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AVOIDED INTERSECTION OF POTENTIAL ENERGY SURFACES: THE ($H^+ + H_2$, $H + H_2^+$) SYSTEM*

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ABSTRACT

Nonempirical electronic structure calculations have been carried out on the two lowest $^1A_1$ states of H_3^+. When one proton is infinitely separated from the other two, these $^1A_1$ potential surfaces cross each other. The nature of this avoided intersection is examined by means of potential curves, contour diagrams, and perspective plots. Surface hopping is discussed within a Landau-Zener-Stuckelberg (LZS) framework, and the LZS assumptions concerning the surfaces are shown to be reasonable near the avoided intersection. Ab initio LZS parameters are compared with those obtained from the semi-empirical diatomics-in-molecules surfaces of Preston and Tully. The agreement is good, better than might have been anticipated.

INTRODUCTION

The avoided crossing of diatomic molecule potential energy curves is a phenomena familiar to most chemical physicists.[1] The most carefully studied[2,3] example of an avoided crossing is probably the E, F, $^1\Sigma_g^+$ "double minimum" state of the hydrogen molecule. Many other theoretical examples are available.[4] The dynamic consequences of the avoided crossing have been the subject of a great deal of theoretical research, most notably the papers of Landau,[5] Zener,[6] and Stuckelberg.[7]

If only from our knowledge of diatomic potential curves, it is clear that the avoided <u>intersection</u> of potential energy <u>surfaces</u> must be a common occurrence in nature. However, it appears that there has not been a single careful <u>ab initio</u> study of an avoided intersection. Studies of the molecular dynamics accompanying an avoided intersection are almost equally scarce.[8-10] In fact, the only concrete example which has been studied is the H_3^+ system, for which examination of the H_2 and H_2^+ ground state potential curves implies[10] the existence of an avoided intersection. Preston and Tully[10] have studied the dynamics of the reaction of H^+ and D_2 using semi-empirical diatomics-in-molecules[11] potential surfaces for the two lowest singlet states. In their work, Preston and Tully adopted a classical trajectory approach. However, in the spirit of Landau-Zener-Stuckelberg, they allowed for the possibility of "surface hopping" (nonadiabatic electronic transitions) at points of avoided intersection of the potential surfaces.

In light of the Preston-Tully research, it seemed sensible to concern the first <u>ab initio</u> study of an avoided intersection with the ($H^+ + H_2$, $H + H_2^+$) pair of potential surfaces. The H_3^+ system has the additional obvious

advantage that the electronic structure calculations may be made sufficiently precise as to allow us to concentrate on the surfaces, rather than the possible deficiencies of the calculations. In addition to learning something about the nature of adiabatic potential surfaces near an avoided intersection, we should be able to evaluate the reliability of the semi-empirical diatomics-in-molecules method[11] for the H_3^+ system.

DESCRIPTION AND RELIABILITY OF THE CALCULATIONS

An uncontracted set of gaussian basis functions, seen in Table I, was used in the present work. The set of five s functions are those found optimum for the hydrogen atom by van Duijneveldt.[12] For the H atom, this basis yields an energy of -0.499 810 hartrees, compared to the exact result, -0.5 hartrees. The p functions were taken from the work of Czismadia and co-workers,[13] and are nearly optimum for the hydrogen molecule. The total number of basis functions is 33, and for the C_{2v} geometries considered herein there will be 16 a_1 functions, 2 a_2 functions, 4 b_1 functions, and 11 b_2 functions.

For the H_2 molecule at 1.4 bohrs internuclear separation, the present basis yields a full configuration interaction (CI) energy of -1.171 140 hartrees. This energy lies 2.1 kcal/mole above the corresponding exact H_2 energy,[14] -1.174 475 hartrees. For H_2^+ at R = 1.4, the calculated and exact energies are -0.569 245 and -0.569 984 hartrees, which differ by 0.5 kcal.

All the H_3^+ calculations reported in the present work are full or complete (within the chosen basis) CI calculations. For C_{2v} geometries the full CI includes 215 configurations, making the computations rather straightforward. Concerning the accuracy of the H_3^+ surfaces, we concur with Csizmadia _et al._[13] in the opinion that the absolute error will be somewhat greater for H^+

infinitely separated from H_2 than for the H_3^+ complex. More concretely, 3 kcal/mole appears to be a reasonable upper limit to the absolute error in the two calculated potential energy surfaces. Relative errors, of course, may be much smaller.

POTENTIAL ENERGY SURFACES

Only isosceles triangle configurations (C_{2v} geometries) were considered in the present work. Although the full three-dimensional surface could be obtained, it was not necessary to fulfill the goals of the present study. The coordinate system is seen in Fig. 1, where r is the separation of the two equivalent H atoms, and R is the distance between the third H atom and the midpoint of the two equivalent atoms.

As pointed out by Preston and Tully,[10] an easy way to envisage the avoided intersection is to set $R = \infty$ and then plot the energy of the two states as a function of r. Two potential energy curves will be obtained in this manner, as can be seen in Fig. 2. The first is that for the ground state of H_2, and the second that for H_2^+. However, the H_2^+ curve is uniformly lowered by 0.5 hartree due to the presence of an H atom at infinite separation. The crossing of the two potential curves only occurs if $R = \infty$. For finite values of R, the curves will avoid each other. The family of curves arising from all possible R values generates a two-dimensional potential energy surface.

The first series of calculations was carried out for R = 2, 4, 6, 8, and 100 and r = 1.0 through 4.0 in 0.2 bohr intervals. In addition r = 2.5 was included. These 85 points give us a broad picture of the two surfaces. In the interest of journal space, these 170 energies are not reproduced here, but may be obtained from the authors.

For R = 100, 8, 6, 4, and 2 bohrs, the potential curves E(r) are shown in Figs. 2, 3, 4, 5, and 6. At R = 100, it is clear that the curves very nearly cross each other. Specifically the avoided crossing occurs at r = 2.456 bohrs and the separation ΔE_o is 0.00002 hartrees. This predicted avoided crossing point may be compared with the true crossing point for R = ∞, which we find to be ~ 2.50 bohrs from the interpolated "exact" potential curves[14,15] for H_2 and H_2^+. For R = 8, the avoided crossing is quite sharp also, but at R = 6 the separation ΔE_o becomes substantial, 0.0264 hartrees = 16.6 kcal. At R = 4, it is no longer clear that the two curves avoid each other. Finally, for R = 2, the upper curve no longer has a minimum, and thus bears no simple relation to the H_2 and/or H_2^+ potential energy curves.

We have plotted the same potential curves of H_3^+ for the diatomics-in-molecules (DIM) surfaces of Preston and Tully. For R = 8 and R = 6 their curves are very similar to Figs. 3 and 4, the only noticeable difference at R = 8 being that the lower curve is slightly (~ 3 kcal) deeper than ours. This is expected since the DIM surface should be quite accurate for large R, and we know that the <u>ab initio</u> calculations yield an H_2 energy 2.1 kcal above the exact result. At R = 4, more noticeable deviations between the semi-empirical and <u>ab initio</u> results begin to appear. The DIM lower curve now lies ~ 5 kcal below the <u>ab initio</u> curve near the bottom of the potential well. The upper $^1A_1$ state results show the DIM curve ~ 3 kcal below the <u>ab initio</u> curve at R = 1.8, but 1 kcal higher at R = 3.4.

