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A HARTREE-FOCK INTERACTION POTENTIAL BETWEEN A RIGID ASYMMETRIC TOP AND A SPHERICAL ATOM: (H_2CO,He)

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ABSTRACT: A basis set of better than "triple zeta plus polarization" quality is used to compute the interaction potential between a rigid $H_2CO(^1A_1)$ and $He(^1S)$. The highly anisotropic energy surface has a slight attraction arising from induction effects at intermolecular separations around 9 a.u. It is fitted to a spherical harmonic expansion to facilitate scattering applications.

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I. INTRODUCTION

The $1_{11} \rightarrow 1_{10}$ rotational transition in formaldehyde has been observed in absorption in interstellar space.[1] This absorption implies an effective temperature for the two levels below both the temperature of the isotropic background radiation and the expected kinetic temperature. Townes and Cheung[2] propose a collisional pumping model to explain the excess population in the lower 1_{11} state. To test their proposition requires the calculation of cross sections for rotational excitation of H_2CO by collision with the likely scattering particles He and H_2.

Classical,[2,3] semi-classical,[3] and quantum-mechanical[4,5] methods have been used to compute the rotational cross sections of interest. These calculations were carried out using hard-sphere[2,4] and Gaussian-shape[3,5] interaction potentials. The validity of these studies is limited by the reliability of the potential energy surfaces employed. The purpose of the present paper is to report progress on an effort to remedy this shortcoming within the Hartree-Fock (HF) approximation.

Because collision energies in interstellar space are small ($\leq$100°K) and the vibrational energy level spacings of H_2CO are sufficiently large (>1600°K for the lowest fundamental), H_2CO should be well approximated by a rigid rotor. Consistent with the rigid rotor model, H_2CO is constrained to a single geometry in the calculations to be described. This results in a smaller number of degrees of freedom that must be treated and thereby significantly reduces the number of points needed to map the region of the interaction potential required for scattering studies.

In order to keep the computational effort at a tractable level, the present study is limited to He as the scattering partner. In line with the computer-time concerns, H_2 was not considered for study because of the additional degrees of freedom that would have to be sampled even treating it as a rigid rotor. It is expected that scattering by He would be similar to collisions involving H_2 in the lowest (j = 0) para rotational state.

A preliminary study[6] of the interaction potential between H_2CO ($^1A_1$) and He (^1S) revealed that the Gordon-Kim (GK) electron gas model differs significantly from HF results for regions of the ground-state energy surface that are important at collision energies occurring in interstellar clouds. In this study, the HF basis set was explicitly chosen comparable to the one used in the GK calculation in order to remove the basis set as a source of difference between results of the two methods. Later tests indicated that the basis set used was deficient, at least for the HF calculation, resulting in a superposition error[7] that was a significant percentage of the well depth. It is further remarked that the use of a larger basis set in the two methods produced an even larger difference in interaction energy due primarily to changes in the HF interaction energy. For this reason, basis sets are further examined in the present study.

At long range, the dispersion energy dominates the interaction of He with H_2CO. Lesk[8] has recently proven that the dispersion energy is unobtainable in the HF approximation so that a reliable determination of the correlation energy contribution is required for scattering studies of the present system. Nevertheless, it is clear that the HF method can

accurately characterize the repulsive anisotropy of atom-diatomic molecule interactions between closed shell systems and yield quantitatively the induction energy at long range for such systems.[9] The present study forms the first of a two-part effort in which the second part - the determination of the dispersion interaction - will be presented in a subsequent paper.

The outline of the present paper is as follows: Section II describes the calculations performed and Section III presents the results and discussion. Section IV summarizes the findings of the study.

II. DESCRIPTION OF CALCULATIONS

Hartree-Fock calculations were carried out following the Roothaan approach with H_2CO constrained to the equilibrium geometry of R_{CO} = 1.208Å, R_{CH} = 1.116Å, and ∠ HCH = 116°31' determined by Takagi and Oka.[10] To facilitate collision studies, interaction energies are presented in a coordinate system with origin at the center-of-mass (c.m.) of H_2CO that is shown in Fig. 1.

The choice of basis set was governed by two criteria. One is that the superposition error[8] be small. The other is that the quantities which determine the leading terms of the induction contribution to the interaction energy at long range (permanent moments of H_2CO, dipole polarizability of He) be reliably characterized.[11]

To test these criteria, preliminary calculations were performed with He constrained to $\theta = 0°$ (O-atom end) and $\theta = 180°$ (C-atom end) approaches to H_2CO, i.e., C_{2v} geometries. Table I lists interaction energies obtained

(1) in the HF model employing the basis sets used in our recent study[12] of ground and excited state properties of H_2CO, and (2) using the multipole theory expression given in Appendix A. The excellent agreement (within 0.1°K) for $R \geq 11$ a.u. between energies computed using both basis sets and perturbation theory indicates that the induction contribution is quite well described and furthermore that the onset of the non-overlap region occurs for $R \simeq 11$ a.u.

Table II lists basis sets A and B for the (H_2CO,He) system omitting formaldehyde basis A which has been given previously.[12] The He basis sets are due to van Duijneveldt[13] augmented by p functions chosen to give an accurate dipole polarizability.[14] The latter functions are required to yield a proper description of the induction contribution to the interaction energy at long range. Figure 2 plots the interaction energy for C_{2v} approaches of He to the O-atom end ($\theta = 0°$) and C-atom end ($\theta = 180°$) for basis sets A and B and indicates the magnitude of the superposition error that accompanies the use of basis set A. Basis set B reduces the superposition error to approximately half the well depth. The close agreement between interaction energies obtained using basis set B and perturbation theory results given in Table I, and the reasonable agreement between the dipole moment determined employing basis set B and experiment, lend support to the notion that basis set B should provide a reliable description of the HF portion of the interaction potential.

