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INTERACTION POTENTIAL BETWEEN TWO RIGID HF MOLECULES*

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ABSTRACT

As a prelude to the study of energy transfer in the HF-HF system, the potential energy surface for the interaction of two rigid HF molecules has been calculated within the ab initio self-consistent-field framework. A H(4s 1p/2s 1p), F(9s 5p 1d/4s 2p 1d) basis set of contracted gaussian function was employed. The number of unique points on the surface is greatly reduced by symmetry, and only 294 points were required to give a fairly complete description of the four-dimensional surface. Parts of the surface are illustrated by a series of contour maps. Some preliminary attempts to fit the surface to an analytic form are described. The equilibrium geometry of $(HF)_2$ is predicted.

INTORDUCTION

Over the past decade, experimental chemical physicists have become increasingly interested in energy transfer processes.[1,2] These processes may involve the excitation or relaxation of rotational, vibrational, or translational degrees of freedom. We subscribe to the view that it should be possible to study energy transfer problems by theoretical methods as well. An a priori theoretical study may readily be divided into two essentially independent parts: a) the determination of the potential energy surface from ab initio electronic wave functions, and b) the use of this surface to describe the collision dynamics, via classical trajectories or some more sophisticated approach. For systems with 30 or fewer electrons and 4 or fewer nuclei, the theoretical solution (to sufficient accuracy to make comparison with experiment meaningful) of both the electronic structure and dynamics problems now seen within reach.

Nevertheless, to date it appears that only the $He-H_2$[3-7] and Li^+-H_2[8-11] systems have succumbed to a priori theoretical energy transfer studies. And even then, in the former case, the long range part of the surface must be parameterized semi-empirically. In the vast majority of theoretical studies of energy transfer processes, a rough model potential surface is adopted and the dynamics are evaluated using any of a wide range of approximations, typical of which might be the discussion of A + BC vibrational excitation in one-dimension. However, this practice is becoming less acceptable as, according to Moore,[2] "experimental facts have forced model calculations out of the one-dimensional rut."

The present paper is the first in a series, the goal of which is to study energy transfer in the HF-HF system by a priori theoretical methods.

The choice of HF-HF is determined by its relative simplicity, as well as the unusual experimental interest[12] in this system. Here we report that part of the HF-HF potential energy surface appropriate to pure rotational excitation and relaxation. Later studies will deal with the remainder of the surface and the treatment of the dynamics by classical trajectory methods.

THEORETICAL APPROACH

A serious problem associated with the a priori calculation of potential energy surfaces is the fact that the dispersion attraction, due to the polarizabilities of the two molecules, is a very subtle correlation effect,[13] which has only been treated with a degree of reliability for very simple systems.[14] With this exception, it appears that the potential energy of two closed shell systems is well accounted for at the single configuration Hartree-Fock level of theory. This can be seen most readily from the work of Gilbert and Wahl[15] on He-He, Ne-Ne, and Ar-Ar. Except in the van der Waals region, their self-consistent-field potential curves provide very good agreement with experimental data.

Fortunately, for the HF-HF system the dispersion attraction is largely concealed by the much greater attraction due to dimer formation, i.e. hydrogen bonding. Hence, one expects the HF-HF potential surface to be rather reliably described at the Hartree-Fock level. And indeed, there is a large body of computational evidence[16] which suggests that single configuration self-consistent field (SCF) theory provides a qualitatively correct description of hydrogen bonding. Unfortunately, it does not at present appear possible to say whether SCF theory yields a quantitative description of hydrogen bonding. This is because the experimental uncertainties in certain crucial hydrogen bond energies, e.g., the H_2O and HF dimers, appear to be at least one kcal/mole.

One disclaimer must be appended to our contention that the HF-HF surface should be reliably obtained at the Hartree-Fock level. This situation will only hold for H-F bond distances (for the two distinguishable diatomics) near equilibrium. In particular, it is well known that for large r(H-F), the Hartree-Fock potential energy curve for the isolated HF molecule bears little resemblence to the experimental potential curve.[17] Hence it would be futile to attempt to use such a surface to describe any process involving the breakage of an HF bond, e.g., $HF + HF \rightarrow H_2 + F_2$. However, for the present project, our primary interest is in the HF molecule in its v = 0 and v = 1 vibrational states, and the HF potential curve is adequately described in this region at the SCF level.[18]

In choosing a set of analytic basis functions for the present work, a compromise was made in order to a) approach the Hartree-Fock limit fairly closely, and yet b) allow a relatively large number of points on the surface to be computed. In addition, reasonable predicted values of the molecular dipole and quadrupole moments were considered desirable. The basis set finally chosen is seen in Table I. The H atom basis is the 4s primitive set of Huzinaga,[19] contracted to 2s via Dunning.[20] A set of 2p functions with $\alpha = 0.7$ was then added as polarization functions.[13] For flourine, the comparable[19,20] (9s 5p/4s 2p) basis has been augmented with a set of d-like functions ($\alpha = 1.0$). In standard terminology,[13] such a basis set is called "double zeta plus polarization."

Using this basis, a potential energy curve was computed using the single-configuration $1\sigma^2\ 2\sigma^2\ 3\sigma^2\ 1\pi^4$ SCF method. This potential curve is seen in Table II. After spline fitting[21] these points, the one-dimensional Schrödinger equation was solved for the v = 0, 1, and 2 levels. These results are seen in Table III. In addition, Table III contains the calculated total energy, dipole moment, and

quadrupole moment at r = 1.733 bohr. Further, the spectroscopic constants[22] r_e, ω_e, B_e, $\omega_e x_e$, and x_e were obtained by fitting the five energetically lowest points to a function of the form $E(r) = a + b(r-r_e)^2 + c(r-r_e)^3 + d(r-r_e)^4$. Finally, these results have been compared with the SCF results, obtained with much larger basis sets, of Cade and Huo[18] and McLean and Yoshimine.[23]

Our calculated electric dipole moment is 0.01 debye greater than the near Hartree-Fock result and 0.12 debye greater than experiment. The calculated quadrupole moment appears to be only 5% less than experiment, but it should be pointed out that the experimental uncertainty is probably at least 10%. Nevertheless the general agreement is encouraging. One property for which the present SCF calculations yield a significantly more accurate result than that of Cade and Huo[18] is the bond distance r_e (and, consequently, B_e). This is a manifestation of the general trend[24] for SCF calculations using very large basis sets to predict bond distances significantly smaller than experiment. The other spectroscopic constants agree rather well with experiment, as do those from the more exhaustive calculations of Cade and Huo. The calculated vibrational energy levels will of course be very pertinent to our future work on vibrational energy transfer. For the present, let us note that the $v = 0 \rightarrow 1$ transition energy is overestimatedby 310 cm^{-1}, an error of about 7.8%. In general then, the results of Table II support our contention that the properties of HF near equilibrium are rather well represented by the single configuration SCF approximation using a double zeta plus polarization basis set.

The HF-HF SCF calculations were carried out in an analogous manner. Considerable savings can be made by fully exploiting symmetry in cases like F—H—H—F ($\theta_1 = 0°$, $\theta_2 = 180°$, $\phi = 0°$), where the point group is $D_{\infty h}$. However, there were sufficiently few of these high symmetry points that only two distinct cases were considered. In the general planar (C_s) case the wave function is of the form

$$1a'^2\ 2a'^2\ 3a'^2\ 4a'^2 5a'^2\ 6a'^2\ 7a'^2\ 8a'^2\ 1a''^2\ 2a''^2.$$

And for completely general geometry (the point group containing only the identity operation)

$$1a^2\ 2a^2\ 3a^2\ 4a^2\ 5a^2\ 6a^2\ 7a^2\ 8a^2\ 9a^2\ 10a^2.$$

THE SURFACE

Figure 1 gives the coordinate system chosen to describe the two rigid HF molecules, with internuclear separation 1.723 bohrs. The nuclear masses were taken to be exactly 1.0 and 19.0.

After some preliminary calculations, it was decided to study the surface for center-of-mass separations R = 3.0, 3.5, 4.0, 5.0, 6.0, and 8.0. For R < 3.0, the surface becomes quite repulsive, and for R > 8.0 it becomes less interesting. For each value of R, θ_1, θ_2, and ϕ were allowed to take on the values 0°, 45°, 90°, 135°, 180°, 225°, 270°, and 315°. If the three angular degrees of freedom were completely independent and unique from 0° - 360°, there would be $8^3 = 512$ points required to describe the surface for each of the six R values.

Fortunately, only 49 of these 512 points are unique and must be computed. Let us consider first the 64 possible planar ($\phi = 0°$) points. Figure 2

illustrates the fact that in general about one-fourth of the planar points are unique. In our case, due to the sparseness of the grid, 21 of the 64 points are unique. The conformations of these 21 unique points are shown in Fig. 3. For $\phi = 45°$ a related analysis shows that 26 of the 64 points are unique. However, for $\phi = 90°$ most of the 64 combinations of θ_1 and θ_2 are equivalent to $\phi = 0°$ points. In fact there are only two unique $\phi = 90°$ points not contained in the $\phi = 0°$ set. Further, all points with $\phi > 90°$ are equivalent to points in the range $0° \leqslant \phi \leqslant 90°$. The precise mapping of the complete 512 points into the unique 49 points is not reproduced here but may be obtained on request from the authors.

The 126 calculated planar energies are given in Table IV. In the same way the 168 unique nonplanar points are shown in Table V. The remainder of this paper consists of an analysis of these data.

Given the surface, our first questions relate to its qualitative features. In particular the relative energies of the planar and nonplanar points are of interest. Let us compare, for example, the 64 planar (ϕ=0°) points at R = 3, 5, and 8 bohrs with the nonplanar points with $\phi = 45°$. At R = 3, 13 of the planar points lie lower, while 47 of the $\phi = 45°$ points are lower, and four points are energetically identical. When $\phi = 0°$ is compared with $\phi = 90°$, only eight of the 64 $\phi = 0°$ points lie lower. Four points are equal and 52 of the $\phi = 90°$ points lie lower. Thus it can reasonably be stated that for short internuclear separations, nonplanar geometries are energetically favored. At R = 3, the nonplanarity provides a mechanism for the nuclei to avoid each other.

At R = 5 bohrs comparison of the $\phi = 0°$ and $\phi = 45°$ points shows 30 of the 0° energies lower, 4 equal, and 30 of the 45° energies lower. Comparing 0° and 90°, the three categories contain 28, 4, and 32 members. It appears then that near the equilibrium R value for the dimer, planar and nonplanar geometries are about equally favored.

Finally, at R = 8, the planar geometries become somewhat favored. Comparison between $\phi = 0°$ and $\phi = 45°$ shows that 33 of the planar points lie lower, 4 are identical, and 27 lie higher than the nonplanar points. The 0° = 90° comparison yields 34, 4, and 26 in the three categories.

