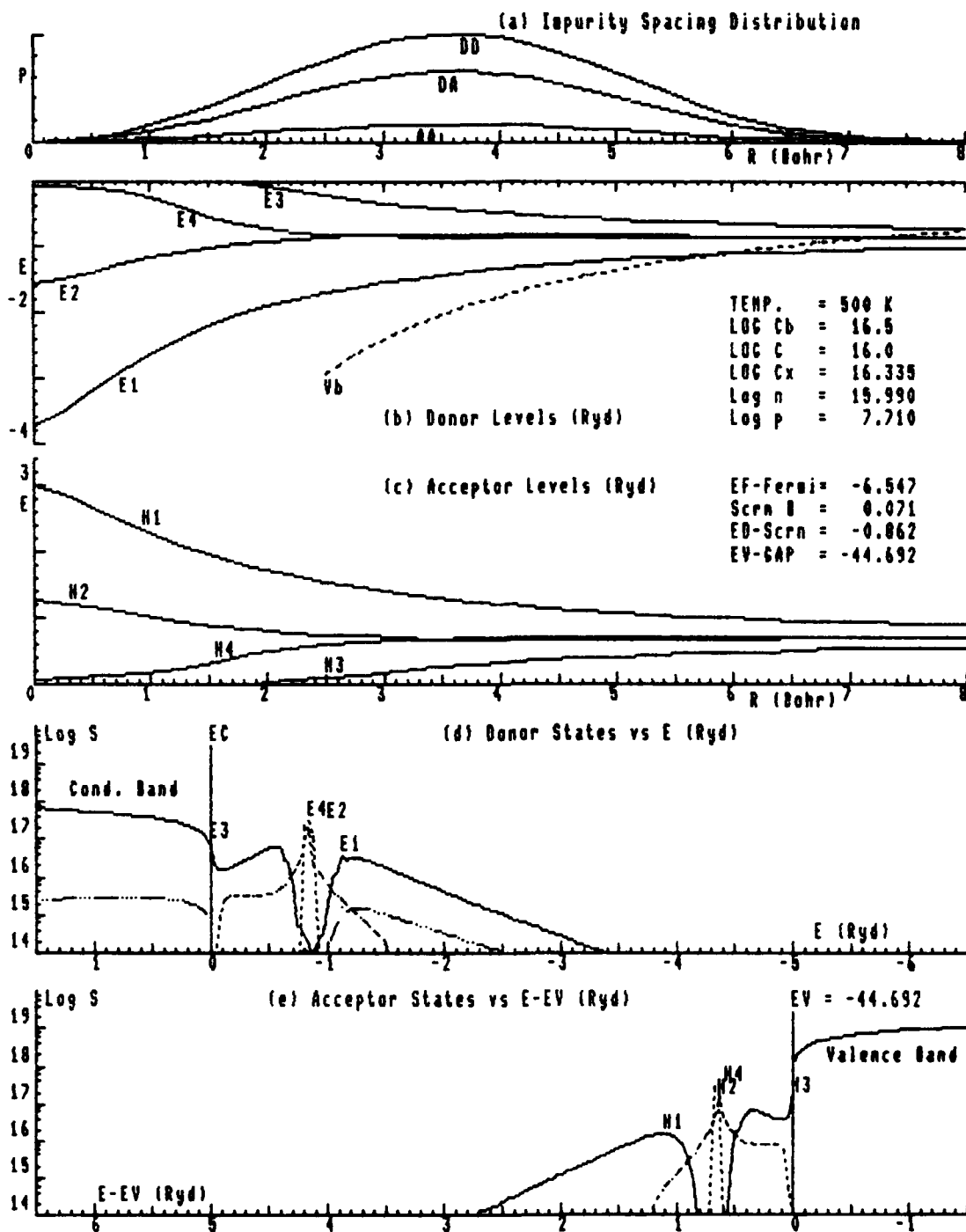


Fig. A 527. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

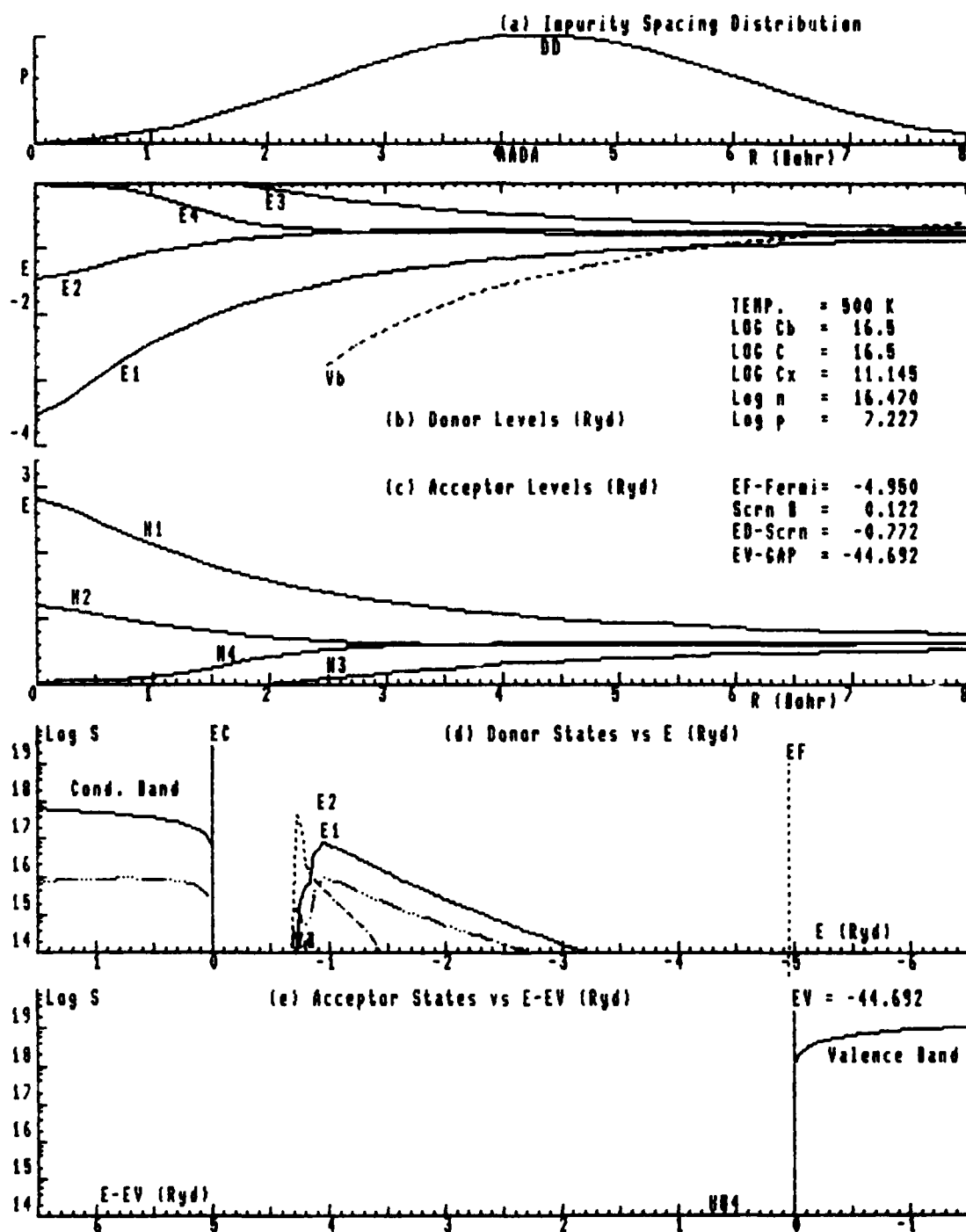


Fig. A 52B. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

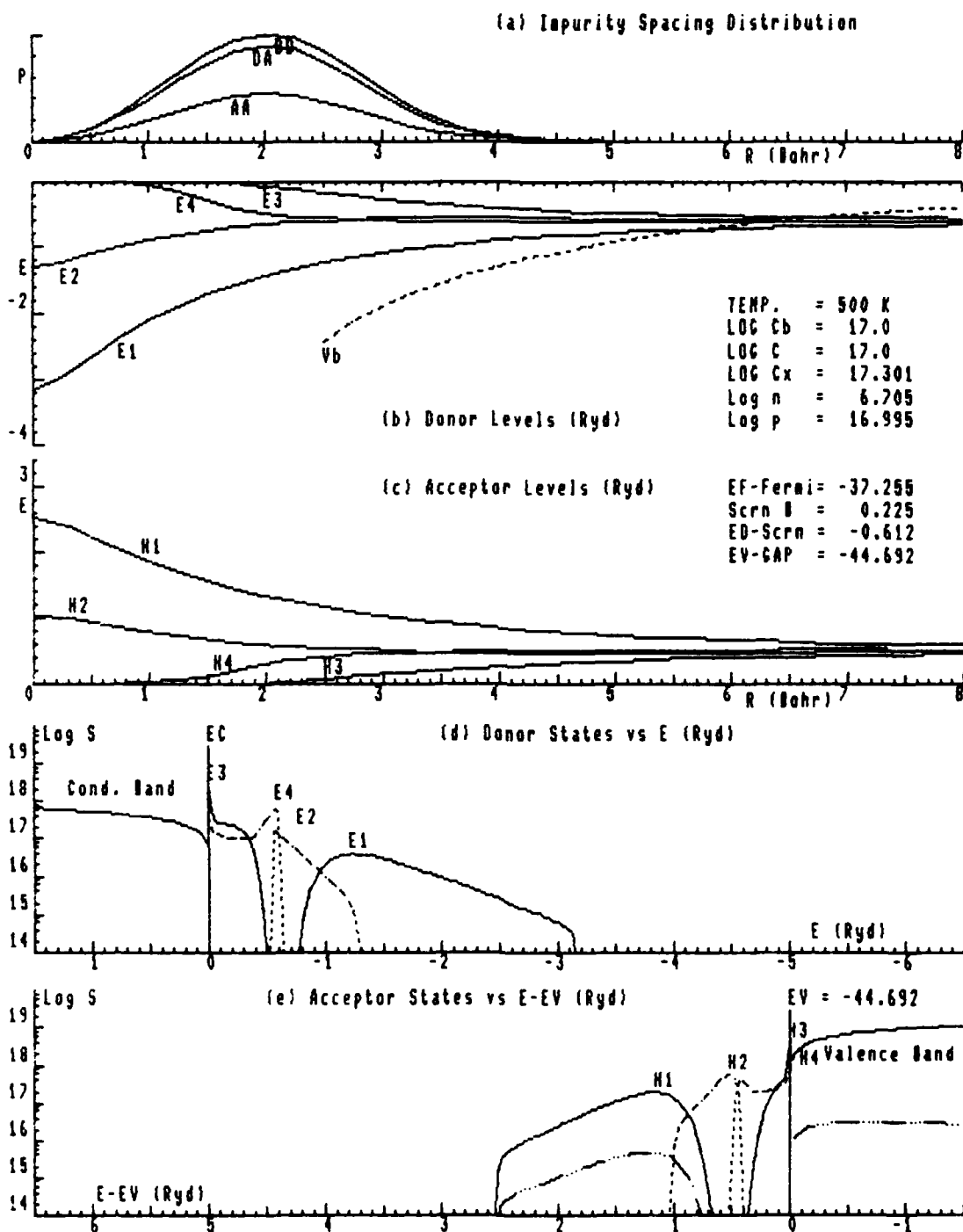


Fig. A 530. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

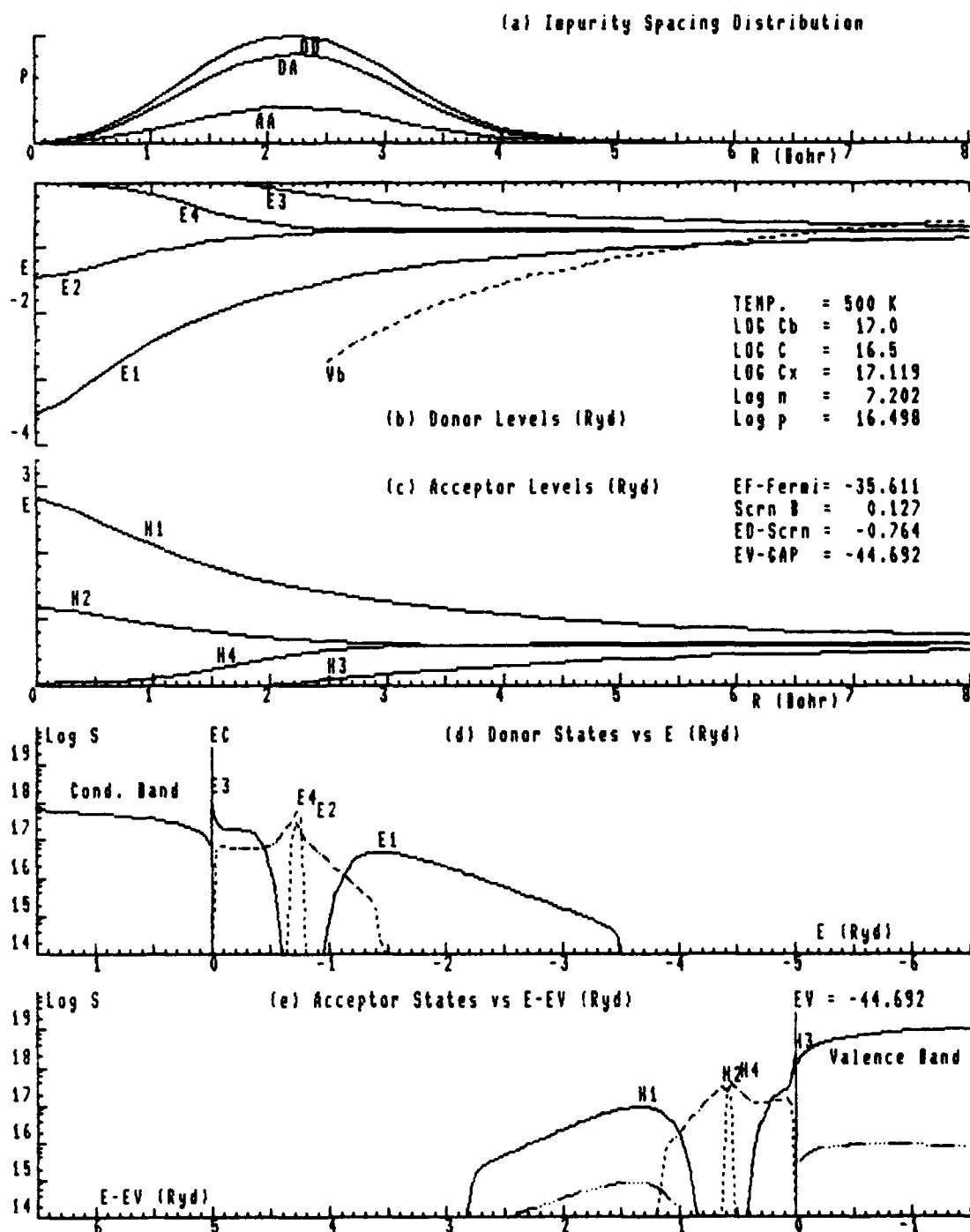


Fig. A 531. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

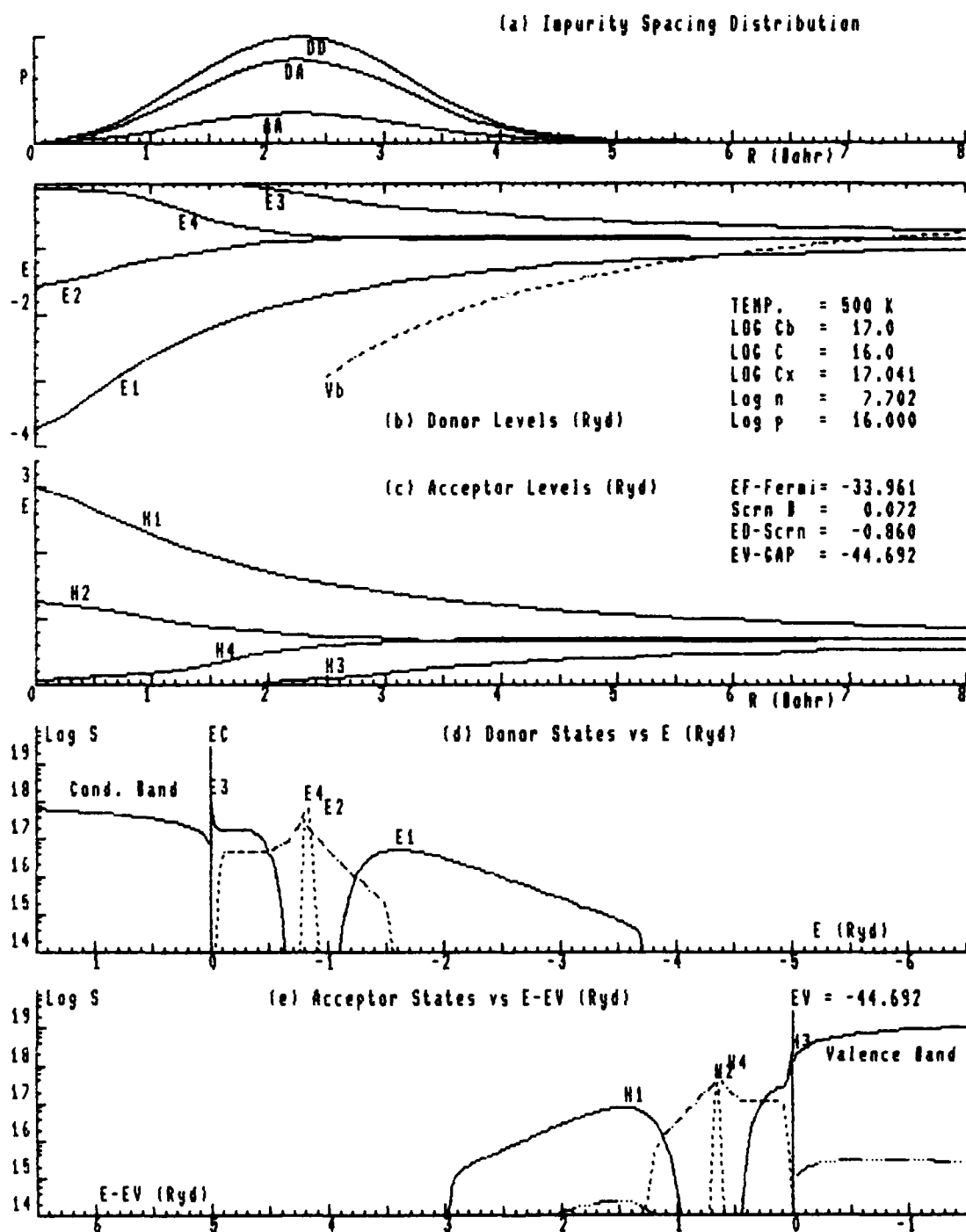


Fig. A 532. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

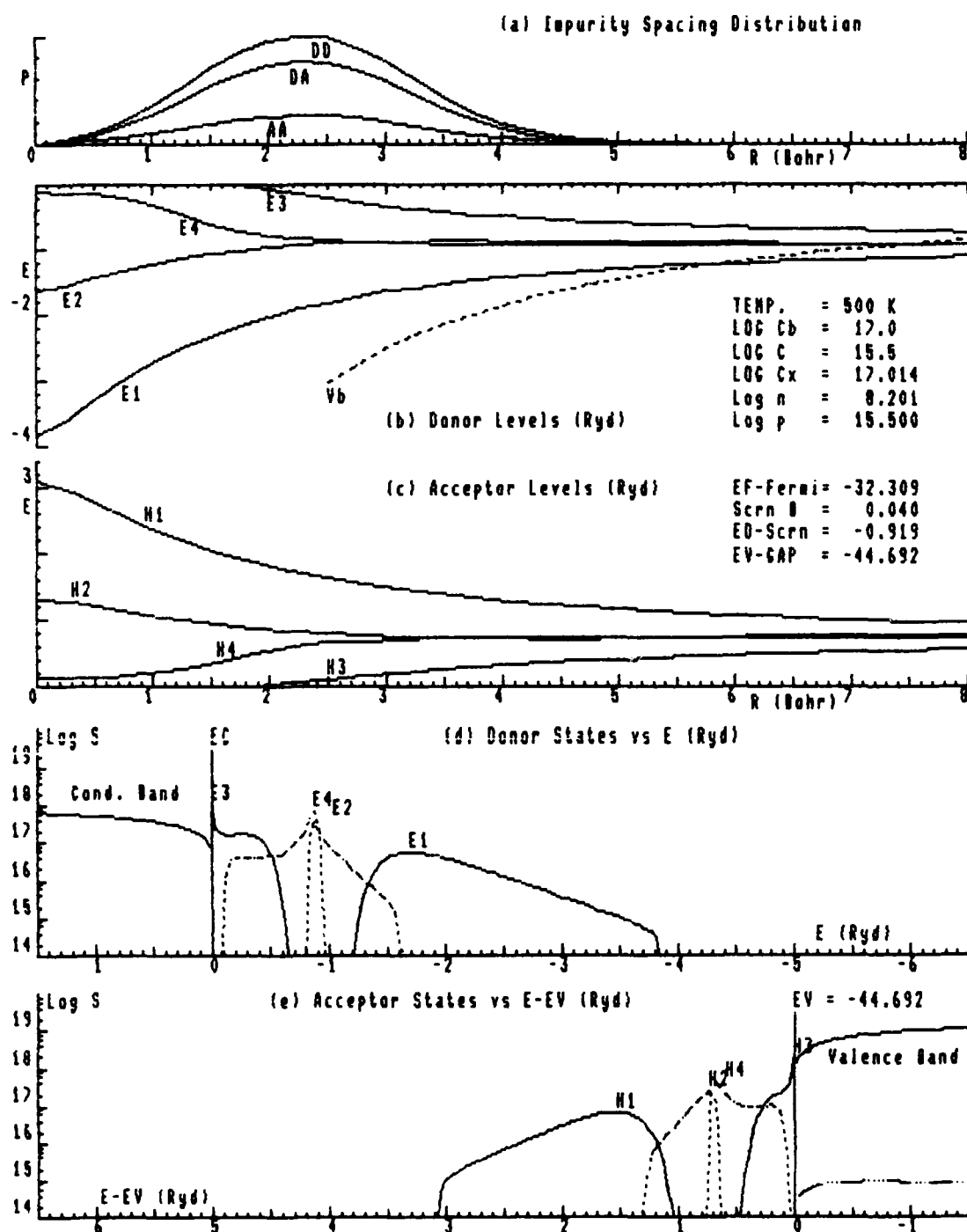


