21

JAERI-Data/Code
98-031

FERMILAB
JAN 6 1999
LIBRARY

JAERI-DATA-CODE-98-031

Fermilab Library
0 1160 0068144 9

POTENTIAL ENERGIES FOR THE TWO LOWEST $^1A'$ ELECTRONIC STATES OF H_3^+

November 1998

Akira ICHIHARA, Keiichi YOKOYAMA and Osamu IWAMOTO

日本原子力研究所
Japan Atomic Energy Research Institute

本レポートは，日本原子力研究所が不定期に公刊している研究報告書です。
入手の問合わせは，日本原子力研究所研究情報部研究情報課（〒319-1195　茨城県那珂郡東海村）あて，お申し越しください。なお，このほかに財団法人原子力弘済会資料センター（〒319-1195　茨城県那珂郡東海村日本原子力研究所内）で複写による実費頒布をおこなっております。

This report is issued irregularly.
Inquiries about availability of the reports should be addressed to Research Information Division, Department of Intellectual Resources, Japan Atomic Energy Research Institute, Tokai-mura, Naka-gun, Ibaraki-ken, 319-1195, Japan.

© Japan Atomic Energy Research Institute, 1998

編集兼発行　　日本原子力研究所

JAERI-Data/Code 98-031

Potential Energies for the Two Lowest $^1A'$ Electronic States of H_3^+

Akira ICHIHARA, Keiichi YOKOYAMA[+] and Osamu IWAMOTO

Department of Nuclear Energy System
Tokai Research Establishment
Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun, Ibaraki-ken

(Received October 1 , 1998)

Potential energies for the two lowest $^1A'$ states of H_3^+ at 701 different spatial geometries are tabulated. These energies have been calculated by the ab initio full configuration interaction method with a [8s6p2d1f] Gaussian type basis set. Features of avoided crossing of two surfaces as well as the potential well in the ground state can be produced by interpolating calculated energies. These ab initio energies are expressed as a function of three internuclear distances in the range from 0.6 to 10.0 bohr, and they are applicable to the molecular dynamics study for the $H^+ + H_2$ system.

Keywords : Three Dimensional Potential Energy Surface, H_3^+, Avoided Crossing, Ab Initio Full Configuration Interaction

---

[+]Department of Materials Science

基底及び第一電子励起 $^1A'$状態における H_3^+のポテンシャルエネルギー

日本原子力研究所東海研究所エネルギーシステム研究部
市原　晃・横山　啓一[+]・岩本　修

（1998年10月1日受理）

基底及び第一電子励起 $^1A'$状態における H_3^+のポテンシャルエネルギーを701の異なる空間構造に対して計算し、その結果を表にまとめた。これらのポテンシャルエネルギーは、[8s6p2d1f]ガウス型基底関数を用いた、非経験的分子軌道論に基づく完全な配置間相互作用法により計算された。ポテンシャルの計算値を内挿することにより、二つのポテンシャル面間の avoided crossing や基底状態ポテンシャル面のエネルギー極小値付近の形状を表現する事が可能である。ポテンシャルエネルギーは三つの核間距離の関数として0.6から10.0ボーアの範囲内で与えられており、$H^+ + H_2$衝突に関する分子動力学の研究に適している。

東海研究所：〒319-1195　茨城県那珂郡東海村白方白根 2-4
[+]物質科学研究部

Contents

1. Introduction 1
2. Description of Calculation 2
   2.1 Basis Set 2
   2.2 Potential Surfaces 5
3. Tables of Potential Energies 8
Acknowledgements 17
References 17

目　次

1. 緒言 1
2. 計算の説明 2
   2.1　基底関数 2
   2.2　ポテンシャル面 5
3. ポテンシャルエネルギーの表 8
謝辞 17
参考文献 17

1. Introduction

The H_3^+ system, being the simplest polyatomic ion, has been attracting the interest of theorists as well as experimentalists. A variety of calculations have been carried out for the H_3^+ equilibrium energy to test the accuracy of computational method[1,2]. Also, the potential energy surface (PES) for the ground $^1A'$ electronic state has been calculated by several groups around the equilibrium geometry in order to identify the H_3^+ vibration-rotation spectra[3-11]. Moreover, global H_3^+ PES's are required to study ion production processes occurring in the $H^+ + H_2$ system and its isotopic variants[12-17]. These collision processes are of great importance for the plasma modeling of fusion reactor divertor[18].

It is known from the theoretical calculation of Baucshlicher et al.[19] that H_3^+ in the equilibrium state produces H^+ and H_2 when a proton is adiabatically separated from the other protons, while H_3^+ in the first excited electronic $^1A'$ state produces H and H_2^+. Consequently, accurate H_3^+ PES's in the two lowest $^1A'$ states are indispensable to the theoretical study on the $H^+ + H_2$ collision processes with electron transfer. However, there is no theoretical three-diemnsional (3D) PES for the first excited state of H_3^+. Bauschlicher et al. calculated ab initio PES's only for the C_{2v} (isosceles triangle) spatial geometry. Due to the lack of theoretical 3D-PES's, semi-empirical PES's based on the diatomics-in-molecules (DIM) model have ever been used to investigate the $H^+ + H_2$ collision process[12-17].

We have calculated ab initio potential energies for the two lowest electonic states of H_3^+ in a wide range of 3D space so that the molecular dynamics calculation with the ab initio 3D-PES's becomes possible. The ab initio potential energies of this report have been calculated at 701 different spatial geometries by using the full configuration interaction (full CI) method with a [8s6p2d1f] Gaussian type basis set. In Sec.2 we give a table of basis set parameters with explanations of the accuracy of calculation and the features of PES's. The calculated potential energies are tabulated in Sec.3 as a function of three internuclear distances.

All ab initio calculations of this study have been carried out with the MOLCAS2[20] program package on the IBM RS6000 system. Detailed description for the geography of PES's and the application to the calculation of ion production cross sections for the $H^+ + H_2$ collisions are given in our recent papers[21,22].

2. Description of Calculation

2.1 Basis Set

The parameters of [8s6p2d1f] Gaussian type basis set for hydrogen are shown in Table1. The basis set comprises Huzinaga (10s) primitive functions[23] augmented with (1s6p2d1f) primitives. The Huzinaga (10s) functions are contracted to (4,1,1,1,1,1,1). This contracted [7s] set yields the hydrogen 1s energy of -0.499999 atomic unit (au). A supplemental s-type function with the exponent of 0.0100437 are added to [7s] set as a diffuse function. Remaining (6p2d1f) primitives are uncontracted and added to the [8s] set. These exponents have been optimized to minimize the potential energy at an equilateral triangle of side 1.65 bohr, where H_3^+ takes the equilibrium geometry. The energy obtained with the optimized basis set is -1.343429 au. This energy is only 0.030 % (0.011 eV) above the corresponding most accurate energy, -1.343835 au[1].

In order to estimate the accuracy of calculation, the potential curve of H_2 in the ground electronic state has also been calculated with the [8s6p2d1f] basis set. Figure 1 shows the deviation of calculated potential energy from the accurate potential of Kolos and Wolnievicz[24]. It can be seen from Fig.1 that the discrepancy is in the range of 0.033 to 0.044 % (0.011 to 0.013 eV). Moreover, the potential energy of the ground state H_2^+ has been calculated at the internuclear distance of 1.4 bohr. The obtained energy, -0.569977 au, is only 0.0012 % (0.00019 eV) above the corresponding exact energy, -0.569984 au[19]. From these calculations and the result for the H_3^+ minimal energy, the absolute error of the H_3^+ ground state PES is expected to be less than 0.06 % (0.02 eV) except for the strongly repulsive region. It is thought that the error which affects the shape of the ground state PES must be less than the absolute error, because the absolute error of H_2 potential is almost independent of the internuclear distance. The upper limit of error for the first excited PES may be slightly larger than the ground state PES, because electrons have broader spatial distribution in the excited state.

Table 1 Parameters of the [8s6p2d1f] Gaussian type basis set*

Type	Exponent	Coefficient
s	1170.498	0.0007
	173.5822	0.0058
	38.65163	0.0318
	10.60720	0.1380
s	3.379649	1.0
s	1.202518	1.0
s	0.463925	1.0
s	0.190537	1.0
s	0.0812406	1.0
s	0.0285649	1.0
s	0.0100437	1.0
p	8.0	1.0
p	2.2	1.0
p	1.8	1.0
p	0.77	1.0
p	0.30	1.0
p	0.12	1.0
d	2.2	1.0
d	1.6	1.0
f	1.4	1.0

*The exponents of s-type orbitals are taken from Ref.[23].

