SUPPORTING INFORMATION

Potential energy surfaces and quasiclassical trajectory study of the O + H_2^+ → OH^+ + H, OH + H^+ proton and hydrogen atom transfer reactions and isotopic variants (D_2^+, HD^+)

Miguel Paniagua,[1,*] Rodrigo Martínez,[2] Pablo Gamallo,[3] and Miguel González[3,*]

[1] Depto. de Química Física Aplicada, Univ. Autónoma de Madrid, Cantoblanco, Spain

[2] Depto. de Química, Univ. de La Rioja, Logroño, Spain

[3] Dept. de Química Física i IQTC, Univ. de Barcelona, Barcelona, Spain

CONTENTS

Table S1. QCT rate constants for the $O + H_2^+ \rightarrow OH^+ + H$ ($1^2A''$ PES), $OH + H^+$ ($1^2A'$ PES) reactions, and global rate constant k_{tot} expressed in units of 10^{-10} $cm^3 \cdot molecule^{-1} \cdot s^{-1}$.[a]

T / K	$k(1^2A'')$	$k(1^2A')$	k(LGS)	k_{tot}	k_{tot}(LGS)
200	3.143(0.009)	0.953(0.003)	1.452	4.096(0.012)	2.905
300	3.682(0.011)	1.156(0.004)	1.599	4.838(0.015)	3.198
500	4.025(0.014)	1.367(0.006)	1.687	5.392(0.020)	3.373
700	4.060(0.015)	1.487(0.006)	1.713	5.547(0.021)	3.425
900	4.000(0.017)	1.565(0.007)	1.724	6.564(0.024)	3.447

[a] The LGS results are also included. The rate constants on the different PESs and from the LGS model are multiplied by the electronic factor f_{el} (see eqs. 8 (f_{el}) and 9 (k) in the paper), which takes the following values 0.0927, 0.1021, 0.1076, 0.1093, and 0.1100 for T=200, 300, 500, 700, and 900 K, respectively. Moreover, $k_{tot} = k(1^2A'') + k(1^2A')$, $k_{tot}(LGS) = 2\ k(LGS)$, and the QCT statistical errors (1σ) are given between parentheses.

Table S2. QCT rate constants for the $O + D_2^+ \rightarrow OD^+ + D$ ($1^2A''$ PES), $OD + D^+$ ($1^2A'$ PES) reactions, and global rate constant k_{tot} expressed in units of 10^{-10} $cm^3 \cdot molecule^{-1} \cdot s^{-1}$.[a]

T / K	$k(1^2A'')$	$k(1^2A')$	k(LGS)	k_{tot}	k_{tot}(LGS)
200	2.344(0.006)	0.710(0.002)	1.083	3.054(0.008)	2.166
300	2.763(0.008)	0.867(0.003)	1.193	3.630(0.011)	2.386
500	3.018(0.011)	1.015(0.004)	1.258	4.033(0.015)	2.516
700	3.029(0.011)	1.107(0.004)	1.278	4.136(0.015)	2.556
900	2.972(0.012)	1.165(0.005)	1.286	4.137(0.017)	2.572

[a] The LGS results are also included. The rate constants on the different PESs and from the LGS model are multiplied by the electronic factor f_{el} (see eqs. 8 (f_{el}) and 9 (k) in the paper), $k_{tot} = k(1^2A'') + k(1^2A')$, and $k_{tot}(LGS) = 2\ k(LGS)$. The QCT statistical errors (1σ) are given between parentheses.

Table S3. QCT rate constants for the O + HD^+ → OH^+ + D and OD^+ + H ($1^2A''$ PES), OH + D^+ and OD + H^+ ($1^2A'$ PES) reactions, and global rate constant k_{tot} expressed in units of 10^{-10} $cm^3 \cdot molecule^{-1} \cdot s^{-1}$.[a]

T / K	$k(1^2A'')$	$k(1^2A')$	k(LGS)	k_{tot}	k_{tot}(LGS)
200	2.631(0.007)	0.800(0.003)	1.219	3.431(0.010)	2.438
300	3.114(0.009)	0.977(0.004)	1.342	4.091(0.013)	2.684
500	3.429(0.012)	1.162(0.005)	1.416	4.591(0.017)	2.832
700	3.459(0.012)	1.266(0.005)	1.438	4.725(0.017)	2.876
900	3.405(0.020)	1.341(0.005)	1.447	4.746(0.025)	2.894

[a] The LGS results are also included. The rate constants on the different PESs and from the LGS model are multiplied by the electronic factor f_{el} (see eqs. 8 (f_{el}) and 9 (k) in the paper), $k_{tot} = k(1^2A'') + k(1^2A')$, and $k_{tot}(LGS) = 2\,k(LGS)$. The QCT statistical errors (1σ) are given between parentheses.

Table S4. QCT rate constants for the O + HD^+ → OH^+ + D and OD^+ + H ($1^2A''$ PES) reactions, expressed in units of 10^{-10} $cm^3 \cdot molecule^{-1} \cdot s^{-1}$.[a]

T / K	$k(1^2A'')$	
	OH^+ + D	OD^+ + H
200	1.399(0.007)	1.220(0.007)
300	1.646(0.009)	1.450(0.008)
500	1.826(0.012)	1.600(0.011)
700	1.835(0.011)	1.612(0.011)
900	1.803(0.018)	1.588(0.017)

[a] The QCT rate constants on the different PESs are multiplied by the electronic factor f_{el}. See eqs. 8 (f_{el}) and 9 (k) in the paper. The QCT statistical errors (1σ) are given between parentheses.

Table S5. QCT rate constants for the O + HD^+ → OH + D^+ and OD + H^+ ($1^2A'$ PES) reactions, expressed in units of 10^{-10} $cm^3 \cdot molecule^{-1} \cdot s^{-1}$.[a]

T / K	$k(1^2A')$	
	OH^+ + D	OD^+ + H
200	0.388(0.003)	0.385(0.003)
300	0.460(0.003)	0.469(0.003)
500	0.590(0.005)	0.535(0.004)
700	0.632(0.005)	0.621(0.005)
900	0.668(0.005)	0.663(0.005)

[a] The QCT rate constants on the different PESs are multiplied by the electronic factor f_{el}. See eqs. 8 (f_{el}) and 9 (k) in the paper. The QCT statistical errors (1σ) are given between parentheses.

Table S6. QCT cross sections for the O + H_2^+ → OH^+ + H ($1^2A''$ PES), OH + H^+ ($1^2A'$ PES) reactions, and global cross section σ expressed in Å^2.[a]

E_{col} / eV	$\sigma(1^2A'')$	$\sigma(1^2A')$	σ(LGS)	σ_{tot}	σ_{tot}(LGS)
0.01	31.382 (0.021)	9.008 (0.009)	16.776	40.390 (0.030)	33.552
0.05	20.282 (0.017)	6.259 (0.006)	7.502	26.541 (0.023)	15.005
0.1	13.641 (0.024)	5.069 (0.007)	5.305	18.710 (0.031)	10.610
0.2	7.983 (0.016)	4.155 (0.006)	3.751	12.138 (0.022)	7.502
0.3	6.095 (0.012)	3.675 (0.006)	3.063	9.770 (0.018)	6.126
0.4	5.137 (0.011)	3.351 (0.006)	2.652	8.488 (0.017)	5.305
0.5	4.661 (0.031)	3.084 (0.006)	2.372	7.745 (0.037)	4.745

[a] The LGS results are also included. The cross sections on the different PESs and from the LGS model are multiplied by the electronic factor f_{el} = 2/18 (see the paper), $\sigma_{tot} = \sigma(1^2A'') + \sigma(1^2A')$, and $\sigma_{tot}(LGS) = 2\,\sigma(LGS)$. The QCT statistical errors (one standard deviation) are given between parentheses.