Fig. A 533. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)+, E3; (DA)-, E4 (DA)+ vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)-, H3; (AD)+, H4 (AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

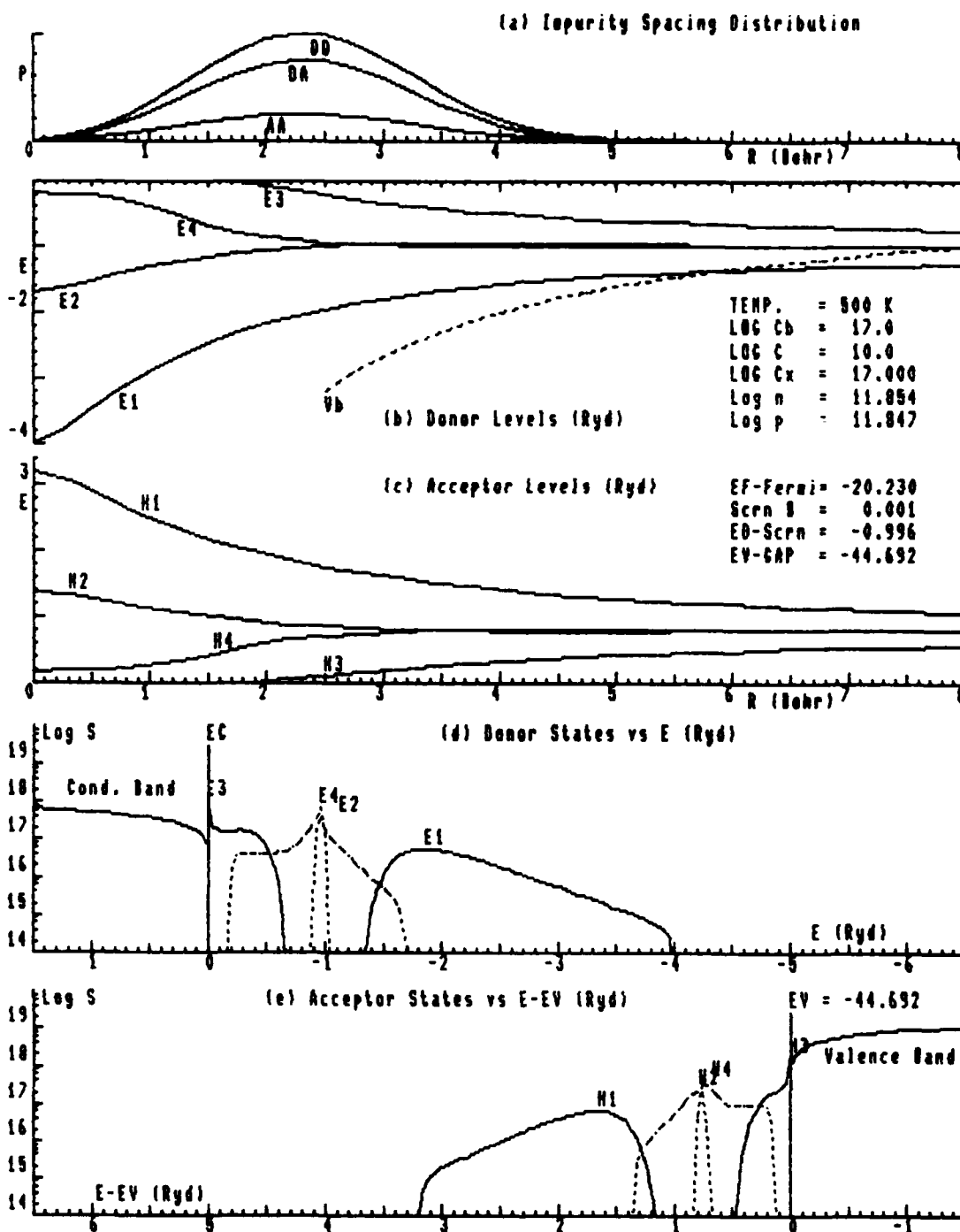


Fig. A 534. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

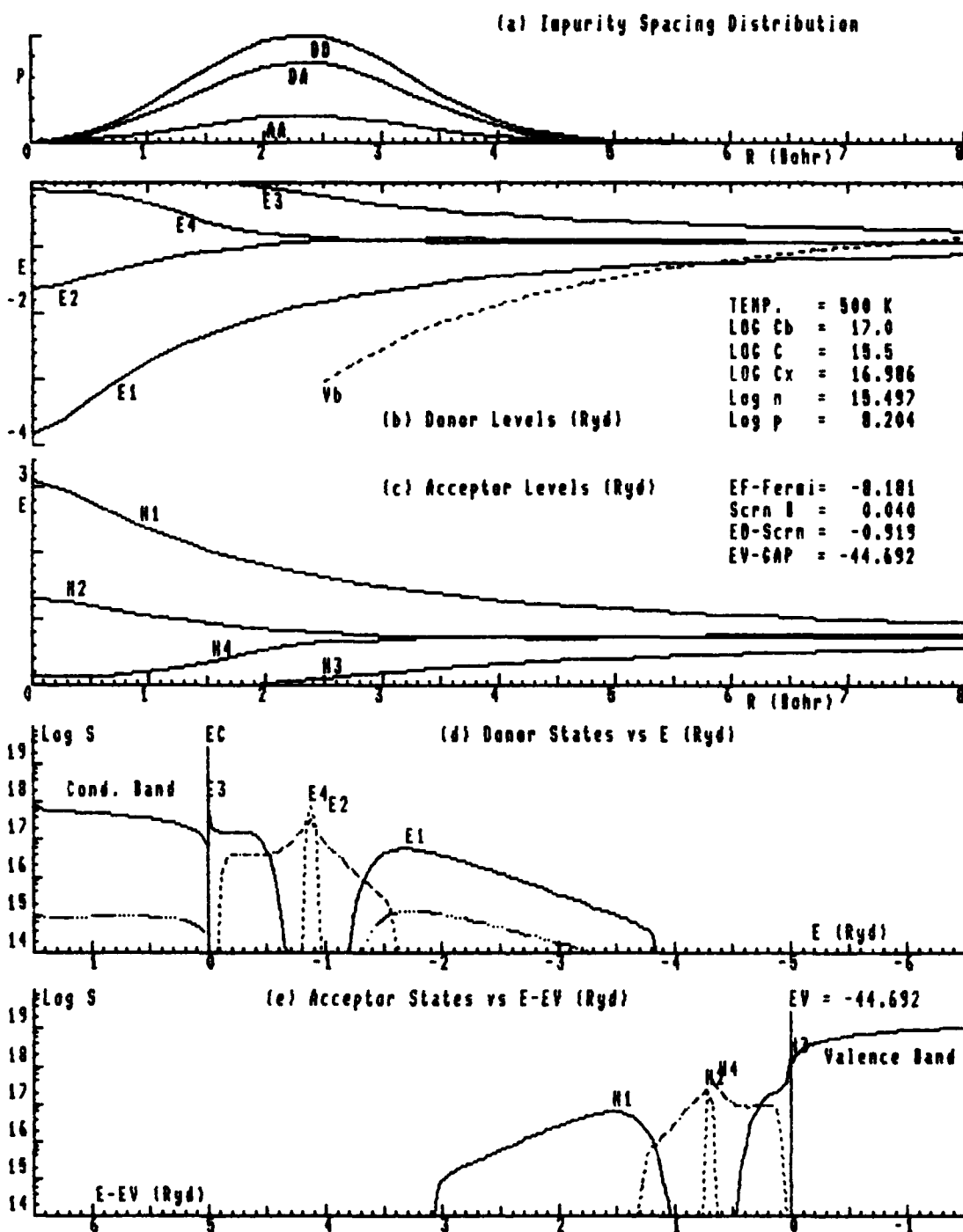


Fig. A 535. (a) Probability, $AA + DA + DD$, of Pairs vs R
 (b) Donor Energy $E1; (DD)^-, E2; (DD)^-, E3; (DA)^-, E4; (DA)^-$ vs R
 (c) Acceptor En. $H1; (AA)^+, H2; (AA)^+, H3; (AD)^+, H4; (AD)^+$ vs R
 (d) Densities of Donor States, $E1, E2, E3$, & $E4$, vs E
 (e) Densities of Acceptor States, $H1, H2, H3$, & $H4$ vs $E-EV$.