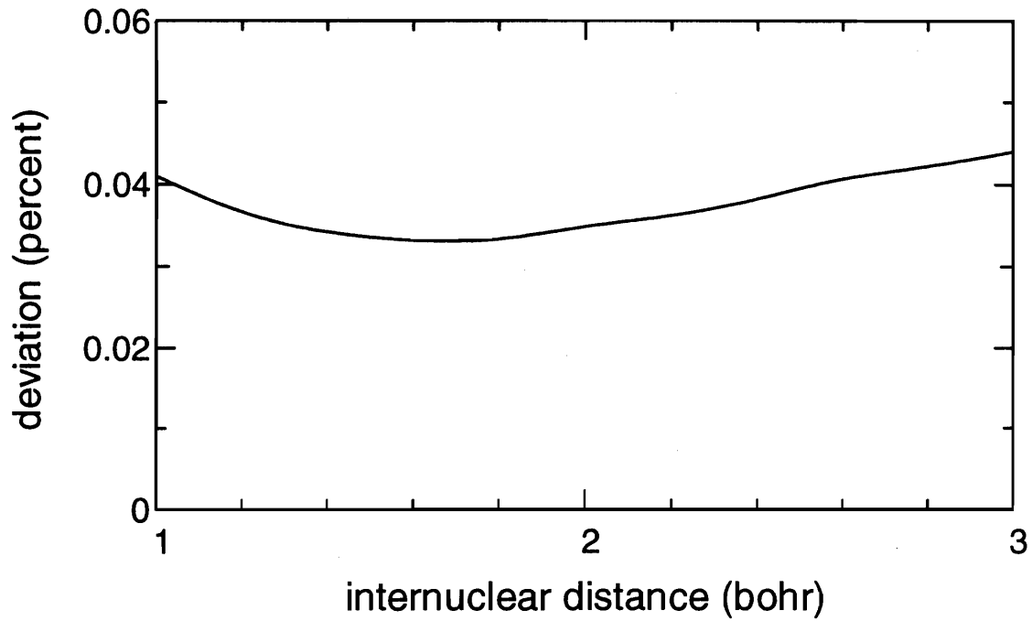

Fig.1 Deviation of the ground state H_2 potential from the accurate potential of Kolos and Wolnievicz [Ref.24].

2.2 Potential Surfaces

The full CI calculation has been carried out for 701 different spatial geometries, 530 of which are triangles, and 171 are collinear geometries. The triangles considered are obtained from physically possible geometries when each of three internuclear distances are given by r=0.6, 0.7, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 2.2, 2.4, 2.6, 2.8, 3.0, 3.5, 4.0, 6.0, 8.0, and 10.0 bohr. The collinear configurations are obtained such that two internuclear distances between nearest neighbor protons are defined by above r values.

The 3D-PES's can be produced from these ab initio energies. For instance, Fig.2 shows contour maps in the C_{2v} (isosceles triangle) spatial geometry for the ground state (lower figure) and the first excited state(upper one). The contours are shown as a function of two coordinates (r, R), where r is the distance between two protons and R is the distance from the midpoint of the proton pair to the third proton. The levels of contours are in eV with respect to zero energy which is selected to be the minimum of the ground state PES. To obtain these contours, potential energy values were evaluated by a linear interpolation with the ab initio energies at eight apexes of a hexahedron surrounding each point.

As can be seen from Fig.2, the ground state PES has a deep minimum around the equilateral triangle of side 1.65 bohr. The PES in the first excited state has no minimum and the features reflect the repulsive interaction between H and H_2^+ in the region of $R < 5.0$ bohr. Dashed lines in Fig.2 show the position of avoided crossing of two PES's. In order to have pictures of the avoided crossing, cross sections of PES's at R=6.0, 7.0, 8.0, and 9.0 bohr are shown in Fig.3. The avoided crossing arises in the region (r= 2.5 bohr, $R \geqq 6.0$ bohr). The presence of avoided crossing can not be clearly recognized for $R < 6.0$ bohr.

It can be seen from Figs. 2 and 3 that the avoided crossing arises in the area far from the H_3^+ equilibrium geometry. When H^+ collides with H_2, rearrangement of protons should take place around the minimum of the ground state PES with a formation of long lived H_3^+ complex. On the other hand, the electron transfer between the $H^+ + H_2$ and $H + H_2^+$ states is characterized by the nonadiabatic electronic transition in the region where the avoided crossing arises. Therefore, it is concluded that the proton rearrangement and electron transfer in the $H^+ + H_2$ collision are brought about in the different area of PES's.

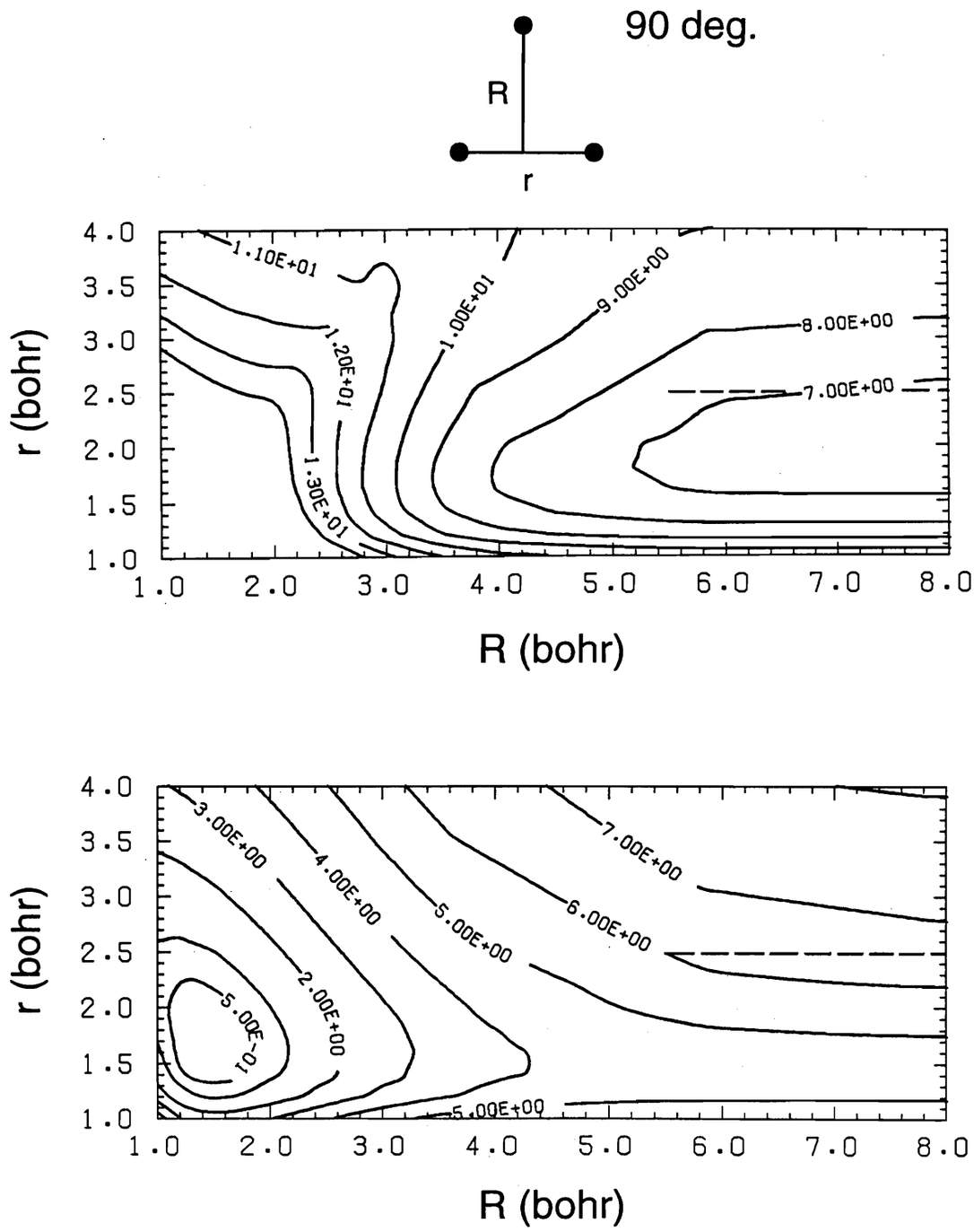

Fig.2 Contour maps of H_3^+ potential energy surfaces for the C_{2v} spatial geometry. The contour for the $^1A'$ ground (first excited) state is shown in the lower (upper) part of the figure. The contour levels are in eV with respect to zero energy which is chosen to be the minimum of the ground state surface. The dashed lines on contours indicate the position where the avoided crossing appears.