Only for R = 2 is there a <u>qualitative</u> difference between the DIM and <u>ab initio</u> potential curves. This is not really surprising since for these geometries the identities of the diatomic molecules become blurred, and one

must contend with an H_3^+ molecule. Although the DIM potential curve for the second $^1A_1$ state remains attractive, the ab initio curve, seen in Fig. 6, takes on an interesting repulsive shape. The two ground state curves remain similar in shape, but the DIM curve is ~ 20 kcal deeper. Since the ab initio surfaces are estimated to have an absolute error of no more than 3 kcal, the DIM curve seems to be seriously in error.

As we shall see in the following section, there is virtually zero probability of surface hopping at R = 2. Thus, the DIM surfaces are qualitatively correct in the region of the avoided intersection. However, classical trajectories will sample the R = 2 region, and detailed studies would be necessary to determine whether the deficiencies of the DIM surfaces affect the dynamics of the $H^+ + H_2$ and $H + H_2^+$ reactions.

Figures 7 and 8 give contour maps of the two lowest $^1A_1$ potential energy surfaces of H_3^+. The ground state surface pertains to the adiabatic approach of H^+ to H_2, while the excited surface refers to $H + H_2^+$. The surprising feature of the two contour maps is that the presence of the avoided intersection is not apparent. Thus, it is clear that the surface cuts of Figs. 2-6 give a more useful picture of the avoided intersection. The lowest $^1A_1$ surface is very attractive, as H_3^+ is bound by ~ 106 kcal/mole[13] relative to $H^+ + H_2$. Our calculations do not include the equilibrium H_3^+ geometry (R ~ 1.44 bohrs, r ~ 1.66 bohrs[13]), since is occurs in a region far from the avoided intersection. The first excited $^1A_1$ surface is very different, its repulsive nature reflecting the relatively unfavorable interaction between H and H_2^+.

A more qualitative view of the two surfaces is given by the perspective plots of Figs. 9 and 10. The primary virtue of these graphical displays is

that they do indicate the presence of the avoided intersection. Although the area shown only goes to R = 10, it is clear that the avoided intersection will become more sharply avoided for larger R; of course the surfaces will cross at $R = \infty$.

PARAMETERS DESCRIBING THE AVOIDED INTERSECTION

In the one-dimensional Landau-Zener-Stuckelberg (LZS) formulation,[5-7] the probability of potential curve hopping is given by

$$P = \exp\left[-\frac{2\pi H_{12}^2}{\hbar v |\Delta H_o'|}\right] \tag{1}$$

where v is the relative velocity of the two particles.

The LZS approximation is formulated in terms of diabatic[16] potential curves, which do not interact and therefore must cross each other. The interaction term H_{12} is just

$$H_{12} = \langle \psi_1 | H | \psi_2 \rangle_{r=r_o} \tag{2}$$

and $|\Delta H_o'|$ is the difference in slopes of the two diabatic curves

$$\Delta H_o' = \frac{\partial}{\partial r} [\langle \psi_2 | H | \psi_2 \rangle - \langle \psi_1 | H | \psi_1 \rangle]_{r=r_o} \tag{3}$$

Since adiabatic potential surfaces result from our <u>ab initio</u> calculations, we transform the LZS expression to an adiabatic framework using the two-state approximation

$$H_{12} \cong \frac{1}{2} \Delta E_o \tag{4}$$

The adiabatic energy difference, a function of r, is

$$\Delta E(r) = \sqrt{(\Delta H)^2 + 4\, H_{12}^2} \tag{5}$$

Assuming $H_{12}(r)$ is constant, this difference may be expanded in a truncated Taylor series about r_o, the point of avoided crossing

$$\Delta E(r) \cong \sqrt{\Delta H_o'(r - r_o)^2 + \Delta E_o^2} \tag{6}$$

Assuming the above relation is exact, one obtains

$$|\Delta H_o'| = \frac{\sqrt{\Delta E(r)^2 - \Delta E_o^2}}{|r - r_o|} \tag{7}$$

Since $\Delta H_o'$ is a constant in the LZS approximation, the deviation of (7) from constancy will provide a measure of the consistency of the LZS approximation.

An alternative expression for $|\Delta H_o'|$ may be obtained by twice differentiating Eq. (6) with respect to r

$$|\Delta H_o'| = \sqrt{\Delta E_o''\, \Delta E_o} \tag{8}$$

The hopping probability P in terms of adiabatic curves is obtained by substituting Eqs. (4) and (8) into (1)

$$P = \exp\left[-\sqrt{\frac{E_c}{E}}\right] \tag{9}$$

In Eq. (9), E is the collision energy and E_c is a "critical" energy

$$E_c = \frac{\pi^2}{8} \frac{\mu}{\hbar^2} \frac{\Delta E_o^3}{\Delta E_o''} \tag{10}$$

E_c is the energy E at which the probability P of hopping is $e^{-1} = 0.37$.

For a specified value of R (the distance between the third proton and the center of mass of the two equivalent protons), the present ($H^+ + H_2$, $H + H_2^+$) problem becomes one-dimensional. The accuracy of the LZS parameters for this series of one-dimensional problems should give a clear picture of the suitability of any pair of potential surfaces for the description of the surface hopping phenomena. To calculate these parameters, it was necessary to carry out an additional series of computations for geometries close to the avoided intersection. For each value of R considered, the value (to within an integer multiple of 0.01 bohr) of r for which ΔE is a minimum was determined. Finally, calculations were performed for this r value ±0.01, and ±0.02 bohr. One feature of the surfaces that should be stated immediately is that the avoided intersection "disappears" between R = 4.0 and R = 5.0 bohrs. That is, for R = 4.0, $\Delta E(r)$ does not pass through a minimum, but rather decreases monotonically from r = 1.0 to r = 4.0.

Table II compares the values of the diabatic quantity $|\Delta H_o'|$ obtained using Eqs. (7) and (8). In the limit of $r = r_o$ it is clear that the value obtained using Eq. (7) must equal that found from Eq. (8). However, the values calculated for neighboring r are also in reasonable agreement with $\sqrt{\Delta E_o'' \, \Delta E_o}$. For R = 5, 6, 7, and 8, the largest deviations are 5.3%, 1.8%, 4.0%, and 2.6%. Thus, it appears that near the avoided crossing, the LZS assumptions of a) linearity of ΔH in $(r - r_o)$ and b) constancy of H_{12} are reasonably valid.

The LZS parameters of interest are summarized in Table III and compared with the diatomics-in-molecules results of Preston and Tully.[10] The distance of closest approach is remarkably constant as a function of R in the ab initio calculations. The r_o values range from 2.469 to 2.478, a span of only 0.009 bohrs. The DIM results for r_o increase monotonically from 2.349 (R = 5.0) to 2.498 (R = 8.0), a span of 0.149 bohrs. At R = 5.0, we expect the ab initio results to be much more reliable. However, at R = 8.0, it seems clear that at least one of the DIM parameters, r_o, is more accurate than the ab initio result. This is because the DIM value of r_o at R = 8 is very close to the exact[14,15] crossing point, ~ 2.50, for R = ∞. Since the avoided crossing is quite sharp at R = 8.0, r_o should be essentially determined by the diatomic curves.