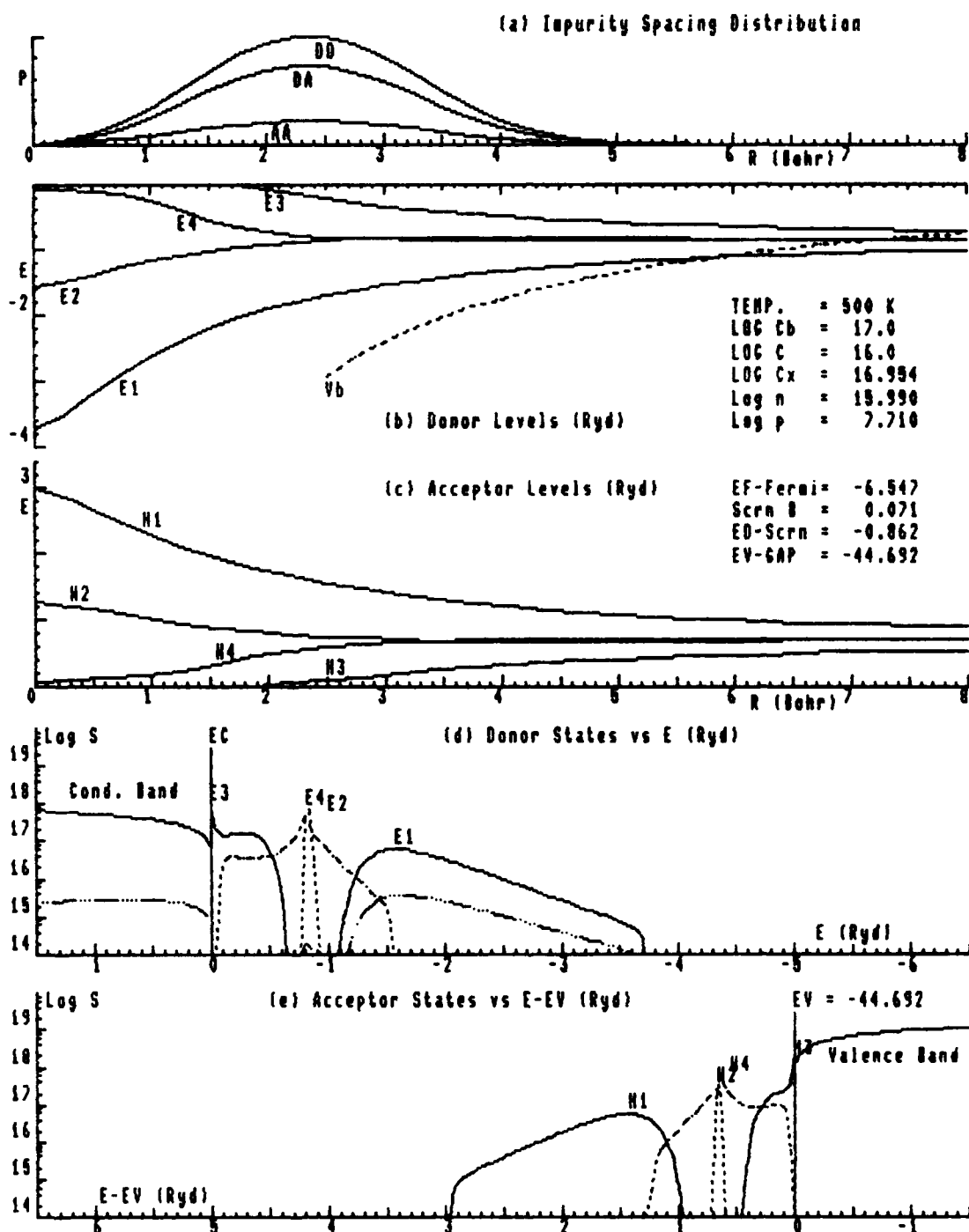


Fig. A 536. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

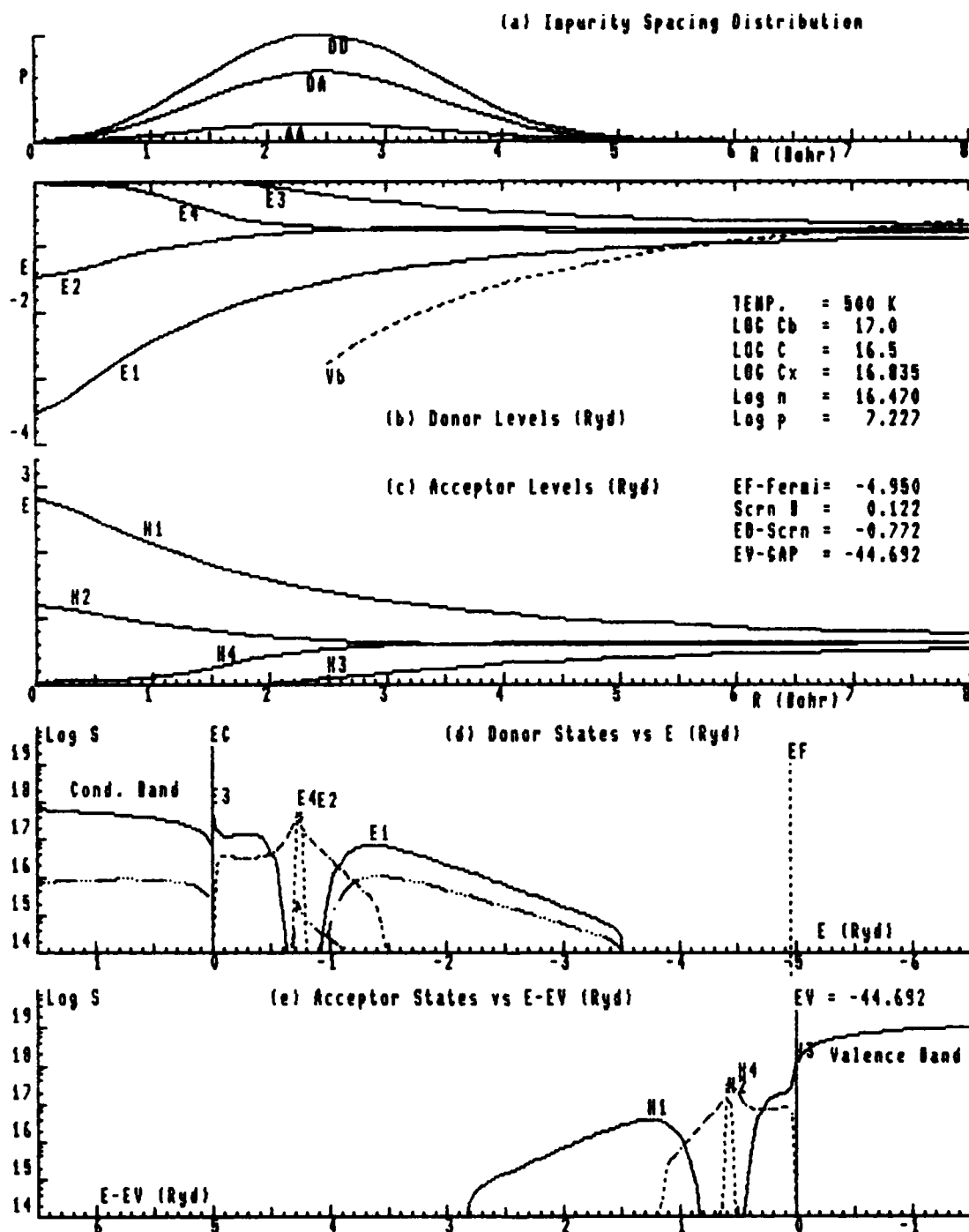


Fig. A 537. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4 (DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4 (AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

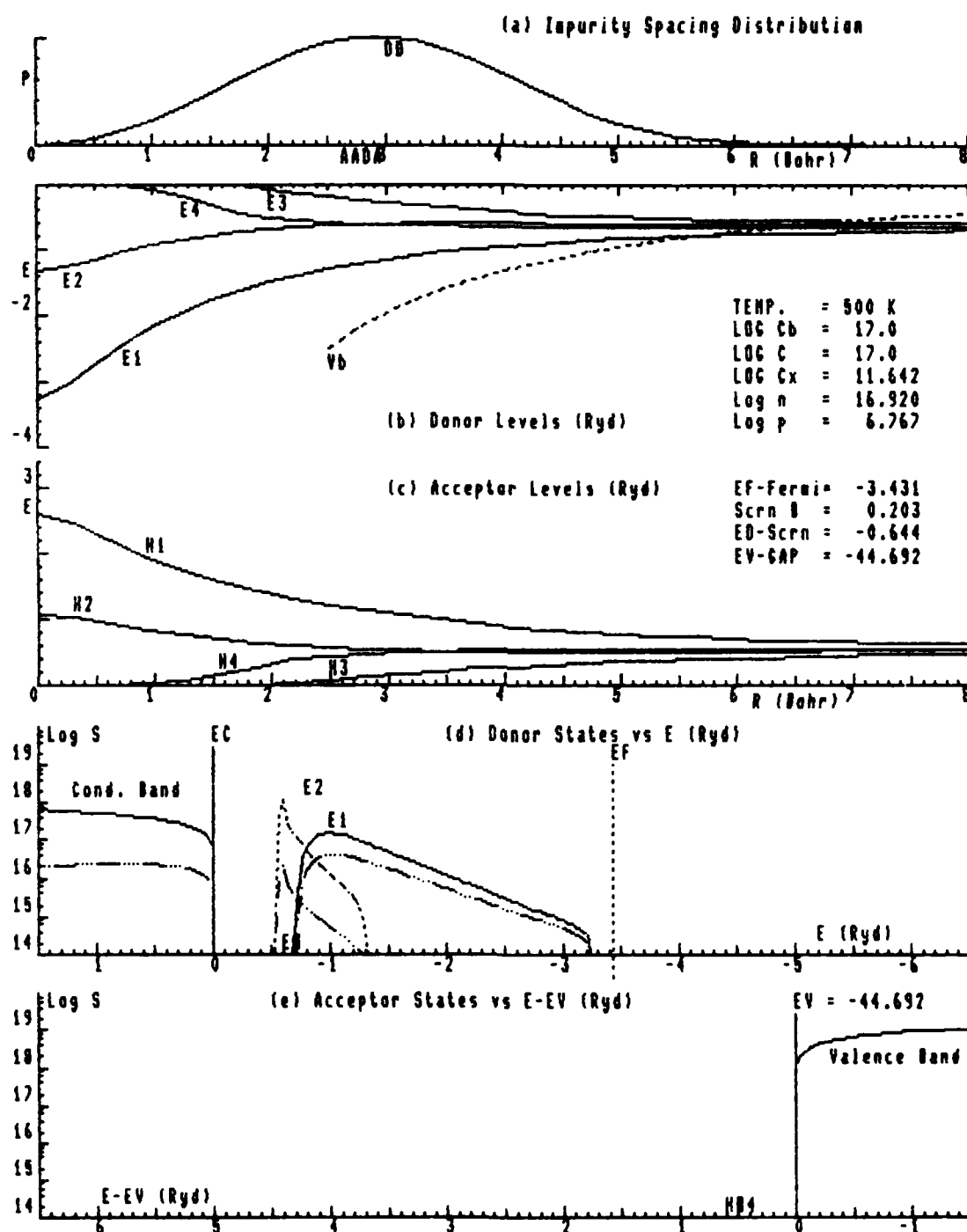


Fig. A 538. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

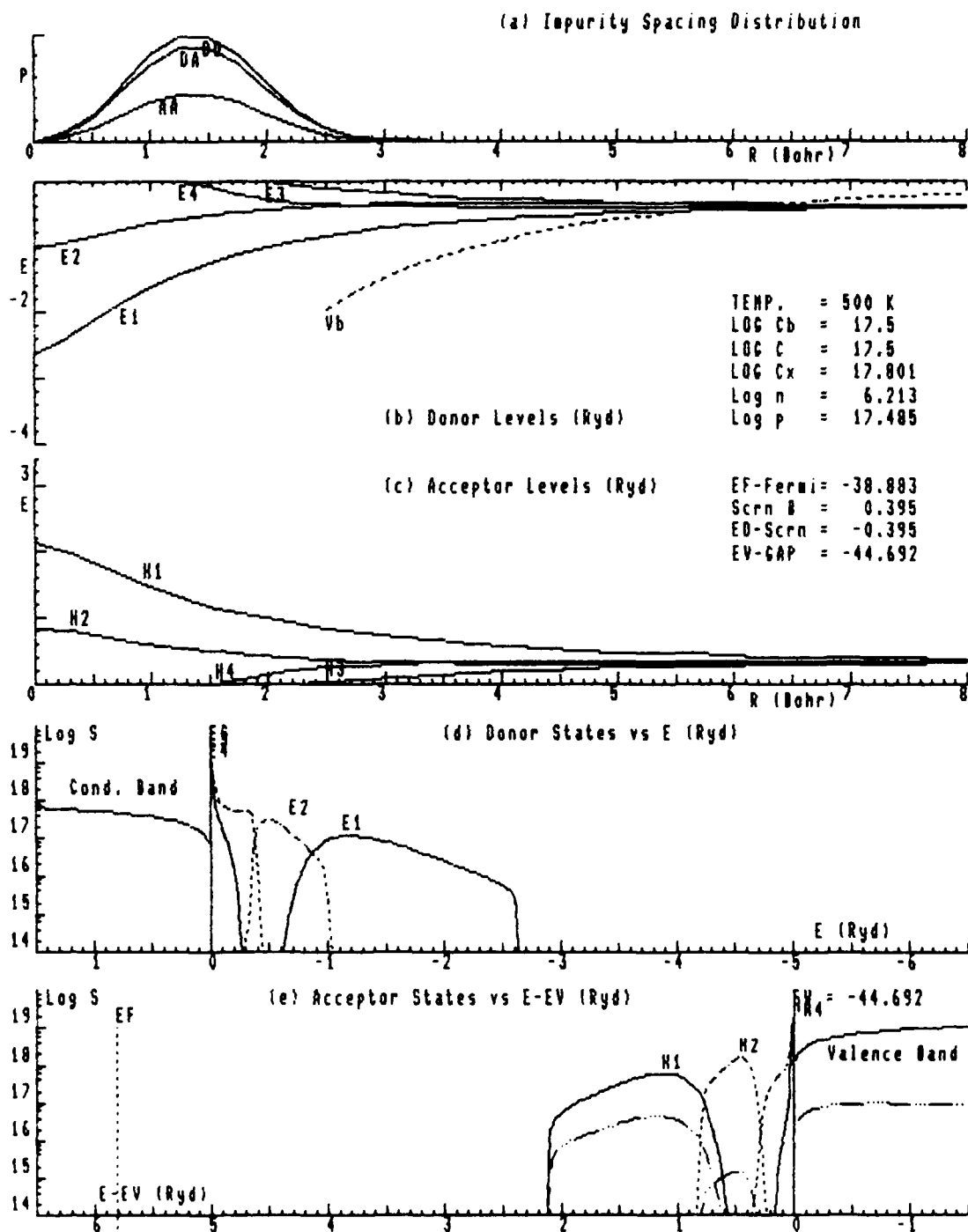


Fig. A 540. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

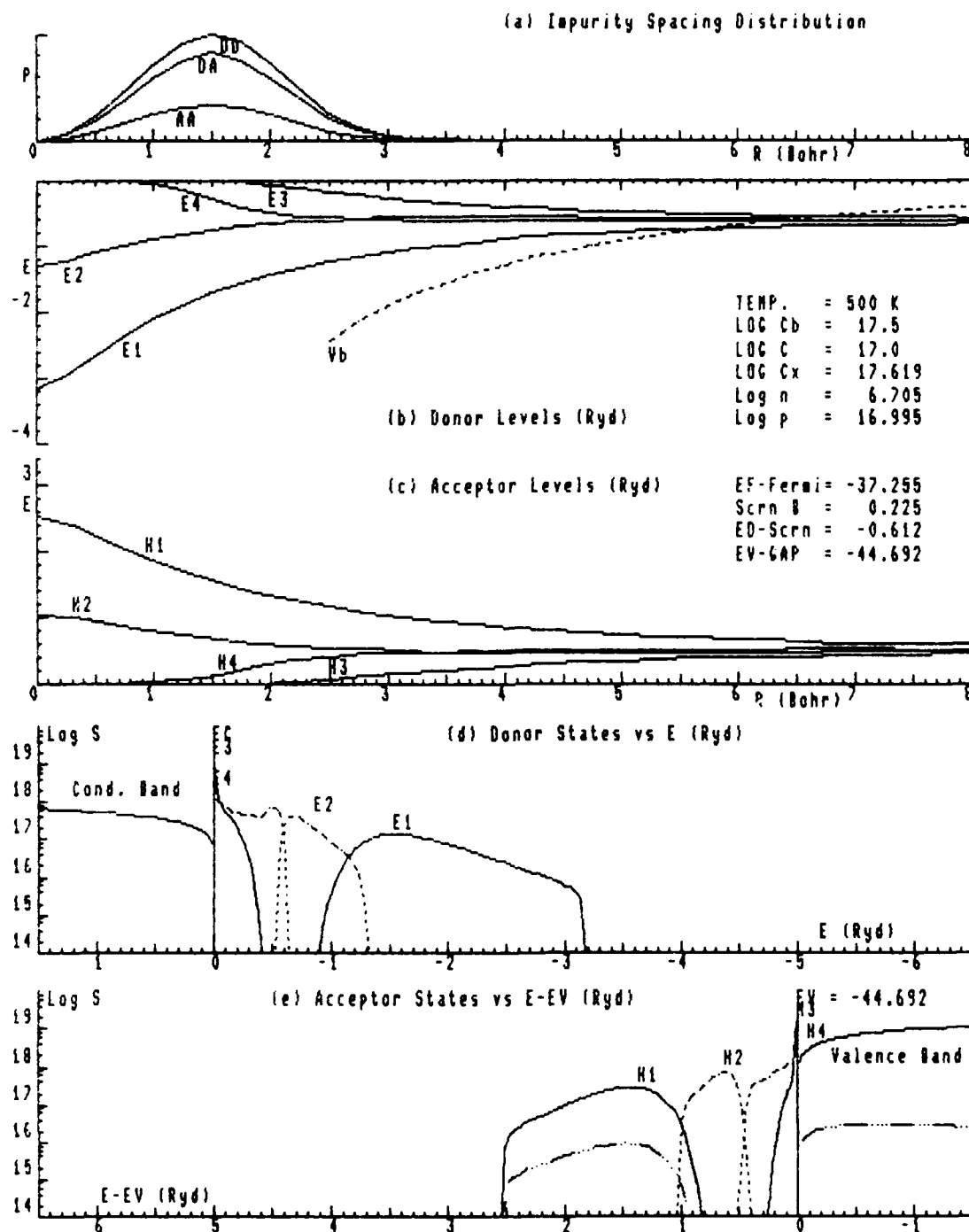


Fig. A 541. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1; (DD)-, E2; (DD)-, E3; (DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1; (AA)+, H2; (AA)+, H3; (AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

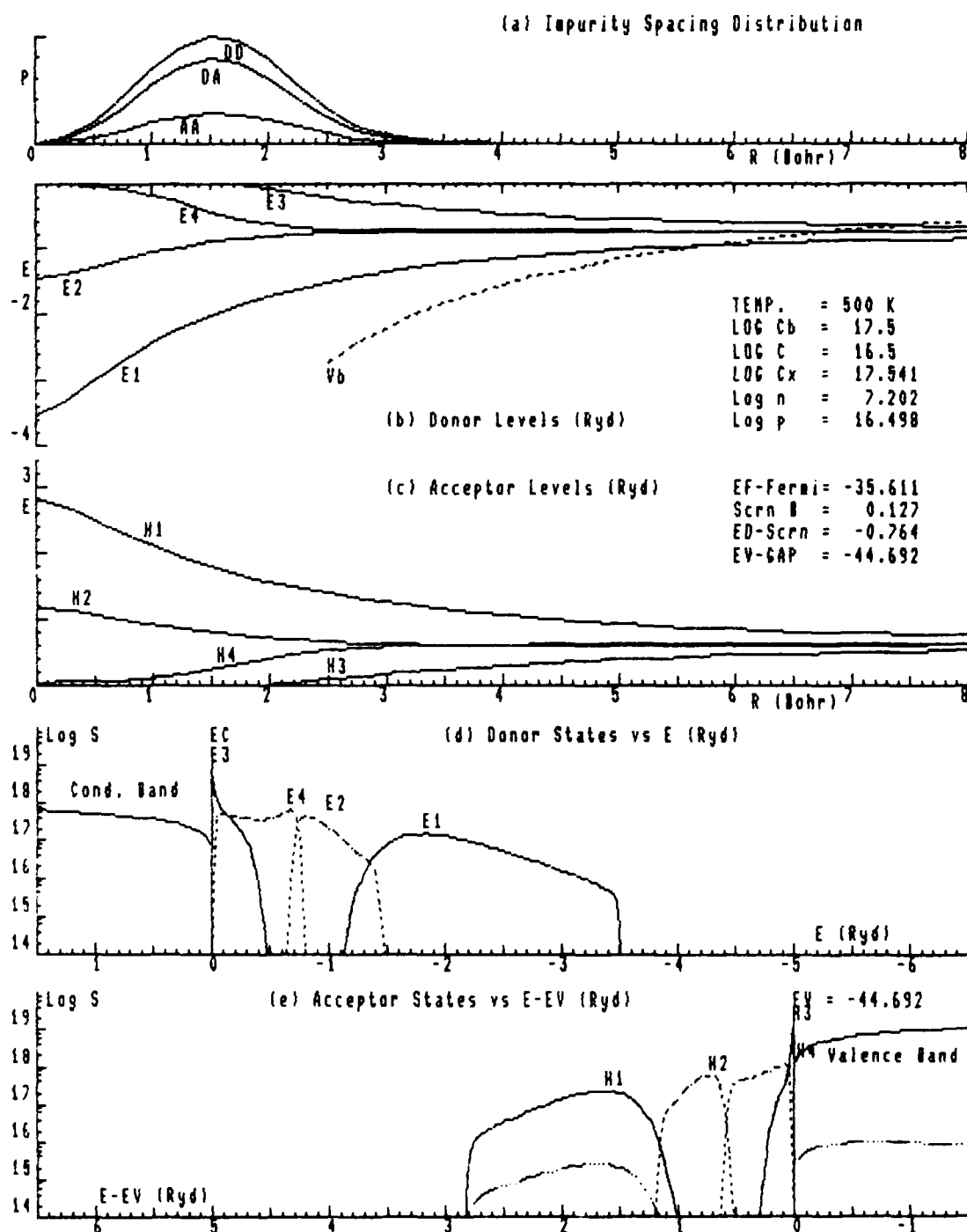


Fig. A 542. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)- vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