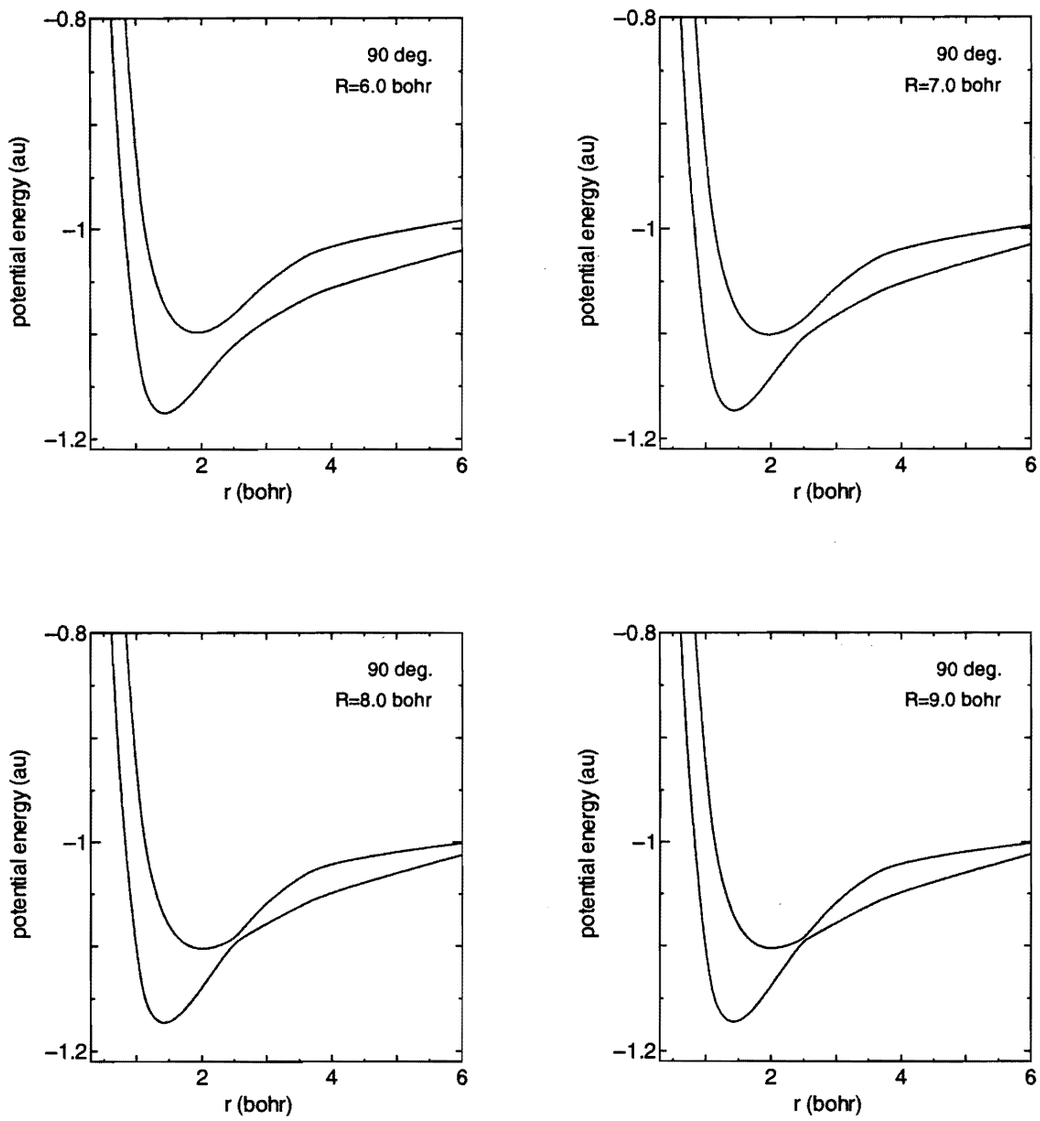

Fig.3 Sections of potential energy surfaces at R=6.0, 7.0, 8.0, and 9.0 bohr.

3.Tables of Potential Energies

The ab initio potential energies for the two lowest $^1A'$ states of H_3^+ at 530 triangular geometries are shown in Table 2 as a function of three internuclear distances (r_1, r_2, r_3, where $r_1 \leqq r_2 \leqq r_3$)[25]. The potential energies for 171 collinear geometries are shown in Table 3 as a function of two internuclear distances($r_1 \leqq r_2$, where $r_3=r_1+r_2$). Moreover, supplemental potential energies at 11 spatial geometries in the region of avoided crossing (r_1=2.5 bohr,4.0 bohr$\leqq r_2 \leqq$10.0 bohr) are shown in Table 4

Table 2. The ab initio potential energies for the two lowest $^1A'$ states of H_3^+ at triangular geometry

r_1	r_2	r_3	potential energy		r_1	r_2	r_3	potential energy	
			ground	excite				ground	excite
bohr	bohr	bohr	au	au	bohr	bohr	bohr	au	au
0.6	0.6	0.6	-0.126681	1.383747	0.6	2.2	2.2	-0.840392	-0.285217
0.6	0.6	0.7	-0.264048	1.212743	0.6	2.2	2.4	-0.833337	-0.310527
0.6	0.6	1.0	-0.428812	0.959508	0.6	2.2	2.6	-0.825467	-0.331523
0.6	0.7	0.7	-0.404320	1.039860	0.6	2.4	2.4	-0.827981	-0.335349
0.6	0.7	1.0	-0.576423	0.782047	0.6	2.4	2.6	-0.821675	-0.355813
0.6	0.7	1.2	-0.600849	0.589699	0.6	2.4	2.8	-0.814892	-0.372755
0.6	1.0	1.0	-0.767738	0.402333	0.6	2.6	2.6	-0.816822	-0.375667
0.6	1.0	1.2	-0.802805	0.299159	0.6	2.6	2.8	-0.811385	-0.391989
0.6	1.0	1.4	-0.808207	0.227283	0.6	2.6	3.0	-0.805654	-0.405471
0.6	1.2	1.2	-0.843901	0.196942	0.6	2.8	2.8	-0.807206	-0.407659
0.6	1.2	1.4	-0.854595	0.124757	0.6	2.8	3.0	-0.802644	-0.420502
0.6	1.2	1.6	-0.850012	0.070016	0.6	3.0	3.0	-0.799178	-0.432705
0.6	1.4	1.4	-0.869978	0.052506	0.6	3.0	3.5	-0.789542	-0.454445
0.6	1.4	1.6	-0.869548	-0.002897	0.6	3.5	3.5	-0.785257	-0.472789
0.6	1.4	1.8	-0.860924	-0.047198	0.6	3.5	4.0	-0.779654	-0.483703
0.6	1.6	1.6	-0.872826	-0.058778	0.6	4.0	4.0	-0.777745	-0.492284
0.6	1.6	1.8	-0.867512	-0.103739	0.6	6.0	6.0	-0.770304	-0.505988
0.6	1.6	2.0	-0.857688	-0.140659	0.6	8.0	8.0	-0.769454	-0.505361
0.6	1.8	1.8	-0.865177	-0.149096	0.6	10.0	10.0	-0.769233	-0.505022
0.6	1.8	2.0	-0.858030	-0.186370	0.7	0.7	0.7	-0.547047	0.865458
0.6	1.8	2.2	-0.848361	-0.217279	0.7	0.7	1.0	-0.725531	0.603724
0.6	2.0	2.0	-0.853314	-0.223717	0.7	0.7	1.2	-0.753428	0.409800
0.6	2.0	2.2	-0.845846	-0.254593	0.7	1.0	1.0	-0.920795	0.226585
0.6	2.0	2.4	-0.836951	-0.280247	0.7	1.0	1.2	-0.958038	0.122850