Figure S1. Distribution of energy deviations, i.e., $\Delta E = E_{analytical} - E_{ic\text{-}MRCI+Q}$, for the ground and excited PESs: (a) $1^2A''$ and (b) $1^2A'$.

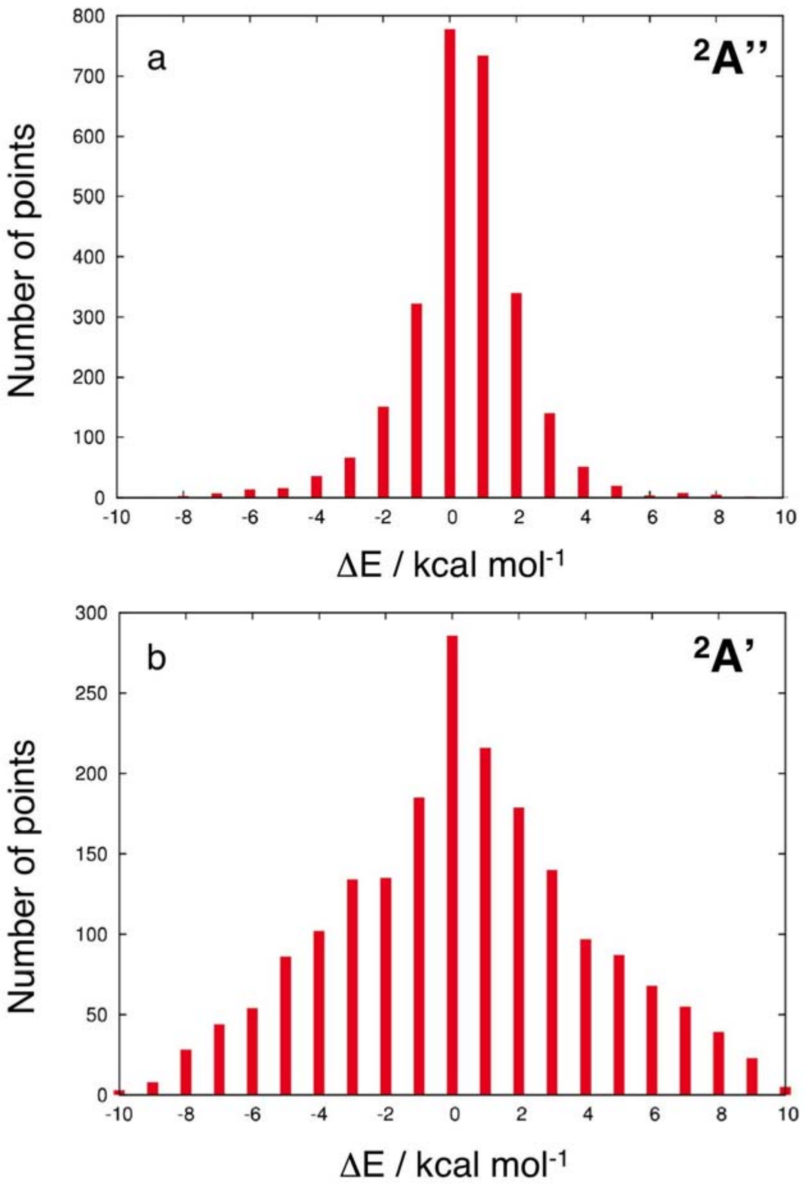
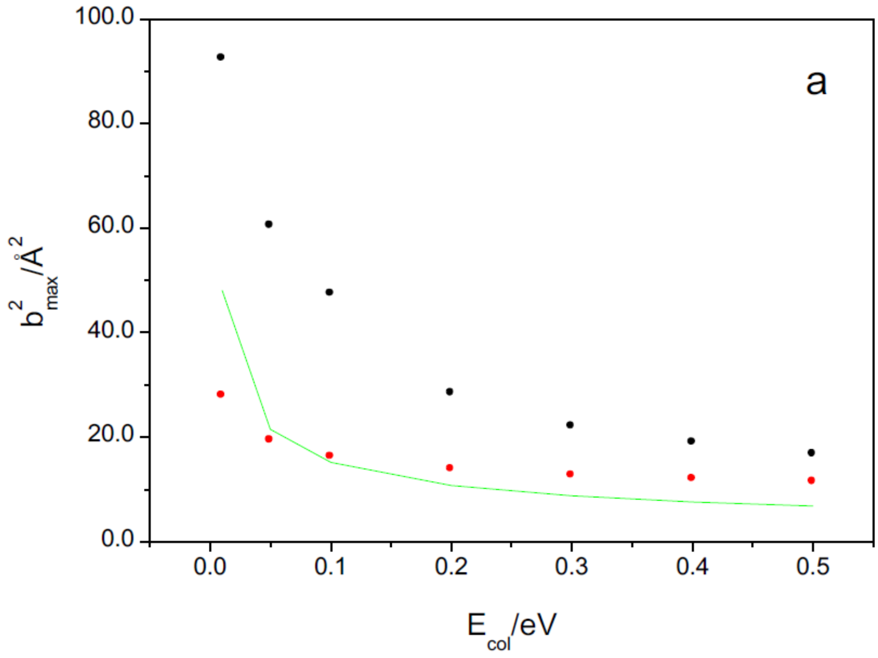


Figure S2: (a) QCT b_{max}^2 for the O + H_2^+(v=0,j=0) → OH^+ + H ($1^2A''$ PES; ●), OH + H^+ ($1^2A'$ PES; ●) reactions, and LGS (—) values; **(b)** Same as in (a) but for b_{max}.



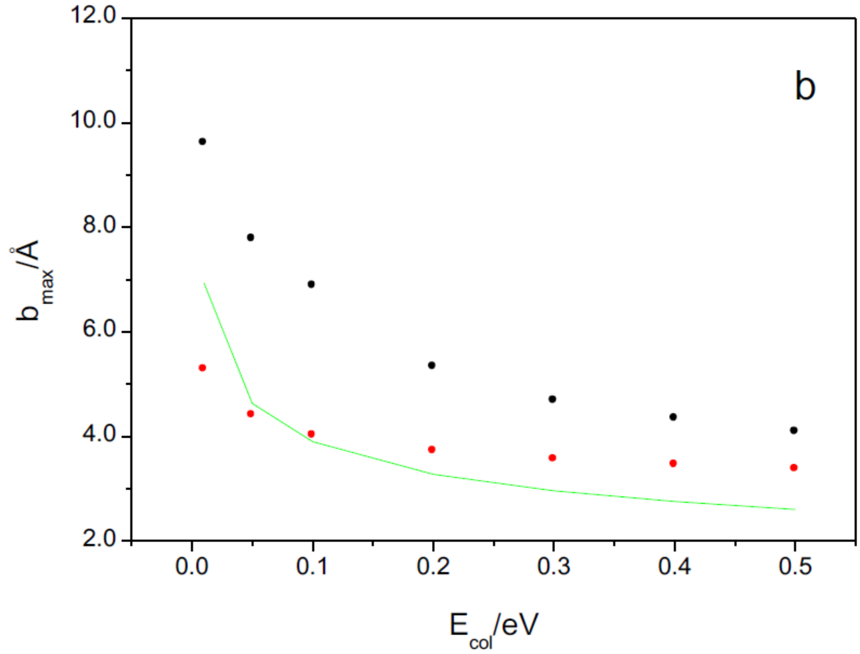


Figure S3: QCT reaction probability for the O + H_2^+(v=0,j=0) → OH^+ + H ($1^2A''$ PES; ●), OH + H^+ ($1^2A'$ PES; ●) reactions. The f_{el} = 2/18 factor was not included here, i.e., these values were directly obtained from the QCT calculations.