III. RESULTS AND DISCUSSION

Hartree-Fock interaction energies obtained using basis set B are presented in Table III for $\phi = 0°$ (He incident in the plane of

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formaldehyde), in Table IV for $\phi = 30°$, in Table V for $\phi = 60°$, and in Table VI for $\phi = 90°$ (He incident in the perpendicular bisector plane of H_2CO). Owing to H_2CO symmetry, only $0° \leq \phi \leq 90°$ need be considered. Because the interaction potential is planned for scattering studies at energies $\leq 100°K$, R = 5 a.u. was arbitrarily chosen as the minimum R for computations. At this separation, the interaction is exponential with repulsion energies ranging up to several thousand degrees K; see Tables III-VI. The maximum R treated was chosen as the onset of agreement between HF and perturbation theory induction energies which, as discussed in relation to Table I, occurs at $\sim$ 11 a.u. Because of the large repulsion at $\theta \simeq 140°$ due to the He-H interaction, θ was sampled at the unevenly spaced values of 0°, 30°, 60°, 90°, 120°, 140°, 160°, and 180°. A total of 156 energy points were computed using basis set B.

Figure 3 broadly summarizes the results contained in Tables III-VI in the form of equipotential plots for He incident in (a) the H_2CO plane ($\phi = 0°$) and (b) the perpendicular bisector plane ($\phi = 90°$). For $\phi = 0°$, a slight attraction at $R \simeq 9$ a.u. is evident as is the large repulsion at small R due to the H atom. At $\phi = 90°$, however, the equipotential plot is very nearly symmetrical about $\theta = 90°$. (Note that the opening of the zero contour is an artifact of having used the spherical harmonic expansion to generate the plots and reflects slight inaccuracies in the fit functions.) These and other features are more clearly shown in the planar projections presented in Figs. 4-7. The reduction of the strong repulsion due to the H atoms as He approaches for increasingly large out-of-(H_2CO) plane angles ϕ is detailed in Fig. 4 for R = 7 a.u., in Fig. 5 for R = 9

a.u., and in Fig. 6 for R = 10 a.u. Figure 7 presents another view of the R dependence of the interaction for He incident in the plane of H_2CO and shows the pronounced decline of the repulsion due to H at $R \simeq 10$ a.u. which portends the onset of the non-overlap region describable by multipole theory. From perturbation theory, the form of the long-range induction energy is $\cos^2\theta$. At R = 9 a.u. (Fig. 5), this functional behavior is perceptible in the bisector plane approach (ϕ=90°). Note that by R = 10 a.u. (Fig. 6), the He-H interaction is much less repulsive and the long-range forces begin to dominate.

The HF interaction energies obtained using basis set B have been fit to an expansion in spherical harmonics, viz.

$$V(R,\theta,\phi) = \sum_{\ell=o}^{\ell_{max}} \sum_{m=-\ell}^{\ell} (4\pi/2\ell+1)^{1/2}\, v_{\ell m}(R)\, Y_{\ell m}(\theta,\phi) \quad .$$

<u>Ab initio</u> energy points were supplemented by additional points determined by the method of splines to yield a dense grid to facilitate the determination of the radial coefficients. The HF energies were accurately reproduced for $\ell_{max} = 12$ using both least-squares and numerical integration procedures. Formaldehyde symmetry leads to $v_{\ell m}(R) = v_{\ell -m}(R)$, for m an even integer , and to 49 unique non-zero terms through $\ell = 12$. The $v_{\ell m}$ coefficients are given in Appendix B.

IV SUMMARY AND REMARKS

Using a basis set of better than triple zeta plus polarization quality, a Hartree-Fock interaction potential for the H_2CO-He system has been

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determined for fixed geometry of H_2CO suitable for rigid rotor scattering studies. The potential energy surface is highly anisotropic for He incident in the plane of H_2CO and has a small ($\leq 3°K$) minimum at $R \simeq 9$ a.u. The ab initio surface agrees closely with interaction energies determined from perturbation theory for $R \geq 11$ a.u. which is indicative of the onset of the non-overlap region.

Since the Hartree-Fock model cannot describe dispersion contributions which from perturbation theory should dominate the long-range interaction in the present system, correlation studies will be needed to complement results presented here. Such studies are in progress and will be reported in a later paper.

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APPENDIX A

The induction contribution to the long range interaction between H_2CO and He may be written,

$$V(R,\theta,\phi) = \sum_{\ell}\sum_{m} (4\pi/2\ell+1)^{1/2}\, v_{\ell m}(R) Y_{\ell m}(\theta,\phi) \tag{A1}$$

The lowest order non-zero terms are

$$v_{00}(R) = -\mu^2\alpha/R^6 \tag{A2}$$

$$v_{20}(R) = v_{00}(R) \tag{A3}$$

$$v_{10}(R) = -18\,\mu\alpha\theta_{zz}/5R^7 \tag{A4}$$

$$v_{30}(R) = (2/3)\, v_{10}(R) \tag{A5}$$

$$v_{32}(R) = -\mu\alpha\,(8/15)^{1/2}(\theta_{xx}-\theta_{yy})/R^7 \tag{A6}$$

Here, α is the dipole polarizability of He, μ is the dipole moment of H_2CO, and θ_{ii} ($ii \equiv xx, yy$, and zz) are the diagonal components of the quadrupole moment tensor of H_2CO. Note that the dipole - induced dipole contribution (R^{-6}) is two orders of magnitude larger than the quadrupole-induced dipole term (R^{-7}).

The values of molecular properties used to construct the entries in the third column of Table I were taken from Ref. 12. They are:

$\mu = -1.1249$ a.u., $\theta_{xx} = 0.1773$ a.u., $\theta_{yy} = -0.1481$ a.u. and $\theta_{zz} = -0.0292$ a.u.

An experimental dipole polarizability (1.397 a.u.) was used for helium.[15]

APPENDIX B

Tabulated below are the $v_{\ell m}(R)$ coefficients of Eq. (1).