0.7	1.0	1.4	-0.965316	0.050356
0.7	1.0	1.6	-0.957732	-0.003288
0.7	1.2	1.2	-1.000618	0.021891
0.7	1.2	1.4	-1.012604	-0.049897
0.7	1.2	1.6	-1.009153	-0.104466
0.7	1.2	1.8	-0.997866	-0.147304
0.7	1.4	1.4	-1.028777	-0.120734
0.7	1.4	1.6	-1.029050	-0.175352
0.7	1.4	1.8	-1.021064	-0.219161
0.7	1.4	2.0	-1.008884	-0.254802
0.7	1.6	1.6	-1.032663	-0.229983
0.7	1.6	1.8	-1.027667	-0.274209
0.7	1.6	2.0	-1.018152	-0.310682
0.7	1.6	2.2	-1.006392	-0.340888
0.7	1.8	1.8	-1.025368	-0.318720
0.7	1.8	2.0	-1.018283	-0.355552
0.7	1.8	2.2	-1.008704	-0.386237
0.7	1.8	2.4	-0.997941	-0.411819
0.7	2.0	2.0	-1.013408	-0.392523
0.7	2.0	2.2	-1.005834	-0.423284
0.7	2.0	2.4	-0.996881	-0.448952
0.7	2.0	2.6	-0.987326	-0.470380
0.7	2.2	2.2	-1.000096	-0.453924
0.7	2.2	2.4	-0.992823	-0.479386
0.7	2.2	2.6	-0.984795	-0.500593
0.7	2.2	2.8	-0.976479	-0.518280
0.7	2.4	2.4	-0.987102	-0.504498
0.7	2.4	2.6	-0.980506	-0.525297
0.7	2.4	2.8	-0.973502	-0.542570
0.7	2.4	3.0	-0.966372	-0.556959
0.7	2.6	2.6	-0.975244	-0.545601
0.7	2.6	2.8	-0.969477	-0.562359
0.7	2.6	3.0	-0.963488	-0.576237
0.7	2.8	2.8	-0.964872	-0.578556
0.7	2.8	3.0	-0.959966	-0.591876
0.7	3.0	3.0	-0.956080	-0.604624
0.7	3.0	3.5	-0.945727	-0.627420
0.7	3.5	3.5	-0.940453	-0.647040
0.7	3.5	4.0	-0.934301	-0.658749
0.7	4.0	4.0	-0.931749	-0.668173
0.7	6.0	6.0	-0.922931	-0.683701
0.7	8.0	8.0	-0.921939	-0.683166
0.7	10.0	10.0	-0.921683	-0.682830
1.0	1.0	1.0	-1.126595	0.053219
1.0	1.0	1.2	-1.169811	-0.148280
1.0	1.0	1.4	-1.182335	-0.223868
1.0	1.0	1.6	-1.179360	-0.279512
1.0	1.0	1.8	-1.168511	-0.322100
1.0	1.2	1.2	-1.216521	-0.242273
1.0	1.2	1.4	-1.232172	-0.314608
1.0	1.2	1.6	-1.231986	-0.370286
1.0	1.2	1.8	-1.223625	-0.413778
1.0	1.2	2.0	-1.211164	-0.448160
1.0	1.4	1.4	-1.250650	-0.380490
1.0	1.4	1.6	-1.253017	-0.433500
1.0	1.4	1.8	-1.246950	-0.476700
1.0	1.4	2.0	-1.236546	-0.511878
1.0	1.4	2.2	-1.224075	-0.540427
1.0	1.6	1.6	-1.257706	-0.483817
1.0	1.6	1.8	-1.253742	-0.525896
1.0	1.6	2.0	-1.245236	-0.561192
1.0	1.6	2.2	-1.234470	-0.590582
1.0	1.6	2.4	-1.222747	-0.614867
1.0	1.8	1.8	-1.251698	-0.567123
1.0	1.8	2.0	-1.244934	-0.602242
1.0	1.8	2.2	-1.235747	-0.632003
1.0	1.8	2.4	-1.225443	-0.657015
1.0	1.8	2.6	-1.214784	-0.677872
1.0	2.0	2.0	-1.239768	-0.637263
1.0	2.0	2.2	-1.232034	-0.667154
1.0	2.0	2.4	-1.223052	-0.692486
1.0	2.0	2.6	-1.213585	-0.713800
1.0	2.0	2.8	-1.204079	-0.731639
1.0	2.2	2.2	-1.225639	-0.697106
1.0	2.2	2.4	-1.217883	-0.722519
1.0	2.2	2.6	-1.209535	-0.743958
1.0	2.2	2.8	-1.201043	-0.761967
1.0	2.2	3.0	-1.192671	-0.777050
1.0	2.4	2.4	-1.211262	-0.747900
1.0	2.4	2.6	-1.203961	-0.769273
1.0	2.4	2.8	-1.196432	-0.787214
1.0	2.4	3.0	-1.188937	-0.802244
1.0	2.6	2.6	-1.197638	-0.790481
1.0	2.6	2.8	-1.191020	-0.808218
1.0	2.6	3.0	-1.184368	-0.823041
1.0	2.6	3.5	-1.168445	-0.850318
1.0	2.8	2.8	-1.185259	-0.825686
1.0	2.8	3.0	-1.179414	-0.840213
1.0	2.8	3.5	-1.165260	-0.866788
1.0	3.0	3.0	-1.174335	-0.854405
1.0	3.0	3.5	-1.161903	-0.880138
1.0	3.5	3.5	-1.153485	-0.903609
1.0	3.5	4.0	-1.145529	-0.913294
1.0	4.0	4.0	-1.140619	-0.930144
1.0	6.0	6.0	-1.126297	-0.952484
1.0	8.0	8.0	-1.124756	-0.952320
1.0	10.0	10.0	-1.124374	-0.951997
1.2	1.2	1.2	-1.265690	-0.317985
1.2	1.2	1.4	-1.283568	-0.395034
1.2	1.2	1.6	-1.285400	-0.452420