In order to graphically depict parts of the planar (ϕ=0°) surface, we have made two-dimensional spline fits to the energies at R = 5,6, and 8. The resulting contour maps are seen in Figs. 4, 5, and 6. The primary trend seen, as expected, is the increasing complexity of the surface with decreasing R. We also obtained a spline fit for the planar surface at R = 4. However the fit was entirely unreasonable, predicting a well depth of 36 kcal/mole at $\theta_1 = 253°$, $\theta_2 = 214°$. This unfortunate result is due to the 45° intervals at which the surface was computed. As long as the surface is reasonably smooth, the spline fit from such a sparse grid is quite well behaved. However, at R = 4 changes of 45° in θ_1 and θ_2 result in severe changes in the potential energy, and although the spline fit reproduces all the calculated points, the regions in between are excessively bumpy. We suspect that a 15° grid would have to be used tc yield a physically reasonable spline fit at R = 4. The same problem arises to a much lesser degree at R = 5, Fig. 4. This is manifested in the predicted minimum (-4.77 kcal/mole) at $\theta_1 = 303.75°$, $\theta_2 = 123.75°$. An actual calculation at that point yields an energy of -3.87 kcal/mole.

Figure 7 gives a contour map of a part (ϕ=45°) of the nonplanar surface for R = 5.0. Comparison with the planar surface of Fig. 5 is interesting, as the two maps have many of the same features. However, the -3.6 kcal/mole and -4.0 kcal/mole contours near the center of the ϕ =0° map are conspicuously absent in the ϕ = 45° surface. This is a consequence of the fact that the ϕ = 45° cut does not have all the symmetry of the planar cuts, as illustrated in Fig. 2. More specifically, inspection of Fig. 7 shows that there is only inversion symmetry about the center (θ_1 = 180°, θ_2 = 180°) of the map.

PRELIMINARY EFFORTS TO FIND AN ANALYTIC REPRESENTATION OF THE SURFACE

In order to perform dynamics studies, e.g. classical trajectories,[25] it is usually necessary to be able to differentiate one's potential surface rapidly. This requirement would appear to eliminate several types of potential surfaces from contention. For example, the use of a four-dimensional (R, θ_1, θ_2, ϕ) spline function[21] would have the highly desirable property of exactly reproducing each of our 292 calculated total energies. However, such a surface would be extremely difficult to manipulate and make the dynamics calculations terribly time-consuming. Hence we turned to simpler forms for the surface.

Recently Berend and Thommarson[26] have reported a planar classical trajectory study of vibrational relaxation of HF and DF by HF and DF. Since their semiempirical surface was available, we decided to see how closely it conformed to our <u>ab initio</u> energies. In the surface of Berend and Thommarson,

the interaction between chemically bonded atoms is represented by Morse functions

$$V(r) = D_e[1 - e^{-\alpha(r-r_e)}]^2$$

with parameters taken from spectroscopic data. The interaction between non-bonded atom pairs is given as a sum of a Morse function and a second function designed to incorporate the effects of hydrogen bonding. The latter Coulomb function is constructed by representing HF as two partial point charges, located at the nuclei, i.e. $H^{+\delta}F^{-\delta}$. δ is chosen to classically reporduce the experimental dipole moment at the equilibrium internuclear separation.

For the Berend-Thommarson surface, the least squares deviation

$$\sqrt{\frac{\sum_{i=1}^{n} (E_{SCF}-E_{FIT})_i}{n-1}}$$

from the 294 <u>ab initio</u> points is 117.0 kcal/mole. However, the surface at R = 3.0 and R = 3.5 is everywhere so repulsive that it is likely to be rather unimportant in describing rotational energy transfer, i.e. that part of the surface is not likely to be sampled in our classical trajectory studies. Therefore it is important to break down the deviations as follows: R = 3.0, 201 kcal/mole; R = 3.5, 194 kcal/mole; R = 4.0, 76 kcal/mole; R = 5.0, 2.7 kcal/mole; R = 6.0, 0.69 kcal/mole; R = 8.0, 0.21 kcal/mole. These results demonstrate that the fit is strongly R dependent, and that the Berend-Thommarson surface appears to fail badly for smaller R values.

Next we attempted to fit the <u>ab initio</u> surface to the Berend-Thommarson[26] form, allowing all parameters - except the Morse functions describing the two HF bonds - to be determined by the fitting procedure. There are ten such parameters. After a few trial fits, all points with R = 3.0 and 3.5 were deleted from the procedure. As may be inferred from the previous paragraph, these repulsive

points (all with $E \geqslant +30$ kcal/mole) are simply not well described by such an analytic form. The remaining 196 points were fit to the Berend-Thommarson form with a least squares deviation of 1.4 kcal/mole. Although we are not particularly pleased with this fit, it does represent more than an order of magnitude in provement over the original form.[26]

A second possible function with which to fit the surface is that of London, Eyring, Polanyi, and Sato (LEPS). This type of valence bond potential surface has been used by Raff, Stivers, Porter, Thompson, and Sims[27] to describe the HI-HI interaction. In their work Raff et al., used a ten parameter function to describe the interaction between each of the three distinct pairs of atoms: HI, H_2, and I_2. If the same r_e value is used for both the singlet and triplet diatomic states, only nine parameters are needed.

There are of course already existing LEPS surfaces[28-32] for the triatomic systems HF_2 and FH_2 and in several cases these surfaces have been calibrated to reproduce the experimentally observed dynamics for the exothermic reactions $F + H_2 \rightarrow FH + H$ and $H + F_2 \rightarrow HF + F$. Further, the qualitative features of these surfaces have been verified by <u>ab initio</u> theory.[33,34] It would of course be extremely encouraging to find that these empirical LEPS parameters could be transferred from HF_2 and FH_2 to the four-atom system HF-HF. Therefore it seemed of value to construct an LEPS surface for HF-HF from Blais' triatomic parameters,[28] which have also been used by Thompson in a trajectory studies[35] of F + HF and H + HF vibrational relazation. For this LEPS surface, the least squares deviation from the 294 <u>ab initio</u> points is 99.0 kcal/mole. Further broken down into separate R values, we find: R = 3.0, 152 kcal/mole; R = 3.5, 181 kcal/mole; R = 4.0, 67 kcal/mole; R = 5.0, 4.9 kcal/mole; R = 6.0, 2.6 kcal/mole;

R = 8.0, 1.1 kcal/mole. The LEPS surface thus displays the same tendency to large deviations for small R as does the Berend-Thommarson[26] form. However, the LEPS form is somewhat more accurate for R = 3.0, 3.5, and 4.0, and less accurate for R = 5.0, 6.0, and 8.0.

If one fixes the ten LEPS parameters of the two bonded HF molecules, there remain 30 additional parameters. Adjusting these 30 parameters to provide the best fit for our 194 ab initio energies ($R \geqslant 4.0$), a least squares deviation of $\sim$ 3.3 kcal/mole was found. This was somewhat of a surprise, since the Berend-Thommarson form, with only ten adjustable parameters, yielded a deviation of 1.4 kcal/mole. This result seemed to imply that the partial-point-charge dipole-dipole term in the latter form might be quite valuable. So this term and the adjustable parameter δ were added to the LEPS form, to give a total of 31 adjustable parameters. The resultant least squares deviation was 1.2 kcal, a large improvement. Thus, it appears that something comparable to the dipole-dipole term in the Berend-Thommarson form is a necessary component of any reasonable analytic fit to the HF-HF potential energy surface.

Our purpose here has not been to present an accurate analytic form for the HF-HF surface. It became clear to us shortly after our fitting procedures began that this is a very difficult job, perhaps one for which we are not best suited. Therefore we have only provided a sketch of our own experience to date. It is our hope that others will be encouraged to search for and find an accurate form for the present ab initio surface.

$(HF)_2$ EQUILIBRIUM GEOMETRY

After the water dimer, the hydrogen fluoride dimer is probably the most frequently cited[16,36] example of hydrogen bonding in the gas phase. Nevertheless, even the dimerization energy has not been definitively established experimentally, although most estimates[37,38] seem to fall in the range 6.0±1.5 kcal/mole. The most interesting experimental work of the past decade is that of Dyke, Howard, and Klemperer,[39] who used the molecular beam electric resonance technique. They determined a good deal about the equilibrium geometry, as well as discovering "a unique hydrogen tunneling motion involving the breaking and reforming of the hydrogen bond."

Ab initio SCF studies of $(HF)_2$ near equilibrium have been reported by Kollman and Allen,[40] Diercksen and Kraemer,[41] and Del Bene and Pople.[42] Diercksen and Kraemers used the largest basis set and (assuming $\theta_1 = 0°$) predict $\theta_2 = 60°$, r(F-F) = 2.85Å, and a dimerization energy of 4.5 kcal/mole. Del Bene, and Pople carried out an exhaustive geometry search using a minimum basis set and predict a planar equilibrium structure with $\theta_1 = 356°$, $\theta_2 = 69°$, R(F-F) = 2.55Å. Their predicted dimerization energy was 5.2 kcal/mole. For comparison, the experimental work of Klemperer and coworkers[40] seems to establish $\theta_1 \approx 0°$, $\theta_2 = 60\text{-}70°$, and R(F-F) = 2.79Å.

Initially, we were reluctant to search for the $(HF)_2$ minimum, since we were concerned that it would distract us from our primary goal, determining the entire surface in terms of a relatively coarse grid. However, in the end, it required relatively little effort to locate the minimum. Table IV shows that the lowest calculated planar energy occurs for R = 5, $\theta_1 = 0°$, $\theta_2 = 45°$.

Since the planar part of the surface was completed before going on to the non-planar points, we decided to search for the minimum starting from the above point. Minimization of the total energy with respect to R yielded R = 5.29 bohrs. Then θ_2 was varied as is shown in Table VI. As expected from Pople's calculations[43] and Klemperer's experimental work,[40] the energy is relatively insensitive to θ_2. The predicted minimum is at $\theta_2 = 52.2°$, in reasonable agreement with the earlier values, all in the range 60-70°. Note that the difference between the energies for $\theta_2 = 50°$ and $\theta_2 = 60°$ is only 0.045 kcal/mole.

Interestingly Table V shows that the lowest nonplanar energy (R = 5, $\theta_1 = 0°$, $\theta_2 = 45°$, $\phi = 45°$) is actually lower by 0.05 kcal than the lowest planar energy. Since this suggests the equilibrium geometry may be nonplanar, the energy was minimized with respect to ϕ for R = 5.29, $\theta_1 = 0°$, and $\theta_2 = 52.2°$. These results are seen in Table VII, which appears to demonstrate that the equilibrium geometry of $(HF)_2$ is planar. It is undeniable that in going from R = 5 to R = 5.29 bohrs, the planar geometries become favored. This is another example of the trend, discussed earlier, for smaller R values to energetically favor nonplanar geometries.