TABLE B1 - Radial Coefficients of Spherical Harmonic Expression (°K)

ℓ	m \ R(a.u.)	5	6	7	8	9	10
0	0	2580.1	374.7	46.91	3.47	-0.93	-0.68
1	0	-3253.8	-531.2	-77.89	-11.50	-2.05	-0.41
2	0	3773.1	527.4	64.57	5.40	-0.83	-0.72
2	2	1144.5	188.8	27.81	3.48	0.29	0.01
3	0	-296.6	-20.8	2.79	2.39	1.00	0.24
3	2	-2139.1	-355.0	-54.02	-8.19	-1.35	-0.23
4	0	-1003.4	-208.0	-37.17	-6.22	-0.87	-0.09
4	2	2383.1	388.2	58.51	8.26	1.00	0.09
4	4	223.7	34.6	4.26	0.31	-0.02	0.00
5	0	1348.7	224.7	35.37	5.66	1.02	0.22
5	2	-1541.8	-241.5	-35.86	-5.39	-0.89	-0.17
5	4	-415.2	-63.7	-8.33	-0.98	-0.09	-0.01
6	0	-827.2	-134.2	-20.57	-3.25	-0.54	-0.09
6	2	764.2	115.6	17.03	2.50	0.35	0.05
6	4	457.9	66.6	8.65	1.05	0.11	0.01
6	6	32.0	3.4	-0.16	-0.15	-0.04	-0.01
7	0	290.0	48.4	7.50	1.12	0.20	0.05
7	2	-185.8	-30.0	-4.49	-0.67	-0.13	-0.03
7	4	-369.9	-49.5	-6.23	-0.73	-0.07	0.00
7	6	-63.1	-7.5	-0.06	0.18	0.04	0.01
8	0	51.8	4.9	0.50	0.14	0.05	0.02
8	2	-65.1	-8.2	-1.12	-0.21	-0.05	-0.01
8	4	253.6	32.6	4.05	0.48	0.05	0.00
8	6	73.1	8.5	0.32	-0.13	-0.03	-0.01
8	8	12.3	1.1	0.23	0.01	0.00	0.00
9	0	-101.9	-16.0	-2.44	-0.41	-0.07	-0.01
9	2	106.3	15.7	2.29	0.35	0.05	0.00
9	4	-145.5	-18.9	-2.37	-0.29	-0.03	0.00
9	6	-64.3	-6.9	-0.45	0.06	0.02	0.00
9	8	-23.9	-3.8	-0.51	-0.06	-0.01	0.00

TABLE B1 (Cont'd)

10	0	39.9	6.0	0.90	0.17	0.03	0.00
10	2	-36.1	-5.3	-0.77	-0.12	-0.02	0.00
10	4	59.0	7.8	0.99	0.13	0.01	0.00
10	6	53.5	5.6	0.45	-0.02	-0.01	0.00
10	8	28.9	4.4	0.57	0.07	0.01	0.00
10	10	1.2	0.1	0.03	0.00	0.00	0.00
11	0	28.2	4.9	0.77	0.10	0.01	0.00
11	2	-25.5	-4.1	-0.62	-0.09	-0.01	0.00
11	4	-11.0	-1.5	-0.20	-0.03	0.00	0.00
11	6	-39.8	-4.2	-0.34	0.01	0.01	0.00
11	8	-29.4	-4.2	-0.54	-0.06	-0.01	0.00
11	10	-2.7	-0.5	-0.07	-0.01	0.00	0.00
12	0	-55.2	-9.3	-1.45	-0.22	-0.03	-0.01
12	2	49.2	7.7	1.15	0.17	0.03	0.00
12	4	-8.0	-1.0	-0.12	0.00	0.00	0.00
12	6	26.1	2.7	0.23	-0.01	0.00	0.00
12	8	28.0	3.9	0.49	0.06	0.01	0.00
12	10	3.7	0.6	0.09	0.01	0.00	0.00
12	12	0.0	0.0	0.00	0.00	0.00	0.00

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TABLE I

Comparison of Hartree-Fock and Multipole Expansion Interaction Energies (°K)[a]

θ = 0°	Basis Set		Multipole Expansion
R(a.u.)	A[b]	B[c]	
5.0	2508.83	2606.14	
6.0	228.96	276.60	
7.0	-11.05	20.58	
7.5	-22.29	1.83	-6.34
8.0	-18.65	-3.05	-4.30
8.5	-11.79	-3.61	-2.99
9.0	-6.33	-2.98	-2.12
9.5	-3.15	-2.15	-1.53
10.0	-1.62	-1.47	-1.13
11.0	-0.63	-0.69	-0.63
12.0		-0.36	-0.38
13.0		-0.22	-0.23
θ = 180°			
5.0	6355.97	6467.19	
6.0	777.87	838.07	
7.0	55.07	85.42	
7.5	4.13	21.36	
8.0	-6.91	1.78	-4.22
8.5	-7.13	-3.03	-2.93
9.0	-5.22	-3.29	-2.08
9.5	-3.39	-2.48	-1.51
10.0	-2.08	-1.67	-1.11
11.0	-0.77	-0.73	-0.63
12.0		-0.37	-0.37
13.0		-0.22	-0.23

a) $1°K = 3.1668 \times 10^{-6}$ a.u.

b) Obtained with formaldehyde geometry of Ref. 16.

c) Obtained with formaldehyde geometry of Ref. 10. The energy differences are attributable to basis set; differences due to geometry are negligible.

TABLE II - Contracted Gaussian Basis Sets for H_2CO and He[a]

Basis A

Atom	Type	Function[b]
He	S	0.002600(233.093) + 0.019628(35.023) + 0.091421(7.9557) + 0.272853(2.2028)
	S	1.0(0.66435)
	S	1.0(0.20825)
	X,Y,Z	1.0(1.0000)
	X,Y,Z	1.0(0.2000)

Basis B

O	S	0.000210(31195.6) + 0.001628(4669.38) + 0.008450(1062.62) + 0.034191(301.426) + 0.110311(98.5153)
	S	1.0(35.4609)
	S	1.0(13.6179)
	S	1.0(5.38618)
	S	1.0(1.53873)
	S	1.0(0.60550)
	S	1.0(0.22054)
	X,Y,Z	0.002266(114.863) + 0.017192(26.8767) 0.075341(8.32077)
	X,Y,Z	1.0 (2.97237)
	X,Y,Z	1.0 (1.12848)
	X,Y,Z	1.0 (0.42360)
	X,Y,Z	1.0 (0.15074)
	X^2,Y^2,Z^2,XY,XZ,YZ	1.0 (2.0)
	X^2,Y^2,Z^2,XY,XZ,YZ	1.0 (0.5)

a) Basis set A for H_2CO has been given previously. See basis set A of Ref. 12.

b) Linear combinations are written in the form $C_1(\alpha_1) + C_2(\alpha_2) + \ldots$ where $C_1, C_2, \ldots$ are coefficients and $\alpha_1, \alpha_2, \ldots$ are Gaussian exponents.