1.2	1.2	1.8	-1.278866	-0.496972
1.2	1.2	2.0	-1.268059	-0.532207
1.2	1.2	2.2	-1.255252	-0.560195
1.2	1.4	1.4	-1.303493	-0.454431
1.2	1.4	1.6	-1.307198	-0.507864
1.2	1.4	1.8	-1.302371	-0.551974
1.2	1.4	2.0	-1.293118	-0.587732
1.2	1.4	2.2	-1.281719	-0.616609
1.2	1.4	2.4	-1.269471	-0.639803
1.2	1.6	1.6	-1.312630	-0.554518
1.2	1.6	1.8	-1.309386	-0.595690
1.2	1.6	2.0	-1.301580	-0.630832
1.2	1.6	2.2	-1.291497	-0.660157
1.2	1.6	2.4	-1.280443	-0.684302
1.2	1.6	2.6	-1.269167	-0.703988
1.2	1.8	1.8	-1.307603	-0.634168
1.2	1.8	2.0	-1.301136	-0.668113
1.2	1.8	2.2	-1.292278	-0.697357
1.2	1.8	2.4	-1.282336	-0.722054
1.2	1.8	2.6	-1.272066	-0.742640
1.2	1.8	2.8	-1.261906	-0.759637
1.2	2.0	2.0	-1.295905	-0.701222
1.2	2.0	2.2	-1.288181	-0.730222
1.2	2.0	2.4	-1.279274	-0.755144
1.2	2.0	2.6	-1.269944	-0.776242
1.2	2.0	2.8	-1.260632	-0.793917
1.2	2.0	3.0	-1.251589	-0.808623
1.2	2.2	2.2	-1.281501	-0.759108
1.2	2.2	2.4	-1.273556	-0.784099
1.2	2.2	2.6	-1.265106	-0.805424
1.2	2.2	2.8	-1.256593	-0.823431
1.2	2.2	3.0	-1.248271	-0.838538
1.2	2.4	2.4	-1.266501	-0.809135
1.2	2.4	2.6	-1.258872	-0.830524
1.2	2.4	2.8	-1.251114	-0.848634
1.2	2.4	3.0	-1.243482	-0.863874
1.2	2.4	3.5	-1.225738	-0.891999
1.2	2.6	2.6	-1.252010	-0.851903
1.2	2.6	2.8	-1.244965	-0.869981
1.2	2.6	3.0	-1.237991	-0.885189
1.2	2.6	3.5	-1.221655	-0.913295
1.2	2.8	2.8	-1.238590	-0.887957
1.2	2.8	3.0	-1.232246	-0.903037
1.2	2.8	3.5	-1.217290	-0.930829
1.2	3.0	3.0	-1.226500	-0.917939
1.2	3.0	3.5	-1.212895	-0.945242
1.2	3.0	4.0	-1.200845	-0.962635
1.2	3.5	3.5	-1.202481	-0.971021
1.2	3.5	4.0	-1.193232	-0.986936
1.2	4.0	4.0	-1.186636	-1.001242
1.2	6.0	6.0	-1.167403	-1.029304
1.2	8.0	8.0	-1.165368	-1.029498
1.2	10.0	10.0	-1.164887	-1.029189
1.4	1.4	1.4	-1.324778	-0.493802
1.4	1.4	1.6	-1.329754	-0.551816
1.4	1.4	1.8	-1.326111	-0.597496
1.4	1.4	2.0	-1.317959	-0.634194
1.4	1.4	2.2	-1.307584	-0.663814
1.4	1.4	2.4	-1.296287	-0.687645
1.4	1.4	2.6	-1.284817	-0.706680
1.4	1.6	1.6	-1.335926	-0.591519
1.4	1.6	1.8	-1.333402	-0.633037
1.4	1.6	2.0	-1.326292	-0.669095
1.4	1.6	2.2	-1.316885	-0.699034
1.4	1.6	2.4	-1.306483	-0.723555
1.4	1.6	2.6	-1.295839	-0.743434
1.4	1.6	2.8	-1.285383	-0.759392
1.4	1.8	1.8	-1.331928	-0.667940
1.4	1.8	2.0	-1.325796	-0.701106
1.4	1.8	2.2	-1.317296	-0.730312
1.4	1.8	2.4	-1.307733	-0.755071
1.4	1.8	2.6	-1.297859	-0.775653
1.4	1.8	2.8	-1.288108	-0.792544
1.4	1.8	3.0	-1.278725	-0.806273
1.4	2.0	2.0	-1.320579	-0.731796
1.4	2.0	2.2	-1.312926	-0.759883
1.4	2.0	2.4	-1.304145	-0.784476
1.4	2.0	2.6	-1.294989	-0.805430
1.4	2.0	2.8	-1.285894	-0.822986
1.4	2.0	3.0	-1.277106	-0.837537
1.4	2.2	2.2	-1.306060	-0.787239
1.4	2.2	2.4	-1.298008	-0.811604
1.4	2.2	2.6	-1.289523	-0.832697
1.4	2.2	2.8	-1.281042	-0.850627
1.4	2.2	3.0	-1.272811	-0.865686
1.4	2.2	3.5	-1.254067	-0.893135
1.4	2.4	2.4	-1.290631	-0.835872
1.4	2.4	2.6	-1.282771	-0.857020
1.4	2.4	2.8	-1.274865	-0.875125
1.4	2.4	3.0	-1.267161	-0.890440
1.4	2.4	3.5	-1.249517	-0.918718
1.4	2.6	2.6	-1.275493	-0.878218
1.4	2.6	2.8	-1.268128	-0.896388
1.4	2.6	3.0	-1.260922	-0.911800
1.4	2.6	3.5	-1.244341	-0.940417
1.4	2.8	2.8	-1.261268	-0.914579
1.4	2.8	3.0	-1.254536	-0.929992
1.4	2.8	3.5	-1.238990	-0.958633
1.4	2.8	4.0	-1.225682	-0.976991
1.4	3.0	3.0	-1.248252	-0.945360

1.4	3.0	3.5	-1.233715	-0.973831
1.4	3.0	4.0	-1.221234	-0.992066
1.4	3.5	3.5	-1.221567	-1.001507
1.4	3.5	4.0	-1.211196	-1.018883
1.4	4.0	4.0	-1.202902	-1.035126
1.4	6.0	6.0	-1.177806	-1.069797
1.4	8.0	8.0	-1.175127	-1.070490
1.4	10.0	10.0	-1.174536	-1.070199
1.6	1.6	1.6	-1.342825	-0.610287
1.6	1.6	1.8	-1.341006	-0.656369
1.6	1.6	2.0	-1.334577	-0.693994
1.6	1.6	2.2	-1.325823	-0.724860
1.6	1.6	2.4	-1.316047	-0.750084
1.6	1.6	2.6	-1.306000	-0.770551
1.6	1.6	2.8	-1.296112	-0.787007
1.6	1.6	3.0	-1.286627	-0.800105
1.6	1.8	1.8	-1.339871	-0.684188
1.6	1.8	2.0	-1.334098	-0.717722
1.6	1.8	2.2	-1.325968	-0.747891
1.6	1.8	2.4	-1.316784	-0.773332
1.6	1.8	2.6	-1.307298	-0.794348
1.6	1.8	2.8	-1.297938	-0.811497
1.6	1.8	3.0	-1.288945	-0.825340
1.6	2.0	2.0	-1.328950	-0.745079
1.6	2.0	2.2	-1.321413	-0.772556
1.6	2.0	2.4	-1.312789	-0.797237
1.6	2.0	2.6	-1.303826	-0.818363
1.6	2.0	2.8	-1.294955	-0.836028
1.6	2.0	3.0	-1.286415	-0.850592
1.6	2.0	3.5	-1.267219	-0.876163
1.6	2.2	2.2	-1.314436	-0.797859
1.6	2.2	2.4	-1.306336	-0.821550
1.6	2.2	2.6	-1.297862	-0.842479
1.6	2.2	2.8	-1.289444	-0.860391
1.6	2.2	3.0	-1.281324	-0.875446
1.6	2.2	3.5	-1.263016	-0.902696
1.6	2.4	2.4	-1.298726	-0.844628
1.6	2.4	2.6	-1.290707	-0.865360
1.6	2.4	2.8	-1.282712	-0.883366
1.6	2.4	3.0	-1.274982	-0.898695
1.6	2.4	3.5	-1.257499	-0.927008
1.6	2.6	2.6	-1.283114	-0.886016
1.6	2.6	2.8	-1.275513	-0.904072
1.6	2.6	3.0	-1.268146	-0.919546
1.6	2.6	3.5	-1.251445	-0.948441
1.6	2.6	4.0	-1.237525	-0.966791
1.6	2.8	2.8	-1.268279	-0.922182
1.6	2.8	3.0	-1.261255	-0.937727
1.6	2.8	3.5	-1.245300	-0.966893
1.6	2.8	4.0	-1.231962	-0.985608
1.6	3.0	3.0	-1.254553	-0.953313
1.6	3.0	3.5	-1.239317	-0.982557
1.6	3.0	4.0	-1.226558	-1.001393
1.6	3.5	3.5	-1.225762	-1.011622
1.6	3.5	4.0	-1.214481	-1.030170
1.6	4.0	4.0	-1.204679	-1.048091
1.6	6.0	6.0	-1.173001	-1.090002
1.6	8.0	8.0	-1.169456	-1.091415
1.6	10.0	10.0	-1.168742	-1.091152
1.8	1.8	1.8	-1.339093	-0.690786
1.8	1.8	2.0	-1.333687	-0.728870
1.8	1.8	2.2	-1.325930	-0.760650
1.8	1.8	2.4	-1.317119	-0.787029
1.8	1.8	2.6	-1.308003	-0.808744
1.8	1.8	2.8	-1.299010	-0.826455
1.8	1.8	3.0	-1.290377	-0.840766
1.8	1.8	3.5	-1.271055	-0.865020
1.8	2.0	2.0	-1.328651	-0.749232
1.8	2.0	2.2	-1.321260	-0.777138
1.8	2.0	2.4	-1.312810	-0.802830
1.8	2.0	2.6	-1.304045	-0.824691
1.8	2.0	2.8	-1.295392	-0.842848
1.8	2.0	3.0	-1.287087	-0.857729
1.8	2.0	3.5	-1.268516	-0.883545
1.8	2.2	2.2	-1.314227	-0.799424
1.8	2.2	2.4	-1.306121	-0.822679
1.8	2.2	2.6	-1.297688	-0.843801
1.8	2.2	2.8	-1.289350	-0.861974
1.8	2.2	3.0	-1.281344	-0.877224
1.8	2.2	3.5	-1.263442	-0.904569
1.8	2.4	2.4	-1.298345	-0.844058
1.8	2.4	2.6	-1.290221	-0.864319
1.8	2.4	2.8	-1.282176	-0.882283
1.8	2.4	3.0	-1.274445	-0.897687
1.8	2.4	3.5	-1.257145	-0.926112
1.8	2.4	4.0	-1.243004	-0.943573
1.8	2.6	2.6	-1.282388	-0.884066
1.8	2.6	2.8	-1.274615	-0.901858
1.8	2.6	3.0	-1.267137	-0.917322
1.8	2.6	3.5	-1.250391	-0.946402
1.8	2.6	4.0	-1.236683	-0.964788
1.8	2.8	2.8	-1.267095	-0.919591
1.8	2.8	3.0	-1.259852	-0.935098
1.8	2.8	3.5	-1.243620	-0.964556
1.8	2.8	4.0	-1.230315	-0.983494
1.8	3.0	3.0	-1.252829	-0.950659
1.8	3.0	3.5	-1.237081	-0.980334
1.8	3.0	4.0	-1.224163	-0.999575
1.8	3.5	3.5	-1.222439	-1.010253
1.8	3.5	4.0	-1.210961	-1.030190