Finally, the energy was varied with respect to θ_1, for R = 5.29, $\theta_2 = 52.2°$, and $\phi = 0°$. The results are seen in Table VIII, which shows the SCF energy at $\theta_2 = 350°$ to be 0.0075 kcal/mole higher than that at $\theta_2 = 0°$. Interpolation gives our final predicted equilibrium geometry: R = 5.29, $\theta_1 = 355.2°$, $\theta_2 = 52.2°$, $\phi = 0°$. The dimer dissociation energy D_e is -4.63 kcal/mole, in essential agreement with experiment,[37,38] 6.0±1.5. Although a further refinement of the predicted equilibrium geometry could be carried out, our final geometry is sufficiently close to that found from the coarse grid that additional changes should be quite small.

FOOTNOTES AND REFERENCES

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Table I. Basis set of contracted gaussian functions for HF-HF.

Atom	Type	Exponent α	Coefficient
H	s	13.3615	0.032 828
	s	2.0133	0.231 207
	s	0.4538	0.817 233
	s	0.1233	1.0
	p_x, p_y, p_z	0.7	1.0
F	s	9994.7900	0.002017
	s	1506.0300	0.015 295
	s	350.2690	0.073 110
	s	104.0530	0.246 420
	s	34.8432	0.612 593
	s	4.3688	0.242 489
	s	12.2164	1.0
	s	1.2078	1.0
	s	0.3634	1.0
	p_x, p_y, p_z	44.3555	0.020 868
	p_x, p_y, p_z	10.0820	0.130 092
	p_x, p_y, p_z	2.9959	0.396 219
	p_x, p_y, p_z	0.9383	0.620 368
	p_x, p_y, p_z	0.2733	1.0
	d_{xx}, d_{yy}, d_{zz}, d_{xy}, d_{xz}, d_{yz}	0.7	1.0

Table II. Potential energy curve for the HF diatomic molecule.

R(H-F), bohrs	E(hartrees)
1.1328	-99.748 794
1.2328	-99.872 032
1.3328	-99.951 091
1.4328	-99.999 846
1.5328	-100.027 661
1.6328	-100.040 948
1.7328	-100.044 156
1.8328	-100.040 419
1.9328	-100.031 962
2.0328	-100.020 372
2.1328	-100.006 780
2.2328	-99.991 985
2.3328	-99.976 549
2.4328	-99.960 864
2.5328	-99.945 207

Table III. Predicted and experimental properties of diatomic HF.

	SCF Present Work	Near Hartree-Fock	Experiment
Total Energy(hartrees) at R = 1.7328	-100.0442	-100.0705[a]	
Dipole moment (debye)	1.94	1.93[a]	1.82[b]
Quadrupole moment (10^{-26} esu cm^2)	2.48	2.33[a]	2.6[c]
r_e (bohrs)	1.723	1.696[d]	1.733[e]
ω_e (cm^{-1})	4460	4469[d]	4139[e]
B_e (cm^{-1})	21.363	21.868[d]	20.956[e]
$\omega_e x_e$ (cm^{-1})	97.92	80.34[d]	90.05[e]
α_e (cm^{-1})	0.753	0.769[d]	0.796[e]
From Solution of Vibrational Schrödinger Equation			
E (v = -1/2)	-2202		
E (v = 0)	0		0
E (v = 1)	4272		3962
E (v = 2)	8383		7751

[a]Ref. 23.

[b]R. Weiss, Phys. Rev. 131, 659 (1963).

[c]D. E. Stogryn and A. P. Stogryn, Mol. Phys. 11, 371 (1966).

[d]Ref. 18.

[e]D. E. Mann, B. A. Thrush, D. R. Lide, J. J. Ball, and N. Acquista, J. Chem. Phys. 34, 420 (1961).

Table IV. Calculated total energies for planar HF-HF. R, θ_1, and θ_2 are defined in Figure 1. The final column gives the energy in kcal/mole relative to two separated HF molecules.

R (bohrs)	θ_1 (degrees)	θ_2 (degrees)	E (hartrees)	E ($\frac{kcal}{mole}$)
3.0	0	0	-199.629107	288.196
		45	-199.668460	263.502
		90	-199.719377	231.552
		135	-199.629684	287.834
		180	-197.267468	1770.125
	45	0	-199.894681	121.549
		45	-199.887396	126.120
		90	-199.847161	151.367
		135	-199.328042	477.115
	90	0	-199.920623	105.270
		45	-199.180032	569.991
		90	-199.902411	116.698
	135	0	-199.912357	110.457
		45	-199.902516	116.632
	180	0	-199.917339	107.331
	225	45	-199.905551	114.728
		90	-199.912258	110.519
		135	-199.883994	128.255
	270	90	-199.923355	103.556
		135	-199.907220	113.680
	315	135	-199.917064	107.503

Table IV. (Cont'd.)

R (bohrs)	θ_1 (degrees)	θ_2 (degrees)	E (hartrees)	E ($\frac{kcal}{mole}$)
3.5	0	0	-199.972143	72.941
		45	-199.984014	65.492
		90	-199.991713	60.661
		135	-199.897943	119.502
		180	-196.772882	2080.478
	45	0	-200.026871	38.599
		45	-200.022011	41.649
		90	-199.998312	56.520
		135	-199.841834	154.710
	90	0	-200.031947	35.414
		45	-200.025546	39.431
		90	-200.019285	43.360
	135	0	-200.028162	37.789
		45	-200.023052	40.996
	180	0	-200.030997	36.010
	225	45	-200.024829	39.881
		90	-200.028176	37.781
		135	-200.022712	41.209
	270	90	-200.034280	33.950
		135	-200.034461	33.837
	315	135	-200.037522	31.916

Table IV. (Cont'd.)

R (bohrs)	θ_1 (degrees)	θ_2 (degrees)	E (hartrees)	E ($\frac{kcal}{mole}$)
4.0	0	0	-200.062561	16.204
		45	-200.066651	13.637
		90	-200.065888	14.116
		135	-200.006444	51.417
		180	-199.568759	326.065
	45	0	-200.072116	10.208
		45	-200.069060	12.126
		90	-200.054047	21.546
		135	-199.990885	61.181
	90	0	-200.069385	11.922
		45	-200.065619	14.285
		90	-200.060938	17.222
	135	0	-200.067029	13.400
		45	-200.064394	15.054
	180	0	-200.068346	12.574
	225	45	-200.065668	14.254
		90	-200.067986	12.800
		135	-200.070749	11.066
	270	90	-200.072157	10.182
		135	-200.077466	6.851
	315	135	-200.078307	6.323

Table IV. (Cont'd.)

R (bohrs)	θ_1 (degrees)	θ_2 (degrees)	E (hartrees)	E ($\frac{kcal}{mole}$)
5.0	0	0	-200.094130	-3.606
		45	-200.095178	-4.263
		90	-200.092621	-2.659
		135	-200.070811	11.027
		180	-200.019175	43.429
	45	0	-200.090814	-1.525
		45	-200.089460	-0.675
		90	-200.082428	3.737
		135	-200.065583	14.308
	90	0	-200.086079	1.446
		45	-200.084544	2.410
		90	-200.082276	3.833
	135	0	-200.084449	2.469
		45	-200.083704	2.937
	180	0	-200.084568	2.395
	225	45	-200.084521	2.424
		90	-200.086361	1.269
		135	-200.091270	-1.811
	270	90	-200.088986	-0.378
		135	-200.093979	-3.511
	315	135	-200.093168	-3.002

Table IV. (Cont'd.)

R (bohrs)	θ_1 (degrees)	θ_2 (degrees)	E (hartrees)	E ($\frac{kcal}{mole}$)
6.0	0	0	-200.094098	-3.586
		45	-200.094411	-3.782
		90	-200.092307	-2.462
		135	-200.082158	3.907
		180	-200.067838	12.893
	45	0	-200.091299	-1.829
		45	-200.090375	-1.249
		90	-200.086567	1.140
		135	-200.079555	5.540
	90	0	-200.087961	0.265
		45	-200.087127	0.789
		90	-200.085925	1.543
	135	0	-200.086739	1.032
		45	-200.086483	1.193
	180	0	-200.086584	1.130
	225	45	-200.087085	0.815
		90	-200.088504	-0.075
		135	-200.091893	-2.202
	270	90	-200.090178	-1.126
		135	-200.092989	-2.890
	315	135	-200.091647	-2.048

Table IV. (Cont'd.)

R (bohrs)	θ_1 (degrees)	θ_2 (degrees)	E (hartrees)	E ($\frac{kcal}{mole}$)
8.0	0	0	-200.090769	-1.497
		45	-200.090693	-1.449
		90	-200.089505	-0.703
		135	-200.086006	1.492
		180	-200.082876	3.456
	45	0	-200.089634	-0.784
		45	-200.089107	-0.454
		90	-200.087582	0.503
		135	-200.085395	1.876
	90	0	-200.088150	0.147
		45	-200.087748	0.399
		90	-200.087267	0.701
	135	0	-200.087492	0.560
		45	-200.087407	0.613
	180	0	-200.087360	0.643
	225	45	-200.087762	0.390
		90	-200.088530	-0.092
		135	-200.089955	-0.986
	270	90	-200.089245	-0.540
		135	-200.090077	-1.062
	315	135	-200.088963	-0.363

Table V. Nonplanar total energies for HF-HF. Coordinates are defined in Figure 1. The final column gives the energy relative to two separated HF molecules.

R(bohrs)	θ_1(degrees)	θ_2(degrees)	ϕ(degrees)	E(hartrees)	E($\frac{kcal}{mole}$)
3.0	0	45	45	-199.690034	249.965
		135	45	-199.696536	245.885
	45	0	45	-199.891502	123.543
		45	45	-199.887690	125.935
		90	45	-199.870563	136.683
		135	45	-199.826666	164.228
		180	45	-199.861678	142.258
	90	0	45	-199.912694	110.245
		45	45	-199.909415	112.303
		90	45	-199.909097	112.503
		135	45	-199.899644	118.434
	135	0	45	-199.905064	115.033
		45	45	-199.903882	115.775
		90	45	-199.910998	111.310
		135	45	-199.907067	113.776
	180	45	45	-199.913228	109.910
		135	45	-199.915023	108.784
	225	45	45	-199.905445	114.794
		90	45	-199.912701	110.241
		135	45	-199.908438	112.916
	270	45	45	-199.913305	109.862
		90	45	-199.922869	103.861
		135	45	-199.921429	104.764
	315	45	45	-199.891944	123.266
		90	45	-199.908026	113.175
		135	45	-199.913480	109.752
	45	0	90	-199.899292	118.655
	90	0	90	-199.918818	106.403

Table V. (Cont'd.)