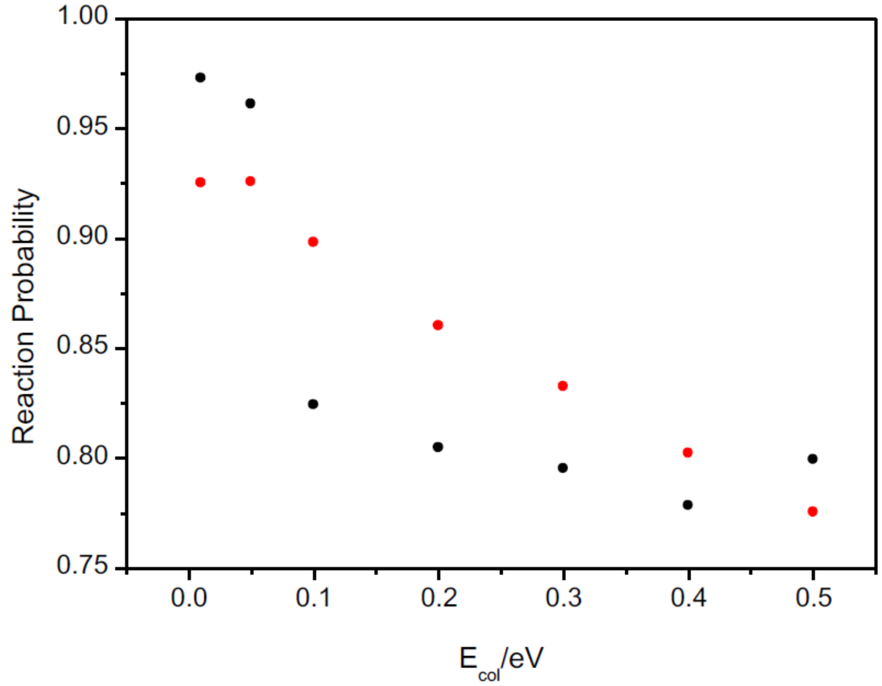
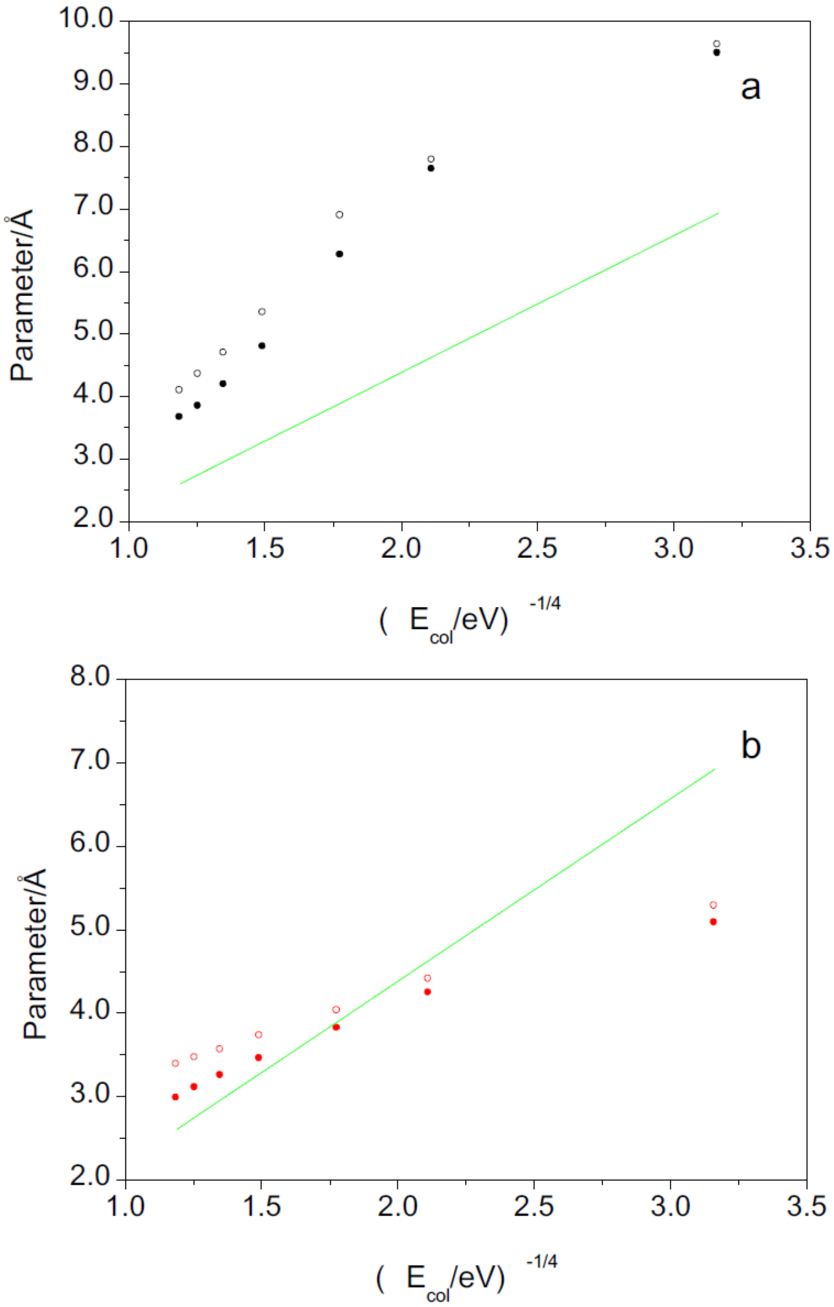


Figure S4: (a) b_0 (—), b_{max} (O), and $b_{max}\ P_r^{1/2}$ (●) for $O + H_2^+(v{=}0,j{=}0) \rightarrow OH^+ + H$ ($1^2A''$ PES), as a function of $E_{col}^{-1/4}$; **(b)** b_0 (—), b_{max} (O), and $b_{max}\ P_r^{1/2}$ (●) for $O + H_2^+(v{=}0,j{=}0) \rightarrow OH + H^+$ ($1^2A'$ PES), as a function of $E_{col}^{-1/4}$. The f_{el} = 2/18 factor was not included here.