TABLE II (Cont'd)

Basis B (Cont'd)

Atom	Type	Function
C	S	0.000242(15469.4) + 0.001879(2316.47)
		+ 0.009743(527.099) + 0.039167(149.438)
		+ 0.123636(48.8562)
	S	1.0 (17.6209)
	S	1.0 (6.81082)
	S	1.0 (2.7276)
	S	1.0 (0.75674)
	S	1.0 (0.30073)
	S	1.0 (0.11409)
	X,Y,Z	0.002734 (51.7233) + 0.018979(12.3397)
		+ 0.080806 (3.77224)
	X,Y,Z	1.0 (1.32487)
	X,Y,Z	1.0 (0.50546)
	X,Y,Z	1.0 (0.19827)
	X,Y,Z	1.0 (0.07731)
	X^2,Y^2,Z^2,XY,XZ,YZ	1.0 (2.0)
	X^2,X^2,Z^2,XY,XZ,YZ	1.0 (0.5)
H	S	0.002006(82.636374) + .015345(12.409558)
		+ 0.075577(2.823854)
	S	1.0 (0.797670)
	S	1.0 (0.258053)
	S	1.0 (0.089891)
	X,Y,Z	1.0 (1.0)
He	S	0.000059(4840.888547) + 0.000463(723.108918)
		+ 0.002422(164.299706) + 0.009995(46.636262)
		+ 0.034249(15.277787) + 0.096302(5.526897)
	S	1.0 (2.132879)
	S	1.0 (0.849674)
	S	1.0 (0.343643)
	S	1.0 (0.138709)
	X,Y,Z	1.0 (1.0)
	X,Y,Z	1.0 (0.2)

TABLE III - Interaction Energies (°K) for $\phi = 0°$[a]

θ \ R(a.u.)	5	6	7	8	9	10
0	2606.14	276.60	20.58	-3.05	-2.98	-1.47
30	2044.04	237.92	20.15	-3.26	-3.55	-1.66
60	837.23	101.05	6.60	-3.67	-2.67	-1.03
90	621.14	76.45	5.52	-1.52	-0.98	-0.37
120	7220.33	1178.99	169.48	21.63	2.02	-0.15
140	15852.93	2474.73	352.67	46.22	4.86	0.01
160	11942.20	1774.97	235.29	25.72	0.82	-0.86
180	6467.19	838.07	85.42	1.78	-3.29	-1.67

a) See footnote a of Table I.

0 0 0 0 4 2 0 5 2 8 1

TABLE IV - Interaction Energies (°K) for $\phi = 30°$[a]

θ \ R(a.u.)	5	6	7	8	9	10
30	1967.52	226.04	18.50	-3.12	-3.29	-1.56
60	840.15	102.82	7.62	-2.92	-2.32	-0.95
90	563.52	70.95	6.26	-0.74	-0.70	-0.33
120	4468.44	735.56	109.13	14.39	1.27	-0.22
140	10343.96	1642.55	236.61	30.93	2.91	-0.23
160	9735.36	1431.19	185.02	18.57	-0.18	-1.01

a) See footnote a of Table I.

0 0 0 0 4 2 0 6 2 8 2

TABLE V - Interaction Energies (°K) for $\phi = 60°$[a]

θ \ R(a.u.)	5	6	7	8	9	10
30	1813.06	202.06	15.16	-2.83	-2.77	-1.35
60	830.64	103.06	8.69	-1.84	-1.77	-0.80
90	555.09	72.21	7.22	-0.21	-0.54	-0.31
120	1608.87	240.09	30.45	2.74	-0.32	-0.44
140	3942.97	590.33	75.57	6.93	-0.55	-0.73
160	6138.00	850.97	97.83	5.87	-2.03	-1.30

a) See footnote a of Table I.

0 0 0 0 4 2 0 6 2 8 3

TABLE VI - Interaction Energies (°K) for $\phi = 90°$[a]

θ \ R(a.u.)	5	6	7	8	9	10
30	1735.15	189.98	13.48	-2.70	-2.50	-1.25
60	819.62	101.86	8.84	-1.47	-1.53	-0.73
90	589.43	80.31	8.63	-0.06	-0.53	-0.31
120	888.84	115.70	11.74	0.09	-0.71	-0.46
140	2060.27	262.98	23.82	-0.87	-1.78	-0.93
160	4670.12	606.53	60.25	0.34	-2.86	-1.44

a) See footnote a of Table I.

0 0 0 0 4 2 0 6 2 8 4

0 0 0 0 4 2 0 6 2 8 5

FIGURE CAPTIONS

Fig. 1 Coordinate system and geometry for the H_2CO-He system. The triads in parenthesis are the x,y, and z coordinates of the atoms.

Fig. 2 Basis set dependence of the interaction energy for C_{2v} geometry: — — — basis A for $\theta = 0°$, ———— basis B for $\theta = 0°$, ------- basis A for $\theta = 180°$, —— —— basis B for $\theta = 180°$.