R(bohrs)	θ_1(degrees)	θ_2(degrees)	ϕ(degrees)	E(hartrees)	E($\frac{kcal}{mole}$)
3.5	0	45	45	-199.989790	61.868
		135	45	-199.957934	81.857
	45	0	45	-200.024959	39.799
		45	45	-200.021621	41.894
		90	45	-200.009593	49.441
		135	45	-199.983317	65.930
		180	45	-199.999714	55.640
	90	0	45	-200.027890	37.960
		45	45	-200.025251	39.616
		90	45	-200.023394	40.781
		135	45	-200.020571	42.553
	135	0	45	-200.024415	40.141
		45	45	-200.023425	40.762
		90	45	-200.026459	38.858
		135	45	-200.027707	38.075
	180	45	45	-200.028287	37.711
		135	45	-200.032410	35.124
	225	45	45	-200.024574	40.041
		90	45	-200.028294	37.706
		135	45	-200.029350	37.044
	270	45	45	-200.028465	37.599
		90	45	-200.033618	34.366
		135	45	-200.035698	33.060
	315	45	45	-200.025824	39.256
		90	45	-200.033471	34.458
		135	45	-200.033759	34.277
	45	0	90	-200.026173	39.037
	90	0	90	-200.030138	36.549

Table V. (Cont'd.)

R(bohrs)	θ_1(degrees)	θ_2(degrees)	ϕ(degrees)	E(hartrees)	E($\frac{kcal}{mole}$)
4.0	0	45	45	-200.068340	12.578
		135	45	-200.041860	29.194
	45	0	45	-200.071243	10.756
		45	45	-200.068590	12.421
		90	45	-200.060267	17.643
		135	45	-200.045233	27.077
		180	45	-200.054184	21.461
	90	0	45	-200.067440	13.142
		45	45	-200.065501	14.359
		90	45	-200.063703	15.487
		135	45	-200.063755	15.455
	135	0	45	-200.065278	14.499
		45	45	-200.064615	14.915
		90	45	-200.066291	13.863
		135	45	-200.069431	11.893
	180	45	45	-200.067114	13.347
		135	45	-200.072053	10.248
	225	45	45	-200.065544	14.332
		90	45	-200.067953	12.820
		135	45	-200.070939	10.947
	270	45	45	-200.068127	12.711
		90	45	-200.071502	10.593
		135	45	-200.074632	8.629
	315	45	45	-200.072158	10.182
		90	45	-200.076143	7.681
		135	45	-200.075126	8.319
	45	0	90	-200.070489	11.229
	90	0	90	-200.068603	12.413

Table V. (Cont'd.)

R(bohrs)	θ_1(degrees)	θ_2(degrees)	ϕ(degrees)	E(hartrees)	E($\frac{kcal}{mole}$)
5.0	0	45	45	-200.095252	-4.310
		135	45	-200.082121	3.930
	45	0	45	-200.090808	-1.521
		45	45	-200.069247	12.008
		90	45	-200.084883	2.197
		135	45	-200.079206	5.759
		180	45	-200.082872	3.459
	90	0	45	-200.085717	1.674
		45	45	-200.084679	2.325
		90	45	-200.083703	2.937
		135	45	-200.084876	2.201
	135	0	45	-200.084202	2.624
		45	45	-200.083970	2.770
		90	45	-200.084944	2.159
		135	45	-200.088011	0.234
	180	45	45	-200.084653	2.341
		135	45	-200.089005	-0.390
	225	45	45	-200.084626	2.358
		90	45	-200.086226	1.354
		135	45	-200.089240	-0.539
	270	45	45	-200.086468	1.202
		90	45	-200.088398	-0.009
		135	45	-200.090868	-1.559
	315	45	45	-200.091623	-2.032
		90	45	-200.092930	-2.853
		135	45	-200.091488	-1.948
	45	0	90	-200.089588	-0.756
	90	0	90	-200.086453	1.212

Table V. (Cont'd.)

R(bohrs)	θ_1(degrees)	θ_2(degrees)	ϕ(degrees)	E(hartrees)	E($\frac{kcal}{mole}$)
6.0	0	45	45	-200.094247	-3.679
		135	45	-200.086845	0.966
	45	0	45	-200.091305	-1.833
		45	45	-200.090286	-1.194
		90	45	-200.087791	0.372
		135	45	-200.084865	2.208
		180	45	-200.086547	1.153
	90	0	45	-200.087940	0.279
		45	45	-200.087305	0.677
		90	45	-200.086749	1.026
		135	45	-200.087553	0.521
	135	0	45	-200.086825	0.978
		45	45	-200.086742	1.030
		90	45	-200.087392	0.622
		135	45	-200.089380	-0.625
	180	45	45	-200.086962	0.892
		135	45	-200.089958	-0.988
	225	45	45	-200.087233	0.722
		90	45	-200.088364	0.013
		135	45	-200.090334	-1.224
	270	45	45	-200.088563	0.112
		90	45	-200.089740	-0.851
		135	45	-200.091076	-1.689
	315	45	45	-200.091881	-2.194
		90	45	-200.092301	-2.458
		135	45	-200.090946	-1.608
	45	0	90	-200.090311	-1.209
	90	0	90	-200.088436	-0.033

Table V. (Cont'd.)

R(bohrs)	θ_1(degrees)	θ_2(degrees)	ϕ(degrees)	E(hartrees)	E($\frac{kcal}{mole}$)
8.0	0	45	45	-200.090501	-1.328
		135	45	-200.087427	0.601
	45	0	45	-200.089568	-0.743
		45	45	-200.089055	-0.421
		90	45	-200.088004	0.238
		135	45	-200.086894	0.935
		180	45	-200.087311	0.673
	90	0	45	-200.088253	0.082
		45	45	-200.087857	0.331
		90	45	-200.087610	0.486
		135	45	-200.087917	0.293
	135	0	45	-200.087596	0.494
		45	45	-200.087563	0.515
		90	45	-200.087880	0.316
		135	45	-200.088743	-0.225
	180	45	45	-200.087629	0.474
		135	45	-200.089064	-0.427
	225	45	45	-200.087850	0.335
		90	45	-200.088433	-0.031
		135	45	-200.089271	-0.557
	270	45	45	-200.088520	-0.085
		90	45	-200.089005	-0.390
		135	45	-200.089385	-0.628
	315	45	45	-200.089818	-0.900
		90	45	-200.089765	-0.867
		135	45	-200.088904	-0.326
	45	0	90	-200.088939	-0.348
	90	0	90	-200.088359	0.016

Table VI. Variation of the total energy (in kcal/mole relative to HF + HF) as a function of θ_2, with the following parameters held fixed: R = 5.29 bohrs, θ_1 = 0°, and ϕ = 0°.

θ_2	Energy (kcal/mole)
25°	-4.2745
30°	-4.3524
35°	-4.4292
40°	-4.4981
45°	-4.5512
50°	-4.5806
55°	-4.5781
60°	-4.5354
65°	-4.4443
70°	-4.2970
75°	-4.0857

Table VII. Variation in the total energy (in kcal/mole relative to HF + HF) as a function of ϕ, with the following parameters held fixed: R = 5.29 bohrs, $\theta_1 = 0°$, and $\theta_2 = 52.2°$.

ϕ	Energy (kcal/mole)
0°	-4.5839
10°	-4.5836
20°	-4.5788
30°	-4.5584
40°	-4.5052
50°	-4.3982
60°	-4.2143
70°	-3.9313
80°	-3.0000
90°	-2.9921

Table VIII. Variation of the SCF energy (in kcal/mole relative to HF + HF) as a function of θ_2 with the following parameters held fixed.

θ_2	Energy (kcal/mole)
330°	-3.5849
340°	-4.1998
350°	-4.5764
0°	-4.5839
10°	-4.1608
20°	-3.3695
30°	-2.3690

FIGURE CAPTIONS

Fig. 1. Coordinate system chosen for HF-HF. R is the distance between the two HF centers of mass. The angle ϕ is defined with respect to the indicated y axis. ϕ is the angle of rotation of the right-hand HF molecule about this y axis.

Fig. 2. Qualitative picture of equivalences among different planar geometries of HF-HF. θ_1 and θ_2 are defined in Fig. 1. The unique points are a) those contained on the four darkened lines, plus b) those in the shaded regions I and II. Points in regions labeled I' are equivalent to those in I, and points in II' are equivalent to those in II. There is inversion symmetry about the center of the square, and mirror symmetry about the indicated diagonals bisecting each quadrant.

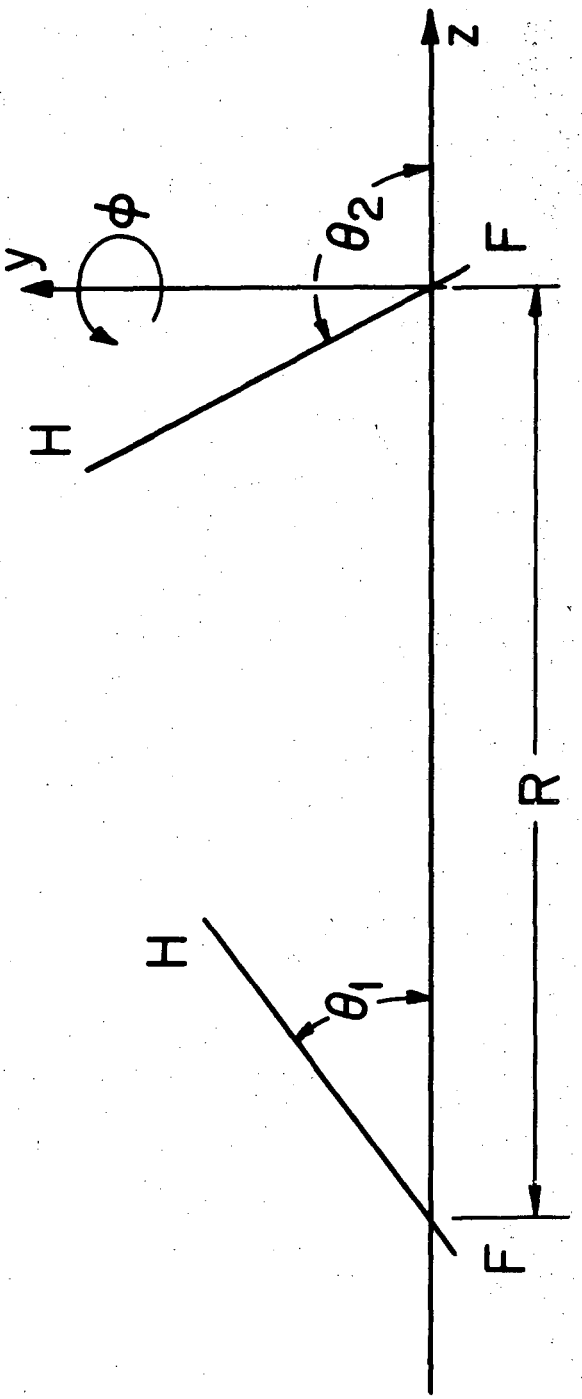
Fig. 3. Unique planar ($\phi = 0°$) geometries for HF-HF, assuming θ_1 and θ_2 both begin at 0° and increase in increments of 45°.