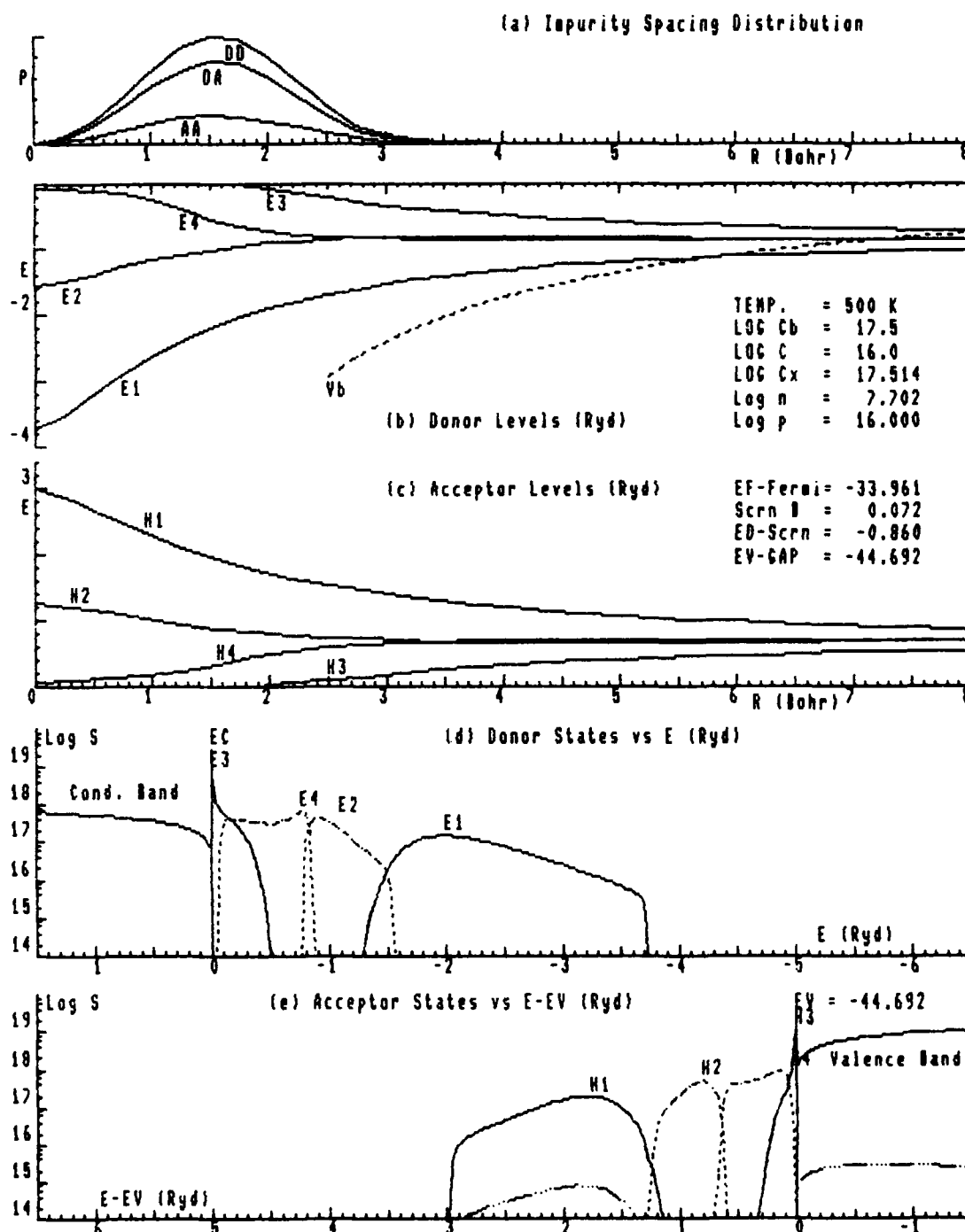


Fig. A 543. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

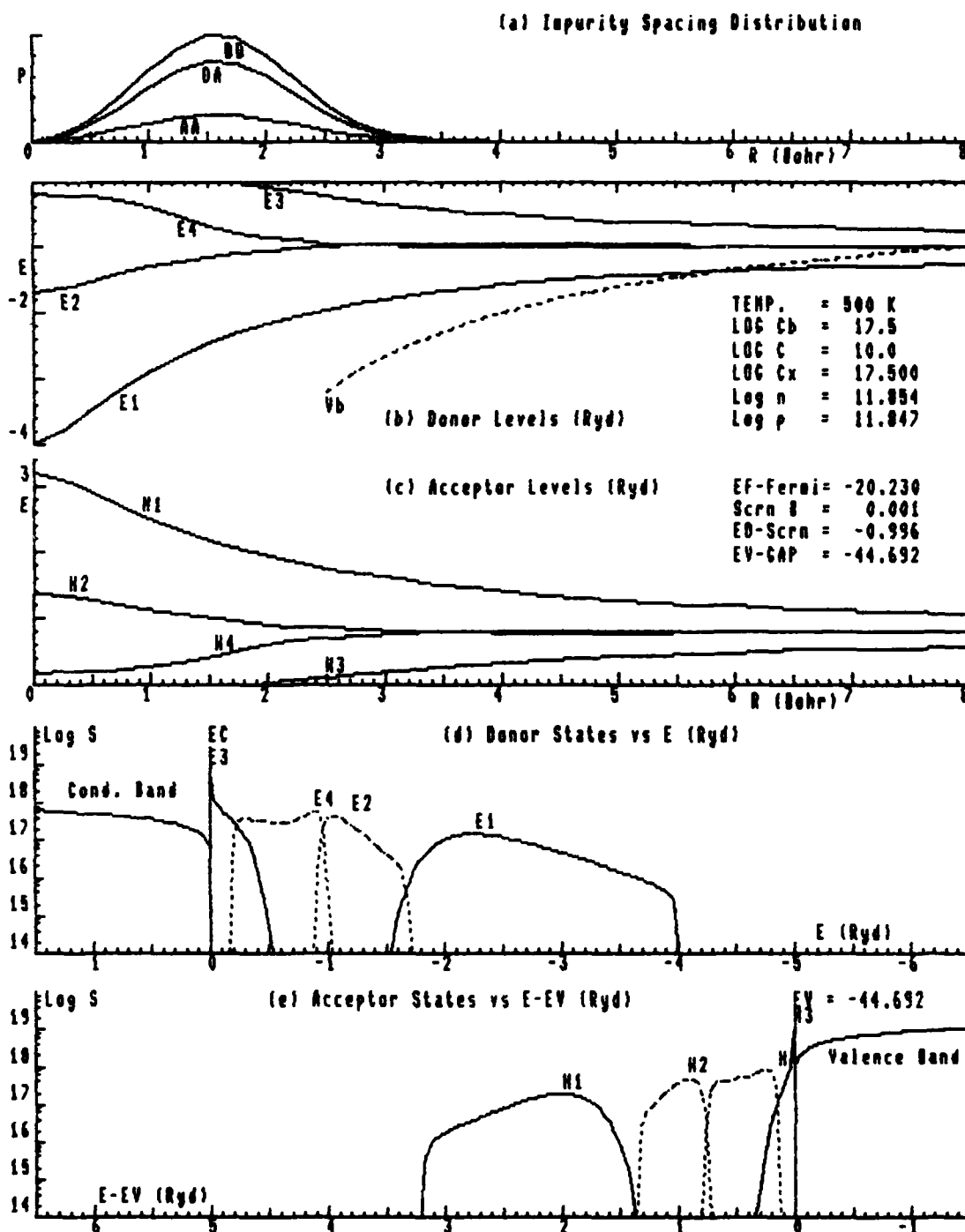


Fig. A 544. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

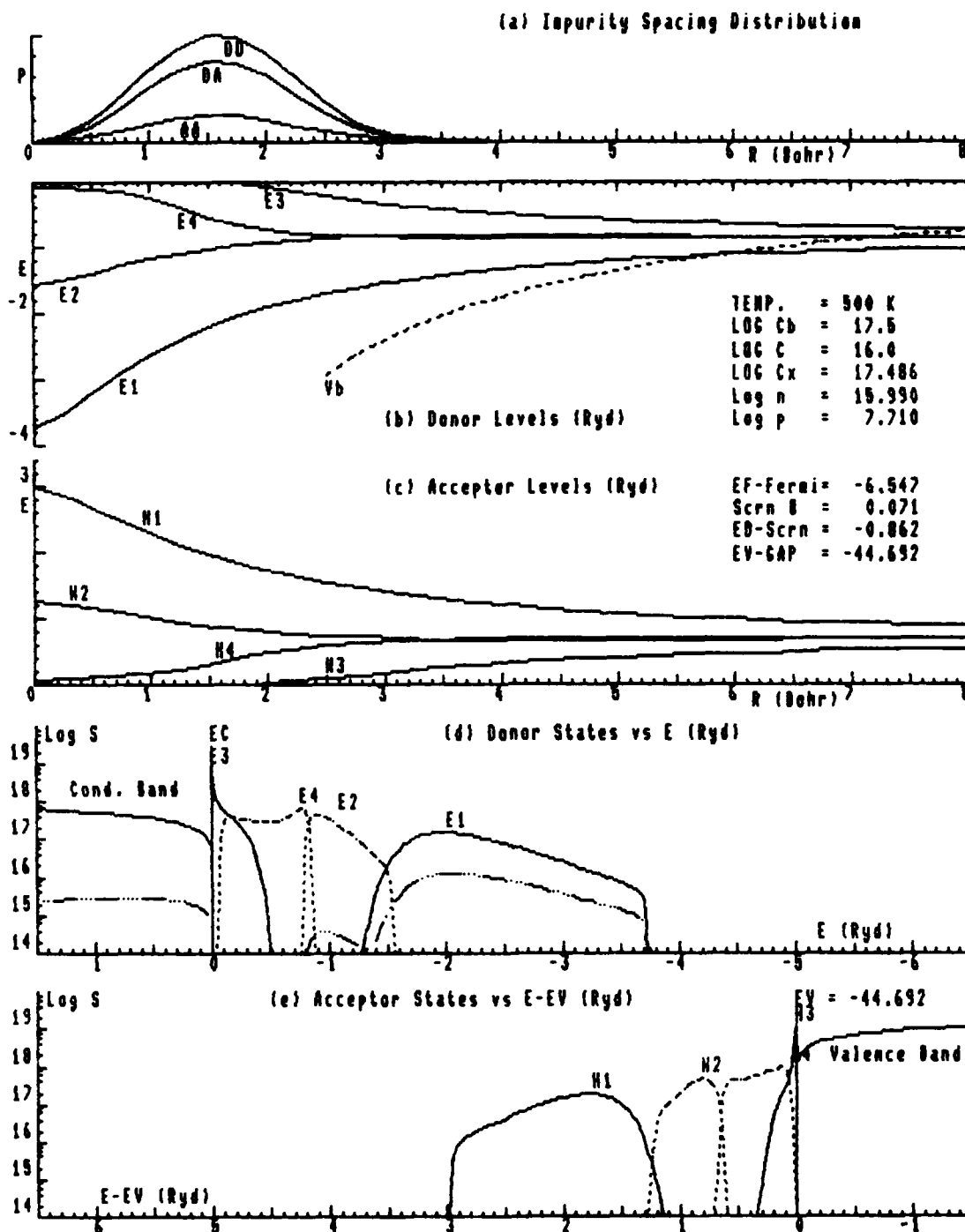


Fig. A 545. (a) Probability, $AA + DA + DD$, of Pairs vs R
 (b) Donor Energy $E_1; (DD)^-, E_2; (DD)^-, E_3; (DA)^-, E_4; (DA)^-$ vs R
 (c) Acceptor En. $H_1; (AA)^+, H_2; (AA)^+, H_3; (AD)^+, H_4; (AD)^+$ vs R
 (d) Densities of Donor States, $E_1, E_2, E_3, \& E_4$, vs E
 (e) Densities of Acceptor States, $H_1, H_2, H_3, \& H_4$ vs $E-EV$.