As is also clear from Figs. 2-6, the separations ΔE_o of Table III increase with decreasing R. In each case the DIM separation is greater than the ab initio, although the results are qualitatively quite similar. At R = 5, 6, and 7, the ab initio results are quite likely to be the more reliable, but at R = 8 the situation is less clear. Although the diatomic potential curves guarantee the avoided crossing point r_o to be accurate for large R, the separation ΔE_o is not related to experimentally known quantities in such a transparent way. The good agreement between the DIM and ab initio values of ΔE_o suggests that the DIM surfaces are more accurate than could have reasonably been expected.

The difference $\Delta E_o''$ in the curvatures of the two curves at the point r_o of avoided intersection is expected to be rather sensitive to the potential energy surfaces. Except at R = 5, where DIM may begin to have serious weaknesses,

the ab initio values of $\Delta E''_o$ are greater than the DIM values. The $\Delta E''_o$ values are reflected through Eq. (10) in the critical energies E_c and therefore in the hopping probabilities P. The critical energies from the ab initio and DIM surfaces are seen to differ significantly, by nearly a factor of four at R = 8.0 and by more than a factor of two at R = 7.0. However, these differences are noticeably damped out in the calculated hopping probabilities, which are in good qualitative agreement. From both the ab initio and DIM surfaces, the hopping probability is found to fall off very sharply below R = 6.0 bohrs. This result is crucial to the viability of the DIM description of the avoided intersection, since as pointed out earlier, the DIM surfaces begin to have serious errors for R < 5.0.

CONCLUDING REMARKS

Potential surfaces for the two lowest $^1A_1$ states of H_3^+ have been obtained ab initio to an absolute accuracy of ~ 3 kcal. The surfaces are appropriate to the $H^+ + H_2$ and $H + H_2^+$ chemical reactions. Near the avoided intersection, the ab initio surfaces are quite similar to the semi-empirical diatomics-in-molecules surfaces. For closer approaches of H^+ to H_2 or H to H_2^+, the semi-empirical surfaces become less accurate.

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FOOTNOTES AND REFERENCES

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†Neshan Zovick Fellow.

††Alfred P. Sloan Fellow.

‡M. H. Fellow.

1. G. Herzberg, Spectra of Diatomic Molecules (D. Van Nostrand Company, Princeton, 1950). See especially pages 295-298.
2. E. R. Davidson, J. Chem. Phys. 33, 1577 (1960); 35, 1189 (1961).
3. W. Kolos and L. Wolniewicz, J. Chem. Phys. 50, 3228 (1969).
4. The $^2\Pi$ states of CN are a particularly interesting case. See H. F. Schaefer and T. G. Heil, J. Chem. Phys. 54, 2573 (1971).
5. L. D. Landau, Physik. Z. Sowjetunion U.R.S.S. 2, 46 (1932).
6. C. Zener, Proc. Roy. Soc. (London) A137, 696 (1932).
7. E. C. G. Stuckelberg, Helv. Phys. Acta 5, 369 (1932).
8. E. E. Nikitin, in Chemische Elementarprozesse, edited by H. Hartmann (Springer, Berlin, 1968).
9. W. H. Miller and T. H. George, J. Chem. Phys. 56, 5637 (1972).
10. R. K. Preston and J. C. Tully, J. Chem. Phys. 54, 4297 (1971); 55, 562 (1971).
11. F. O. Ellison, J. Am. Chem. Soc. 85, 3540, 3544 (1963).
12. F. B. van Duijneveldt, Report RJ 945, IBM Research Laboratory, San Jose, California.
13. I. G. Csizmadia, R. E. Kari, J. C. Polanyi, A. C. Roach, and M. A. Robb, J. Chem. Phys. 52, 6205 (1970).
14. W. Kolos and L. Wolniewicz, J. Chem. Phys. 49, 404 (1968).
15. D. R. Bates, K. Ledsham, and A. L. Stewart, Phil. Trans. Roy. Soc. A246, 215 (1953).
16. F. T. Smith, Phys. Rev. 179, 111 (1969).

Table I. Basis set of gaussian functions centered on each proton.

Type	Gaussian exponent α
1s	33.865 014
1s	5.094 788
1s	1.158 786
1s	0.325 840
1s	0.102 741
$2p_x, 2p_y, 2p_z$	2.0
$2p_x, 2p_y, 2p_z$	0.5

Table II. Evaluation of the Landau-Zener-Stuckelberg quantity $|\Delta H'_o|$ by two methods. Results are in hartrees (1 hartree = 627.5 kcal/mole).

	R = 5.0	R = 6.0	R = 7.0	R = 8.0
Eq. (7)				
r = 2.45	0.05228	0.05 461	0.05 488	0.05 558
r = 2.46	0.05303	0.05 425	0.05 436	0.05 532
r = 2.47	0.05026	0.05 354	0.05 299	0.05 538
r = 2.48	0.04916	0.05 417	0.05 269	0.05 421
r = 2.49	0.04948	0.05 344	0.05 406	0.05 408
r = 2.50	0.05036	0.05 304	0.05 374	0.05 371
Eq. (8)	0.05038	0.05403	0.05277	0.05512

Table III. *Ab initio* parameters related to the avoided intersection of the $H^+ + H_2$ and $H + H_2^+$ potential energy surfaces. 1 hartree = 627.5 kcal. Results obtained from the semi-empirical surfaces of Preston and Tully[10] are given in parentheses.

R(bohrs)	5.0	6.0	7.0	8.0
Distance r_o (bohrs) of closest approach	2.469 (2.349)	2.478 (2.458)	2.477 (2.491)	2.472 (2.498)
Separation ΔE_o (kcal) at r_o	37.08 (39.41)	16.59 (18.13)	7.20 (8.34)	3.01 (3.84)
Curvature $\Delta E''_o$ (kcal/bohr^2)	27.0 (37.7)	69.3 (57.0)	152.3 (113.7)	397.1 (236.1)
Slope $\partial E/\partial r$ (kcal/bohrs) at r_o	35.17 (34.66)	35.23 (34.67)	35.25 (34.55)	35.28 (34.52)
Critical energy E_c (kcal)	3413.27 (2931.01)	118.83 (188.47)	4.42 (9.20)	0.124 (0.434)
Hopping probability P for E = 1 eV = 23.06 kcal	5.2×10^{-6} (1.3×10^{-5})	0.1033 (0.0573)	0.6455 (.5317)	0.9292 (.8718)

FIGURE CAPTIONS

Fig. 1. Coordinate system used to describe that part of the H_3^+ potential surfaces considered in the present work.

Fig. 2. Potential curves for the lowest two $^1A_1$ states of H_3^+ for R = 100 bohrs.

Fig. 3. Potential curves for the lowest two $^1A_1$ states of H_3^+ for R = 8 bohrs.

Fig. 4. Potential curves for the lowest two $^1A_1$ states of H_3^+ for R = 6 bohrs.

Fig. 5. Potential curves for the lowest two $^1A_1$ states of H_3^+ for R = 4 bohrs.