Fig. 4. Contour map of that part of the HF-HF potential surface with R = 5 bohrs and $\phi = 0°$ (planar). θ_1 and θ_2 are defined in Fig. 1, and contours are marked in kcal/mole relative to two infinitely separated HF molecules. Each HF molecule has fixed internuclear separation 1.723 bohrs.

Fig. 5. HF-HF potential surface: R = 6 bohrs, $\phi = 0°$ (planar).

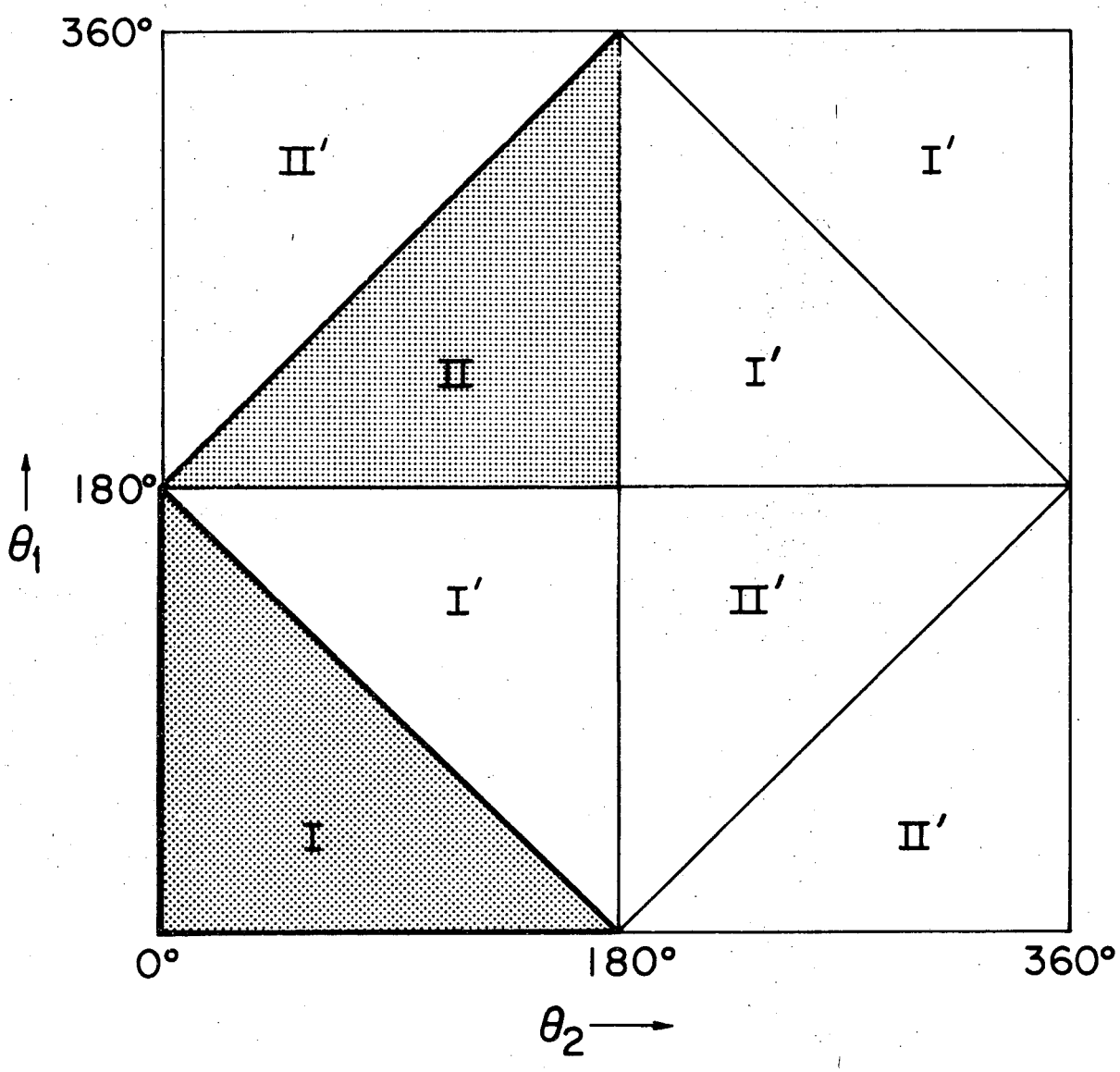
Fig. 6. HF-HF potential surface: R = 8 bohrs, $\phi = 0°$ (planar).

Fig. 7. A nonplanar cut ($\phi = 45°$) of the HF-HF potential surface for R = 5 bohrs.



XBL738-3761

Fig. 1



XBL737-3454

Fig. 2

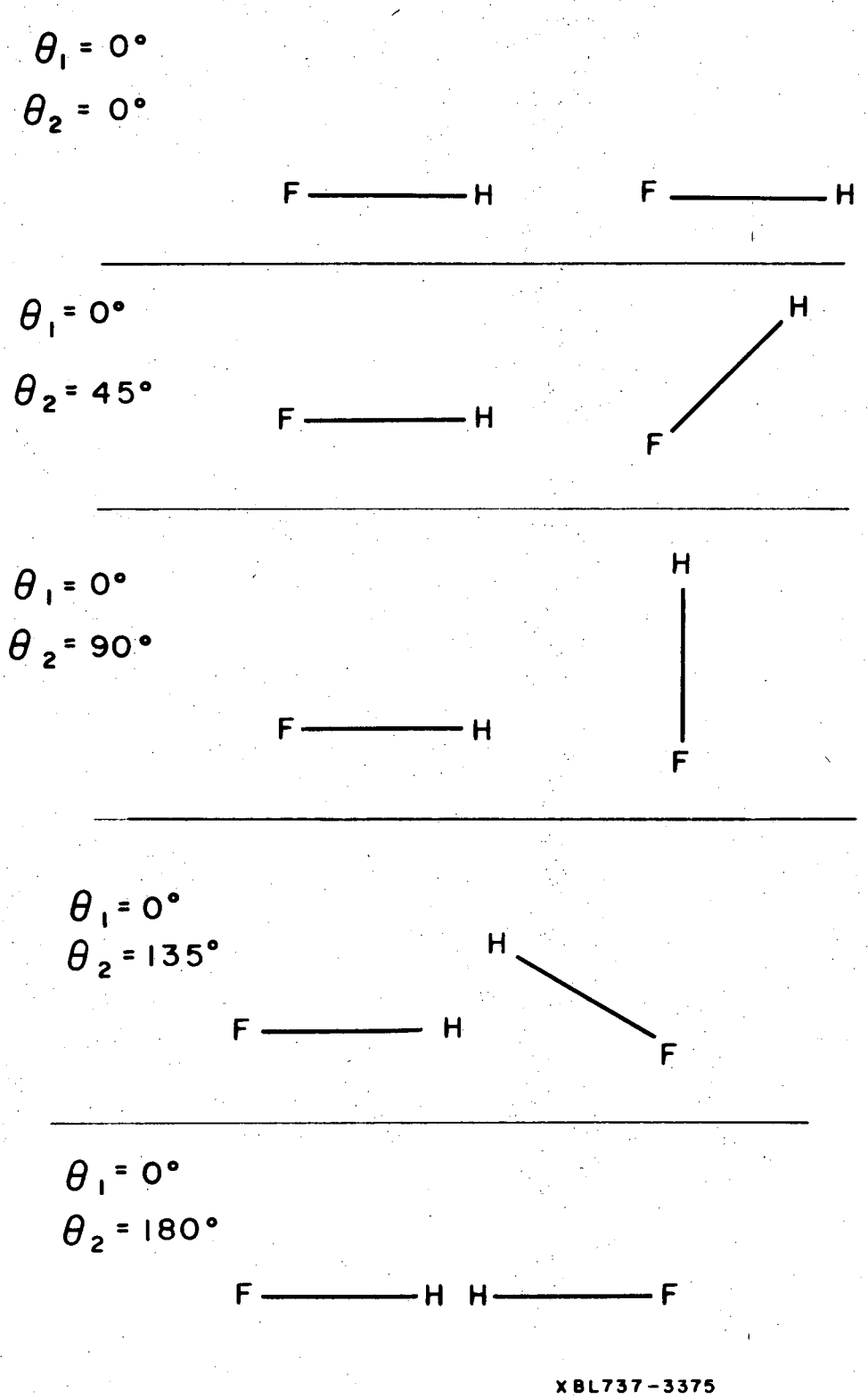

θ1 = 0°
θ2 = 0°
F H
F H
θ1 = 0°
θ2 = 45°
F H
H
F
θ1 = 0°
θ2 = 90°
F H
H
F
θ1 = 0°
θ2 = 135°
F H
H
F
θ1 = 0°
θ2 = 180°
F H H F
XBL737-3375