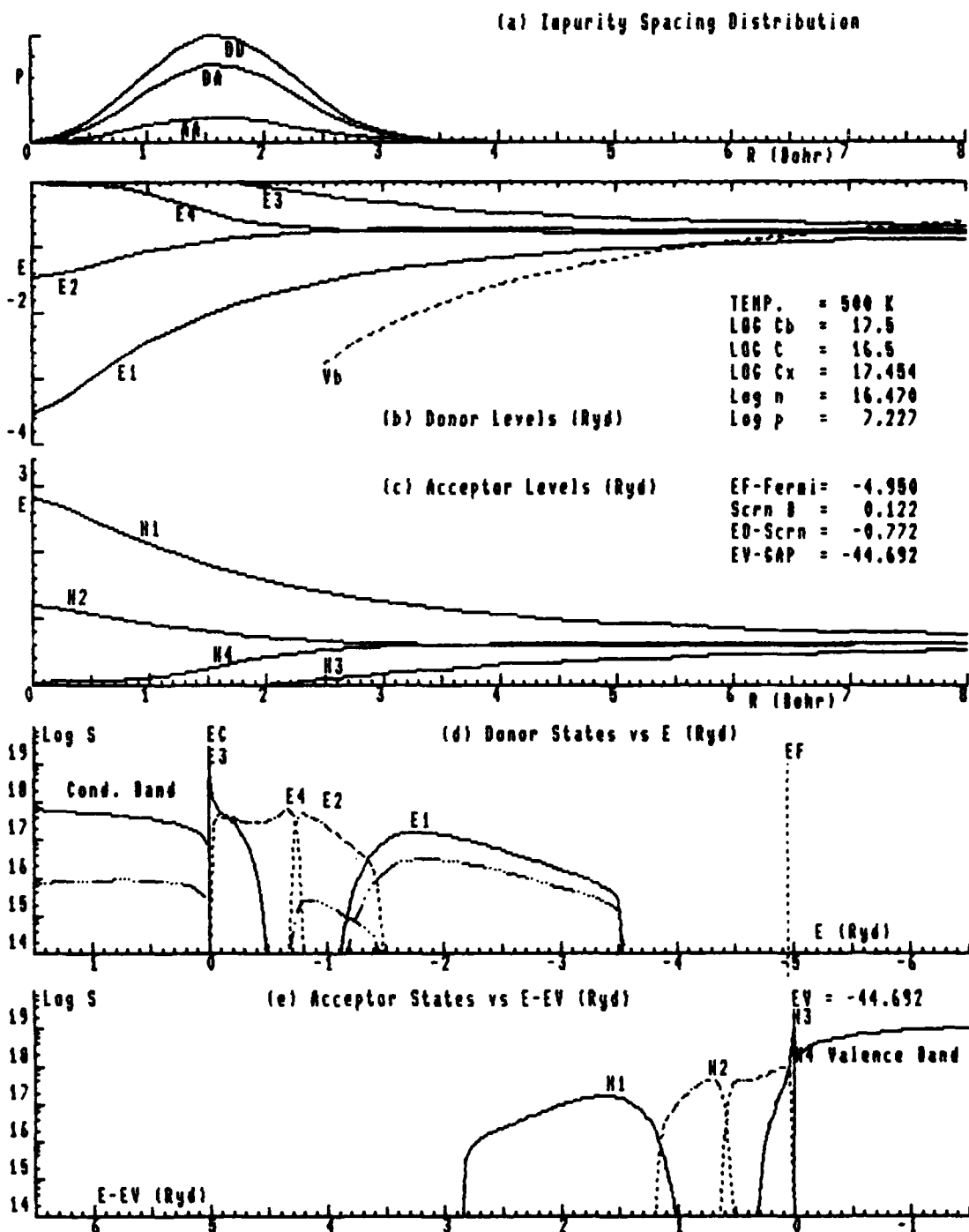


Fig. A 546. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

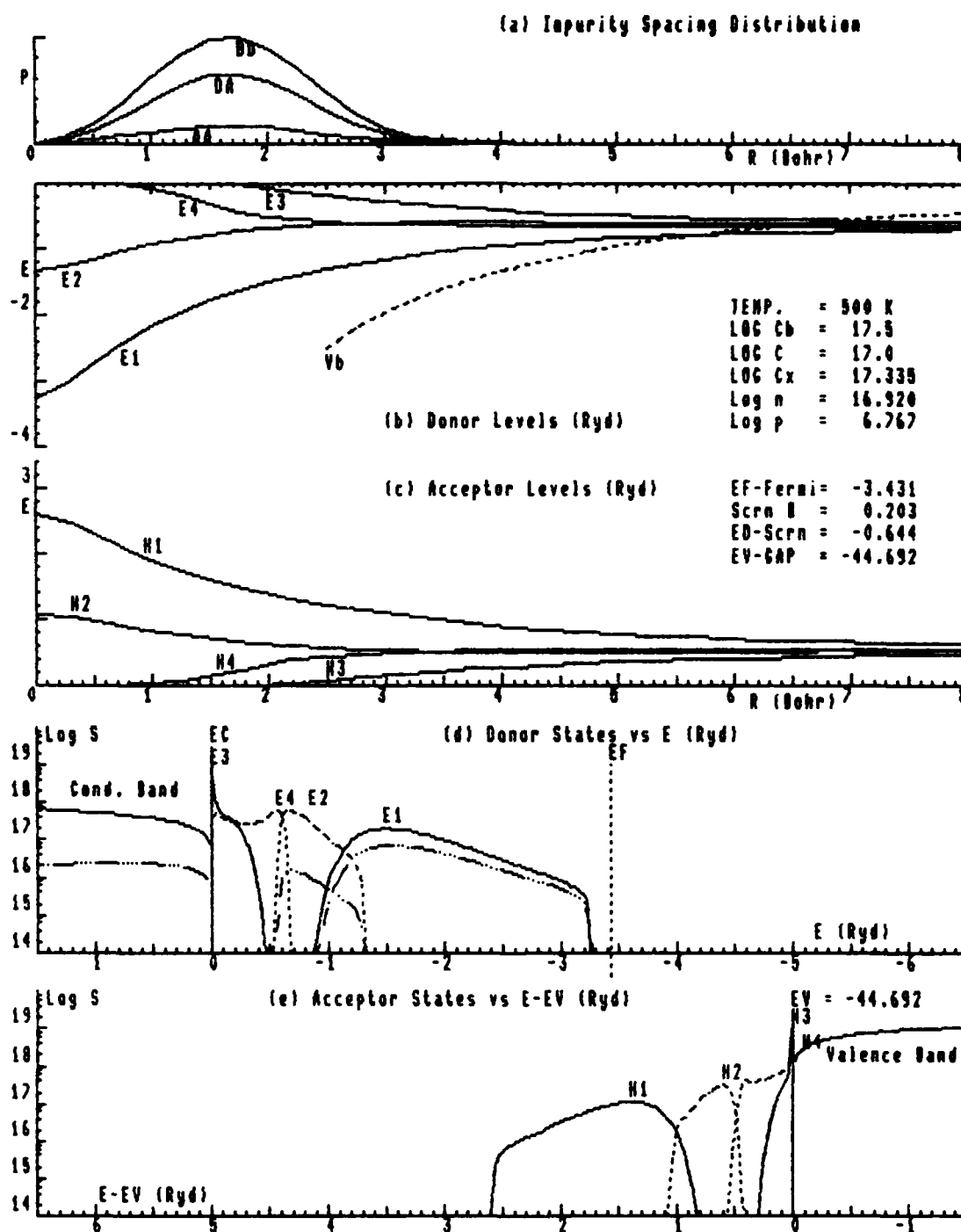


Fig. A 547. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

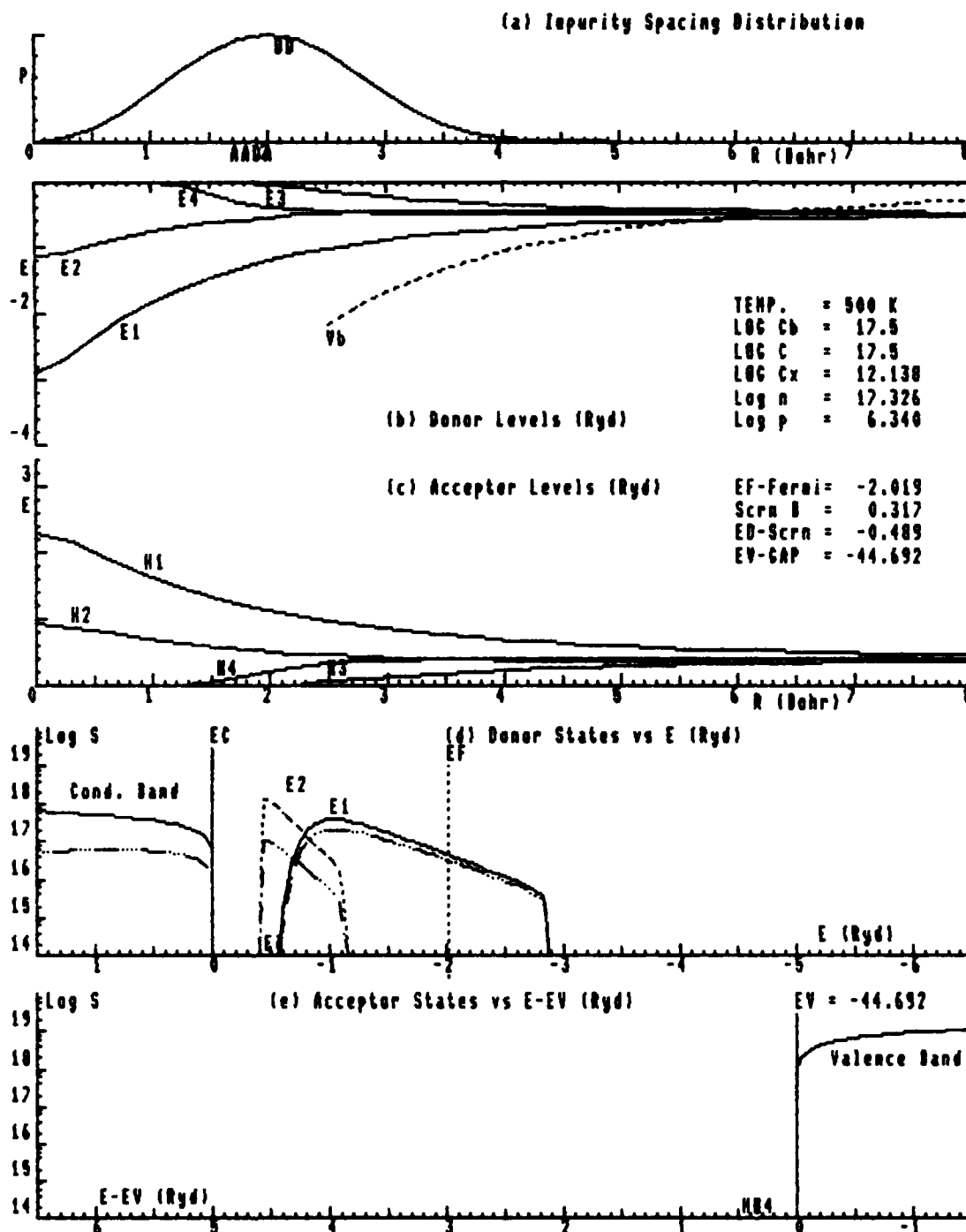


Fig. A 548. (a) Probability, AA + DA + DD, of Pairs vs R
 (b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R
 (c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD)+ vs R
 (d) Densities of Donor States, E1, E2, E3, & E4, vs E
 (e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.

APPENDIX B

Theoretical Basis

Donor-Donor Pair Energy Calculations

The procedure makes use of a variation type calculation similar to that used by Slater in calculating the ground-state energies of H_2 and H_2^+ . The impurity centers are located at points a and b separated by a distance R. Distances from these centers to electrons at points 1 and 2 are denoted by r_{1a} , r_{1b} , r_{2a} , and r_{2b} . The inter-electron distance is r_{12} . Two angles ϕ_1 , and ϕ_2 locate the azimuthal positions.

Four normalized 1s wave functions of the form $a(1) = (\alpha^3/\pi)^{1/2} \exp(-\alpha r_{1a})$ are used to form the system wave function along with appropriate spin functions. For the H_2 type system, the ground state function has the form:

$$\psi U_A = [a(1)b(2) + a(2)b(1)]U_A \quad (1)$$

where U_A is an antisymmetric spin function. The spin function does not enter into the energy integral but determines the symmetry of the orbital function for the ground state (the Hamiltonian is spin independent). In the H_2^+ case the orbital function has the form:

$$\psi = a(1) + b(1) \quad (2)$$

The Hamiltonian for the H_2 type system (in units of Bohr radii and Rydbergs) has the form:

$$H = -\nabla_1^2 - \nabla_2^2 - v_{1a} - v_{1b} - v_{2a} - v_{2b} + v_{12} \quad (3)$$

where the potential energy terms are of the form $V_{1a} = 2\exp(-\beta r_{1a})/r_{1a}$, etc., and β is the inverse screening range. For the H_2^+ system, terms with subscript 2 are omitted.

The integrals to be calculated come from the expression

$$E = \int \psi^* H \psi dv / \int \psi^* \psi dv \quad (4)$$

for each of the two systems. The parameter α in the basis function is the variation parameter. It, of course, has the value unity for an isolated hydrogen-like atom, but, in the case of a molecule-like system it is adjusted by minimizing the energy with respect to a variation of α . The above integrals can be expressed in terms of the following integrals over the basis functions: ($w = \alpha R$)

$$\int a(1) (-\nabla_1^2) a(1) dv_1 = \alpha^2 \quad (5)$$

$$\int a(1) b(1) dv_1 = S = e^{-w} (1 + w + w^2/3) \quad (6)$$

$$\int a(1) (-\nabla_1^2) b(1) dv_1 = -\alpha^2 (K + S) = \alpha^2 e^{-w} (1 + w - w^2/3) \quad (7)$$

$$\int a^2(1) (-V_{1a}) dv_1 = -2\alpha / (1 + \beta/2\alpha)^2 \quad (8)$$

$$\int a^2(1) (-V_{1b}) dv_1 = \alpha J_s \quad (9)$$

$$\int a(1) b(1) (-V_{1b}) dv_1 = \alpha K_s \quad (10)$$

$$\int a^2(1) b^2(2) V_{12} dv_1 dv_2 = \alpha J_s' \quad (11)$$

$$\int a(1)b(1)a(2)b(2)V_{12}dv_1dv_2 = \alpha K_s' \quad (12)$$

Other integrals encountered in the evaluation of Equation (4) can be reduced to those above by interchanging indices. Expressions for the first four relatively simple integrals are included above. Expressions for Equations (9), (10), and (11) are long and cumbersome and will be treated in another section. Equation (12) cannot be integrated in closed analytical form and requires numerical evaluation.

The first three of the above integrals do not depend explicitly on β in contrast to the remaining five. The last four are functions of α , β , and R , however, if the substitutions $g = \beta/2\alpha$ and $w = \alpha R$ are made, then J_s , K_s , J'_s and K'_s are functions of g and w only. In the process of minimizing the energy by varying α , the final value of α depends on β so that the first three integrals depend implicitly on β . The last five depend both explicitly and implicitly on β . The numerical evaluation of K'_s , to be treated in detail later, covered an array of 1025 values, with $0 \leq g \leq 2.4$ in steps of 0.1, and $0 \leq w \leq 8.0$ with steps of 0.2. A series of the form $G(g)e^{-2w}(1 + A_1w + A_2w^2 + A_3w^3 + A_4w^4)$ with $G(g) = (f^2/2 + f^3 + f^4)/2$, was fitted to this array by least square adjustment of the A 's for each g , good to four decimal places ($f = 1/(1 + g)$).

In terms of the above expressions, the energy becomes, with $f = (1 + \beta/2\alpha)^{-1}$,

$$E_1(\alpha) = (1 + S)^{-1}(\alpha^2(1 - S - K) + \alpha(-2f^2 + J_s + 2K_s)) \quad (13)$$

for the H_2^+ - type system, and

$$E_{12}(\alpha) = (1 + S^2)^{-1} (2\alpha^2(1 - KS - S^2) + \alpha(-4f^2 + 2J_s + 4SK_s + J_s' + K_s')) \quad (14)$$

for the two electron H_2 - type system.

These expressions must be minimized independently with respect to a variation of α for each value of β and R selected. This procedure for calculating molecular binding energies has been shown to give results within 2 or 3 percent of correct values over the mid-range of R and even better accuracy at large and small R .

This calculation leads to two binding energies of interest; first E_1 the energy of one electron bound to a pair of impurities at separation R and concentration c , second $E_2 = E_{12} - E_1$ the energy for binding a second electron to the same system.

Density of States for E_1 and E_2

Because of the variation of the binding energies, E_1 and E_2 , with impurity spacing, R , and with screening, β , the donor level (or acceptor level) cannot be considered as a constant, independent of impurity concentration. The resulting band of levels can be described by two distributions, one for E_1 and one for E_2 , which can be calculated from E_1 and E_2 (as functions of R and c), and $P(R, c)$, where c here is the total concentration, i.e., $c = C_1 + C_2$.

The value of $P(R, c')$ is given by

$$P(R, c')dR = (4\pi c')R^2 dR \exp(-4\pi c'R^3/3) \quad (15)$$

where R is in effective Bohr radii and c' is concentration in corresponding units. If c is the concentration in $(\text{cm})^{-3}$, then, the frequency of pairs with separation between R and $R + dR$ per cm^3 is

$$N(R)dR = (c/2)P(R, c')dR = (c/2)P_R \quad (16)$$

From the values of E_1 (say) at R and at $R + dR$ (where dR is small but finite) the corresponding values of E_1 and $E_1 + dE_1$ are determined. Consequently, the frequency in Equation (16) is identified with the frequency falling between E_1 and $E_1 + dE_1$, thus

$$S_1(E_1) = (c/2)P(R, c')dR/dE_1 \quad (17)$$

All of the quantities on the right side are known at least in numerical form so that a plot of $S_1(E_1)$ and similarly $S_2(E_2)$ can be produced with an appropriate computer program. Care must be exercised in implementing this program because of the behavior of dE_1 and dE_2 which may occasionally become zero.

The calculation produces two overlapping band-like distributions of donor levels (or acceptor levels) which, upon increasing concentration, broaden and form a "tail" which extends deep into the band gap. There is an accompanying decrease in the energy separation between the conduction band and the peak of the impurity band distribution.

Recalculation of Fermi-level and Screening Factor

The starting values for the screening parameter, β , and the Fermi-level, $E_F = kT\eta_F$ are obtained from the charge-balance equation

$$n = N^+ + p \quad (\text{donor case}) \quad (18)$$

and the relation

$$\beta^2 = (q^2/\epsilon kT) dn/d\eta_F \quad (19)$$

based on the Thomas-Fermi approximation. The conduction electron concentration, n , has the form

$$n = 2\pi^{-1/2} N_c F_{1/2}(\eta_F) \quad (20)$$

with N_c the effective density of states in the conduction band and $F_{1/2}(\eta_F)$ the Fermi integral

$$F_{1/2}(\eta_F) = \int_0^\infty \eta^{1/2} (1 + \exp(\eta - \eta_F))^{-1} d\eta \quad (21)$$

Equation (20) can be put in the form

$$n = N_c \exp(\eta_F) S_F \quad (22)$$

where S_F has the form

$$S_F = (\pi^{1/2}/2) \int_0^\infty \eta^{1/2} d\eta / (\exp \eta_F + \exp \eta). \quad (23)$$

The factor S_F has the effect of correcting the Boltzman statistics, which applies in the expression $n = N_c \exp(\eta_F)$ for the non-degenerate case, to Fermi statistics for the general case. A similar expression can be developed for p . In the initial calculation the expression for N^+ is

$$\begin{aligned} N^+ &= N_D (1 - F(E)) \\ N^+ &= N_D (1 + g \exp((E_F - E_D)/kT))^{-1} \end{aligned} \quad (24)$$

where $N_D = c$ is the number of donor impurities and E_D is the donor energy level, assumed to be constant. The spin degeneracy, g , is 2 for this case. Equation 24 is valid for low concentrations where the impurities are isolated from one another and the donor (acceptor) energy level is unperturbed.

At the medium and high impurity concentrations, the ground state energies, $E_1(R)$ and $E_2(R)$, as calculated above, show substantial variation from E_D (as much as $4E_D$) and vary from site to site. Consequently, the expression for N^+ takes the form of a sum over contributions with different energies. Since the energies are known as functions of R as well as the frequencies of occurrence, $N(R)$, it is convenient to form the sum over incremental values of R such that

$$N_R = N(R)dR, \quad (25)$$

where dR is small but finite, is the number of impurity pairs with separation between R and $R + dR$. Among these N_R pairs are n_2 neutral, n_1 singly ionized (charge = +1), and n_0 doubly ionized (charge = +2) for the donor case. From statistical mechanics the Fermi statistics relations are

$$n_0/n_1 = g_1 \exp((E_1 - E_F)/kT) = p_1(R) \quad (26)$$

$$n_1/n_2 = g_2 \exp((E_2 - E_F)/kT) = p_2(R) \quad (27)$$

$$N_R = n_0 + n_1 + n_2 \quad (28)$$

which, along with the charge relation

$$N_R^+ = 0 \cdot n_2 + 1 \cdot n_1 + 2 \cdot n_0 \quad (29)$$

and Equation (16), lead to

$$N^+ = c \sum_R P_R (1/2 + p_1)/(1 + p_1 + 1/p_2) \quad (30)$$

The factors g_1 and g_2 are spin degenerate values and are 1/2, and 2 respectively for the present case. Equation (30) is evaluated numerically from $N_R = N(R)dR$, calculated earlier, and tabular values of $E_1(R)$ and $E_2(R)$, also from the previous calculation.

This new value for N^+ is inserted in Equation (18) along with the expression for n from Equation (22), leading to a value for $\exp(E_F/kT)$ by means of successive approximations of Equation (18) by an iterative procedure.

The new values of E_F and n are then used to obtain, from Equation (19), a new value for the screening parameter, β . At this point, if β changes noticeably from the previous value, the values of $E_1(R)$ and $E_2(R)$ must be redone and this overall procedure iterated until a self-consistent set of quantities results, i.e., E_F , n , β , $E_1(R)$, $E_2(R)$. This must be done, of course, for each selected value of concentration and temperature.

Distributions of donor (acceptor) levels that are occupied by localized electrons (holes) are calculated after the above conditions are met. These come from procedures similar to those used for $S_1(E_1)$ and $S_2(E_2)$, Equation (17), except that the quantities p_1 and p_2 (Equations 26-27) are incorporated in the numerical calculation.

In compensated materials, the expression, P_R , appearing in Equation 30, above, is multiplied by the factors, P_E in the case of donor-donor pairs, and P_D in the case of donor-acceptor pairs, where $P_E = (1-q)^2$, $P_D = 2a(1-q)$, and $q = C_2/(C_1+C_2)$. This serves to adjust the total impurity concentration, $c = C_T = C_1 + C_2$, to the appropriate value for the type of impurity pair under consideration.