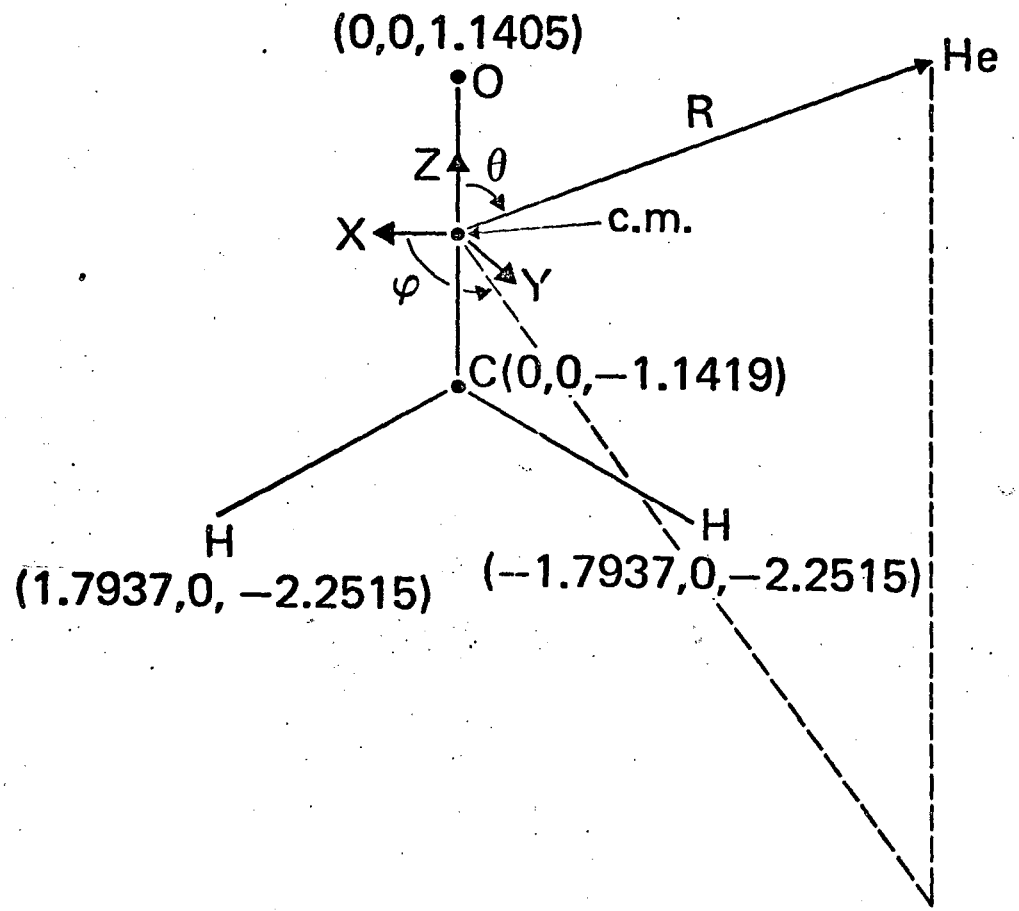
Fig. 3 Contour plots of the interaction potential for He incident in the plane of H_2CO ($\phi = 0°$) and He incident in the bisector plane ($\phi = 90°$). Energies in °K. c.m. denotes center of mass.

Fig. 4 Interaction energy vs. θ for selected angles ϕ at R = 7 a.u.

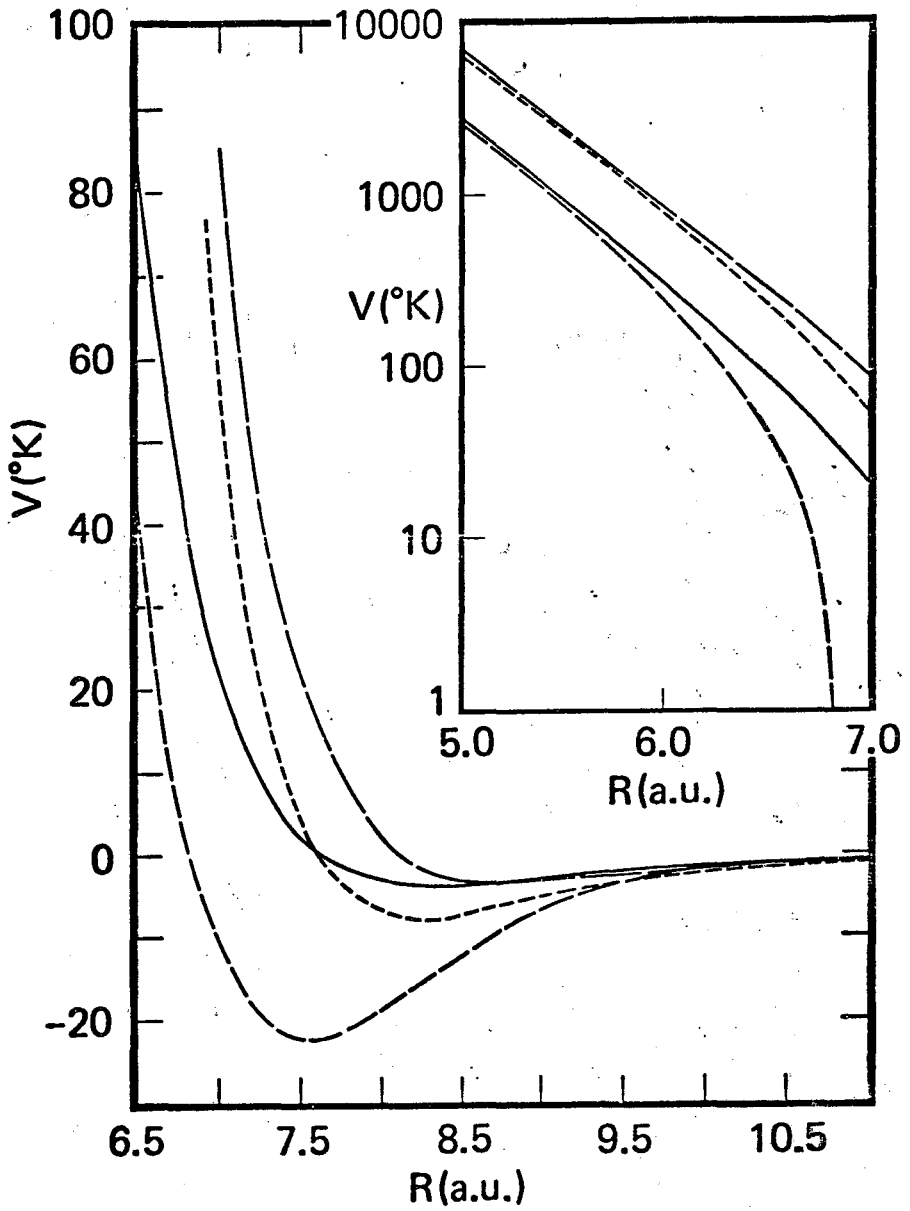
Fig. 5 Interaction energy vs. θ for selected angles ϕ at R = 9 a.u.