Fig. 3a

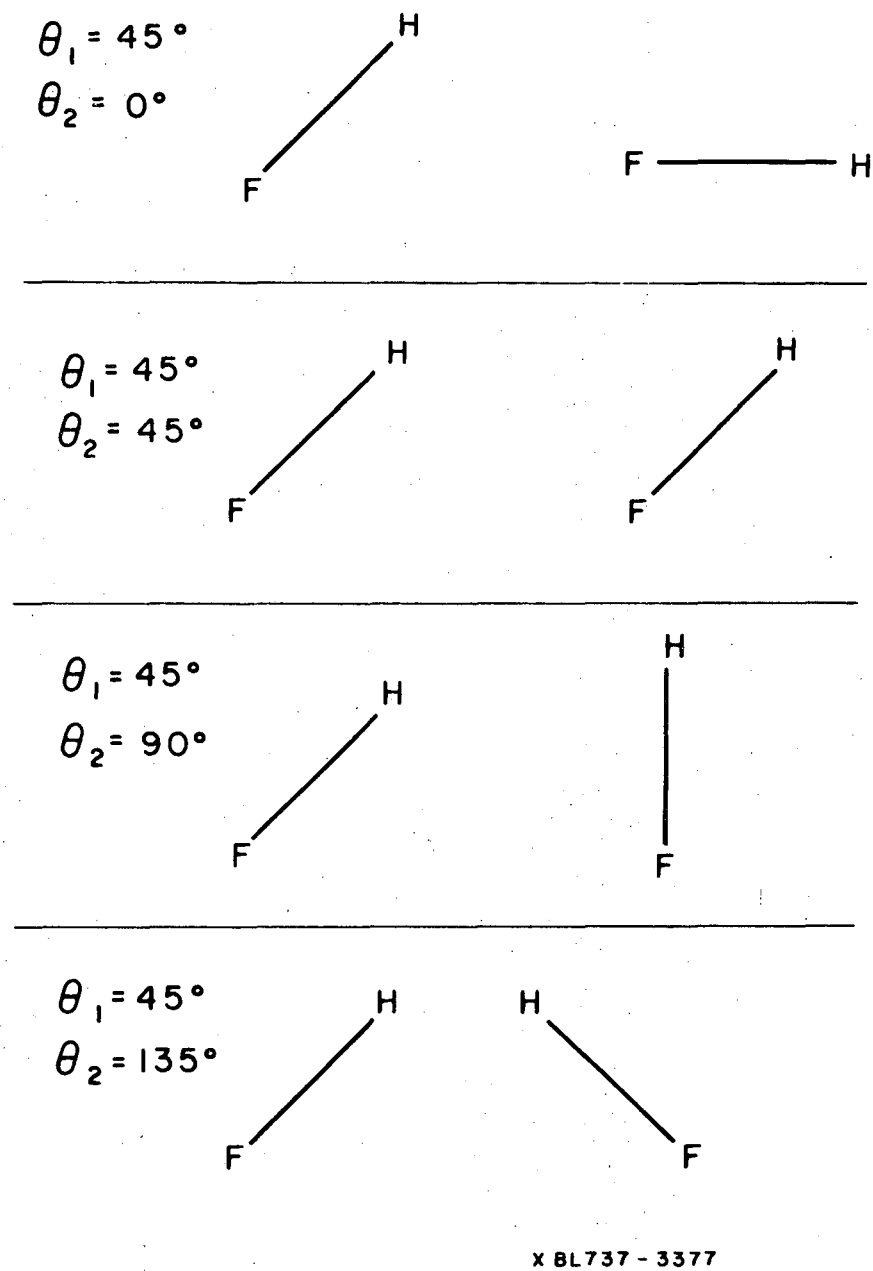

θ1 = 45°
θ2 = 0°
H
F
F
H
θ1 = 45°
θ2 = 45°
H
F
H
F
θ1 = 45°
θ2 = 90°
H
F
H
F
θ1 = 45°
θ2 = 135°
H
F
H
F
X BL737-3377

Fig. 3b

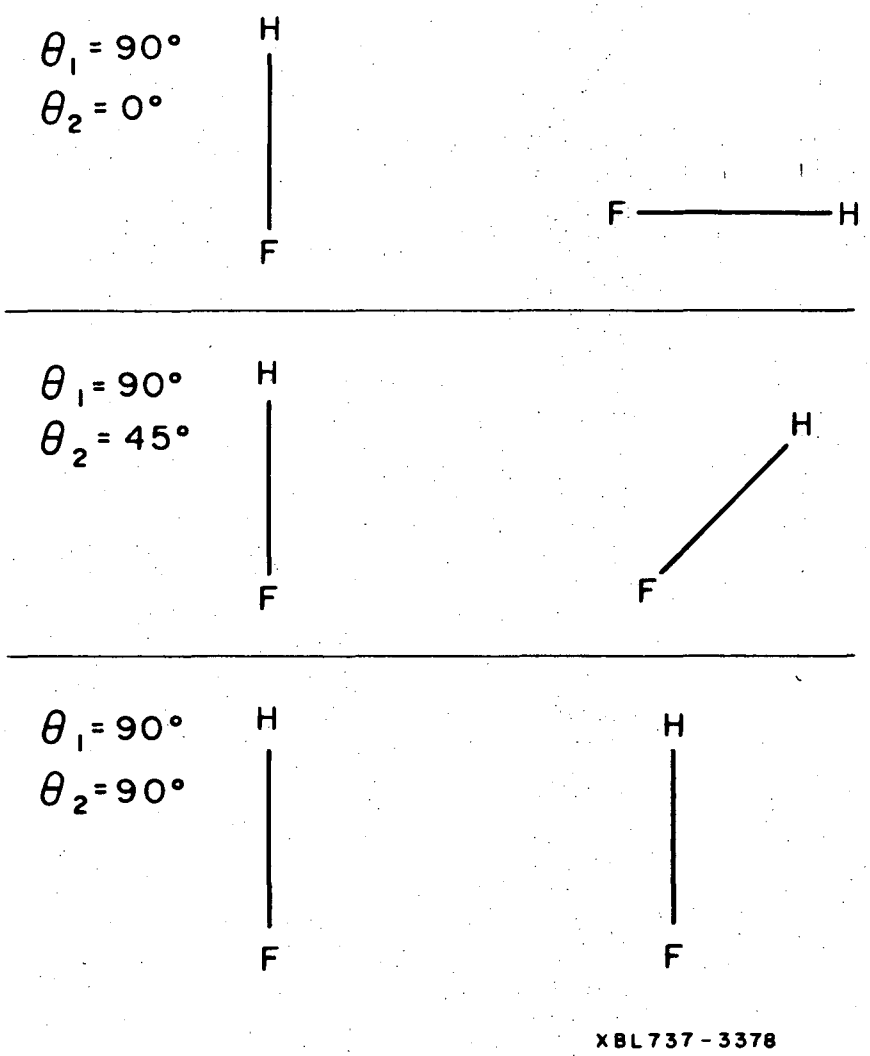


Fig. 3c

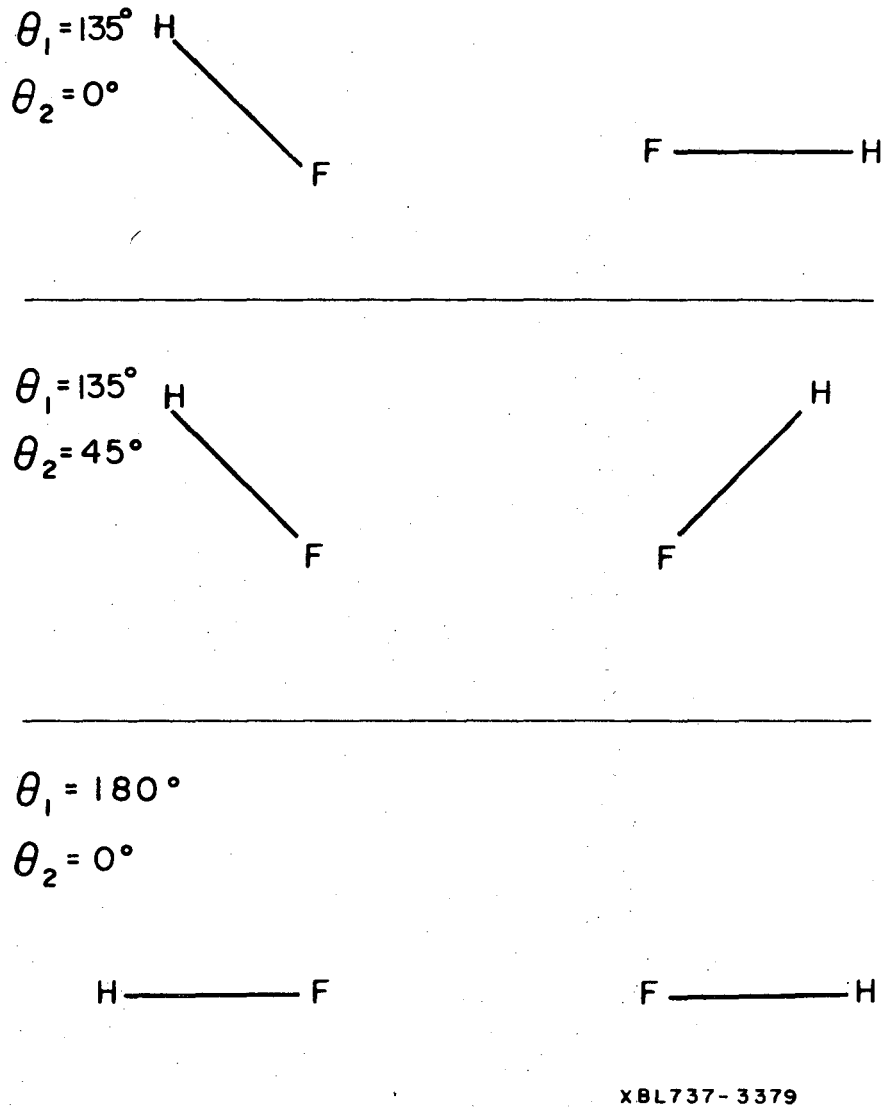


Fig. 3d

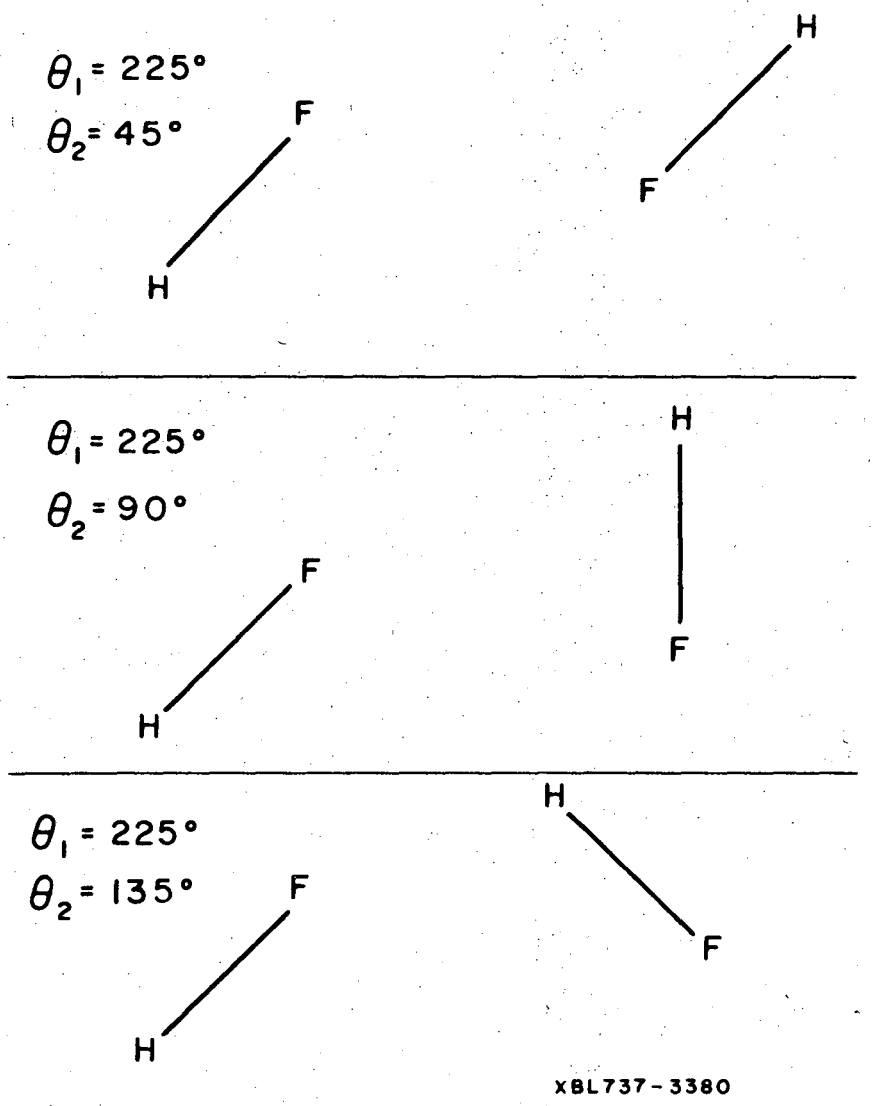

θ1 = 225°
θ2 = 45°
F
H
H
F
θ1 = 225°
θ2 = 90°
F
H
H
F
θ1 = 225°
θ2 = 135°
F
H
H
F
XBL737-3380