Donor-Acceptor Pair Energy Calculation

In this procedure, two systems are considered, first a donor-acceptor impurity pair with a single localized carrier, either an electron or a hole, and second the pair with both localized carriers present. The first system has a groundstate energy called D_1 and the second D_{12} . From these the quantity $D_2 = D_{12} - D_1$ is obtained representing the energy needed to remove one of the two from the system. In the first case it is convenient to fix attention on an electron bound to a donor impurity with an acceptor ion located at a distance R . As before, donor ion to electron distance is r_{1a} and the acceptor ion to electron is r_{1b} . In this case the center of the isotropic electron cloud (origin of the wave function) is assumed to be offset from the donor ion by a small distance L along the direction of the line of centers of the donor-acceptor pair, opposite from the acceptor ion being positive. This step serves to allow for polarization of the neutral donor impurity by the acceptor ion, thus improving the approximation to the system energy, but complicating the computation by introducing a second variation parameter. The energy is minimized with respect to both the offset, L , and the inverse Bohr radius, α , thus adjusting both the polarization and the size of the electron cloud. The distance from the offset origin to the electron is r_1 , so that, in the Hamiltonian, (Equation 3 with terms omitted having subscript 2) the first (kinetic energy) term involves differentiation with respect to r_1 , the second, $-V_{1a}$, remains the same and the third, $+V_{1b}$, has the sign reversed since the acceptor ion is negative. With $V_{1a} = 2 \exp(-\beta r_{1a}) / r_{1a}$, etc.,

$$H = \nabla_1^2 - V_{1a} + V_{1b} \quad (31)$$

The wave function assumed for this case is the (1s) basis function centered at the offset origin,

$$\psi = (\alpha^3/\pi)^{1/2} \exp(-\alpha r_1) \quad (32)$$

The resulting expression for the energy before it is minimized can be stated in terms of the integrals (Equations 5-12) developed earlier, except that they become functions of L and (L+R) rather than R as in the earlier case.

$$E_1 = \alpha^2 + \alpha J_S(L) - \alpha J_S(L+R) \quad (33)$$

In case both the electron and the hole are present, procedures similar to those above are used. The wave functions of both particles are assumed to have their origins offset by equal magnitudes and in opposite directions along the line of centers of the impurity ions. The modified Hamiltonian for this system is

$$H = -\nabla_1^2 - \nabla_2^2 - V_{1a} + V_{1b} + V_{2a} - V_{2b} - V_{12} \quad (34)$$

and the assumed wave function consists of a product of the $1s(r_1)$ and the $1s(r_2)$ basis functions centered at the offset origins near the donor ion and the acceptor ion, respectively,

$$\psi = (\alpha^3/\pi) \exp(-\alpha r_1) \exp(-\alpha r_2) \quad (35)$$

Again, the expression for the energy before minimizing can be written in terms of the integrals (Equations 5-12) as functions of L, (L+R), and (2L+R),

$$E_{12} = 2\alpha^2 + \alpha(2J_s(L) - 2J_s(L+R) - J_s'(2L+R)) \quad . \quad (36)$$

The minimized values of the expressions in Equations 33 and 36 are the energies of interest, D_1 and D_{12} , from which $D_2 = D_{12} - D_1$ is also found. In Appendix A, these energies, as well as those for donor-donor pairs, are plotted as a function of R for an array of temperatures and concentrations.

APPENDIX C

Interaction Integrals

APPENDIX C

$$\int a(1)(-\nabla_1^2)a(1)dV_1 = \alpha^2 \quad (C.1)$$

$$\int a(1)b(1)dV_1 = S = e^{-w}(1 + w + w^2/3) \quad (C.2)$$

$$\int a(1)(-\nabla_1^2)b(1)dV_1 = -\alpha^2(K+S) = \alpha^2 e^{-w}(1+w-w^2/3) \quad (C.3)$$

$$\int a^2(1)(-V_{1a})dV_1 = -2\alpha(1 + \beta/2\alpha)^{-2} = -2\alpha f^2 \quad (C.4)$$

where $f = (1 + g)^{-1}$, $g = \beta/2\alpha$

$$\int a^2(1)(-V_{1b})dV_1 = \alpha J_s \text{ where}$$

$$\alpha J_s = 2\alpha\gamma(e^{-2w} - \gamma(e^{-\beta R} - e^{-2w})/w) \quad (C.5)$$

and $\gamma = (1 - g^2)^{-2}$

Let $Y = (2\alpha - \beta)/R$

$$Y_1 = (1 - e^{-Y})/Y$$

$$Y_2 = (1 - Y - e^{-Y})/Y^2$$

$$Y_3 = (1 - Y + .5Y^2 - e^{-Y})/Y^3$$

$$Y_4 = (1 - Y + .5Y^2 - Y^3/6 - e^{-Y})/Y^4$$

Then

$$Y_3 = Y \cdot Y_4 + 1/6$$

$$Y_2 = Y \cdot Y_3 - 1/2$$

$$Y_1 = Y \cdot Y_2 + 1$$

By using the above definitions, the expression reduces to

$$\alpha J_s = -2\alpha f e^{-\beta R}(2w(2fY_2 + Y_1) + f)$$

$$\int a(1)b(1)(-v_{1b})dv_1 = \alpha K_s \text{ where}$$

$$\alpha K_s = -2\alpha f^2 e^{-w} (1+2w(e^{-\beta R} - (1-\beta R))/\beta^2 R^2) \quad (C.6)$$

$$\text{Let } B_2 = (1 - \beta R - e^{-\beta R})/\beta^2 R^2$$

$$\text{Then } \alpha K_s = -2\alpha f^2 e^{-w} (1 - 2wB_2)$$

$$\int a^2(1)b^2(2)v_{12}dv_1dv_2 = \alpha J_s' \text{ where}$$

$$\begin{aligned} \alpha J_s' &= -\alpha w^3 \gamma(e^{-2w}(2w^2+2w+1)/4w^3 - e^{-2w}/6w + e^{-2w}\gamma(2w+1)/2w^3 \\ &\quad - \gamma((\alpha+.5\beta)R+1)e^{-(\alpha+.5\beta)R}/wR^2(\alpha+.5\beta)^2 \\ &\quad \times (e^{(\alpha-.5\beta)R} - e^{-(\alpha-.5\beta)R})/(\alpha-.5\beta)R \\ &\quad - 2fe^{-(\alpha+.5\beta)R}/wR(\alpha+.5\beta) [(e^{(\alpha-.5\beta)R} - e^{-(\alpha-.5\beta)R}) \\ &\quad /2(\alpha-.5\beta)^2 R^2 - (e^{(\alpha-.5\beta)R} + e^{-(\alpha-.5\beta)R})/2(\alpha-.5\beta)R]) \\ &= \alpha f^2 e^{-\beta R} (-w^2(4f-1)/3 - w(2f^2-1)/2 + (2f^2+2f+1)/4) \\ &\quad + \alpha f w e^{-\beta R} (.5+w+2w^2/3)Y_1 + 2fw(1+2w)Y_2 \\ &\quad + 8f^2 w((h+2w)Y_3 + 2wY_4)) \end{aligned} \quad (C.7)$$

$$\int a(1)b(1)a(2)b(2)v_{12}dv_1dv_2 = \alpha K_s' \quad (C.8)$$

This integral does not have a closed analytic expression. The procedure for numerically evaluating this integral is given in appendix C

Reference (30)

Integrals needed for energy calculation, Heitler-London method for H_2 . The atomic orbitals $a(1)$ and $b(1)$ refer to the normalized functions $\sqrt{a^3/\pi} e^{-a^3/r}$, $\sqrt{a^3/\pi} e^{-a^3/r}$, centered on the atoms a and b . The quantity a is a variation parameter. Energies are expressed in Rydbergs, distances in atomic units. The quantity $w = aR$, where R is the internuclear distance.

$$\begin{aligned} \int a(1)(-\nabla_1^2)a(1) dv_1 &= a^3 \\ \int a^2(1)(-2/r_{1a}) dv_1 &= -2a \end{aligned}$$

$$\int a(1)b(1) dv_1 = S = e^{-w} \left(1 + w + \frac{w^2}{3} \right) = 1 - \frac{1}{6}w^3 + \frac{1}{24}w^4 - \dots$$

$$\int a^2(1)(-2/r_{1a}) dv_1 = aJ = a \left[-\frac{2}{w} + e^{-w} \left(2 + \frac{2}{w} \right) \right]$$

$$= a(-2 + \frac{1}{3}w^3 - \frac{1}{6}w^4 + \frac{1}{24}w^5 - \dots)$$

$$\int a(1)b(1)(-2/r_{1a}) dv_1 = aK = -ae^{-w}(2 + 2w)$$

$$= a(-2 + w^3 - \frac{1}{6}w^4 + \frac{1}{24}w^5 - \dots)$$

$$\begin{aligned} \int a(1)(-\nabla_1^2)b(1) dv_1 &= -a^3(K + S) = a^3(1 + w - \frac{1}{6}w^3) \\ &= a^3(1 - \frac{1}{6}w^3 + \frac{1}{24}w^4 - \frac{1}{24}w^5 + \dots) \end{aligned}$$

$$\begin{aligned} \int a^2(1)b^2(2)(2/r_{1a}) dv_1 dv_2 &= [aa|bb] = aJ' \\ &= a \left[\frac{2}{w} - e^{-2w} \left(\frac{2}{w} + \frac{1}{4} + \frac{1}{2}w + \frac{1}{24}w^3 \right) \right] \\ &= a(\frac{1}{2} - \frac{1}{6}w^3 + \frac{1}{24}w^4 - \dots) \end{aligned}$$

$$\begin{aligned} \int a(1)b(1)a(2)b(2)(2/r_{1a}) dv_1 dv_2 &= [ab|ab] = aK' \\ &= \frac{2}{3}a \left\{ -e^{-2w}(-\frac{2}{3} + \frac{1}{2}w + 3w^3 + \frac{1}{24}w^4) \right. \\ &\quad \left. + \frac{6}{w} [S'(C + \ln w) + S'^2 E_1(-4w) - 2SS'E_1(-2w)] \right\} \\ &= a(\frac{1}{3} - \frac{1}{6}w^3 + (\frac{2}{3}C + \frac{1}{24} \ln 4)w^4 - \dots) \end{aligned}$$

where $S' = e^{-w}(1 + w + \frac{1}{6}w^3) = 1 - \frac{1}{6}w^3 + \frac{1}{24}w^4 - \dots$

C = Euler's constant

$$\int_0^1 \frac{1-e^{-t}}{t} dt = \int_1^\infty \frac{e^{-t}}{t} dt = 0.57722$$

$E_1(x)$ = integral logarithm

$$E_1(-x) = - \int_x^\infty \frac{e^{-t}}{t} dt$$

where $x > 0$.

This function is tabulated in Jahneke-Emde, "Tables of Functions," Dover Publications, New York, 1933.

Procedure for evaluating K'_s

$$\alpha K'_s = \int l s(\alpha_1, \vec{r}_{1a}) l s(\alpha_2, \vec{r}_{1b}) (\exp(-\beta r_{12}) / r_{12}) l s(\alpha_3, \vec{r}_{2a}) l s(\alpha_4, \vec{r}_{2b}) \\ \times dv_1 dv_2$$

$$l s(\alpha, \vec{r}) = (\alpha^3 / \pi)^{1/2} \exp(-\alpha r)$$

Expand all functions in spherical harmonics about center a using

$$(\alpha r_b)^{n-1} \exp(-\alpha r_b) = \sum_{\ell=0}^{\infty} (2\ell+1) \zeta_{\ell n}(\alpha r_a, \alpha R) P_{\ell}(\cos \theta_a)$$

$$\alpha K'_s = \beta ((\alpha_1 \alpha_2 \alpha_3 \alpha_4)^{3/2} / \pi^2) \int \exp(-\alpha_1 r_{1a}) \exp(-\alpha_2 r_{1b}) \times$$

$$\sum_{\ell=0}^{\infty} (2\ell+1) \zeta_{\ell 0}(\beta r_{1a}, \beta r_{2a}) P_{\ell}(\cos \theta_{1a}) \exp(-\alpha_3 r_{2a}) \times$$

$$\sum_{\ell_2=0}^{\infty} (2\ell_2+1) \zeta_{\ell_2 1}(\alpha_4 r_{2a}, \alpha_4 R) P_{\ell_2}(\cos \theta_{2a}) d\omega_2 r_2^2 dr_2 dv_1 =$$

$$4\beta ((\alpha_1 \alpha_2 \alpha_3 \alpha_4)^{3/2} / \pi^2) \sum_{\ell=0}^{\infty} (2\ell+1) \int \exp(-\alpha_1 r_{1a}) \exp(-\alpha_2 r_{1b}) \times$$

$$\zeta_{\ell 0}(\beta r_{1a}, \beta r_{2a}) \exp(-\alpha_3 r_{2a}) \zeta_{\ell 1}(\alpha_4 r_{2a}, \alpha_4 R) \times$$

$$P_{\ell}(\cos \theta_{1a}) r_2^2 dr_2 dv_1$$

$$\begin{aligned}
&= 4\beta((\alpha_1\alpha_2\alpha_3\alpha_4)^{3/2}/\pi) \sum_{\ell=0}^{\infty} (2\ell+1) \int \exp(-\alpha_1 r_{1a}) \times \\
&\quad \sum_{\ell_1=0}^{\infty} (2\ell_1+1) \zeta_{\ell_1 1}(\alpha_2 r_{1a}, \alpha_2 R) P_{\ell_1}(\cos\theta_{1a}) \zeta_{\ell 0}(\beta r_{1a}, \beta r_{2a}) \times \\
&\quad \exp(-\alpha_3 r_{2a}) \zeta_{\ell 1}(\alpha_4 r_{2a}, \alpha_4 R) P_{\ell}(\cos\theta_{1a}) r_2^2 dr_2 d\omega_1 r_1^2 dr_1 = \\
&16\beta(\alpha_1\alpha_2\alpha_3\alpha_4)^{3/2} \sum_{\ell=0}^{\infty} (2\ell+1) \int \exp(-\alpha_1 r_{1a}) \zeta_{\ell 1}(\alpha_2 r_{1a}, \alpha_2 R) \times \\
&\quad \zeta_{\ell 0}(\beta r_{1a}, \beta r_{2a}) \exp(-\alpha_3 r_{2a}) \zeta_{\ell 1}(\alpha_4 r_{2a}, \alpha_4 R) r_2^2 dr_2 r_1^2 dr_1
\end{aligned}$$

$$\zeta_{\ell 0}(t_1, t_2) = i_{\ell}(t_{<}) k_{\ell}(t_{>})$$

$$\zeta_{\ell 1}(t_1, t_2) = t_{>} i_{\ell}(t_{<}) k_{\ell-1}(t_{<}) - t_{<} i_{\ell+1}(t_{<}) k_{\ell}(t_{>})$$

where $i_{\ell}(x)$ and $k_{\ell}(x)$ are spherical modified Bessel functions for which the simplest are

$$i_0(x) = \sinh x/x; \quad i_{-1}(x) = \cosh x/x$$

$$k_0(x) = k_{-1}(x) = e^{-x}/x$$

and the recursion relations are

$$i_{\ell-1}(x) = i_{\ell+1}(x) + ((2\ell+1)/x) i_{\ell}(x)$$

$$k_{\ell+1}(x) = k_{\ell-1}(x) + ((2\ell+1)/x) k_{\ell}(x)$$

The subroutines SSIBFN and SSKBFN compute the scaled spherical Bessel Functions

$$i_{\ell}^s(x) = ((2\ell+1)!!/x^{\ell}) \exp(-x) i_{\ell}(x)$$

$$k_{\ell}^s(x) = (x^{\ell+1}/(2\ell-1)!!) \exp(x) k_{\ell}(x)$$

where $(2\ell+1)!! = 1 \cdot 3 \cdot \dots \cdot (2\ell+1)$ is the "odd number factorial".