Potential energy surface code of the $1^2A''$ ground PES

```
      subroutine fit3d(r12,r13,r23,e,der)
      implicit real*8 (a-h,o-z)
      dimension der(3)
      call diat12(r12,e12,d12)
      call diat12(r13,e13,d13)
      call diat23(r23,e23,d23)
      call triabb(r12,r13,r23,e123,der)
      e=e12+e13+e23+e123
      der(1)=d12+der(1)
      der(2)=d13+der(2)
      der(3)=d23+der(3)
      return
      end
************************************************************************
      subroutine diat12(r,ener,der)
************************************************************************
*     This subroutine computes the energies of a diatomic potential
*     fitted to    35 points
*     rms =      0.10550678 kcal/mol
*     emax =      0.35841842 kcal/mol
************************************************************************
      implicit real*8 (a-h,o-z)
      dimension cf(  8)
      data cf(  1)/0.2626237017073542D+02/
      data cf(  2)/-.3929145755534524D-01/
      data cf(  3)/-.5576266275447588D+00/
      data cf(  4)/0.1370194009011547D+01/
      data cf(  5)/-.4985728768218186D+01/
      data cf(  6)/0.9631514590749279D+01/
      data cf(  7)/-.8675246871602640D+01/
      data cf(  8)/0.1352199732169882D+01/
      e0=0.0000000000000000D+00
      der=0.d0
      vex1=0.5927029020100841D+00
      vex2=0.3624077177579942D+01
      aux = 1.d0/r
      bux = dexp(-vex2*r)*aux
      cux = dexp(-vex1*r)
      ener=e0+cf(1)*bux
      dux=1.d0
      eux=r*cux
      do 1 i=2,  8
        der=der+(i-1)*cf(i)*dux
        dux=dux*eux
        ener=ener+cf(i)*dux
    1 continue
```

```
      der=der*(1.d0-vex1*r)*cux
      der=der-cf(1)*(vex2+aux)*bux
      return
      end
**********************************************************************
      subroutine diat23(r,ener,der)
**********************************************************************
*     This subroutine computes the energies of a diatomic potential
*     fitted to    45 points
*     rms =      0.01346773 kcal/mol
*     emax =      0.04994773 kcal/mol
**********************************************************************
      implicit real*8 (a-h,o-z)
      dimension cf(  6)
      data cf(  1)/0.1024646811738351D+01/
      data cf(  2)/-.5576114537251855D+00/
      data cf(  3)/0.9322189826747831D+00/
      data cf(  4)/-.1867817145831745D+01/
      data cf(  5)/0.2323792364460492D+01/
      data cf(  6)/-.1160064267732280D+01/
      e0=0.0000000000000000D+00
      der=0.d0
      vex1=0.9327861347791375D+00
      vex2=0.1672196347900614D+01
      aux = 1.d0/r
      bux = dexp(-vex2*r)*aux
      cux = dexp(-vex1*r)
      ener=e0+cf(1)*bux
      dux=1.d0
      eux=r*cux
      do 1 i=2,  6
        der=der+(i-1)*cf(i)*dux
        dux=dux*eux
        ener=ener+cf(i)*dux
    1 continue
      der=der*(1.d0-vex1*r)*cux
      der=der-cf(1)*(vex2+aux)*bux
      return
      end
************************************************************
      subroutine triabb(r12,r13,r23,ener,der)
************************************************************
*     This subroutine computes the energies of a 3D PES
*     for the ABB system class fitted to 2698 points
*     rms =      1.79309179 kcal/mol
*     emax =      9.96480771 kcal/mol
************************************************************
      implicit real*8(a-h,o-z)
      dimension i1(  106),i2(  106),i3(  106),i4(  106),cf(  106)
      dimension f12(0: 8),f13(0: 8),f23(0: 8)
```

```
dimension der(3)
data cf(  1)/0.4642116587944736D+02/
data i1(  1)/ 1/,i2(  1)/ 1/,i3(  1)/ 0/,i4(  1)/ 2/
data cf(  2)/0.9623395869455374D+02/
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data cf(  3)/-.1699393251382325D+04/
data i1(  3)/ 1/,i2(  3)/ 1/,i3(  3)/ 1/,i4(  3)/ 1/
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data i1( 65)/ 5/,i2( 65)/ 2/,i3( 65)/ 1/,i4( 65)/ 2/
data cf( 66)/0.2675474090653573D+07/
data i1( 66)/ 5/,i2( 66)/ 1/,i3( 66)/ 2/,i4( 66)/ 2/
data cf( 67)/0.2038862755945507D+07/
data i1( 67)/ 1/,i2( 67)/ 5/,i3( 67)/ 2/,i4( 67)/ 2/
data cf( 68)/0.1392166333171824D+07/
data i1( 68)/ 5/,i2( 68)/ 3/,i3( 68)/ 0/,i4( 68)/ 2/
data cf( 69)/0.1801474397096452D+06/
data i1( 69)/ 5/,i2( 69)/ 0/,i3( 69)/ 3/,i4( 69)/ 2/
data cf( 70)/-.9827945481010350D+06/
data i1( 70)/ 0/,i2( 70)/ 5/,i3( 70)/ 3/,i4( 70)/ 2/
data cf( 71)/-.2103312124188606D+07/
data i1( 71)/ 6/,i2( 71)/ 1/,i3( 71)/ 1/,i4( 71)/ 2/
data cf( 72)/0.2631860714096408D+07/
data i1( 72)/ 1/,i2( 72)/ 6/,i3( 72)/ 1/,i4( 72)/ 1/
data cf( 73)/-.1392610504945040D+07/