1.8	4.0	4.0	-1.199458	-1.048887
1.8	6.0	6.0	-1.160941	-1.098189
1.8	8.0	8.0	-1.156167	-1.100686
1.8	10.0	10.0	-1.155316	-1.100466
2.0	2.0	2.0	-1.323757	-0.748547
2.0	2.0	2.2	-1.316532	-0.780953
2.0	2.0	2.4	-1.308265	-0.808291
2.0	2.0	2.6	-1.299697	-0.831108
2.0	2.0	2.8	-1.291251	-0.849958
2.0	2.0	3.0	-1.283161	-0.865382
2.0	2.0	3.5	-1.265138	-0.892161
2.0	2.2	2.2	-1.309485	-0.796492
2.0	2.2	2.4	-1.301404	-0.820240
2.0	2.2	2.6	-1.293028	-0.842400
2.0	2.2	2.8	-1.284776	-0.861345
2.0	2.2	3.0	-1.276881	-0.877128
2.0	2.2	3.5	-1.259337	-0.905129
2.0	2.2	4.0	-1.245144	-0.921258
2.0	2.4	2.4	-1.293510	-0.838951
2.0	2.4	2.6	-1.285318	-0.858930
2.0	2.4	2.8	-1.277248	-0.877166
2.0	2.4	3.0	-1.269530	-0.892890
2.0	2.4	3.5	-1.252404	-0.921785
2.0	2.4	4.0	-1.238579	-0.939253
2.0	2.6	2.6	-1.277303	-0.877296
2.0	2.6	2.8	-1.269401	-0.894776
2.0	2.6	3.0	-1.261846	-0.910282
2.0	2.6	3.5	-1.245089	-0.939668
2.0	2.6	4.0	-1.231573	-0.958135
2.0	2.8	2.8	-1.261658	-0.911815
2.0	2.8	3.0	-1.254251	-0.927163
2.0	2.8	3.5	-1.237825	-0.956821
2.0	2.8	4.0	-1.224579	-0.975940
2.0	3.0	3.0	-1.246980	-0.942456
2.0	3.0	3.5	-1.230856	-0.972300
2.0	3.0	4.0	-1.217852	-0.991825
2.0	3.5	3.5	-1.215392	-1.002541
2.0	3.5	4.0	-1.202943	-1.022523
2.0	4.0	4.0	-1.191019	-1.042647
2.0	6.0	6.0	-1.146082	-1.098794
2.0	8.0	8.0	-1.139478	-1.102984
2.0	10.0	10.0	-1.138457	-1.102844
2.2	2.2	2.2	-1.302458	-0.791560
2.2	2.2	2.4	-1.294423	-0.819691
2.2	2.2	2.6	-1.286114	-0.843498
2.2	2.2	2.8	-1.277949	-0.863397
2.2	2.2	3.0	-1.270158	-0.879856
2.2	2.2	3.5	-1.252921	-0.908981
2.2	2.2	4.0	-1.239075	-0.925782
2.2	2.4	2.4	-1.286451	-0.832024
2.2	2.4	2.6	-1.278216	-0.852546
2.2	2.4	2.8	-1.270136	-0.871821
2.2	2.4	3.0	-1.262438	-0.888324
2.2	2.4	3.5	-1.245461	-0.918295
2.2	2.4	4.0	-1.231887	-0.936131
2.2	2.6	2.6	-1.270062	-0.868589
2.2	2.6	2.8	-1.262063	-0.885913
2.2	2.6	3.0	-1.254449	-0.901737
2.2	2.6	3.5	-1.237691	-0.931869
2.2	2.6	4.0	-1.224331	-0.950624
2.2	2.8	2.8	-1.254144	-0.901833
2.2	2.8	3.0	-1.246608	-0.916981
2.2	2.8	3.5	-1.230035	-0.946971
2.2	2.8	4.0	-1.216843	-0.966353
2.2	3.0	3.0	-1.239141	-0.931737
2.2	3.0	3.5	-1.222729	-0.961609
2.2	3.0	4.0	-1.209675	-0.981390
2.2	3.5	3.5	-1.206643	-0.991616
2.2	3.5	4.0	-1.193855	-1.011939
2.2	4.0	4.0	-1.181286	-1.032581
2.2	4.0	6.0	-1.154070	-1.062982
2.2	6.0	6.0	-1.131174	-1.094172
2.2	6.0	8.0	-1.123793	-1.098360
2.2	8.0	8.0	-1.121805	-1.101005
2.2	8.0	10.0	-1.119953	-1.101113
2.2	10.0	10.0	-1.120522	-1.101042
2.4	2.4	2.4	-1.278430	-0.824819
2.4	2.4	2.6	-1.270175	-0.849530
2.4	2.4	2.8	-1.262094	-0.870408
2.4	2.4	3.0	-1.254416	-0.887837
2.4	2.4	3.5	-1.237559	-0.919152
2.4	2.4	4.0	-1.224174	-0.937751
2.4	2.6	2.6	-1.261913	-0.859658
2.4	2.6	2.8	-1.253840	-0.877548
2.4	2.6	3.0	-1.246180	-0.894380
2.4	2.6	3.5	-1.229416	-0.926029
2.4	2.6	4.0	-1.216167	-0.945422
2.4	2.8	2.8	-1.245780	-0.891466
2.4	2.8	3.0	-1.238138	-0.906546
2.4	2.8	3.5	-1.221442	-0.937386
2.4	2.8	4.0	-1.208286	-0.957278
2.4	3.0	3.0	-1.230514	-0.920388
2.4	3.0	3.5	-1.213869	-0.950331
2.4	3.0	4.0	-1.200772	-0.970483
2.4	3.5	3.5	-1.197303	-0.979448
2.4	3.5	4.0	-1.184269	-0.999941
2.4	4.0	4.0	-1.171249	-1.020756
2.4	4.0	6.0	-1.144004	-1.051753
2.4	6.0	6.0	-1.117896	-1.085680
2.4	6.0	8.0	-1.109842	-1.090752