In terms of these scaled functions

$$(2\ell+1)\beta \zeta_{\ell 0}(\beta r_{1a}, \beta r_{2a}) = (r_{<}/r_{>})^{\ell+1} i_{\ell}^s(\beta r_{<}) k_{\ell}^s(\beta r_{>}) \times \\ \exp(-\beta(r_{>} - r_{<}))$$

$$\zeta_{\ell 1}(\alpha_4 r_{2a}, \alpha_4 R) = \alpha_4 \exp(-\alpha_4(r_{>} - r_{<})) \times$$

$$[(1/(2\ell-1)(2\ell+1))(r_{<}/r_{>})^{\ell+1} i_{\ell}^s(\alpha_4 r_{<}) k_{\ell-1}^s(\alpha_4 r_{>})]$$

$$-[(1/(2\ell+1)(2\ell+2))(r_{<}/r_{>})^{\ell+2} i_{\ell+1}^s(\alpha_4 r_{<}) k_{\ell}^s(\alpha_4 r_{>})]$$

In order to avoid negative indices, use is made of $k_0 = k_{-1}$ so

that for the $\ell = 0$ case

$$\zeta_{01}(\alpha_4 r_{2a}, \alpha_4 R) = (i_0^s(\alpha_4 r_{<}) \alpha_4 r_{>} - i_1^s(\alpha_4 r_{<}) \alpha_4 r_{<}^2/3r_{>}) \times$$

$$k_0^s(\alpha_4 r_{>}) \exp(-\alpha_4(r_{>} - r_{<}))$$

APPENDIX D

Computer Programs

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100   T=300\TI=.01*T-1\ REM .....CALCULATE EL2 DATA
101   FOR C1I=0 TO 4\ FOR CI=4 TO 8\ GOSUB 102\ NEXT CI\ NEXT C1I\ RETURN
102   DIM LC1(4),LC(8),PF(3)\ GOSUB 120\ GOSUB 252\ GOSUB 254
110   GOSUB 200
112   GOSUB 300\BL=B\ GOSUB 260
114   IF ABS((BL-B)/B)>.005 THEN 112
116   GOSUB 130\ GOSUB 400\ GOSUB 140\ RETURN
120   PRINT ' T; LC1; LC; LC2; C1I; CI;';
121   PRINT C1I,CI
122   FOR I=0 TO 4\LC1(I)=15.5+.5*I\ NEXT I
123   FOR I=0 TO 3\LC(I)=LC1(C1I)-.5*I\ NEXT I\LC(4)=10
124   FOR I=5 TO 7\LC(I)=LC1(C1I)-4+.5*I\ NEXT I
125   LC(8)=LC1(C1I)*.9999999
126   LC1=LC1(C1I)\LC=LC(CI)\C=10^LC\C1=10^LC1
127   C2=C1-C\LC2=LOG10(1+C2)\CT=C1+C2\R=C1/CT\PF(0)=R*R
128   PF(1),PF(3)=2*R*(1-R)\PF(2)=(1-R)*(1-R)\ RETURN
130   DIM #2,XFNPB(4,4,4,8)\ OPEN 'XFNPB' AS FILE #2, VIRTUAL
131   XFNPB(0,TI,C1I,CI)=XF\XFNPB(1,TI,C1I,CI)=EF
132   XFNPB(2,TI,C1I,CI)=LN\XFNPB(3,TI,C1I,CI)=LP
133   XFNPB(4,TI,C1I,CI)=B\ CLOSE \ RETURN
140   DIM #3,EV%(3,4,4,8,33)
141   OPEN 'EV' AS FILE #3, VIRTUAL \K=8000\ FOR Q=0 TO 3
142   FOR I=0 TO 32\EV%(Q,TI,C1I,CI,I)=K*EL(Q,I)
143   NEXT I\ NEXT Q\ CLOSE \ RETURN
198   OPEN 'LP:' AS FILE #1\ PRINT #1,DATE$(0%),TIME$(0)
199   CLOSE \ RETURN

```

```

200 REM ...CALC. PRELIM. EF, LN, LP & B. (Host = GaAs)
202 DIM E(2)\ GOSUB 232\ IF FF<>51 THEN GOSUB 246
204 KT=.08617*T/ED\XK=2*EXP(1/KT)\N0=4.8293*10^15\B0=.0209983*N0
206 NC=N0*MC*(ME*T)^1.5\NV=N0*MV*(MH*T)^1.5\ IF LC>9 THEN 212
208 EF=.5*(EG+KT*LOG(NV/NC))\XF=EXP(EF/KT)\LN=LOG10(NC)+LOG10(XF)
210 B=10^-6\LP=LOG10(NV)+.4343*(EG-EF)/KT\ GOSUB 250\ RETURN
212 CC=C/NC\ IF CC<.0001 THEN XF=CC/(1-CC/4)\ GOTO 216
214 TM=.5*(1-CC/4)/SQR(CC*XK)\XF=SQR(CC/XK)*(SQR(TM*TM+1)-TM)
216 FOR M=0 TO 2\ GOSUB 224\E(M)=XF\ NEXT M\ GOSUB 244
218 GOSUB 240\LN=LOG10(NC)+LOG10(XF)+LOG10(S1)\ GOSUB 242
220 B=SQR(B0*MC*ME^1.5*SQR(T)*S2/KE)*RB\EF=KT*LOG(XF)
222 LP=LOG10(NV)+.4343*(EG-EF)/KT\ GOSUB 250\ RETURN
224 GOSUB 240\Y=EG/KT\ GOSUB 288
226 KP=(MV/MC)*(MH/ME)^1.5*EXP(Y)/(XF*S1)
228 XF=CC/S1/(1+XK*XF)+KP\ RETURN
230 ED=44\RB=20*10^-8\EG=-(1160-.702*T^2/(T+1108))/ED
232 MC=6\MV=1\KE=11.8\ME=.327\MH=.559\ RETURN
234 ED=30\EA=28\RB=40*10^-8\EG=-(1522-.58*T^2/(T+300))/ED
236 MC=1\MV=1\KE=13.1\ME=.067\MH=.473\ RETURN
238 ED=12\RB=37*10^-8\EG=-(741-.456*T^2/(T+210))/ED
240 MC=5\MV=1\KE=16\ME=.221\MH=.31\ RETURN
242 S1=0\ FOR J=0 TO FF\S1=S1+NX(J)/(XF+EX(J))\ NEXT J\ RETURN
244 S2=0\ FOR J=0 TO FF\D=XF+EX(J)\S2=S2+NX(J)*EX(J)/(D*D)
246 NEXT J\S2=XF*S2\ RETURN
248 TM=2*E(1)-E(0)-E(2)\ IF TM=0 THEN XF=E(2)\ RETURN
250 XF=E(2)+ABS(E(1)-E(2))^2/TM\ RETURN
252 FF,I=51\D=.02\ DIM EX(I),NX(I)\A=2*D/3/SQR(PI)\ FOR K=1 TO 26
254 I=2*K-2\X=K*K*D\EX(I)=EXP(X)\NX(I)=SQR(X)*4*K*A\X=K*(K+1)*D
256 EX(I+1)=EXP(X)\NX(I+1)=SQR(X)*(2*K+1)*A\ NEXT K\ RETURN
258 OPEN 'LP:' AS FILE #1\ PRINT #1,LC1;LC;B,EF,LN,LP\ CLOSE
260 PRINT LC1;LC,B,EF,LN,LP\ RETURN
262 OPEN 'LP:' AS FILE #1\ PRINT #1,'Temp';'LogC1';'LogC';'LogC2'
264 PRINT #1,T;LC1;LC;LC2\ CLOSE #1\ PRINT T;LC1;LC;LC2\ RETURN
266 OPEN 'LP:' AS FILE #1\ PRINT #1,'LC1 '; 'LC','B','EF','LN','LP'
268 CLOSE #1\ PRINT 'LC1 '; 'LC','B','EF','LN','LP'\ RETURN
270 REM ____RECALCULATE EF, LN, LP & B, USING EL(Q,I)
272 CB=C*RB^3\CR=CB*4*PI/3\ IF SF<>51 THEN GOSUB 246
274 E(0)=XF\ FOR M=1 TO 2\S=0\AC=1\ GOSUB 274\ GOSUB 224
276 GOSUB 290\E(M)=XF\ NEXT M\ GOSUB 244\ GOSUB 218\ RETURN
278 FOR I=1 TO 32\R=.25*I\ GOSUB 282\ NEXT I\I=33
280 A=AC\EL(0,33),EL(1,33)=.5*(EL(0,32)+EL(1,32))\ GOTO 284
282 AL=AC\Y=-CR*R^3\ GOSUB 288\AC=EXP(Y)\A=AL-AC
284 Y=EL(0,I)/KT\ GOSUB 288\Y1=.5*EXP(Y)/XF
286 Y=EL(1,I)/KT\ GOSUB 288\Y2=.5*EXP(-Y)*XF
288 S=S+A*(.5+Y1)/(1+Y1+Y2)\ RETURN
290 IF Y<-40 THEN Y=-40\ RETURN ELSE RETURN
292 XF=CC*S/S1+KP\ RETURN

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300 REM ____ENERGY EL(Q) VS R (SCRN. POT., VAR.) 1/86
302 IF KF<>1 THEN GOSUB 364
304 FOR Q=0 TO 1\A=(2-Q*5/16)*(1-B^2/8)\AC=A+.06
306 FOR I=0 TO 32\R=.25*I\ GOSUB 330
308 AT=A\ FOR M=0 TO 2\A=AT+.08*(M-1)\ GOSUB 336\E(M)=E\ NEXT M
310 GOSUB 318\ IF ABS(A-AT)>.02 THEN 308 ELSE GOSUB 336\AL=AC\AC=A
312 IF Q=0 THEN EL(0,I)=E\ IF EL(0,I)>0 THEN EL(0,I)=0
314 IF Q=1 THEN EL(1,I)=E-EL(0,I)\ IF EL(1,I)>0 THEN EL(1,I)=0
316 A=2*AC-AL\ GOSUB 322\ NEXT I\ NEXT Q\ RETURN
318 DX=E(0)-2*E(1)+E(2)\ IF DX<.01 THEN DX=.01
320 A=AT+.04*(E(0)-E(2))/DX
322 IF A<.01 THEN A=.01\ RETURN ELSE RETURN
324 E=(Q+1)*(AA-4*AA*HH)+Q*.5*AA*HH*(.5+H+HH)\ RETURN
326 E=(AA*(1+SK)+A*(2*K-2*HH+J))/(1+S)\ RETURN
328 E=(2*AA*(1+S*SK)+A*(2*J-4*HH+JP+4*S*K+KP))/(1+S*S)\ RETURN
330 U=B*R\BE=EXP(-U)\ IF U>.2 THEN B2=(1-BE-U)/(U*U)\ RETURN
332 B2=-(360-U*(120-U*(30-U*(6-U))))/720\ RETURN
336 AA=AA\H=A/(A+.5*B)\HH=H*H\W=A*R\WW=W*W\ IF R=0 GOTO 324
338 W3=WW/3\AX=EXP(-W)\Y=2*W-U\YY=Y*Y
340 S=AX*(1+W+W3)\SK=S-2*AX*W3\ IF YY>.25 THEN 344
342 Y4=-(1680-336*Y+56*YY-8*Y*YY+YY*YY)/40320\ GOTO 346
344 Y4=(1-EXP(-Y)-Y+.5*YY-Y*YY/6)/YY/YY
346 Y3=Y*Y4+1/6\Y2=Y*Y3-.5\Y1=Y*Y2+1\K=-2*HH*AX*(1-2*W*B2)
348 J=-2*H*BE*(2*W*(2*H*Y2+Y1)+H)\ IF Q=0 GOTO 326
350 TM=(.5+W+2*W3)*Y1+2*H*(W+6*W3)*Y2+8*HH*W*(H+2*W)*Y3+2*W*Y4)
352 JP=BE*(W*H*TM+HH*(.5*(HH+H+.5)-W*(HH-.5)-W3*(4*H-1)))
354 G=ABS(5*B/A)\X=INT(G)\D=G-X\ GOSUB 360\SM=TM*(1-D)\X=X+1
356 GOSUB 360\SM=SM+TM*D\KP=.5*HH*(.5+H+HH)*AX*AX*(1+W*SM)\ GOTO 328
360 P=X\ IF P>24 THEN P=24
362 TM=C1(P)+W*(C2(P)+W*(C3(P)-W*C4(P)))\ RETURN
364 DIM EL(3,33),LE(2),A(2)
365 DIM C1(24),C2(24),C3(24),C4(24)\ RESTORE 367
366 FOR P=0 TO 24\ READ C1(P),C2(P),C3(P),C4(P)\ NEXT P\KF=1\ RETURN
367 DATA 2.00243,1.58709,.55446,-.01856,2.00196,1.56891,.51171,.00428
368 DATA 2.00011,1.55993,.46202,.01720,1.99791,1.55498,.41181,.02403
369 DATA 1.99577,1.55152,.36420,.02712,1.99391,1.54822,.32063,.02795
370 DATA 1.99240,1.54452,.28158,.02743,1.99124,1.54018,.24706,.02616
371 DATA 1.99038,1.53523,.21676,.02449,1.98978,1.52975,.19029,.02265
372 DATA 1.98939,1.52385,.16723,.02078,1.98915,1.51768,.14716,.01895
373 DATA 1.98904,1.51133,.12970,.01721,1.98900,1.50492,.11449,.01559
374 DATA 1.98902,1.49854,.10123,.01410,1.98906,1.49224,.08964,.01273
375 DATA 1.98912,1.48609,.07949,.01149,1.98917,1.48013,.07057,.01036
376 DATA 1.98921,1.47438,.06273,.00933,1.98923,1.46887,.05580,.00840
377 DATA 1.98924,1.46361,.04966,.00755,1.98922,1.45859,.04422,.00679
378 DATA 1.98918,1.45383,.03936,.00609,1.98912,1.44931,.03502,.00546
379 DATA 1.98905,1.44504,.03114,.00489

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400 REM ____ENERGY E1 & E2 VS R (COMPENSATED) 8/84
402 IF KF<>1 THEN GOSUB 364
404 DA=.04\DL=.04
406 FOR Q=2 TO 3\A=1-B^2/8\L=0\E=-1
408 FOR I=32 TO 0 STEP -1\ IF E>=0 THEN E,A,L=0\ GOTO 414
410 R=.25*I\ GOSUB 420
414 EL(Q,I)=E-(Q-2)*EL(Q-1,I)\ IF EL(Q,I)>0 THEN EL(Q,I)=0
416 NEXT I\ NEXT Q\ RETURN
420 LT=L\ FOR N=0 TO 2\L=LT+(N-1)*DL\ GOSUB 430\LE(N)=E\A(N)=A\ NEXT N
422 D=LE(0)-2*LE(1)+LE(2)\ IF D<.001 THEN D=.001
424 L=LT+.5*DL*(LE(0)-LE(2))/D
426 IF ABS(LT-L)>DL THEN 420
428 A=A(1)+.5*(L-LT)*(A(2)-A(0))/DL\ GOSUB 440\ RETURN
430 AT=A\ FOR M=0 TO 2\A=AT-(M-1)*DA\ GOSUB 440\E(M)=E\ NEXT M
432 D=E(0)-2*E(1)+E(2)\ IF D<.001 THEN D=.001
434 A=AT+.5*DA*(E(2)-E(0))/D\ IF A<DA+.001 THEN A=DA+.001
436 IF ABS(AT-A)>DA THEN 430 ELSE GOSUB 440\ RETURN
440 AA=AA\A\H=A/(A+.5*B)\HH=H*H\X=ABS(L)\ GOSUB 460\ GOSUB 466\J1=J
442 X=ABS(L+R)\ GOSUB 460\ GOSUB 466\J2=J\ IF Q=2 THEN 456
444 X=ABS(2*L+R)\ GOSUB 460\W3=W*W/3\ IF YY>.25 THEN 448
446 Y4=-(1680-Y*(336-Y*(56-Y*(8-Y))))/40320\Y3=Y*Y4+1/6\ GOTO 450
448 Y4=(1-EXP(-Y)-Y+.5*YY-Y*YY/6)/YY\Y3=Y*Y4+1/6
450 TM=(.5+W+2*W3)*Y1+2*H*(W+6*W3)*Y2+8*HH*W*((H+2*W)*Y3+2*W*Y4)
452 JP=BE*(W*H*TM+HH*(.5*(HH+H+.5)-W*(HH-.5)-W3*(4*H-1)))
454 E=2*AA+A*(2*J1-2*J2-JP)\ RETURN
456 E=AA+A*(J1-J2)\ RETURN
460 U=B*X\BE=EXP(-U)\W=A*X\Y=2*W-U\YY=Y*Y
462 IF YY>.25 THEN Y2=(1-EXP(-Y)-Y)/YY\Y1=Y*Y2+1\ RETURN
464 Y2=-(360-Y*(120-Y*(30-Y*(6-Y))))/720\Y1=Y*Y2+1\ RETURN
466 J=-2*H*BE*(2*W*(2*H*Y2+Y1)+H)\ RETURN
490 PRINT L,A,E(0),E(1),E(2),N\ RETURN
491 PRINT L,A,,E,,R\ RETURN
492 PRINT N,,LE(0),LE(1),LE(2)\ RETURN
493 PRINT L,A,,E,,R\ RETURN