data i1( 73)/ 6/,i2( 73)/ 2/,i3( 73)/ 0/,i4( 73)/ 2/
data cf( 74)/0.1664662120468682D+07/
data i1( 74)/ 6/,i2( 74)/ 0/,i3( 74)/ 2/,i4( 74)/ 2/
data cf( 75)/-.1226870612511497D+07/
```

```
data i1( 75)/ 0/,i2( 75)/ 6/,i3( 75)/ 2/,i4( 75)/ 2/
data cf( 76)/0.5058239999097900D+07/
data i1( 76)/ 7/,i2( 76)/ 1/,i3( 76)/ 0/,i4( 76)/ 2/
data cf( 77)/0.5975327285150377D+07/
data i1( 77)/ 7/,i2( 77)/ 0/,i3( 77)/ 1/,i4( 77)/ 2/
data cf( 78)/-.8922342227688523D+06/
data i1( 78)/ 0/,i2( 78)/ 7/,i3( 78)/ 1/,i4( 78)/ 2/
data cf( 79)/0.6271006095520789D+07/
data i1( 79)/ 3/,i2( 79)/ 3/,i3( 79)/ 3/,i4( 79)/ 1/
data cf( 80)/-.3070175693205085D+07/
data i1( 80)/ 4/,i2( 80)/ 3/,i3( 80)/ 2/,i4( 80)/ 2/
data cf( 81)/-.1534861890100859D+07/
data i1( 81)/ 4/,i2( 81)/ 2/,i3( 81)/ 3/,i4( 81)/ 2/
data cf( 82)/-.3389421768830984D+07/
data i1( 82)/ 2/,i2( 82)/ 4/,i3( 82)/ 3/,i4( 82)/ 2/
data cf( 83)/-.2774055374289952D+07/
data i1( 83)/ 4/,i2( 83)/ 4/,i3( 83)/ 1/,i4( 83)/ 2/
data cf( 84)/0.1533753115567217D+07/
data i1( 84)/ 4/,i2( 84)/ 1/,i3( 84)/ 4/,i4( 84)/ 1/
data cf( 85)/0.2208788009860749D+07/
data i1( 85)/ 5/,i2( 85)/ 2/,i3( 85)/ 2/,i4( 85)/ 2/
data cf( 86)/0.2826792158254851D+07/
data i1( 86)/ 2/,i2( 86)/ 5/,i3( 86)/ 2/,i4( 86)/ 1/
data cf( 87)/0.4551683382165137D+07/
data i1( 87)/ 5/,i2( 87)/ 3/,i3( 87)/ 1/,i4( 87)/ 2/
data cf( 88)/-.2901049431864413D+07/
data i1( 88)/ 5/,i2( 88)/ 1/,i3( 88)/ 3/,i4( 88)/ 2/
data cf( 89)/0.2071665859994505D+07/
data i1( 89)/ 1/,i2( 89)/ 5/,i3( 89)/ 3/,i4( 89)/ 2/
data cf( 90)/0.3845377121748019D+06/
data i1( 90)/ 5/,i2( 90)/ 4/,i3( 90)/ 0/,i4( 90)/ 2/
data cf( 91)/-.1219805601611841D+06/
data i1( 91)/ 5/,i2( 91)/ 0/,i3( 91)/ 4/,i4( 91)/ 2/
data cf( 92)/0.2812895264386767D+06/
data i1( 92)/ 0/,i2( 92)/ 5/,i3( 92)/ 4/,i4( 92)/ 2/
data cf( 93)/-.4687933525298683D+07/
data i1( 93)/ 6/,i2( 93)/ 2/,i3( 93)/ 1/,i4( 93)/ 2/
data cf( 94)/-.2412134610698914D+07/
data i1( 94)/ 6/,i2( 94)/ 1/,i3( 94)/ 2/,i4( 94)/ 2/
data cf( 95)/-.2949110696437190D+07/
data i1( 95)/ 1/,i2( 95)/ 6/,i3( 95)/ 2/,i4( 95)/ 2/
data cf( 96)/-.2119482766626543D+07/
data i1( 96)/ 6/,i2( 96)/ 3/,i3( 96)/ 0/,i4( 96)/ 2/
data cf( 97)/0.1340645138369760D+06/
data i1( 97)/ 6/,i2( 97)/ 0/,i3( 97)/ 3/,i4( 97)/ 2/
data cf( 98)/0.6378630682734155D+06/
data i1( 98)/ 0/,i2( 98)/ 6/,i3( 98)/ 3/,i4( 98)/ 2/
data cf( 99)/0.3313216667929404D+07/
data i1( 99)/ 7/,i2( 99)/ 1/,i3( 99)/ 1/,i4( 99)/ 2/
data cf(100)/-.6345983805759210D+06/
```

```
      data i1(100)/ 1/,i2(100)/ 7/,i3(100)/ 1/,i4(100)/ 1/
      data cf(101)/0.3006186103841881D+07/
      data i1(101)/ 7/,i2(101)/ 2/,i3(101)/ 0/,i4(101)/ 2/
      data cf(102)/-.7346505032867929D+06/
      data i1(102)/ 7/,i2(102)/ 0/,i3(102)/ 2/,i4(102)/ 2/
      data cf(103)/0.9116690891925898D+06/
      data i1(103)/ 0/,i2(103)/ 7/,i3(103)/ 2/,i4(103)/ 2/
      data cf(104)/-.5126249523014837D+07/
      data i1(104)/ 8/,i2(104)/ 1/,i3(104)/ 0/,i4(104)/ 2/
      data cf(105)/-.5005952467094528D+07/
      data i1(105)/ 8/,i2(105)/ 0/,i3(105)/ 1/,i4(105)/ 2/
      data cf(106)/0.4057774024848143D+06/
      data i1(106)/ 0/,i2(106)/ 8/,i3(106)/ 1/,i4(106)/ 2/
      vex1=0.1206097656187775D+01
      vex2=0.1022113059073411D+01
      f12(0)=1.d0
      f13(0)=1.d0
      f23(0)=1.d0
      bux12=r12*dexp(-vex1*r12)
      bux13=r13*dexp(-vex1*r13)
      bux23=r23*dexp(-vex2*r23)
      do 1 i=1, 8
        f12(i)=f12(i-1)*bux12
        f13(i)=f13(i-1)*bux13
        f23(i)=f23(i-1)*bux23
1     continue
      ener = 0.d0
      der12 = 0.d0
      der13 = 0.d0
      der23 = 0.d0
      do 2 l=1,106
        if (i4(l).eq.1) then
          aux=f12(i1(l))*f13(i3(l))*f23(i2(l))
          dux12=i1(l)*f12(i1(l)-1)*f13(i3(l))*f23(i2(l))
          dux13=i3(l)*f12(i1(l))*f13(i3(l)-1)*f23(i2(l))
          dux23=i2(l)*f12(i1(l))*f13(i3(l))*f23(i2(l)-1)
        else
          aux1=f12(i1(l))*f13(i3(l))
          aux2=f12(i3(l))*f13(i1(l))
          aux=(aux1+aux2)*f23(i2(l))
          dux23=(aux1+aux2)*i2(l)*f23(i2(l)-1)
          dux1=i1(l)*f12(i1(l)-1)*f13(i3(l))
          dux2=i3(l)*f12(i3(l)-1)*f13(i1(l))
          dux12=(dux1+dux2)*f23(i2(l))
          dux1=i3(l)*f12(i1(l))*f13(i3(l)-1)
          dux2=i1(l)*f12(i3(l))*f13(i1(l)-1)
          dux13=(dux1+dux2)*f23(i2(l))
        endif
        ener=ener+cf(l)*aux
        der12=der12+cf(l)*dux12
```

```
    der13=der13+cf(l)*dux13
    der23=der23+cf(l)*dux23
2 continue
  der(1)=der12*(1.d0-vex1*r12)*dexp(-vex1*r12)
  der(2)=der13*(1.d0-vex1*r13)*dexp(-vex1*r13)
  der(3)=der23*(1.d0-vex2*r23)*dexp(-vex2*r23)
  return
  end
```