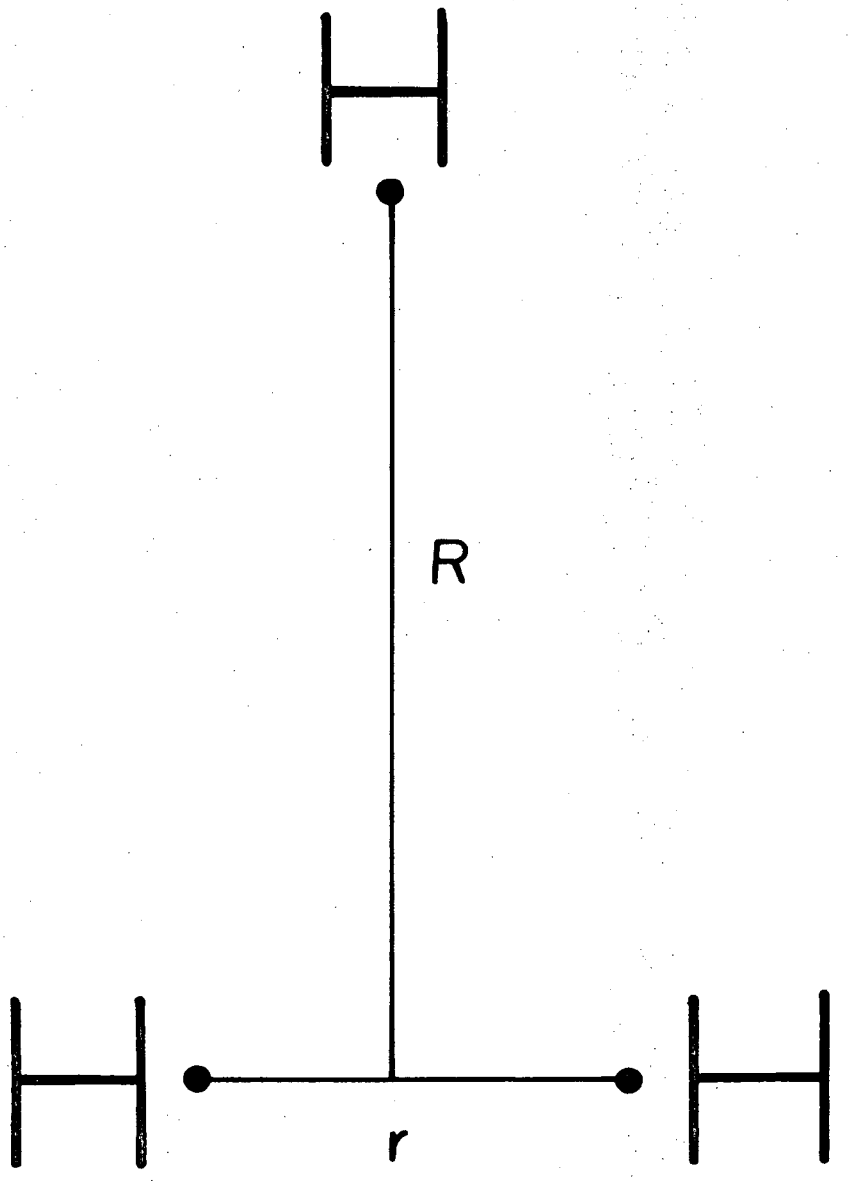
Fig. 6. Potential curves for the lowest two $^1A_1$ states of H_3^+ for R = 2 bohrs.

Fig. 7. Contour map of the lowest $^1A_1$ potential energy surface of H_3^+. r is the distance between the two equivalent protons, and R the distance between the midpoint of the two equivalent protons and the third proton. This surface pertains to the adiabatic approach of H^+ to H_2.

Fig. 8. Contour map of the first excited $^1A_1$ potential surface of H_3^+. This surface pertains to the adiabatic approach of H to H_2^+.

Fig. 9. Perspective plot of the lowest $^1A_1$ potential energy surface of H_3^+.

Fig. 10. Perspective plot of the first excited $^1A_1$ potential surface of H_3^+.



XBL733-2391

Fig. 1

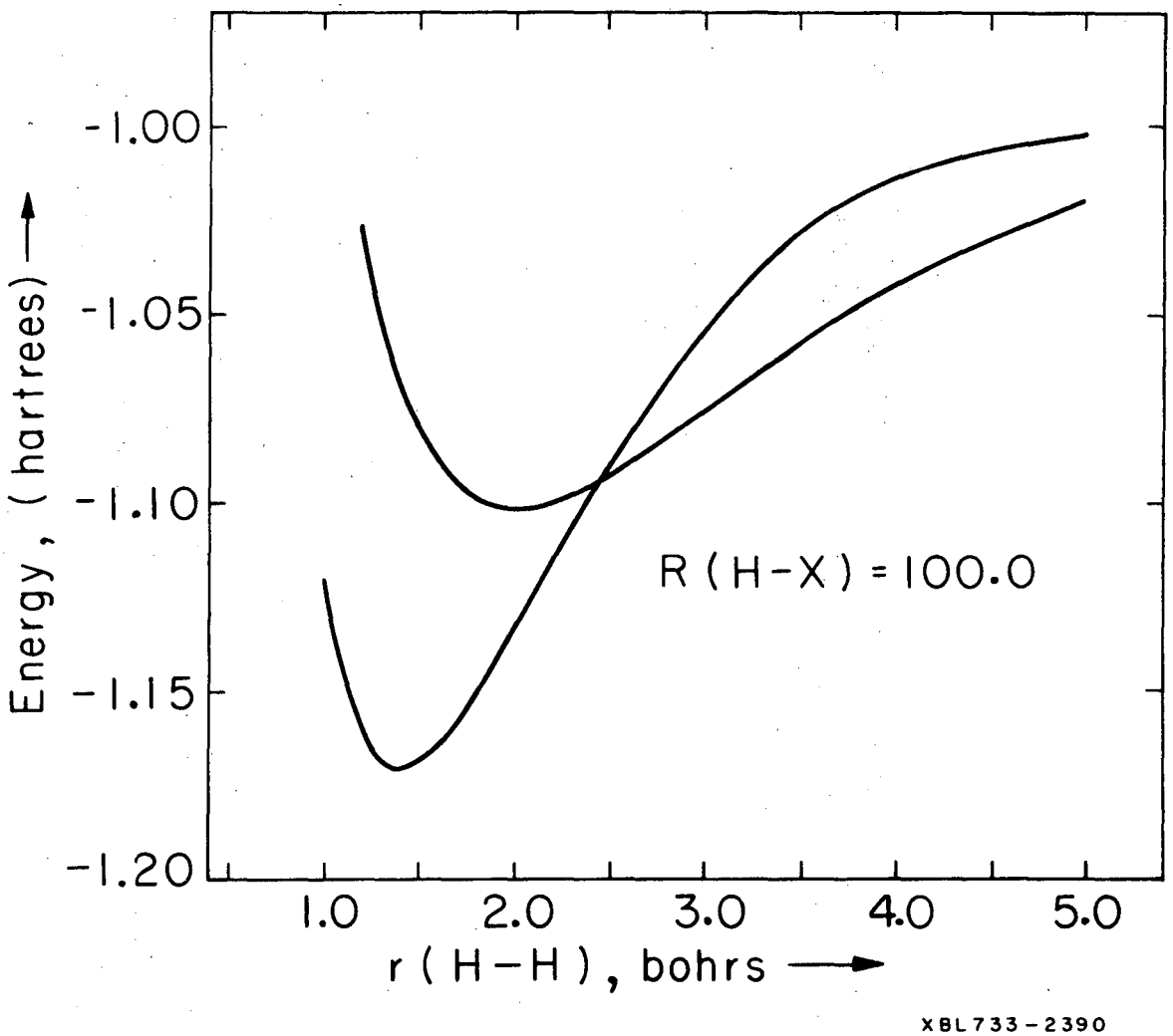
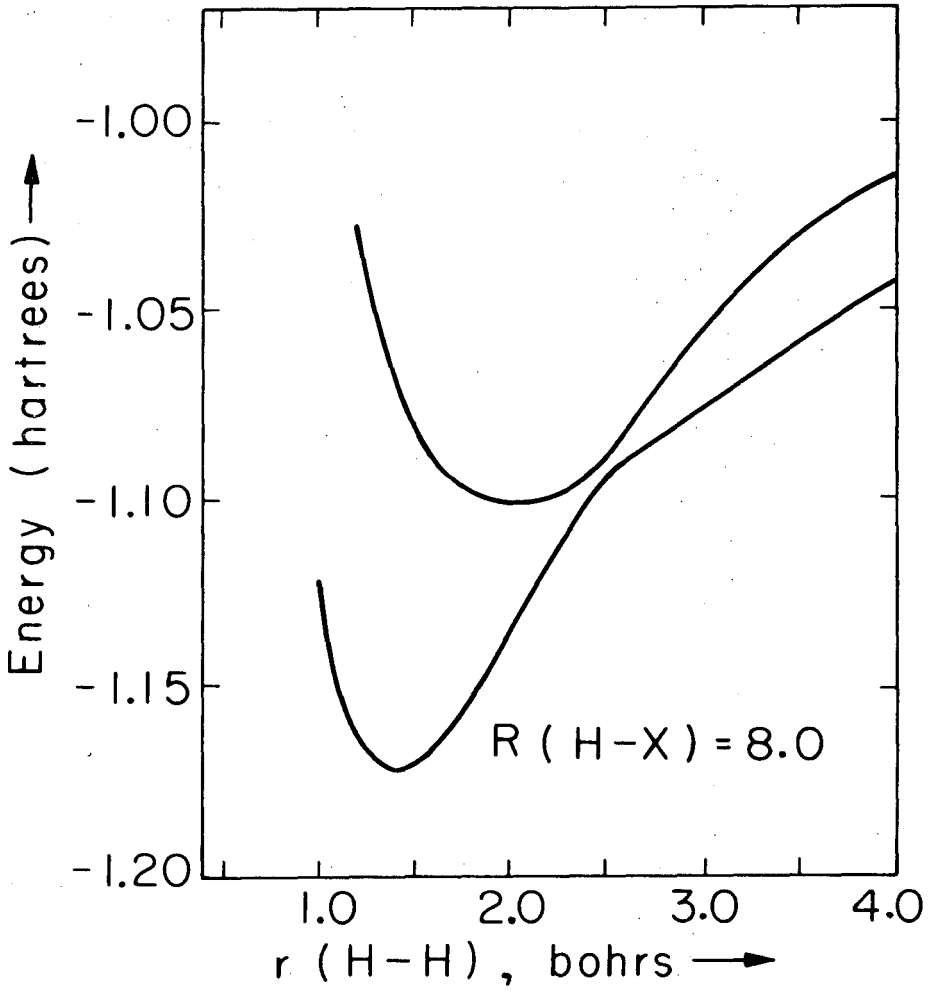