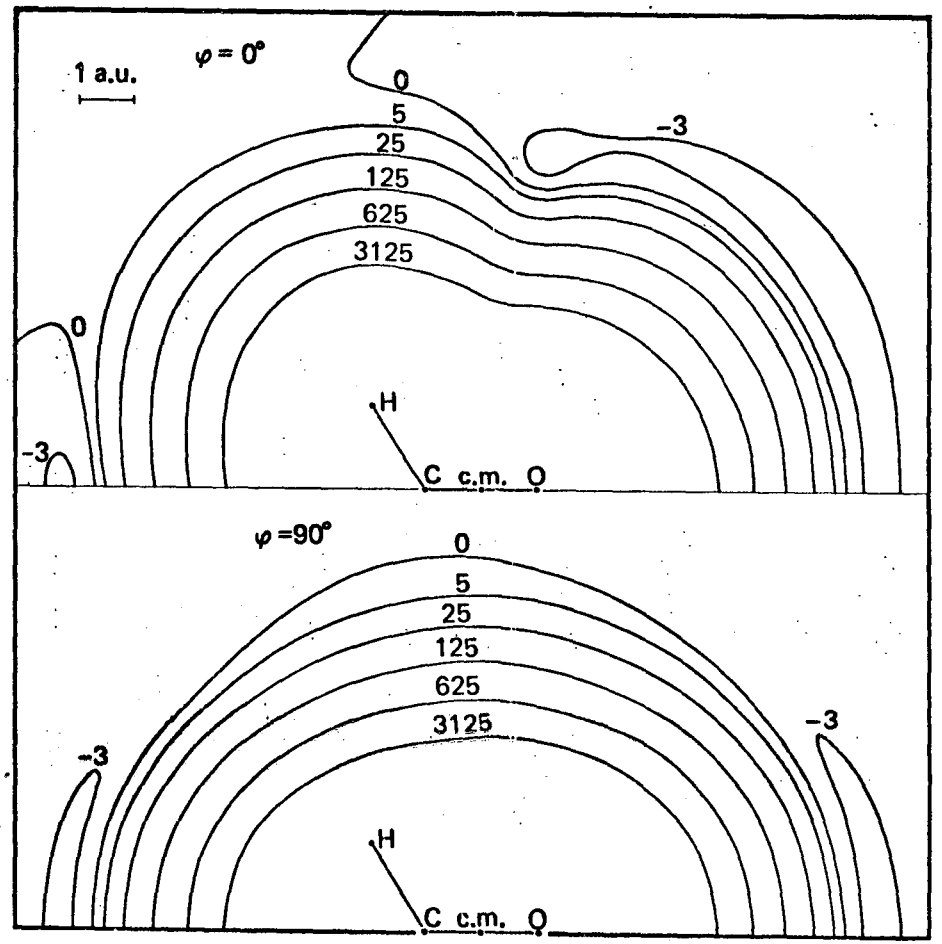
Fig. 6 Interaction energy vs. θ for selected angles ϕ at R = 10 a.u.

Fig. 7 Interaction energy vs. θ for selected R at $\phi = 0°$.


(0,0,1.1405)
O
He
R
Z
θ
X
c.m.
φ
Y
C(0,0,−1.1419)
H
(1.7937,0, −2.2515)
H
(−1.7937,0,−2.2515)