Potential energy surface code of the $1^2A'$ excited PES

```
      subroutine fit3d(r12,r13,r23,e,der)
      implicit real*8 (a-h,o-z)
      dimension der(3)
      call diat12(r12,e12,d12)
      call diat12(r13,e13,d13)
      call diat23(r23,e23,d23)
      call triabb(r12,r13,r23,e123,der)
      eux=e12+e13+e23+e123
      if((r12.lt.1.d0.or.r13.lt.1.d0.or.r23.lt.0.5d0).and.eux.lt.0.0d0)
     -then
         e=10.d0
      else
         e=eux
      endif
      der(1)=d12+der(1)
      der(2)=d13+der(2)
      der(3)=d23+der(3)
      return
      end
************************************************************************
      subroutine diat12(r,ener,der)
************************************************************************
*     This subroutine computes the energies of a diatomic potential
*     fitted to    33 points
*     rms =      0.03432140 kcal/mol
*     emax =      0.09428875 kcal/mol
************************************************************************
      implicit real*8 (a-h,o-z)
      dimension cf(  6)
      data cf(  1)/0.2312363757805886D+01/
      data cf(  2)/-.3238015091667107D+00/
      data cf(  3)/-.6859352457365980D+00/
      data cf(  4)/-.2712016498649659D+02/
      data cf(  5)/0.9072983862782986D+02/
      data cf(  6)/-.1159262159333812D+03/
      e0=0.0000000000000000D+00
      der=0.d0
      vex1=0.9366029160670712D+00
      vex2=0.6700681367513983D+00
      aux = 1.d0/r
      bux = dexp(-vex2*r)*aux
      cux = dexp(-vex1*r)
      ener=e0+cf(1)*bux
      dux=1.d0
      eux=r*cux
      do 1 i=2,  6
```

```
        der=der+(i-1)*cf(i)*dux
        dux=dux*eux
        ener=ener+cf(i)*dux
    1 continue
      der=der*(1.d0-vex1*r)*cux
      der=der-cf(1)*(vex2+aux)*bux
      return
      end
************************************************************************
      subroutine diat23(r,ener,der)
************************************************************************
*     This subroutine computes the energies of a diatomic potential
*     fitted to    45 points
*     rms =      0.01397275 kcal/mol
*     emax =      0.04525281 kcal/mol
************************************************************************
      implicit real*8 (a-h,o-z)
      dimension cf(  6)
      data cf(  1)/0.1039653928417118D+01/
      data cf(  2)/-.5421382121969676D+00/
      data cf(  3)/0.8015288054007554D+00/
      data cf(  4)/-.1233232421797747D+01/
      data cf(  5)/0.8057485350462035D+00/
      data cf(  6)/0.3045632850471855D+00/
      e0=0.0000000000000000D+00
      der=0.d0
      vex1=0.9284835390000000D+00
      vex2=0.1694606420000000D+01
      aux = 1.d0/r
      bux = dexp(-vex2*r)*aux
      cux = dexp(-vex1*r)
      ener=e0+cf(1)*bux
      dux=1.d0
      eux=r*cux
      do 1 i=2,  6
        der=der+(i-1)*cf(i)*dux
        dux=dux*eux
        ener=ener+cf(i)*dux
    1 continue
      der=der*(1.d0-vex1*r)*cux
      der=der-cf(1)*(vex2+aux)*bux
      return
      end
************************************************************
      subroutine triabb(r12,r13,r23,ener,der)
************************************************************
*     This subroutine computes the energies of a 3D PES
*     for the ABB system class fitted to 2000 points
*     rms =      3.97833582 kcal/mol
*     emax =     16.27539230 kcal/mol
```

```
******************************************************************
      implicit real*8(a-h,o-z)
      dimension i1(  106),i2(  106),i3(  106),i4(  106),cf(  106)
      dimension f12(0: 8),f13(0: 8),f23(0: 8)
      dimension der(3)
      data cf(  1)/-.3841766274678932D+02/
      data i1(  1)/ 1/,i2(  1)/ 1/,i3(  1)/ 0/,i4(  1)/ 2/
      data cf(  2)/-.6484108013436645D+05/
      data i1(  2)/ 1/,i2(  2)/ 0/,i3(  2)/ 1/,i4(  2)/ 1/
      data cf(  3)/0.1984164703388390D+07/
      data i1(  3)/ 1/,i2(  3)/ 1/,i3(  3)/ 1/,i4(  3)/ 1/
      data cf(  4)/-.1530587336684808D+04/
      data i1(  4)/ 2/,i2(  4)/ 1/,i3(  4)/ 0/,i4(  4)/ 2/
      data cf(  5)/-.4473022959271920D+06/
      data i1(  5)/ 2/,i2(  5)/ 0/,i3(  5)/ 1/,i4(  5)/ 2/
      data cf(  6)/0.5395781023299511D+04/
      data i1(  6)/ 0/,i2(  6)/ 2/,i3(  6)/ 1/,i4(  6)/ 2/
      data cf(  7)/0.4748835387029239D+08/
      data i1(  7)/ 2/,i2(  7)/ 1/,i3(  7)/ 1/,i4(  7)/ 2/
      data cf(  8)/-.2972812168240410D+08/
      data i1(  8)/ 1/,i2(  8)/ 2/,i3(  8)/ 1/,i4(  8)/ 1/
      data cf(  9)/-.3212398598026111D+06/
      data i1(  9)/ 2/,i2(  9)/ 2/,i3(  9)/ 0/,i4(  9)/ 2/
      data cf( 10)/-.1354333604706873D+09/
      data i1( 10)/ 2/,i2( 10)/ 0/,i3( 10)/ 2/,i4( 10)/ 1/
      data cf( 11)/0.3285706676511578D+06/
      data i1( 11)/ 3/,i2( 11)/ 1/,i3( 11)/ 0/,i4( 11)/ 2/
      data cf( 12)/-.9217993951359890D+08/
      data i1( 12)/ 3/,i2( 12)/ 0/,i3( 12)/ 1/,i4( 12)/ 2/
      data cf( 13)/-.6097221151930420D+05/
      data i1( 13)/ 0/,i2( 13)/ 3/,i3( 13)/ 1/,i4( 13)/ 2/
      data cf( 14)/-.5051678796753177D+09/
      data i1( 14)/ 2/,i2( 14)/ 2/,i3( 14)/ 1/,i4( 14)/ 2/
      data cf( 15)/0.6264339853611868D+09/
      data i1( 15)/ 2/,i2( 15)/ 1/,i3( 15)/ 2/,i4( 15)/ 1/
      data cf( 16)/0.5007319869617210D+09/
      data i1( 16)/ 3/,i2( 16)/ 1/,i3( 16)/ 1/,i4( 16)/ 2/
      data cf( 17)/0.2311096721646887D+09/
      data i1( 17)/ 1/,i2( 17)/ 3/,i3( 17)/ 1/,i4( 17)/ 1/
      data cf( 18)/0.1266899590369634D+08/
      data i1( 18)/ 3/,i2( 18)/ 2/,i3( 18)/ 0/,i4( 18)/ 2/
      data cf( 19)/0.3812367084288307D+10/
      data i1( 19)/ 3/,i2( 19)/ 0/,i3( 19)/ 2/,i4( 19)/ 2/
      data cf( 20)/0.1643760683502171D+07/
      data i1( 20)/ 0/,i2( 20)/ 3/,i3( 20)/ 2/,i4( 20)/ 2/
      data cf( 21)/-.1672261558487688D+08/
      data i1( 21)/ 4/,i2( 21)/ 1/,i3( 21)/ 0/,i4( 21)/ 2/
      data cf( 22)/0.1750109007890343D+10/
      data i1( 22)/ 4/,i2( 22)/ 0/,i3( 22)/ 1/,i4( 22)/ 2/
      data cf( 23)/0.4423640298293427D+06/
```

```
data i1( 23)/ 0/,i2( 23)/ 4/,i3( 23)/ 1/,i4( 23)/ 2/
data cf( 24)/-.6200841393117799D+10/
data i1( 24)/ 2/,i2( 24)/ 2/,i3( 24)/ 2/,i4( 24)/ 1/
data cf( 25)/-.2341257093147368D+10/
data i1( 25)/ 3/,i2( 25)/ 2/,i3( 25)/ 1/,i4( 25)/ 2/
data cf( 26)/0.2241649660266273D+11/
data i1( 26)/ 3/,i2( 26)/ 1/,i3( 26)/ 2/,i4( 26)/ 2/
data cf( 27)/0.2567230434233534D+10/
data i1( 27)/ 1/,i2( 27)/ 3/,i3( 27)/ 2/,i4( 27)/ 2/
data cf( 28)/-.4712068787351490D+08/
data i1( 28)/ 3/,i2( 28)/ 3/,i3( 28)/ 0/,i4( 28)/ 2/
data cf( 29)/-.2687242963072511D+12/
data i1( 29)/ 3/,i2( 29)/ 0/,i3( 29)/ 3/,i4( 29)/ 1/
data cf( 30)/-.7667777551001298D+10/
data i1( 30)/ 4/,i2( 30)/ 1/,i3( 30)/ 1/,i4( 30)/ 2/
data cf( 31)/-.1006556339514249D+10/
data i1( 31)/ 1/,i2( 31)/ 4/,i3( 31)/ 1/,i4( 31)/ 1/
data cf( 32)/-.2686436861324064D+09/
data i1( 32)/ 4/,i2( 32)/ 2/,i3( 32)/ 0/,i4( 32)/ 2/
data cf( 33)/-.9657749780814454D+11/
data i1( 33)/ 4/,i2( 33)/ 0/,i3( 33)/ 2/,i4( 33)/ 2/
data cf( 34)/-.4358051249976448D+07/
data i1( 34)/ 0/,i2( 34)/ 4/,i3( 34)/ 2/,i4( 34)/ 2/
data cf( 35)/0.4333297678193090D+09/
data i1( 35)/ 5/,i2( 35)/ 1/,i3( 35)/ 0/,i4( 35)/ 2/
data cf( 36)/-.1127311193166904D+11/
data i1( 36)/ 5/,i2( 36)/ 0/,i3( 36)/ 1/,i4( 36)/ 2/
data cf( 37)/-.2056263820627286D+07/
data i1( 37)/ 0/,i2( 37)/ 5/,i3( 37)/ 1/,i4( 37)/ 2/
data cf( 38)/-.3218661757605578D+12/
data i1( 38)/ 3/,i2( 38)/ 2/,i3( 38)/ 2/,i4( 38)/ 2/
data cf( 39)/0.5860576722235122D+11/
data i1( 39)/ 2/,i2( 39)/ 3/,i3( 39)/ 2/,i4( 39)/ 1/
data cf( 40)/0.1505488098970710D+11/
data i1( 40)/ 3/,i2( 40)/ 3/,i3( 40)/ 1/,i4( 40)/ 2/
data cf( 41)/0.1503216209234348D+13/
data i1( 41)/ 3/,i2( 41)/ 1/,i3( 41)/ 3/,i4( 41)/ 1/
data cf( 42)/0.1912355707709086D+11/
data i1( 42)/ 4/,i2( 42)/ 2/,i3( 42)/ 1/,i4( 42)/ 2/
data cf( 43)/0.2478886549916408D+12/
data i1( 43)/ 4/,i2( 43)/ 1/,i3( 43)/ 2/,i4( 43)/ 2/
data cf( 44)/-.8252491216884988D+10/
data i1( 44)/ 1/,i2( 44)/ 4/,i3( 44)/ 2/,i4( 44)/ 2/
data cf( 45)/0.1422445371167246D+10/
data i1( 45)/ 4/,i2( 45)/ 3/,i3( 45)/ 0/,i4( 45)/ 2/
data cf( 46)/0.2649398926732705D+13/
data i1( 46)/ 4/,i2( 46)/ 0/,i3( 46)/ 3/,i4( 46)/ 2/
data cf( 47)/-.6594545666295499D+08/
data i1( 47)/ 0/,i2( 47)/ 4/,i3( 47)/ 3/,i4( 47)/ 2/
data cf( 48)/-.2945615120164689D+11/
```