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500 IF QX<>3 THEN GOSUB 560\ REM CALC. DS2 DATA
502 T=300\TI=.01*T-1\ FOR C1I=0 TO 4\ FOR CI=4 TO 8\ GOSUB 504
503 NEXT CI\ NEXT C1I\ RETURN
504 FOR I=0 TO 4\LC1(I)=15.5+.5*I\ NEXT I
505 FOR I=0 TO 3\LC(I)=LC1(C1I)-.5*I\ NEXT I\LC(4)=10
506 FOR I=5 TO 7\LC(I)=LC1(C1I)-4+.5*I\ NEXT I
507 LC(8)=LC1(C1I)*.9999999
508 LC1=LC1(C1I)\LC=LC(CI)\C=10^LC\C1=10^LC1
509 C2=C1-C\LC2=LOG10(1+C2)\CT=C1+C2\R=C1/CT\PF(0)=R*R
510 PF(1),PF(3)=2*R*(1-R)\PF(2)=(1-R)*(1-R)
520 GOSUB 530\ GOSUB 800\ GOSUB 700\ GOSUB 810\ GOSUB 710
521 GOSUB 660\ PRINTSCREEN \ GOSUB 600\ GOSUB 820\ GOSUB 720
522 GOSUB 830\ GOSUB 730\ GOSUB 605\ GOSUB 735
523 PRINTSCREEN \ GOSUB 610\ GOSUB 840\ GOSUB 740
524 GOSUB 790\ PRINTSCREEN \ GOSUB 597\ RETURN
530 OPEN 'XFNPB' FOR INPUT AS FILE #2, VIRTUAL
531 OPEN 'EV' FOR INPUT AS FILE #3, VIRTUAL
532 EF=XFNPB(1,TI,C1I,CI)\LN=XFNPB(2,TI,C1I,CI)
533 LP=XFNPB(3,TI,C1I,CI)\B=XFNPB(4,TI,C1I,CI)\K=.000125
534 XF=XFNPB(0,TI,C1I,CI)\ FOR Q=0 TO 3\ FOR I=0 TO 32
535 EL(Q,I)=K*EV*(Q,TI,C1I,CI,I)\ NEXT I\ NEXT Q\ CLOSE
536 ES=EL(1,32)\ IF ES<-1 THEN ES=-1
537 FOR Q=0 TO 3\EL(Q,33)=ES\ NEXT Q\EF(2),EF(3)=.8
538 EF(0),EF(1)=1\RF(0),RF(1)=1\RF(2),RF(3)=1.25\ GOTO 542
540 ED=44\RB=20*10^-8\EG=-(1160-.702*T^2/(T+1108))/ED
541 MC=6\MV=1\KE=11.8\ME=.327\MH=.559
542 ED=30\EA=28\RB=40*10^-8\EG=-(1522-.58*T^2/(T+300))/ED
543 MC=1\MV=1\KE=13.1\ME=.067\MH=.473
544 KT=.08617*T/ED
545 CB=CT*RB^3\CR=CB*4*PI/3\M=2/3\PM=(CR/M)^M*EXP(M)
546 FOR I=0 TO 32\R=.25*I\Y=-CR*R^3\ GOSUB 648
547 P=PM*R^2*EXP(Y)\P(I)=P\R(I)=R\RH(I)=RF(2)*R\ NEXT I
548 RM=(2/3/CR)^(1/3)\FG%=100*TI+10*C1I+CI+100
550 N0=4.8293*10^15\NC=N0*MC*(ME*T)^1.5\NV=N0*MV*(MH*T)^1.5
551 LNCO=LOG10(NC)-1.5*LOG10(KT)\LNVO=LOG10(NV)-1.5*LOG10(KT)
552 RETURN
560 DIM EL(3,33),P(32),PF(3),EF(3),RF(3),R(32),E(200),X(3)
561 DIM L$(3)\ DIM #2,XFNPB(4,4,4,8)\ DIM #3,EV$(3,4,4,8,33)
562 FOR I=0 TO 200\E(I)=.02*I\ NEXT I\QX=3\IX=200\RX=32\LX=13
563 DIM LC1(4),LC(8),Y(RX),S(IX),RH(RX),L(LX)
564 DIM #4,SF$(1,4,4,8,13)\ DIM #5,SD$(3,4,4,8,13)
565 DIM #6,SA$(3,4,4,8,13)\ RETURN
570 OPEN 'SF' AS FILE #4, VIRTUAL \K=1000\ FOR I=0 TO LX
571 SF$(Q,TI,C1I,CI,I)=K*L(I)\ NEXT I\ CLOSE \ RETURN
572 OPEN 'SD' AS FILE #5, VIRTUAL \K=1000\ FOR I=0 TO LX
573 SD$(Q,TI,C1I,CI,I)=K*L(I)\ NEXT I\ CLOSE \ RETURN
574 OPEN 'SA' AS FILE #6, VIRTUAL \K=1000\ FOR I=0 TO LX
575 SA$(Q,TI,C1I,CI,I)=K*L(I)\ NEXT I\ CLOSE \ RETURN
597 OPEN 'LP:' AS FILE #1\ PRINT #1,CHR$(12)\ CLOSE \ RETURN
598 OPEN 'LP:' AS FILE #1\ PRINT #1,DATE$(0%),TIME$(0%)
599 CLOSE \ RETURN

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600 DIM DS(QX,IX)\ REM ... DEN. OF (DD) ELECTRON STATES
601 SW=3\F=0\ FOR Q=0 TO 1\ GOSUB 620\ NEXT Q\ REM (--)
602 F=1\ FOR Q=2 TO 3\ GOSUB 620\ NEXT Q\ GOTO 616\ REM (++)
605 DIM DS(QX,IX)\ REM ... DEN. OF FILLED (DD) STATES
606 SW=1\F=0\ FOR Q=0 TO 1\ GOSUB 620\ NEXT Q\ GOTO 616
610 DIM DS(QX,IX)\ REM ... DEN. OF HOLE STATES
612 SW=3\F=2\ FOR Q=0 TO 1\ GOSUB 620\ NEXT Q\ REM (++)
614 F=3\ FOR Q=2 TO 3\ GOSUB 620\ NEXT Q\ REM (++)
616 GOSUB 652\ RETURN
620 A2=PF(F)*CT\AC=0\E2=-EF(F)*EL(Q,0)\EC=INT(50*E2)
622 FOR I=0 TO 33\ R=RF(F)*.25*(I+.5)\TM=CR*R*R*R\E1=E2
624 E2=-EF(F)*EL(Q,I)\DX=ABS(E2-E1)\ IF DX<.02 THEN DX=.02
626 A1=A2\ IF TM<25 AND I<33 THEN A2=CT*PF(F)*EXP(-TM) ELSE A2=0
628 AL=AC\AC=(A1-A2)/DX\ IF SW=3 THEN 636
630 Y=EF(F)*EL(0,I)/KT\ GOSUB 648\Y1=.5*EXP(Y)/XF
632 Y=EF(F)*EL(1,I)/KT\ GOSUB 648\Y2=.5*EXP(-Y)*XF
634 IF Q=0 THEN AC=AC*(1+Y2)/(1+Y1+Y2) ELSE AC=AC*Y2/(1+Y1+Y2)
636 EL=EC\EC=INT(50*E2)\D=EC-EL\ IF I=0 THEN 646
638 IF D=0 THEN E=EL\A=AC\ GOSUB 650\ GOTO 646
640 M=(AC-AL)/ABS(D)\ IF D<0 THEN D=-D\ GOTO 644
642 FOR X=1 TO D\E=EL+X\A=AL+X*M\ GOSUB 650\ NEXT X\ GOTO 646
644 FOR X=1 TO D\E=EL-X\A=AL+X*M\ GOSUB 650\ NEXT X
646 NEXT I\ RETURN
648 IF Y<-40 THEN Y=-40\ RETURN ELSE RETURN
650 DS(Q,E)=A+DS(Q,E)\ RETURN
652 L=.25\M=.5\N=.25\ FOR Q=0 TO SW
654 Y=DS(Q,0)\Z=DS(Q,1)\ FOR I=2 TO IX\X=Y\Y=Z\Z=DS(Q,I)
656 DS(Q,I-1)=L*X+M*Y+N*Z\ NEXT I\ NEXT Q\ RETURN
660 SET LINE STYLE 4\D=.125*B\ FOR I=10 TO 32
661 PLOT (.25*I,-32*EXP(-D*I)/I),\ NEXT I\ SET LINE STYLE 1
662 X=.25*10\Y=-32*EXP(-D*10)/10-.4\L$(3)='Vb'\ GOSUB 728\ RETURN
670 SET LINE STYLE 2\ FOR I=2 TO 74 STEP 2\ GOSUB 674
671 PLOT (-E(I),S),\ NEXT I\ PLOT (-E(I),S),\ SET LINE STYLE 1
672 FOR I=1 TO 75\ GOSUB 673\ PLOT (-E(I),S),\ NEXT I\ PLOT \ RETURN
673 E=.02*I\S=A+.5*LOG10(E)\ RETURN
674 E=.02*I\S=A+.5*LOG10(E)-LOG10(1+EXP((E-EF)/KT))
675 IF S<14 THEN S=14\ RETURN ELSE RETURN

700 DIM Y(RX)\X=RM-.3\ IF X>7.25 THEN X=7.25\ REM .....PROBABILITY
701 L$(0)='AA'\L$(1)=' DA'\L$(2)=' DD'
702 FOR Q=0 TO 2\ FOR I=0 TO RX\Y(I)=Y(I)+PF(2-Q)*P(I)\ NEXT I
703 Y=Y/(4*X+2)-.24\ GOSUB 717\ GOSUB 728\ NEXT Q\X=4\Y=1
704 L$(2)='(a) Impurity Spacing Distribution'\ GOSUB 728\ RETURN

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710 L$(0)='E1'\L$(1)='E2'\L$(2)='E3'\ REM .....DONOR LEVELS
711 L$(3)='E4'\X(0)=3\X(1)=1\X(2)=8\X(3)=5
712 FOR Q=0 TO 3\ FOR I=0 TO RX\Y(I)=EL(Q,I)\ NEXT I
713 J=X(Q)\X=R(J)\Y=Y(J)-.4\ GOSUB 717\ GOSUB 728\ NEXT Q
714 X=3\Y=-3.8\L$(3)='(b) Donor Levels (Ryd)'\ GOSUB 728\ RETURN
715 SET LINE STYLE 2\ FOR I=0 TO 200 STEP 2\ PLOT (E(I),S(I)),
716 NEXT I\ PLOT \ SET LINE STYLE 1\ RETURN
717 FOR I=0 TO 32\ PLOT (R(I),Y(I)),\ NEXT I\ PLOT \ RETURN
718 FOR I=0 TO 32\ PLOT (RH(I),Y(I)),\ NEXT I\ PLOT \ RETURN
720 L$(0)='H1'\L$(1)='H2'\L$(2)='H3'\ REM .....ACCEPTOR LEVELS
721 L$(3)='H4'\ FOR Q=0 TO 3\ FOR I=0 TO RX\Y(I)=-EF(2)*EL(Q,I)
722 NEXT I\J=X(Q)\X=RH(J)\Y=Y(J)\ GOSUB 718\ GOSUB 728\ NEXT Q
723 X=3\Y=2.8\L$(3)='(c) Acceptor Levels (Ryd)'\ GOSUB 728\ RETURN
725 IF (Q=0) OR (Q=2) THEN PLOT CURVE (E(),S(),201,0)\ RETURN
726 SET LINE STYLE 4\ FOR I=0 TO 200 STEP 2\ PLOT (E(I),S(I)),
727 NEXT I\ PLOT \ SET LINE STYLE 1\ RETURN
728 SET POSITION (X,Y)\ GRAPHIC PRINT L$(Q)\ RETURN
730 L$(0)='E1'\L$(1)=' E2'\ REM .....DONOR STATES
731 L$(2)='E3'\L$(3)='E4'\ FOR Q=0 TO SW\ GOSUB 750
732 GOSUB 725\ GOSUB 728\ GOSUB 572\ NEXT Q\A=LNC0\ GOSUB 670
733 X=-1.2\Y=18\L$(SW)='Cond. Band'\ GOSUB 728\X=2\Y=19.5
734 L$(SW)='(d) Donor States vs E (Ryd)'\ GOSUB 728\ RETURN
735 FOR Q=0 TO SW\ GOSUB 750\ REM .....FILLED STATES
736 GOSUB 715\ GOSUB 570\ NEXT Q\ RETURN
740 L$(0)='H1'\L$(1)='H2'\L$(2)='H3'\ REM .....ACCEPTOR STATES
741 L$(3)=' H4'\ GOSUB 745\ FOR Q=0 TO SW\ GOSUB 750\ GOSUB 725
742 GOSUB 728\ GOSUB 574\ NEXT Q\A=LNVO\ GOSUB 672\ GOSUB 745
743 X=.3\Y=18\L$(SW)='Valence Band'\ GOSUB 728\X=-4.5\Y=19.5
744 L$(SW)='(e) Acceptor States vs E-EV (Ryd)'\ GOSUB 728\ RETURN
745 FOR I=0 TO IX\E(I)=-E(I)\ NEXT I\ RETURN
750 Y=14\ FOR I=0 TO IX\S(I)=LOG10(100+DS(Q,I))
751 IF S(I)<14 THEN S(I)=14 ELSE IF Y<S(I) THEN Y=S(I)\IM=I
752 NEXT I\X=E(IM)\ DIM L(LX)\L(0)=Y\L(7)=X\L2=INT(Y)
753 L=6\ FOR I=IM TO 0 STEP -1
754 IF S(I)>L2-6+L THEN 755 ELSE L(L)=E(I)\L=L-1\ IF L>=1 THEN 754
755 NEXT I\L=8\ FOR I=IM+1 TO IX
756 IF S(I)>L2+8-L THEN 757 ELSE L(L)=E(I)\L=L+1\ IF L<=13 THEN 756
757 NEXT I\ RETURN
790 SET CHARACTER SIZE .12,.6\ SET CHARACTER SPACING .12,0
791 SET POSITION (-6.65,12.5)\ GRAPHIC PRINT USING 'Fig. A ###.',FG%;
792 FOR Y=1 TO 5\ GOSUB 793\ SET POSITION (-6.25,12.5-.6*Y)\ NEXT Y\ RETURN
793 ON Y GOSUB 794,795,796,797,798\ GRAPHIC PRINT L$\ RETURN
794 L$=' (a) Probability, AA + DA + DD , of Pairs vs R'\ RETURN
795 L$='(b) Donor Energy E1;(DD)-, E2;(DD)-, E3;(DA)-, E4(DA+)- vs R'\ RETURN
796 L$='(c) Acceptor En. H1;(AA)+, H2;(AA)+, H3;(AD)+, H4(AD-)+ vs R'\ RETURN
797 L$='(d) Densities of Donor States, E1, E2, E3, & E4, vs E'\ RETURN
798 L$='(e) Densities of Acceptor States, H1, H2, H3, & H4 vs E-EV.\ RETURN

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800  CLEAR \ SET VIEWPORT .1,1,0,.625\A1=.03\ REM ....PROBABILITY AXES
801  SET WINDOW -.2,8,-3,2\ SET CHARACTER SIZE .1,.25\Y1=0\Y2=1
802  SET CHARACTER SPACING .1,0\ GOSUB 850
803  SET POSITION (-.1,.5)\ GRAPHIC PRINT 'P'\ RETURN
810  SET WINDOW -.2,8,-4.2,3.8\Y1=-4\Y2=0\A1=-.05\ REM DONOR ENERGY AXES
811  GOSUB 852\ GOSUB 860\ RETURN
820  CLEAR \ SET WINDOW -.2,8,-4.6,3.4\A1=.05\ REM ACCEPTOR ENERGY AXES
821  Y1=0\Y2=3.6\ GOSUB 850\ GOSUB 880\ RETURN
830  SET WINDOW -1.7,6.5,13.1,27.1\ REM ....DONOR DENSITY OF STATE AXES
831  X1=-1.5\X2=6.5\ GOSUB 870\ GOSUB 845
832  SET POSITION (5.2,14.2)\ GRAPHIC PRINT 'E (Ryd)'
833  SET POSITION (0,19.5)\ GRAPHIC PRINT 'EC'\ RETURN
840  CLEAR \ SET WINDOW -6.7,1.5,6.1,20.1\ REM ACCEPTOR DEN. OF ST. AXES
841  X1=-6.5\X2=1.5\ GOSUB 870
842  SET POSITION (0,19.5)\ GRAPHIC PRINT USING 'EV = ###.###',EG
843  SET POSITION (-5.95,14.2)\ GRAPHIC PRINT 'E-EV (Ryd)'\ RETURN
845  SET LINE STYLE 4\ PLOT (-EF,13.4),(-EF,19)\ SET LINE STYLE 1
846  GRAPHIC PRINT 'EF'\ RETURN
850  FOR X=-0 TO 8\ SET POSITION (X-.15,-7*A1)\ GRAPHIC PRINT X\ NEXT X
851  SET POSITION (6.15,-9*A1)\ GRAPHIC PRINT 'R (Bohr)'\ PLOT
852  PLOT (0,0),(8,0)\ FOR X=0 TO 8\ PLOT (X,0),(X,3*A1)
853  FOR Y=.1 TO 1 STEP .1\ PLOT (X+Y,0),(X+Y,A1)\ NEXT Y\ NEXT X
854  FOR X=.5 TO 8\ PLOT (X,0),(X,2*A1)\ NEXT X\ PLOT (0,Y1),(0,Y2)
855  FOR Y=Y1 TO Y2\ PLOT (0,Y),(1,Y)\ NEXT Y\ FOR Y=Y1 TO Y2 STEP .2
856  PLOT (0,Y),(1.03,Y)\ NEXT Y
857  SET POSITION (-.1,Y1+2.5)\ GRAPHIC PRINT 'E'\ RETURN
860  SET POSITION (6,-2.05)\ GRAPHIC PRINT USING 'TEMP. = ### K',T
861  SET POSITION (6,-2.4)\ GRAPHIC PRINT USING 'LOG Cb = ###.##',LC1
862  SET POSITION (6,-2.75)\ GRAPHIC PRINT USING 'LOG C = ###.##',LC
863  SET POSITION (6,-3.1)\ GRAPHIC PRINT USING 'LOG Cx = ###.###',LC2
864  SET POSITION (6,-3.45)\ GRAPHIC PRINT USING 'Log n = ###.###',LN
865  SET POSITION (6,-3.8)\ GRAPHIC PRINT USING 'Log p = ###.###',LP
866  SET POSITION (-.2,-4)\ GRAPHIC PRINT -4
867  SET POSITION (-.2,-2)\ GRAPHIC PRINT -2\ RETURN
870  PLOT (X1,14),(X2,14)\ FOR X=X1+.5 TO X2\ PLOT (X,14),(X,14.3)
871  NEXT X\ FOR X=X1 TO X2\ PLOT (X,14),(X,14.2)\ NEXT X
872  FOR X=X1 TO X2 STEP .1\ PLOT (X,14),(X,14.1)\ NEXT X
873  FOR X=X1+.5 TO X2\ SET POSITION (X-.1,13.4)\ GRAPHIC PRINT -X\ NEXT X
874  PLOT (0,14),(0,19.5)\ PLOT (X1,14),(X1,20)\ FOR Y=14 TO 19
875  PLOT (X1,Y),(X1+.08,Y)\ SET POSITION (X1-.3,Y)\ GRAPHIC PRINT Y
876  FOR X=1 TO 4\ S=Y+LOG10(2*X)\ PLOT (X1,S),(X1+.04,S)\ NEXT X\ NEXT Y
877  SET POSITION (X1+.1,19.5)\ GRAPHIC PRINT 'Log S'\ RETURN
880  SET POSITION (6,2.8)\ GRAPHIC PRINT USING 'EF-Fermi= ###.###',EF
881  SET POSITION (6,2.45)\ GRAPHIC PRINT USING 'Scrn B = ###.###',B
882  SET POSITION (6,2.1)\ GRAPHIC PRINT USING 'ED-Scrn = ###.###',ES
883  SET POSITION (6,1.75)\ GRAPHIC PRINT USING 'EV-GAP = ###.###',EG
884  SET POSITION (-.2,3)\ GRAPHIC PRINT 3\ RETURN

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