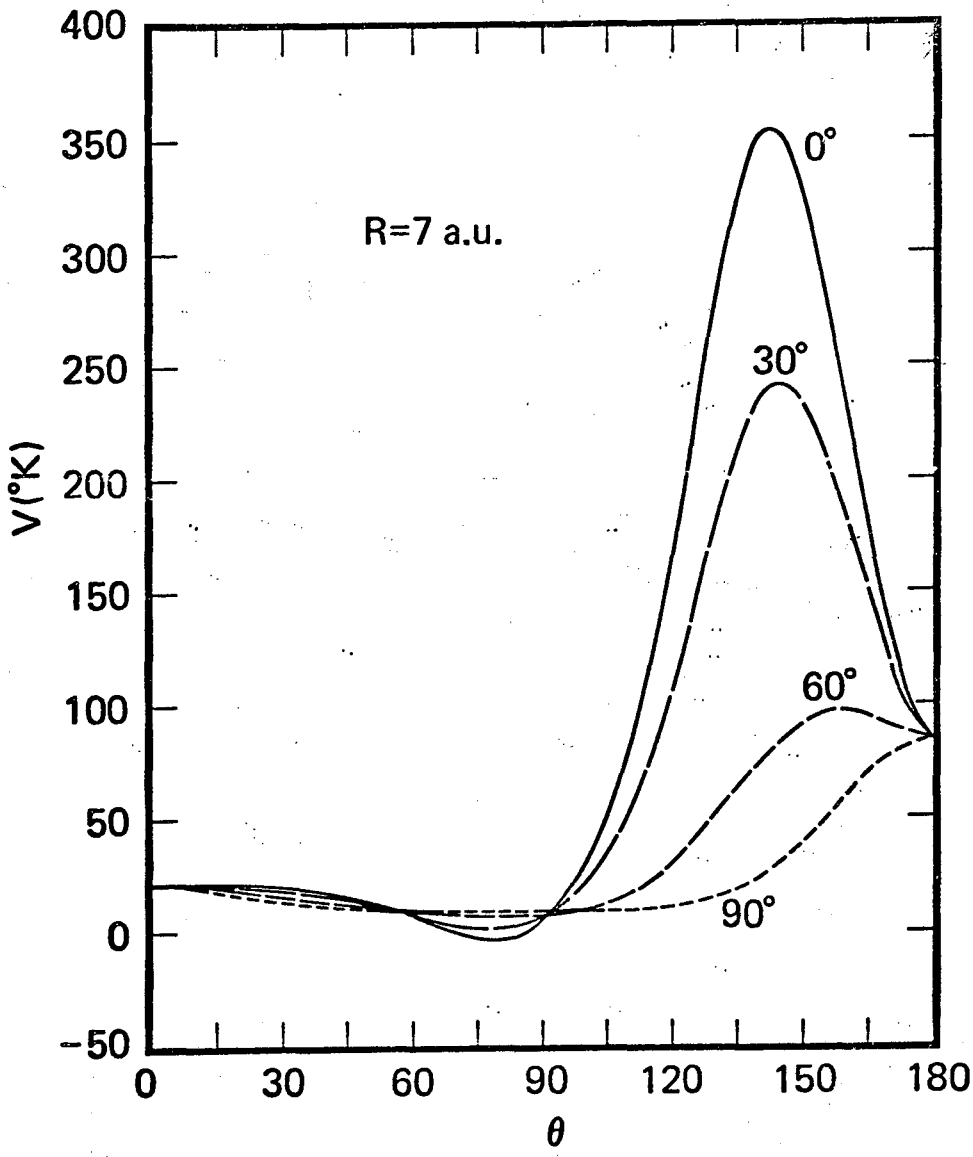
0 0 0 0 4 2 0 6 2 8 7

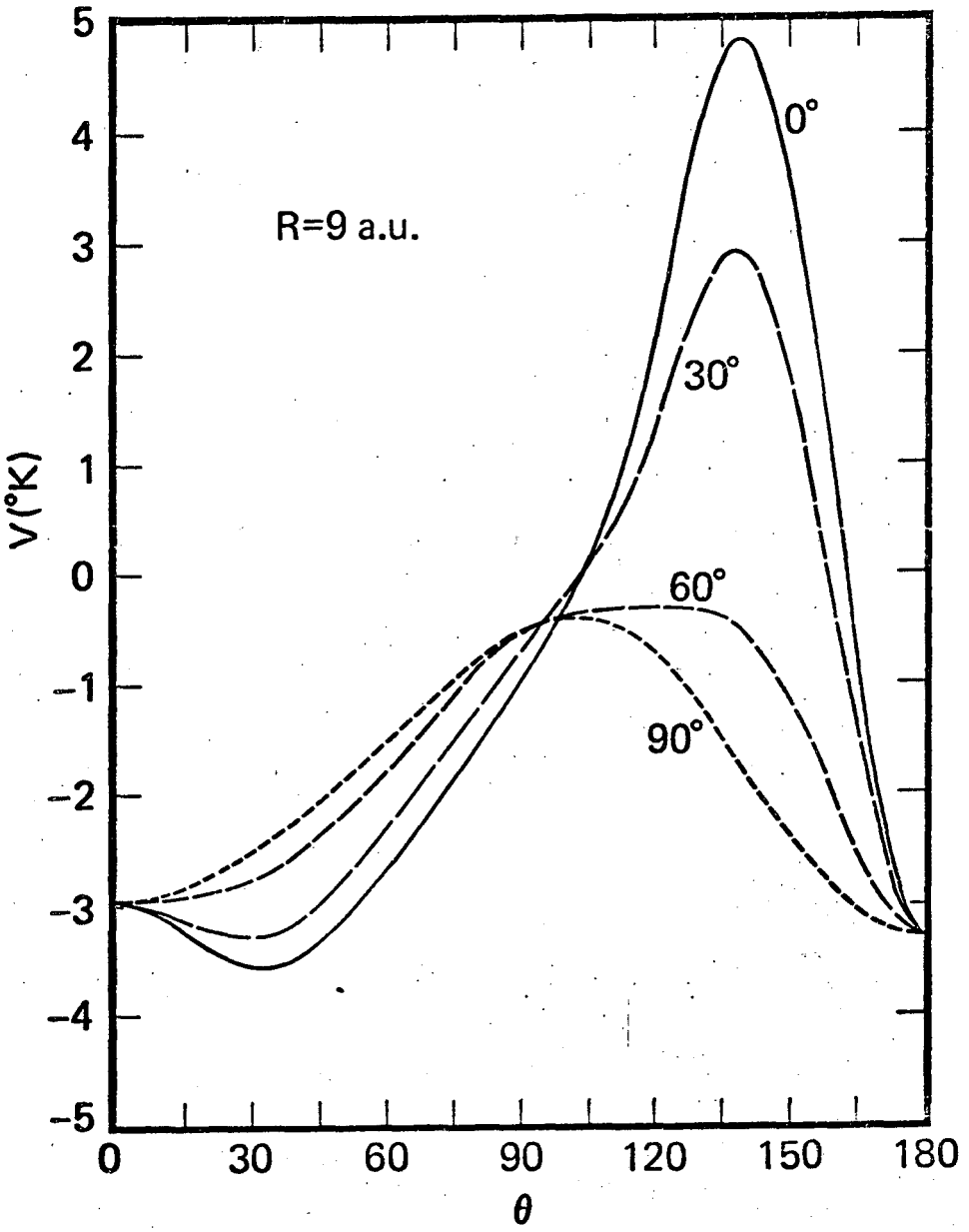


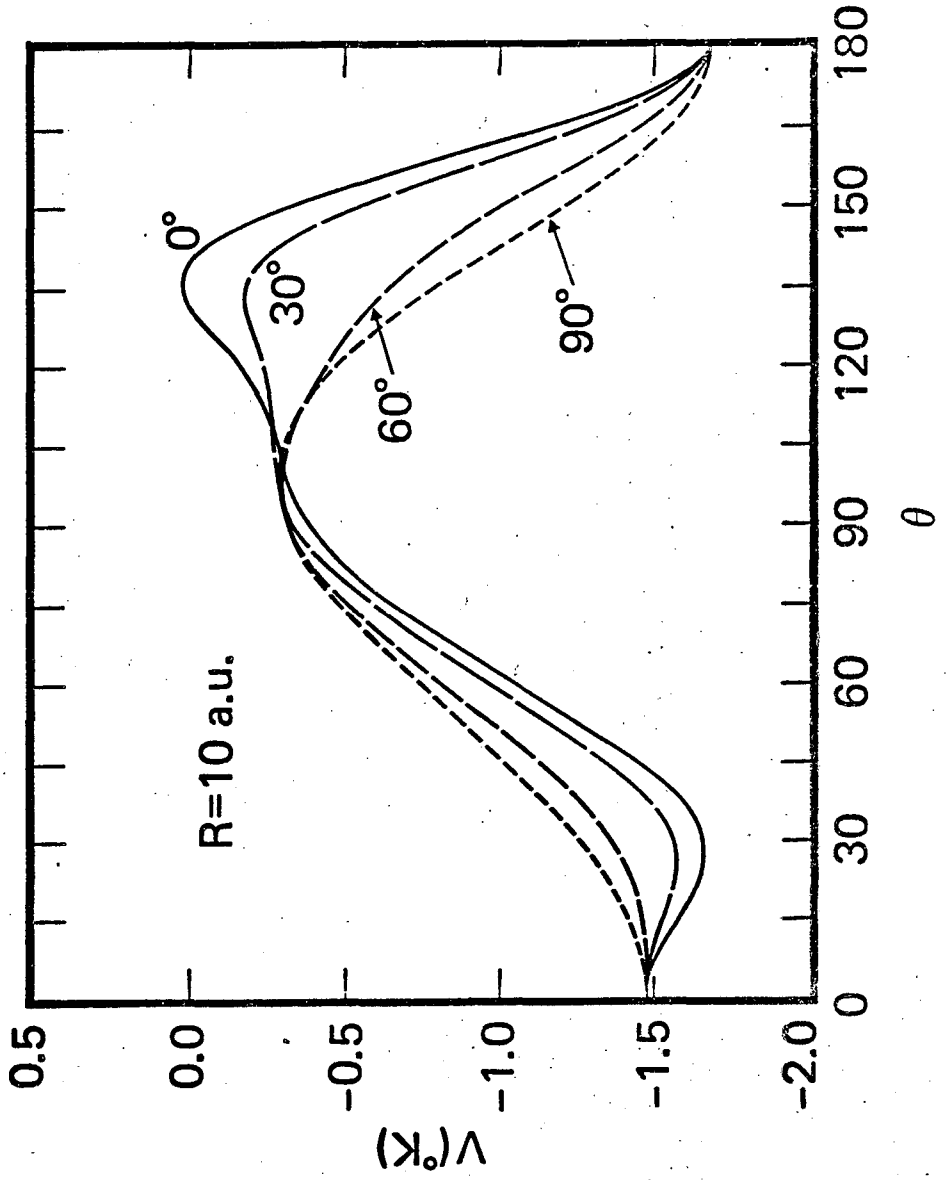

1 a.u.
φ = 0°
0
5
25
125
625
3125
-3
0
-3
H
C c.m. O
φ =90°
0
5
25
125
625
3125
-3
-3
H
C c.m. O

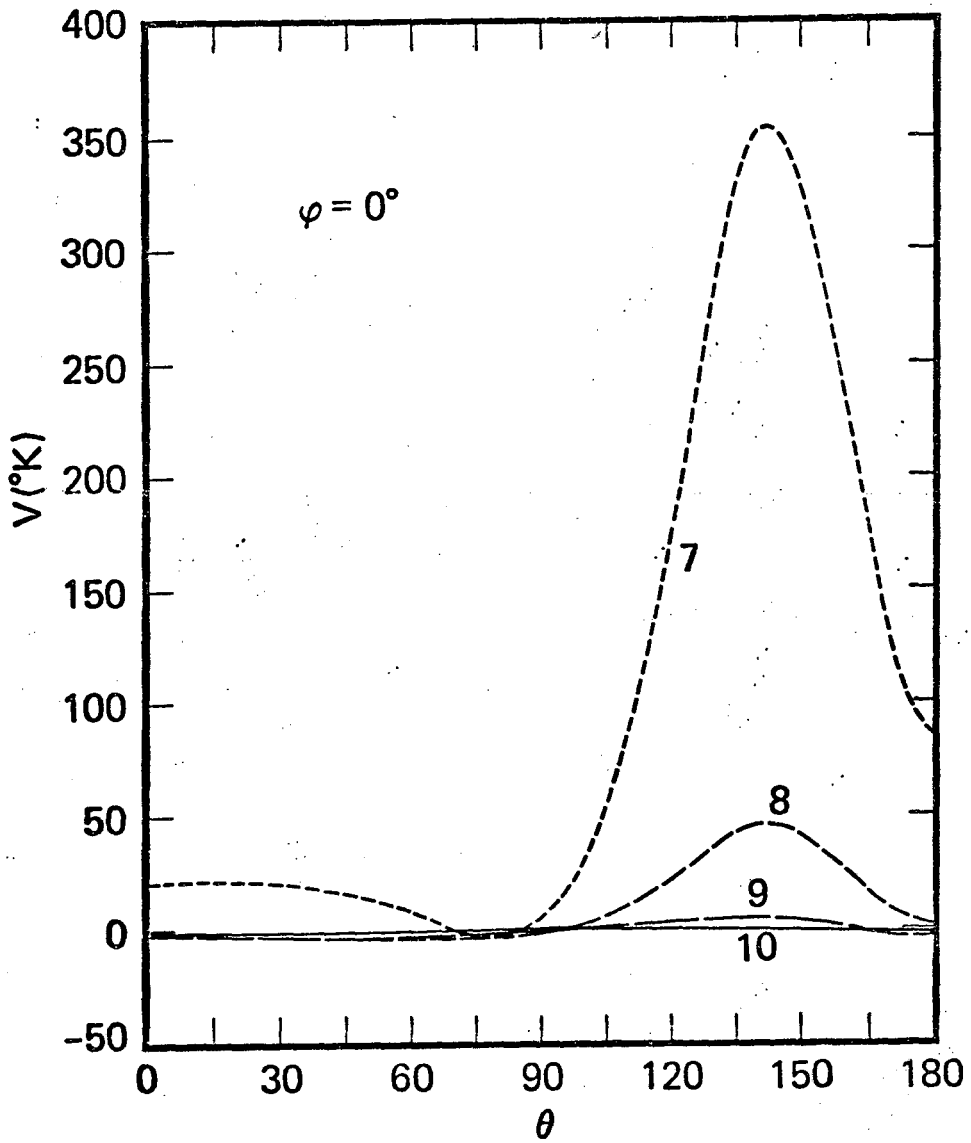
0 0 0 0 4 2 0 2 8 8

0 0 0 0 4 2 0 6 2 8 9




R=9 a.u.
0°
30°
60°
90°
V(°K)
θ
5
4
3
2
1
0
−1
−2
−3
−4
−5
0
30
60
90
120
150
180


0.5
0.0
-0.5
-1.0
-1.5
-2.0
V(°K)
0
30
60
90
120
150
180
θ
R=10 a.u.
0°
30°
60°
90°


400
350
300
250
200
150
100
50
0
-50
V(°K)
φ = 0°
7
8
9
10
0
30
60
90
120
150
180
θ

0 0 0 0 4 2 0 6 2 9 3

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