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data i1( 48)/ 5/,i2( 48)/ 1/,i3( 48)/ 1/,i4( 48)/ 2/
data cf( 49)/0.2536382205500813D+10/
data i1( 49)/ 1/,i2( 49)/ 5/,i3( 49)/ 1/,i4( 49)/ 1/
data cf( 50)/0.1458891572583787D+10/
data i1( 50)/ 5/,i2( 50)/ 2/,i3( 50)/ 0/,i4( 50)/ 2/
data cf( 51)/0.9677044270556626D+12/
data i1( 51)/ 5/,i2( 51)/ 0/,i3( 51)/ 2/,i4( 51)/ 2/
data cf( 52)/0.2038277892693508D+08/
data i1( 52)/ 0/,i2( 52)/ 5/,i3( 52)/ 2/,i4( 52)/ 2/
data cf( 53)/-.4760445263608564D+10/
data i1( 53)/ 6/,i2( 53)/ 1/,i3( 53)/ 0/,i4( 53)/ 2/
data cf( 54)/0.9041511452377247D+11/
data i1( 54)/ 6/,i2( 54)/ 0/,i3( 54)/ 1/,i4( 54)/ 2/
data cf( 55)/0.5340745985685655D+07/
data i1( 55)/ 0/,i2( 55)/ 6/,i3( 55)/ 1/,i4( 55)/ 2/
data cf( 56)/0.1171481416789141D+13/
data i1( 56)/ 3/,i2( 56)/ 3/,i3( 56)/ 2/,i4( 56)/ 2/
data cf( 57)/-.4887152823568205D+13/
data i1( 57)/ 3/,i2( 57)/ 2/,i3( 57)/ 3/,i4( 57)/ 1/
data cf( 58)/-.7520932307707256D+12/
data i1( 58)/ 4/,i2( 58)/ 2/,i3( 58)/ 2/,i4( 58)/ 2/
data cf( 59)/-.2110643758711737D+12/
data i1( 59)/ 2/,i2( 59)/ 4/,i3( 59)/ 2/,i4( 59)/ 1/
data cf( 60)/0.3957293223625313D+10/
data i1( 60)/ 4/,i2( 60)/ 3/,i3( 60)/ 1/,i4( 60)/ 2/
data cf( 61)/-.9235694316699592D+12/
data i1( 61)/ 4/,i2( 61)/ 1/,i3( 61)/ 3/,i4( 61)/ 2/
data cf( 62)/-.5391409693850448D+11/
data i1( 62)/ 1/,i2( 62)/ 4/,i3( 62)/ 3/,i4( 62)/ 2/
data cf( 63)/-.2937830340008920D+10/
data i1( 63)/ 4/,i2( 63)/ 4/,i3( 63)/ 0/,i4( 63)/ 2/
data cf( 64)/-.4321547541853360D+14/
data i1( 64)/ 4/,i2( 64)/ 0/,i3( 64)/ 4/,i4( 64)/ 1/
data cf( 65)/0.3253529638717998D+11/
data i1( 65)/ 5/,i2( 65)/ 2/,i3( 65)/ 1/,i4( 65)/ 2/
data cf( 66)/-.2315164814267487D+12/
data i1( 66)/ 5/,i2( 66)/ 1/,i3( 66)/ 2/,i4( 66)/ 2/
data cf( 67)/0.1653628144130604D+11/
data i1( 67)/ 1/,i2( 67)/ 5/,i3( 67)/ 2/,i4( 67)/ 2/
data cf( 68)/-.5055801345105738D+10/
data i1( 68)/ 5/,i2( 68)/ 3/,i3( 68)/ 0/,i4( 68)/ 2/
data cf( 69)/-.1906908630786933D+14/
data i1( 69)/ 5/,i2( 69)/ 0/,i3( 69)/ 3/,i4( 69)/ 2/
data cf( 70)/0.5619673188122544D+09/
data i1( 70)/ 0/,i2( 70)/ 5/,i3( 70)/ 3/,i4( 70)/ 2/
data cf( 71)/0.3550333595825049D+12/
data i1( 71)/ 6/,i2( 71)/ 1/,i3( 71)/ 1/,i4( 71)/ 2/
data cf( 72)/-.3528395909948593D+10/
data i1( 72)/ 1/,i2( 72)/ 6/,i3( 72)/ 1/,i4( 72)/ 1/
data cf( 73)/-.4091135790846155D+10/
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data i1( 73)/ 6/,i2( 73)/ 2/,i3( 73)/ 0/,i4( 73)/ 2/
data cf( 74)/-.6459892698550041D+13/
data i1( 74)/ 6/,i2( 74)/ 0/,i3( 74)/ 2/,i4( 74)/ 2/
data cf( 75)/-.7211904126874657D+08/
data i1( 75)/ 0/,i2( 75)/ 6/,i3( 75)/ 2/,i4( 75)/ 2/
data cf( 76)/0.2528911183962991D+11/
data i1( 76)/ 7/,i2( 76)/ 1/,i3( 76)/ 0/,i4( 76)/ 2/
data cf( 77)/-.5631856172582240D+12/
data i1( 77)/ 7/,i2( 77)/ 0/,i3( 77)/ 1/,i4( 77)/ 2/
data cf( 78)/-.6643777983316355D+07/
data i1( 78)/ 0/,i2( 78)/ 7/,i3( 78)/ 1/,i4( 78)/ 2/
data cf( 79)/0.7173686566170956D+13/
data i1( 79)/ 3/,i2( 79)/ 3/,i3( 79)/ 3/,i4( 79)/ 1/
data cf( 80)/0.2478085230911072D+13/
data i1( 80)/ 4/,i2( 80)/ 3/,i3( 80)/ 2/,i4( 80)/ 2/
data cf( 81)/-.1131467841871041D+14/
data i1( 81)/ 4/,i2( 81)/ 2/,i3( 81)/ 3/,i4( 81)/ 2/
data cf( 82)/-.1493024519929416D+13/
data i1( 82)/ 2/,i2( 82)/ 4/,i3( 82)/ 3/,i4( 82)/ 2/
data cf( 83)/-.1108466333107508D+12/
data i1( 83)/ 4/,i2( 83)/ 4/,i3( 83)/ 1/,i4( 83)/ 2/
data cf( 84)/0.5760758663422305D+14/
data i1( 84)/ 4/,i2( 84)/ 1/,i3( 84)/ 4/,i4( 84)/ 1/
data cf( 85)/-.9196398505062127D+13/
data i1( 85)/ 5/,i2( 85)/ 2/,i3( 85)/ 2/,i4( 85)/ 2/