-1.00
-1.05
-1.10
-1.15
-1.20
Energy, (hartrees) ⟶
R (H-X) = 100.0
1.0
2.0
3.0
4.0
5.0
r (H-H), bohrs ⟶
XBL733-2390

Fig. 2



XBL 733-2389

Fig. 3

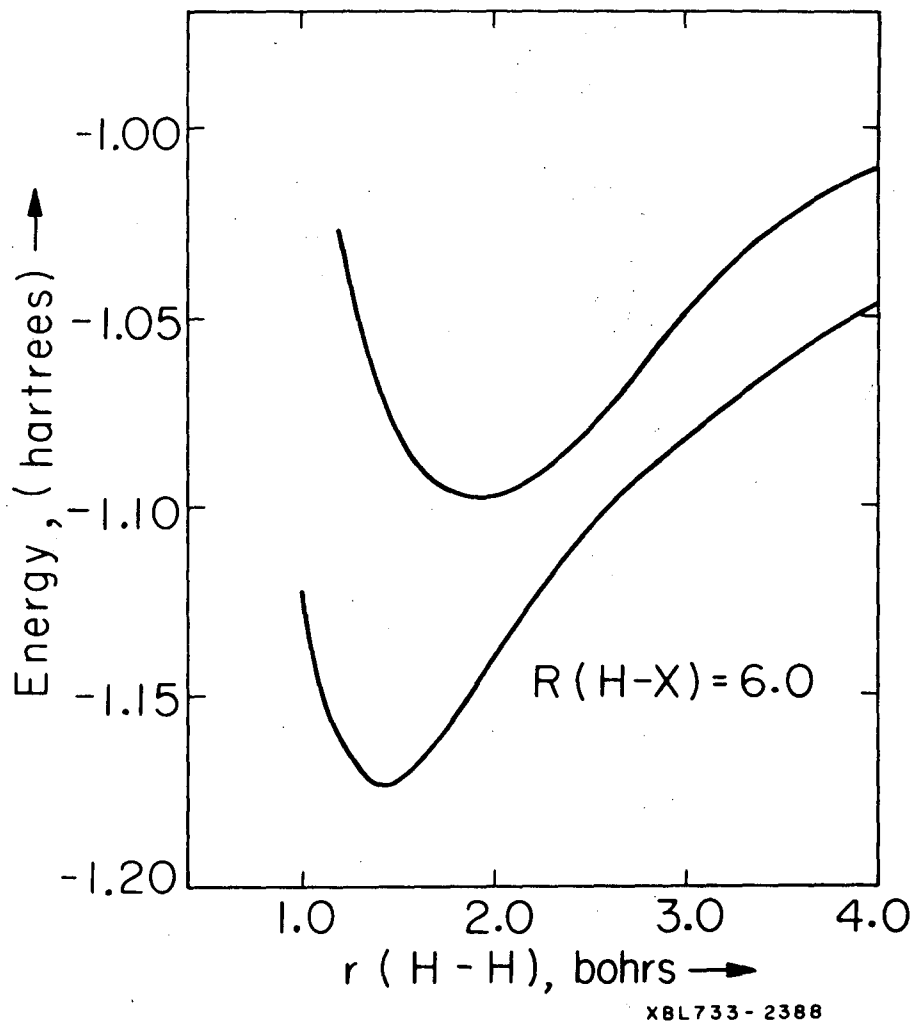
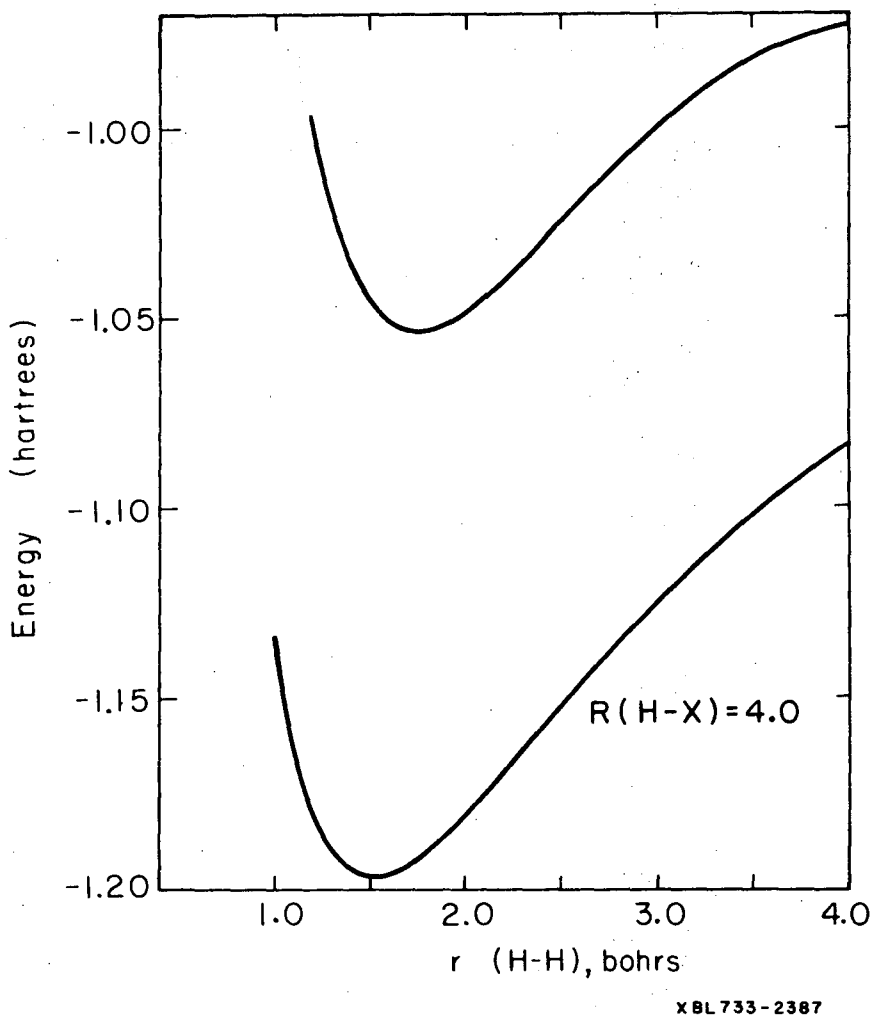