Fig. 3e

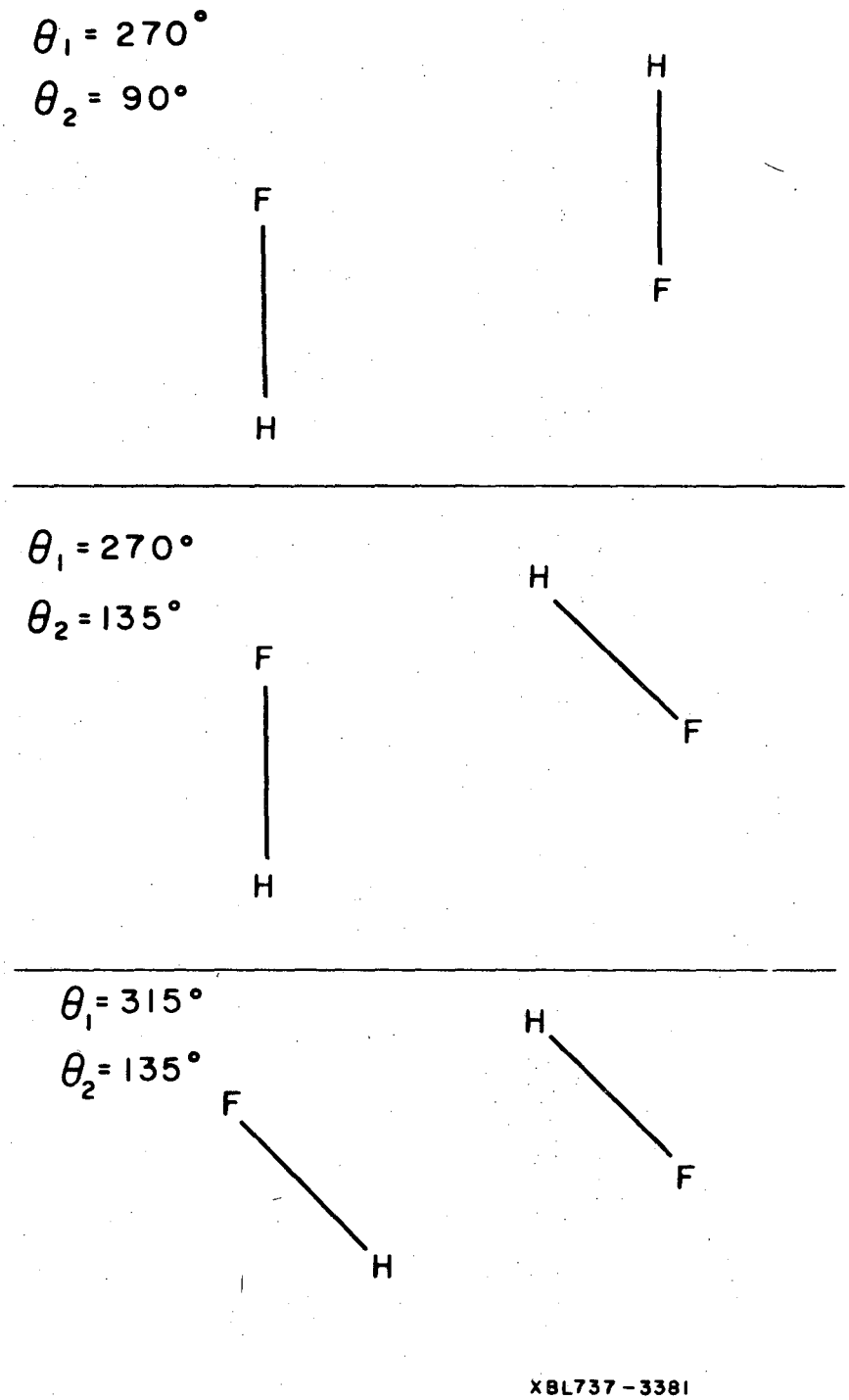

θ1 = 270°
θ2 = 90°
H
F
F
H
θ1 = 270°
θ2 = 135°
H
F
F
H
θ1 = 315°
θ2 = 135°
H
F
F
H
XBL737-3381

Fig. 3f

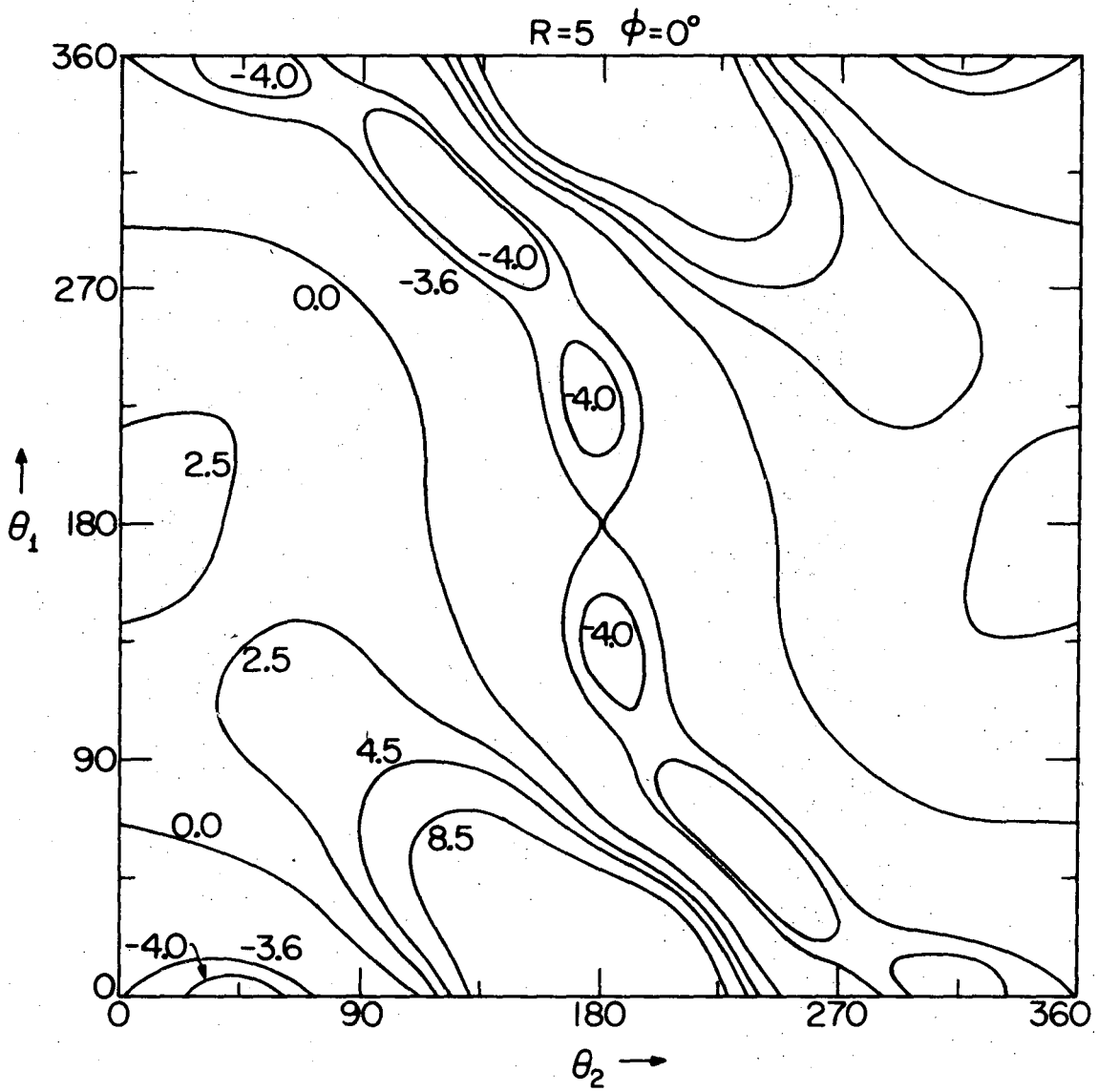
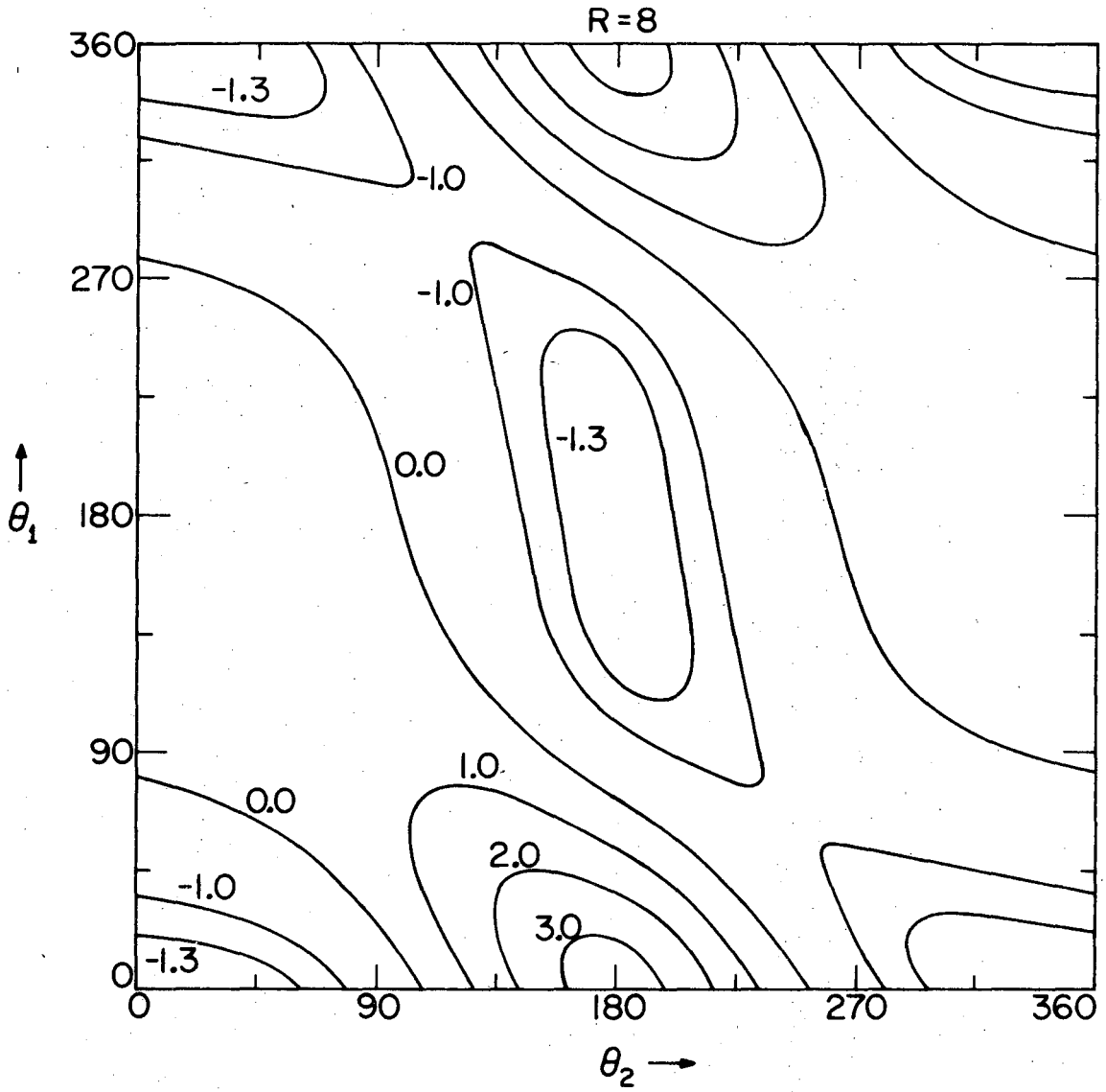