2.4	8.0	8.0	-1.104896	-1.096035
2.4	8.0	10.0	-1.102778	-1.096500
2.4	10.0	10.0	-1.102885	-1.096727
2.6	2.6	2.6	-1.253570	-0.851502
2.6	2.6	2.8	-1.245440	-0.873308
2.6	2.6	3.0	-1.237742	-0.891654
2.6	2.6	3.5	-1.220962	-0.925009
2.6	2.6	4.0	-1.207782	-0.945262
2.6	2.8	2.8	-1.237266	-0.881836
2.6	2.8	3.0	-1.229537	-0.897478
2.6	2.8	3.5	-1.212728	-0.930264
2.6	2.8	4.0	-1.199580	-0.951048
2.6	3.0	3.0	-1.221784	-0.909597
2.6	3.0	3.5	-1.204938	-0.940035
2.6	3.0	4.0	-1.191792	-0.960860
2.6	3.5	3.5	-1.187990	-0.967306
2.6	3.5	4.0	-1.174766	-0.987866
2.6	3.5	6.0	-1.147850	-1.017580
2.6	4.0	4.0	-1.161422	-1.008525
2.6	4.0	6.0	-1.134292	-1.039855
2.6	6.0	6.0	-1.106724	-1.074674
2.6	6.0	8.0	-1.099096	-1.079531
2.6	8.0	8.0	-1.092917	-1.085750
2.6	8.0	10.0	-1.091709	-1.085399
2.6	10.0	10.0	-1.091091	-1.086197
2.8	2.8	2.8	-1.229000	-0.873601
2.8	2.8	3.0	-1.221199	-0.892817
2.8	2.8	3.5	-1.204281	-0.928069
2.8	2.8	4.0	-1.191113	-0.949826
2.8	3.0	3.0	-1.213336	-0.900104
2.8	3.0	3.5	-1.196312	-0.932294
2.8	3.0	4.0	-1.183102	-0.954263
2.8	3.5	3.5	-1.179048	-0.956005
2.8	3.5	4.0	-1.165663	-0.976628
2.8	3.5	6.0	-1.139031	-1.006910
2.8	4.0	4.0	-1.152078	-0.996760
2.8	4.0	6.0	-1.125084	-1.028311
2.8	6.0	6.0	-1.097170	-1.062763
2.8	6.0	8.0	-1.090446	-1.066921
2.8	8.0	8.0	-1.085565	-1.071571
2.8	8.0	10.0	-1.084952	-1.070722
2.8	10.0	10.0	-1.084576	-1.071138
3.0	3.0	3.0	-1.205382	-0.892329
3.0	3.0	3.5	-1.188196	-0.929331
3.0	3.0	4.0	-1.174907	-0.952438
3.0	3.5	3.5	-1.170664	-0.946055
3.0	3.5	4.0	-1.157134	-0.966906
3.0	3.5	6.0	-1.130659	-0.998161
3.0	4.0	4.0	-1.143356	-0.986011
3.0	4.0	6.0	-1.116457	-1.017796
3.0	6.0	6.0	-1.088642	-1.051203
3.0	6.0	8.0	-1.082653	-1.054822
3.0	8.0	8.0	-1.078557	-1.058447
3.0	8.0	10.0	-1.078089	-1.057553
3.0	10.0	10.0	-1.077768	-1.057790
3.5	3.5	3.5	-1.152618	-0.928457
3.5	3.5	4.0	-1.138754	-0.954264
3.5	3.5	6.0	-1.112221	-0.989764
3.5	4.0	4.0	-1.124600	-0.965235
3.5	4.0	6.0	-1.097651	-0.998721
3.5	6.0	6.0	-1.070194	-1.027411
3.5	6.0	8.0	-1.065072	-1.030618
3.5	8.0	8.0	-1.061678	-1.033056
3.5	8.0	10.0	-1.061302	-1.032319
3.5	10.0	10.0	-1.061018	-1.032286
4.0	4.0	4.0	-1.110159	-0.953227
4.0	4.0	6.0	-1.082863	-0.992900
4.0	6.0	6.0	-1.055207	-1.011935
4.0	6.0	8.0	-1.050192	-1.015450
4.0	8.0	8.0	-1.046835	-1.017461
4.0	8.0	10.0	-1.046465	-1.016942
4.0	10.0	10.0	-1.046185	-1.016775
6.0	6.0	6.0	-1.024875	-0.992462
6.0	6.0	8.0	-1.018718	-0.988750
6.0	6.0	10.0	-1.017647	-1.001372
6.0	8.0	8.0	-1.013095	-1.001211
6.0	8.0	10.0	-1.012452	-1.001429
6.0	10.0	10.0	-1.012032	-1.001226
8.0	8.0	8.0	-1.005061	-0.999184
8.0	8.0	10.0	-1.003890	-1.000476
8.0	10.0	10.0	-1.002820	-1.000399
10.0	10.0	10.0	-1.001106	-1.000123

Table 3. The ab initio potential energies for the two lowest $^1A'$ states of H_3^+ at collinear geometry

r_1	r_2	potential energy		r_1	r_2	potential energy	
		ground	excite			ground	excite
bohr	bohr	au	au	bohr	bohr	au	au
0.6	0.6	-0.449256	0.770786	1.0	1.8	-1.204210	-0.695172
0.6	0.7	-0.601303	0.552375	1.0	2.0	-1.194795	-0.746518
0.6	1.0	-0.798984	0.174033	1.0	2.2	-1.184571	-0.789661
0.6	1.2	-0.837718	0.026999	1.0	2.4	-1.174602	-0.825359
0.6	1.4	-0.848155	-0.083223	1.0	2.6	-1.165441	-0.854463
0.6	1.6	-0.845622	-0.171181	1.0	2.8	-1.157356	-0.877869
0.6	1.8	-0.837483	-0.242991	1.0	3.0	-1.150439	-0.896445
0.6	2.0	-0.827411	-0.301610	1.0	3.5	-1.138009	-0.926801
0.6	2.2	-0.817256	-0.349003	1.0	4.0	-1.131071	-0.941941
0.6	2.4	-0.807925	-0.386846	1.0	6.0	-1.124532	-0.952752
0.6	2.6	-0.799815	-0.416671	1.0	8.0	-1.124079	-0.952241
0.6	2.8	-0.793038	-0.439874	1.0	10.0	-1.124030	-0.951965
0.6	3.0	-0.787543	-0.457692	1.2	1.2	-1.241726	-0.582331
0.6	3.5	-0.778438	-0.485330	1.2	1.4	-1.257118	-0.658283
0.6	4.0	-0.773815	-0.498127	1.2	1.6	-1.258104	-0.719897
0.6	6.0	-0.769575	-0.506036	1.2	1.8	-1.252105	-0.773567
0.6	8.0	-0.769171	-0.505307	1.2	2.0	-1.242958	-0.820793
0.6	10.0	-0.769091	-0.505002	1.2	2.2	-1.232710	-0.861647
0.7	0.7	-0.752612	0.339841	1.2	2.4	-1.222469	-0.896253
0.7	1.0	-0.950882	-0.025127	1.2	2.6	-1.212835	-0.925039
0.7	1.2	-0.990625	-0.165318	1.2	2.8	-1.204118	-0.948625
0.7	1.4	-1.001967	-0.270095	1.2	3.0	-1.196464	-0.967695
0.7	1.6	-1.000100	-0.353990	1.2	3.5	-1.182065	-0.999857
0.7	1.8	-0.992370	-0.422966	1.2	4.0	-1.173498	-1.016702
0.7	2.0	-0.982475	-0.479730	1.2	6.0	-1.164994	-1.029781
0.7	2.2	-0.972306	-0.525999	1.2	8.0	-1.164465	-1.029414
0.7	2.4	-0.962817	-0.563237	1.2	10.0	-1.164427	-1.029152
0.7	2.6	-0.954450	-0.592815	1.4	1.4	-1.273602	-0.721722
0.7	2.8	-0.947362	-0.616001	1.4	1.6	-1.275360	-0.772064
0.7	3.0	-0.941541	-0.633941	1.4	1.8	-1.269844	-0.817328
0.7	3.5	-0.931718	-0.662083	1.4	2.0	-1.260923	-0.859275
0.7	4.0	-0.926633	-0.675321	1.4	2.2	-1.250674	-0.897207
0.7	6.0	-0.921977	-0.683784	1.4	2.4	-1.240229	-0.930387
0.7	8.0	-0.921568	-0.683105	1.4	2.6	-1.230214	-0.958659
0.7	10.0	-0.921496	-0.682807	1.4	2.8	-1.220964	-0.982297
1.0	1.0	-1.153836	-0.355250	1.4	3.0	-1.212654	-1.001775
1.0	1.2	-1.196857	-0.475399	1.4	3.5	-1.196319	-1.035726
1.0	1.4	-1.210828	-0.563478	1.4	4.0	-1.185889	-1.054511
1.0	1.6	-1.210817	-0.634795	1.4	6.0	-1.174661	-1.070585