-1.00
-1.05
-1.10
-1.15
-1.20
Energy, (hartrees) →
R(H-X) = 6.0
1.0
2.0
3.0
4.0
r (H - H), bohrs →
XBL733-2388

Fig. 4


-1.00
-1.05
-1.10
-1.15
-1.20
Energy (hartrees)
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2.0
3.0
4.0
r (H-H), bohrs
XBL733-2387

Fig. 5

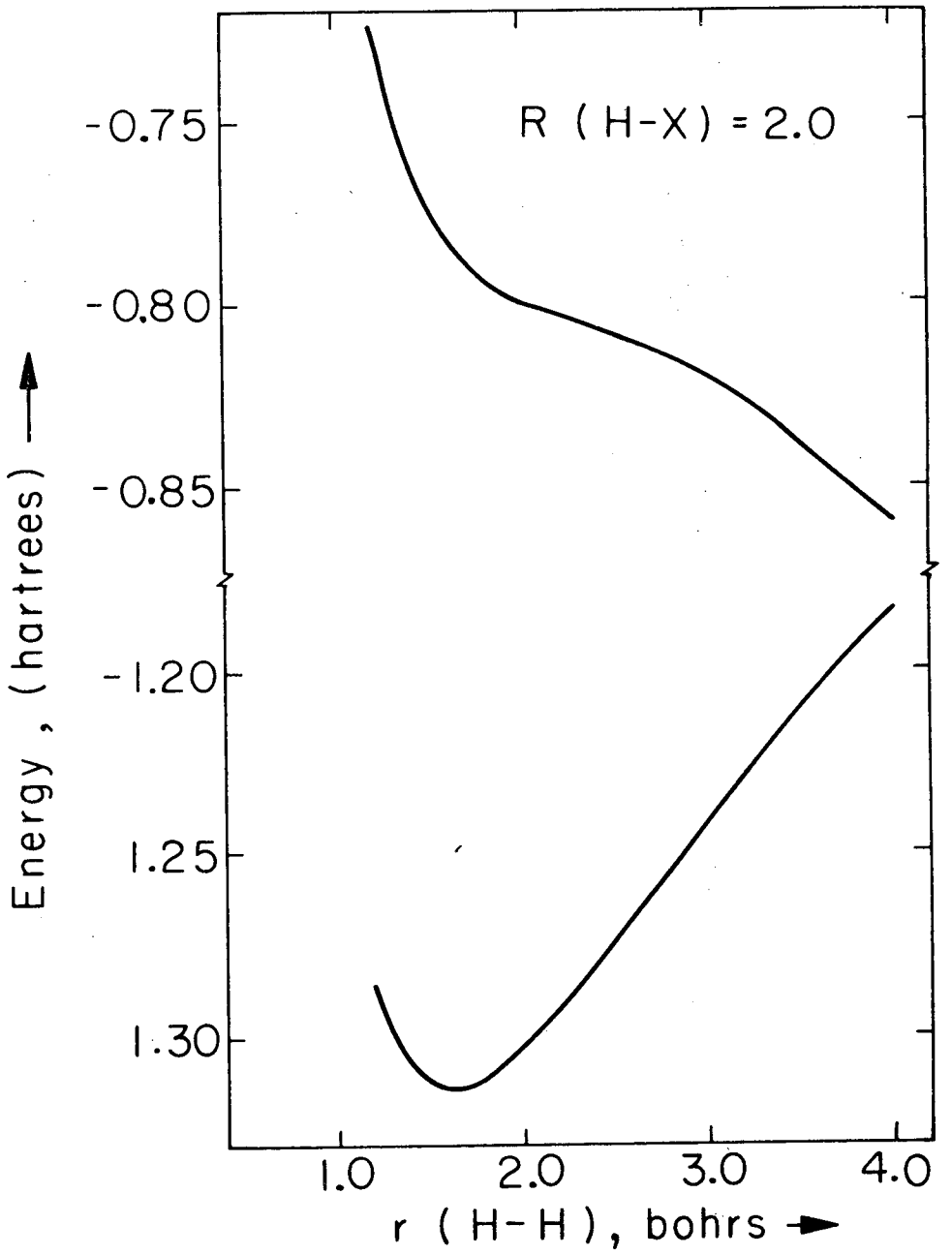

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Fig. 6

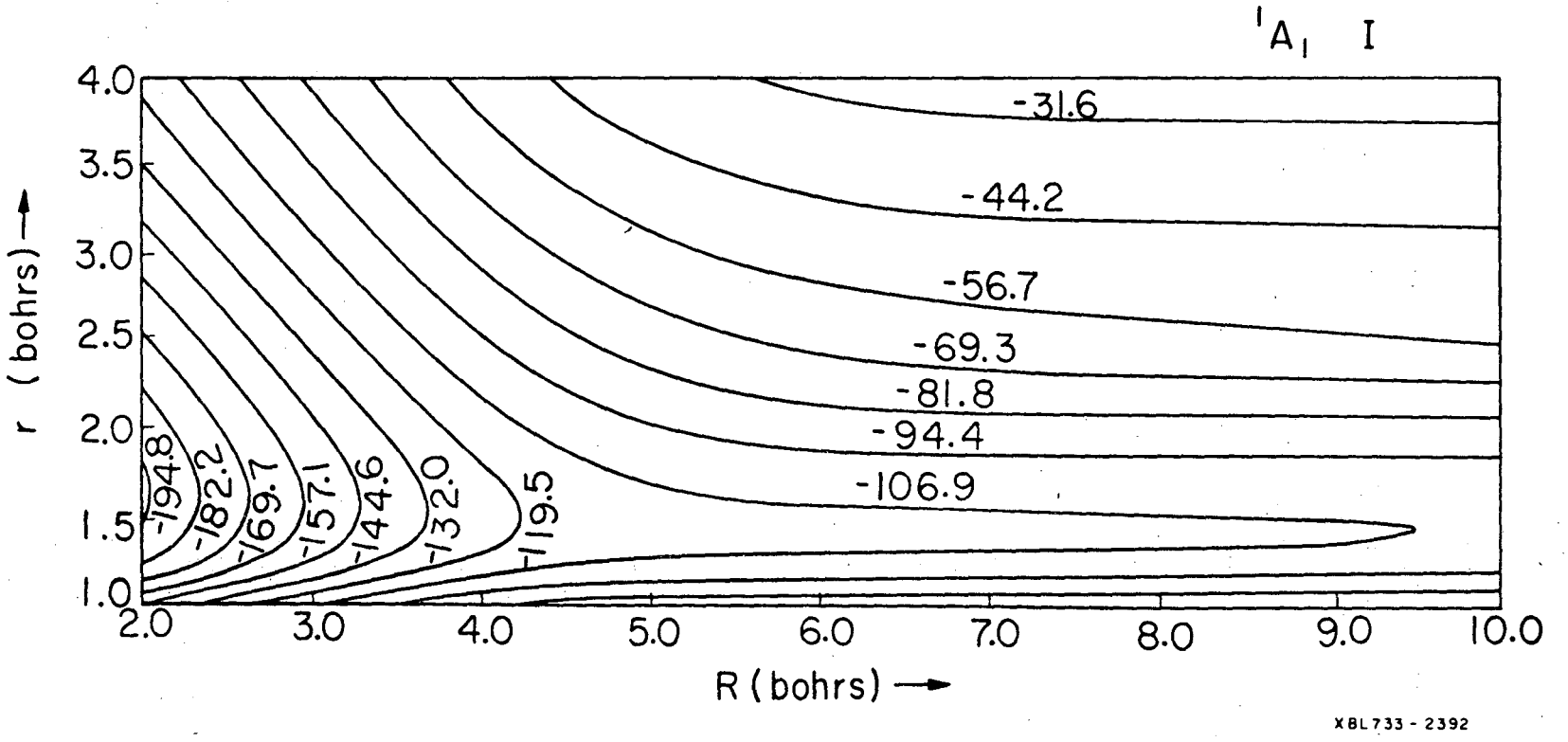

$^1A_1$ I
-31.6
-44.2
-56.7
-69.3
-81.8
-94.4
-106.9
-119.5
-132.0
-144.6
-157.1
-169.7
-182.2
-194.8
r (bohrs)
R (bohrs)
4.0
3.5
3.0
2.5
2.0
1.5
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
XBL733-2392