R=5 ϕ=0°
360
270
180
90
0
θ_1
0
90
180
270
360
θ_2
-4.0
-4.0
-3.6
0.0
-4.0
2.5
-4.0
2.5
4.5
0.0
8.5
-4.0
-3.6
XBL738-3659

Fig. 4



XBL 738-3660

Fig. 5

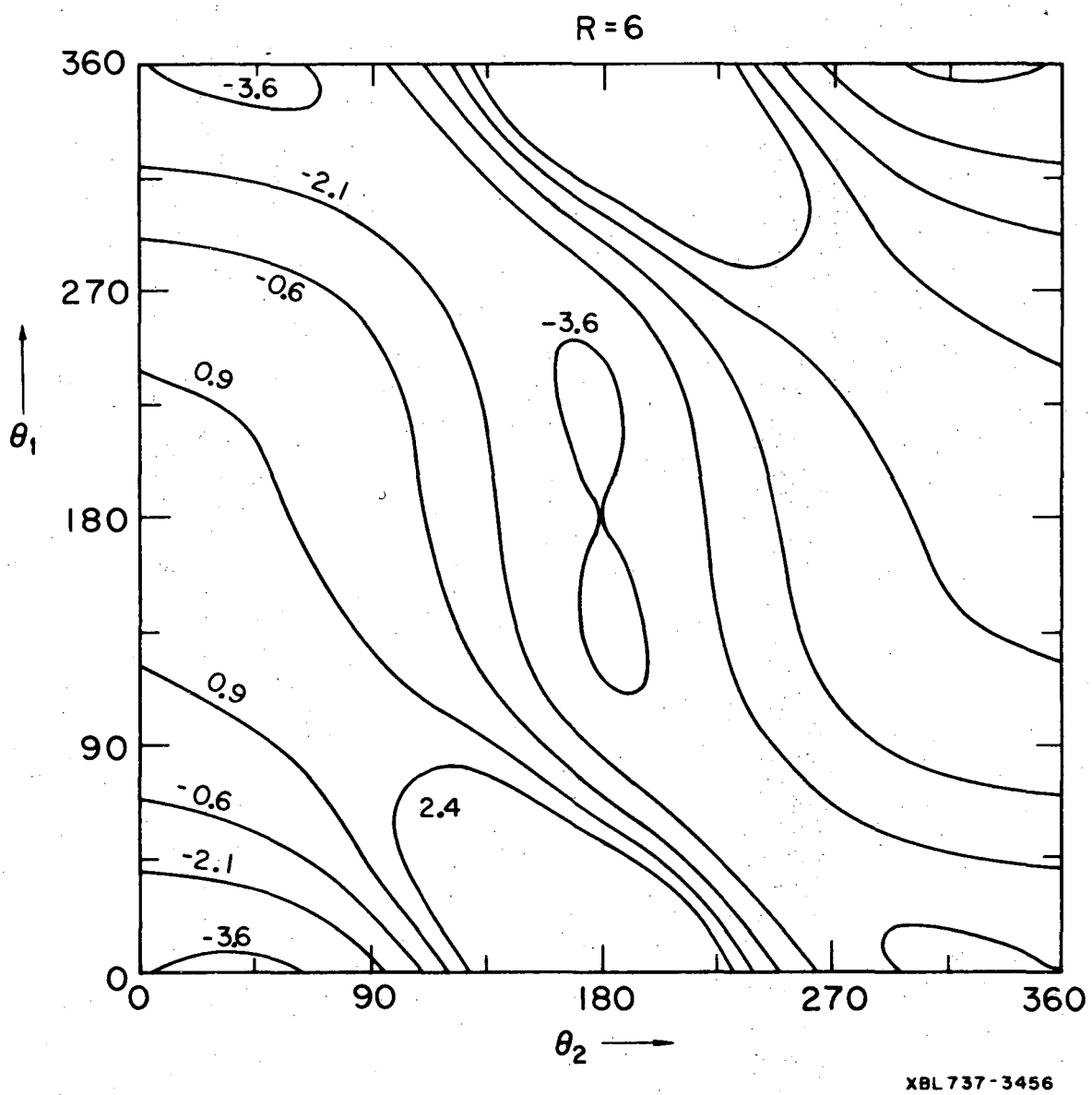

R = 6
360
270
180
90
0
0
90
180
270
360
θ_1
θ_2
-3.6
-2.1
-0.6
0.9
-3.6
0.9
-0.6
2.4
-2.1
-3.6
XBL 737-3456

Fig. 6

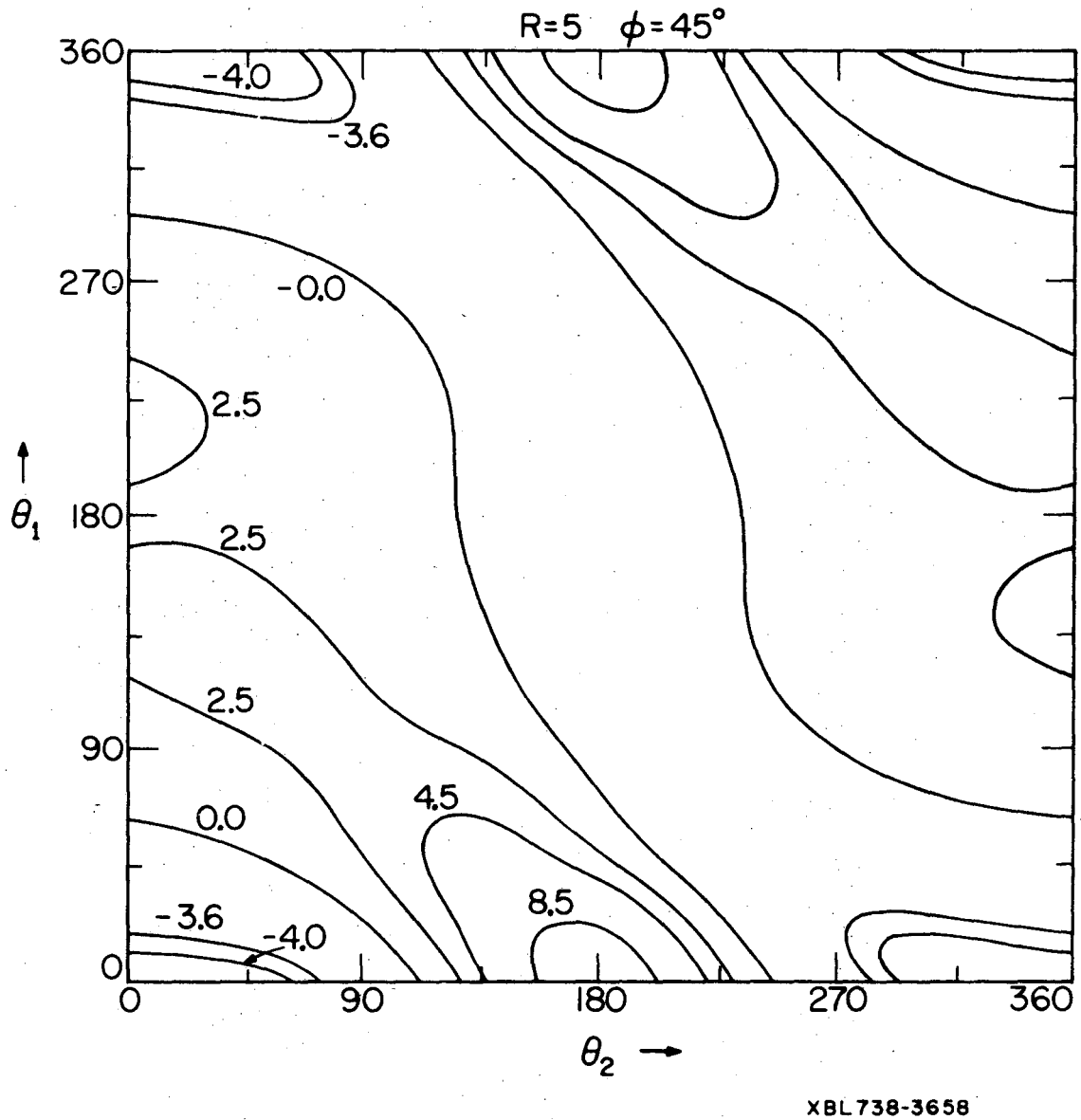

R=5 ϕ=45°
360
270
180
90
0
θ_1
0
90
180
270
360
θ_2
-4.0
-3.6
-0.0
2.5
2.5
2.5
0.0
4.5
8.5
-3.6
-4.0
XBL738-3658

Fig. 7

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