data cf( 86)/0.2533831640671766D+12/
data i1( 86)/ 2/,i2( 86)/ 5/,i3( 86)/ 2/,i4( 86)/ 1/
data cf( 87)/0.5075750374361757D+12/
data i1( 87)/ 5/,i2( 87)/ 3/,i3( 87)/ 1/,i4( 87)/ 2/
data cf( 88)/0.3484412985407782D+14/
data i1( 88)/ 5/,i2( 88)/ 1/,i3( 88)/ 3/,i4( 88)/ 2/
data cf( 89)/0.6963057826311577D+11/
data i1( 89)/ 1/,i2( 89)/ 5/,i3( 89)/ 3/,i4( 89)/ 2/
data cf( 90)/0.4216518886893633D+09/
data i1( 90)/ 5/,i2( 90)/ 4/,i3( 90)/ 0/,i4( 90)/ 2/
data cf( 91)/0.1234627563403959D+15/
data i1( 91)/ 5/,i2( 91)/ 0/,i3( 91)/ 4/,i4( 91)/ 2/
data cf( 92)/0.2868418612344957D+10/
data i1( 92)/ 0/,i2( 92)/ 5/,i3( 92)/ 4/,i4( 92)/ 2/
data cf( 93)/-.2279669563634061D+13/
data i1( 93)/ 6/,i2( 93)/ 2/,i3( 93)/ 1/,i4( 93)/ 2/
data cf( 94)/0.2713770156238207D+14/
data i1( 94)/ 6/,i2( 94)/ 1/,i3( 94)/ 2/,i4( 94)/ 2/
data cf( 95)/-.1484535641763099D+11/
data i1( 95)/ 1/,i2( 95)/ 6/,i3( 95)/ 2/,i4( 95)/ 2/
data cf( 96)/0.2281503692727367D+11/
data i1( 96)/ 6/,i2( 96)/ 3/,i3( 96)/ 0/,i4( 96)/ 2/
data cf( 97)/0.5203699237478941D+13/
data i1( 97)/ 6/,i2( 97)/ 0/,i3( 97)/ 3/,i4( 97)/ 2/
data cf( 98)/-.7558759717718658D+09/
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      data i1( 98)/ 0/,i2( 98)/ 6/,i3( 98)/ 3/,i4( 98)/ 2/
      data cf( 99)/0.2822877783658420D+13/
      data i1( 99)/ 7/,i2( 99)/ 1/,i3( 99)/ 1/,i4( 99)/ 2/
      data cf(100)/0.2130552814489880D+10/
      data i1(100)/ 1/,i2(100)/ 7/,i3(100)/ 1/,i4(100)/ 1/
      data cf(101)/-.2250727982887412D+11/
      data i1(101)/ 7/,i2(101)/ 2/,i3(101)/ 0/,i4(101)/ 2/
      data cf(102)/-.1024446072220024D+14/
      data i1(102)/ 7/,i2(102)/ 0/,i3(102)/ 2/,i4(102)/ 2/
      data cf(103)/0.8779604134700395D+08/
      data i1(103)/ 0/,i2(103)/ 7/,i3(103)/ 2/,i4(103)/ 2/
      data cf(104)/-.3484300048456994D+11/
      data i1(104)/ 8/,i2(104)/ 1/,i3(104)/ 0/,i4(104)/ 2/
      data cf(105)/-.1088425829371763D+13/
      data i1(105)/ 8/,i2(105)/ 0/,i3(105)/ 1/,i4(105)/ 2/
      data cf(106)/0.2759580834034137D+07/
      data i1(106)/ 0/,i2(106)/ 8/,i3(106)/ 1/,i4(106)/ 2/
      vex1=0.3099385676605541D+01
      vex2=0.9647236550306560D+00
      f12(0)=1.d0
      f13(0)=1.d0
      f23(0)=1.d0
      bux12=r12*dexp(-vex1*r12)
      bux13=r13*dexp(-vex1*r13)
      bux23=r23*dexp(-vex2*r23)
      do 1 i=1, 8
        f12(i)=f12(i-1)*bux12
        f13(i)=f13(i-1)*bux13
        f23(i)=f23(i-1)*bux23
1     continue
      ener = 0.d0
      der12 = 0.d0
      der13 = 0.d0
      der23 = 0.d0
      do 2 l=1,106
        if (i4(l).eq.1) then
          aux=f12(i1(l))*f13(i3(l))*f23(i2(l))
          dux12=i1(l)*f12(i1(l)-1)*f13(i3(l))*f23(i2(l))
          dux13=i3(l)*f12(i1(l))*f13(i3(l)-1)*f23(i2(l))
          dux23=i2(l)*f12(i1(l))*f13(i3(l))*f23(i2(l)-1)
        else
          aux1=f12(i1(l))*f13(i3(l))
          aux2=f12(i3(l))*f13(i1(l))
          aux=(aux1+aux2)*f23(i2(l))
          dux23=(aux1+aux2)*i2(l)*f23(i2(l)-1)
          dux1=i1(l)*f12(i1(l)-1)*f13(i3(l))
          dux2=i3(l)*f12(i3(l)-1)*f13(i1(l))
          dux12=(dux1+dux2)*f23(i2(l))
          dux1=i3(l)*f12(i1(l))*f13(i3(l)-1)
          dux2=i1(l)*f12(i3(l))*f13(i1(l)-1)
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        dux13=(dux1+dux2)*f23(i2(l))
      endif
      ener=ener+cf(l)*aux
      der12=der12+cf(l)*dux12
      der13=der13+cf(l)*dux13
      der23=der23+cf(l)*dux23
2 continue
  der(1)=der12*(1.d0-vex1*r12)*dexp(-vex1*r12)
  der(2)=der13*(1.d0-vex1*r13)*dexp(-vex1*r13)
  der(3)=der23*(1.d0-vex2*r23)*dexp(-vex2*r23)
  return
  end
```