Fig. 7

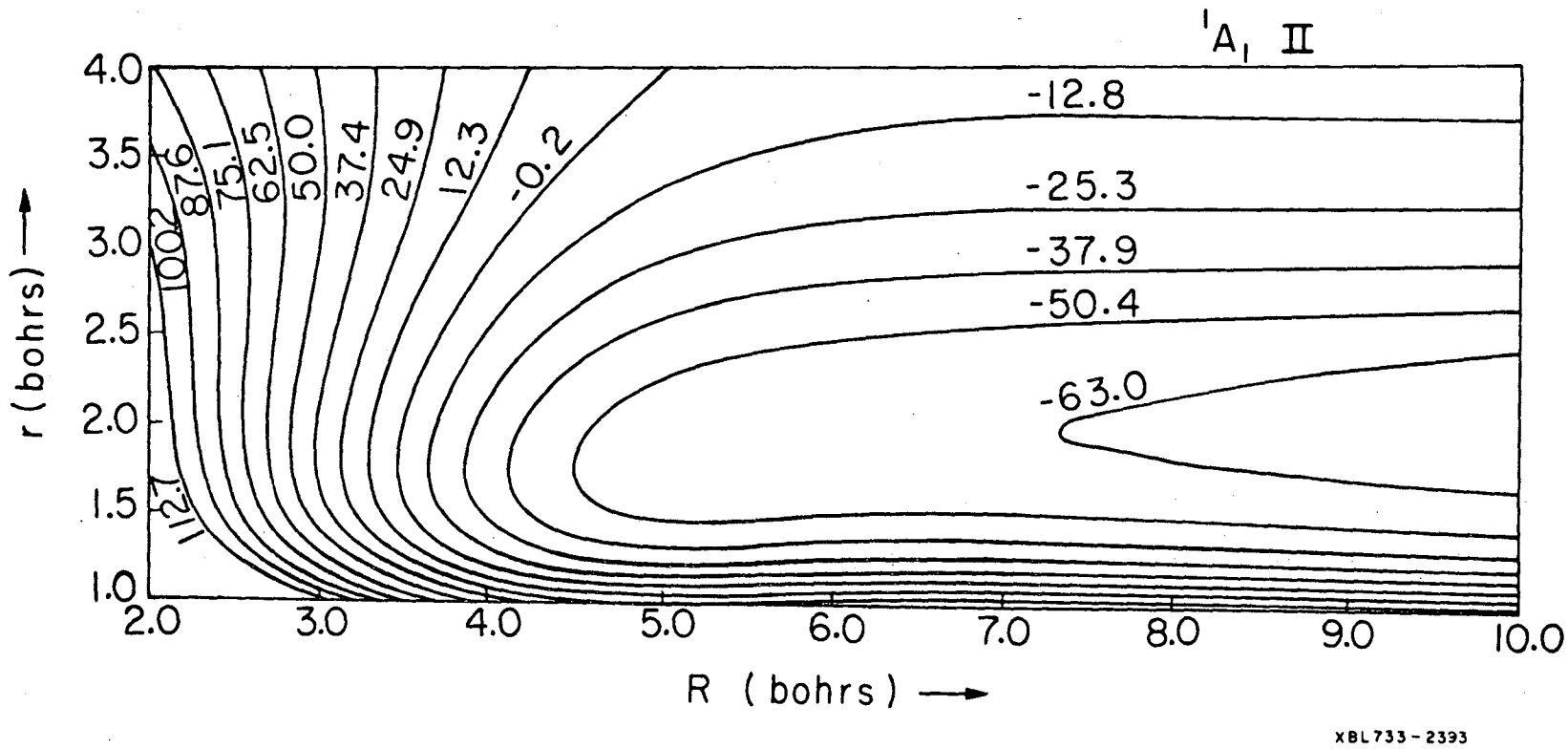
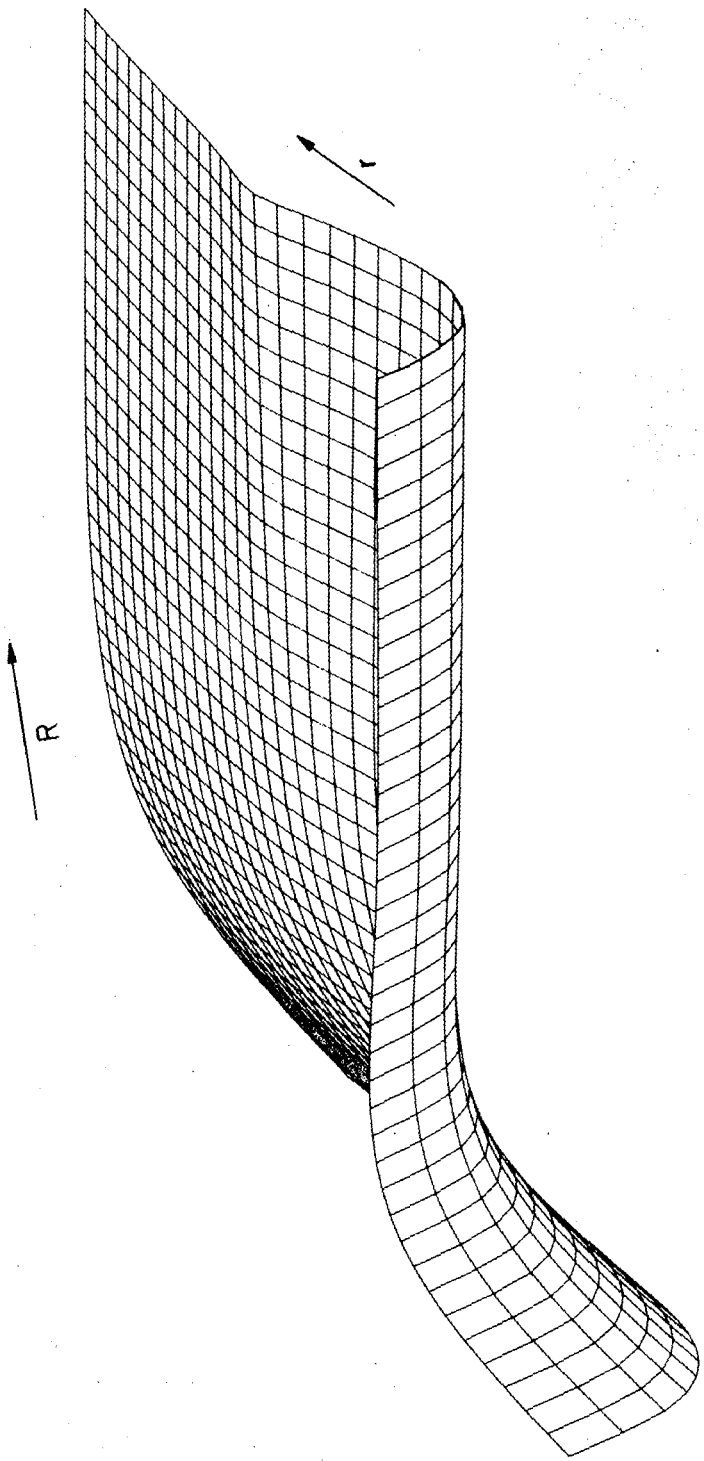
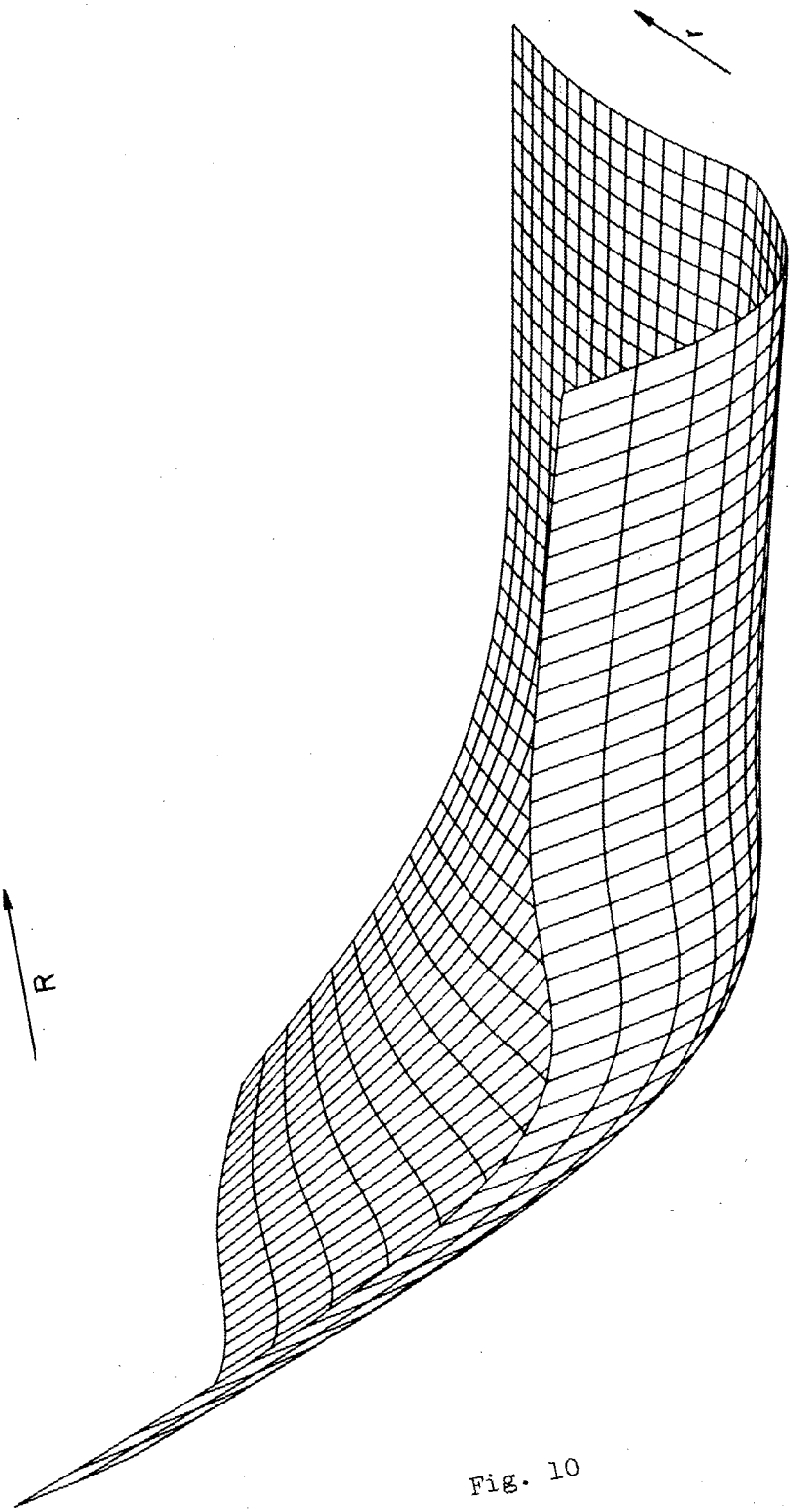

$^1A_1$ II
-12.8
-25.3
-37.9
-50.4
-63.0
100.2
87.6
75.1
62.5
50.0
37.4
24.9
12.3
-0.2
112.7
4.0
3.5
3.0
2.5
2.0
1.5
1.0
r (bohrs)
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
R (bohrs)
XBL733-2393

Fig. 8



XBL 733-2468

Fig. 9



XBL 733-2469

Fig. 10

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