1.4	8.0	-1.173991	-1.070405
1.4	10.0	-1.173958	-1.070158
1.6	1.6	-1.277675	-0.810390
1.6	1.8	-1.272521	-0.845125
1.6	2.0	-1.263783	-0.879788
1.6	2.2	-1.253553	-0.913544
1.6	2.4	-1.242977	-0.944622
1.6	2.6	-1.232689	-0.971998
1.6	2.8	-1.223039	-0.995435
1.6	3.0	-1.214210	-1.015132
1.6	3.5	-1.196182	-1.050586
1.6	4.0	-1.183844	-1.071342
1.6	6.0	-1.168997	-1.091254
1.6	8.0	-1.168087	-1.091339
1.6	10.0	-1.168049	-1.091107
1.8	1.8	-1.267611	-0.868308
1.8	2.0	-1.259010	-0.893163
1.8	2.2	-1.248811	-0.920608
1.8	2.4	-1.238164	-0.948342
1.8	2.6	-1.227707	-0.974156
1.8	2.8	-1.217789	-0.996998
1.8	3.0	-1.208597	-1.016633
1.8	3.5	-1.189278	-1.053080
1.8	4.0	-1.175245	-1.075558
1.8	6.0	-1.155892	-1.100135
1.8	8.0	-1.154571	-1.100631
1.8	10.0	-1.154515	-1.100419
2.0	2.0	-1.250493	-0.906990
2.0	2.2	-1.240325	-0.925372
2.0	2.4	-1.229650	-0.947633
2.0	2.6	-1.219103	-0.970712
2.0	2.8	-1.209031	-0.992330
2.0	3.0	-1.199620	-1.011516
2.0	3.5	-1.179455	-1.048302
2.0	4.0	-1.164161	-1.072006
2.0	6.0	-1.139713	-1.101765
2.0	8.0	-1.137653	-1.102977
2.0	10.0	-1.137560	-1.102795
2.2	2.2	-1.230174	-0.933370
2.2	2.4	-1.219494	-0.947355
2.2	2.6	-1.208911	-0.965675
2.2	2.8	-1.198769	-0.984990
2.2	3.0	-1.189249	-1.003149
2.2	3.5	-1.168625	-1.039501
2.2	4.0	-1.152580	-1.063825
2.2	6.0	-1.123249	-1.098471
2.2	8.0	-1.119717	-1.101114
2.2	10.0	-1.119545	-1.100994
2.4	2.4	-1.208815	-0.951747
2.4	2.6	-1.198229	-0.962616
2.4	2.8	-1.188071	-0.977774
2.4	3.0	-1.178517	-0.993934
2.4	3.5	-1.157715	-1.028865
2.4	4.0	-1.141348	-1.053223
2.4	6.0	-1.108895	-1.090895
2.4	8.0	-1.102337	-1.096505
2.4	10.0	-1.101834	-1.096694
2.6	2.6	-1.187655	-0.964830
2.6	2.8	-1.177511	-0.973390
2.6	3.0	-1.167969	-0.985903
2.6	3.5	-1.147167	-1.017927
2.6	4.0	-1.130758	-1.041776
2.6	6.0	-1.098106	-1.079420
2.6	8.0	-1.091594	-1.084916
2.6	10.0	-1.090991	-1.085178
2.8	2.8	-1.167398	-0.974344
2.8	3.0	-1.157892	-0.981118
2.8	3.5	-1.137188	-1.007832
2.8	4.0	-1.120887	-1.030578
2.8	6.0	-1.089557	-1.066486
2.8	8.0	-1.084890	-1.070065
2.8	10.0	-1.084499	-1.070085
3.0	3.0	-1.148436	-0.981392
3.0	3.5	-1.127876	-0.999550
3.0	4.0	-1.111743	-1.020373
3.0	6.0	-1.081837	-1.054169
3.0	8.0	-1.078033	-1.056809
3.0	10.0	-1.077693	-1.056748
3.5	3.5	-1.107724	-0.992328
3.5	4.0	-1.092009	-1.002278
3.5	6.0	-1.064295	-1.029845
3.5	8.0	-1.061242	-1.031536
3.5	10.0	-1.060942	-1.031369
4.0	4.0	-1.076578	-0.997785
4.0	6.0	-1.049360	-1.014950
4.0	8.0	-1.046397	-1.016279
4.0	10.0	-1.046104	-1.016055
6.0	6.0	-1.001453	-0.987659
6.0	8.0	-1.012318	-1.001306
6.0	10.0	-1.011927	-1.000997
8.0	8.0	-1.000609	-0.998106
8.0	10.0	-1.002653	-1.000297
10.0	10.0	-1.000819	-0.999870

Table 4 The ab initio potential energies near the avoided crossing seam

r_1	r_2	r_3	potential energy	
			ground	excite
bohr	bohr	bohr	au	au
2.5	4.0	4.0	-1.166288	-1.014627
2.5	4.0	6.0	-1.139092	-1.045814
2.5	6.0	6.0	-1.112065	-1.080390
2.5	6.0	8.0	-1.104097	-1.085482
2.5	8.0	8.0	-1.097842	-1.091922
2.5	8.0	10.0	-1.095737	-1.092421
2.5	10.0	10.0	-1.094726	-1.093687
2.5	4.0	6.5	-1.135965	-1.047527
2.5	6.0	8.5	-1.103088	-1.085529
2.5	8.0	10.5	-1.095411	-1.092225
2.5	10.0	12.5	-1.094062	-1.093247

Acknowledgements

The authors would like to thank Dr.T.Takayanagi of Japan Atomic Research Institute for his helpful advice.

References

[1] J.B.Anderson, J.Chem.Phys.**96**,3702(1992), and the related references therein.

[2] R.Rohse, W.Klopper, and W.Kutzelnigg, J.Chem.Phys.**99**,8830(1993).

[3] W.Meyer, P.Botschwina, and P.Burton, J.Chem.Phys.**84**,891(1986).

[4] D.Frye, A.Preiskorn, G.C.Lie, and E.Clementi, J.Chem.Phys.**92**,4948(1990).

[5] R.Rohse, W.Kutzelnigg, R.Jaquet, and W.Klopper, J.Chem.Phys.**101**,2231(1994).

[6] G.C.Lie and D.Frye, J.Chem.Phys.**96**,6784(1992).

[7] M.J.Bramley, J.R.Henderson, J.Tennyson, and B.T.Sutcliffe, J.Chem.Phys. **98**, 10104 (1993).

[8] S.Carter and W.Meyer, J.Chem.Phys.**100**, 2104(1994).

[9] L.Wolniewicz and J.Hinze, J.Chem.Phys.**101**,9817(1994).

[10] R.Prosmiti, O.L.Polyansky, and J.Tennyson, Chem.Phys.Lett.**273**,107(1997).

[11] W.Cencek, J.Rychlewski, R.Jaquet, and W.Kutzelnigg, J.Chem.Phys.**108**,2831 (1998).

[12] J.C. Tully and R.K. Preston, J.Chem.Phys. **55**, 562 (1971).

[13] G.Ochs and E.Teloy, J.Chem.Phys. **61**, 4930 (1974).

[14] Ch. Schlier, U. Nowotny, and E. Teloy, Chem.Phys. **111**, 401 (1987).

[15] J.R. Krenos, R.K. Preston, R. Wolfgang, and J.C. Tully, J.Chem.Phys. **60**, 1634 (1974).

[16] F.O. Ellison, J.Am.Chem.Soc. **85**, 3540, 3544 (1963).

[17] S. Chapman, Adv.Chem.Phys. **82**, 423 (1992).

[18] R.K.Janev, "Atomic, molecular and particle-surface interaction data for divertor physics design studies", INDC(NDS)-331(1995).

[19] C.W. Bauschlicher, Jr., S.V. O'Neil, R.K. Preston, H.F. Schaefer III, and C.F. Bender, J.Chem.Phys. **59**, 1286 (1973).

[20] K.Andersson, M.R.A.Blomberg, M.P.Fulscher, Y.Kello, R.Lindh, P.A.Malmqvist, J.Noga, J.Olsen, B.O.Roos, A.J.Sadlej, P.E.M.Siebbahn, M.Urvan, and P.O.Widmark, MOLCAS version 2, University of Lund, Sweden, 1991.

[21] A.Ichihara and K. Yokoyama, J.Chem.Phys. **103**, 2109 (1995).

[22] A. Ichihara, T.Shirai, and K. Yokoyama, J.Chem.Phys. **105**, 1857 (1996). It should be noted that the square root of the hopping coefficient E_c is given as a function of ΔE_0 in Fig.1 of this reference.

[23] S.Huzinaga, J.Chem.Phys.**42**,1293(1965).

[24] W.Kolos and L.Wolniewicz, J.Chem.Phys.**49**,404(1968).

[25] It should be noted that the potential energies at (r_1, r_2, r_3)=(1.0, 3.5, 4.0) and (1.8, 3.5, 4.0) are interpolated using ab initio energies around these points, because the ab initio calculations did not converge.