

SUPPLEMENTAL MATERIAL

Leading order nonadiabatic corrections to rovibrational levels of H_2 , D_2 , and T_2

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I. NUMERICAL VALUES OF THE NONADIABATIC POTENTIALS

Numerical values of the nonadiabatic potentials (in a.u.) corresponding to the mass-independent form evaluated at 88 internuclear distances R . $\mathcal{U}(R)$, $\mathcal{V}(R)$, and $\delta\mathcal{V}(R)$ were obtained with $\Omega = 18$, $\mathcal{W}_{\parallel}(R)$ – with $\Omega = 17$, and $\mathcal{W}_{\perp}(R)$ – with $\Omega_0 = 19$ and $\Omega_1 = 15$.

$R/\text{a.u.}$	$\mu_n^2 \mathcal{W}_{\parallel}(R)$	$\mu_n^2 \mathcal{W}_{\perp}(R)$	$\mu_n^2 \mathcal{U}(R)$	$\mu_n^2 \mathcal{V}(R)$	$\mu_n^2 \delta\mathcal{V}(R)$
0.1000	-3.396942005475E-02	-2.0977588203800148E-04	-8.4052748884040529	+0.5298385333534346	-1.490159828569
0.2000	-8.182790812740E-02	-8.0843438642341219E-04	-4.7361936665320927	+0.6139991785266204	-8.948376905770E-01
0.3000	-1.185449214584E-01	-1.7403016648231127E-03	-2.9552915391540457	+0.5795582873423691	-5.639978343598E-01
0.3500	-1.323241461359E-01	-2.3155927289172384E-03	-2.4096414802041228	+0.5504705625341966	-4.541036286685E-01
0.4000	-1.435508601977E-01	-2.9571702597364046E-03	-2.0000795149714974	+0.5197635568113762	-3.683741982208E-01
0.4500	-1.526442234763E-01	-3.6611131492133179E-03	-1.6863973348304808	+0.4894305909440212	-3.007033668827E-01
0.5000	-1.599833066257E-01	-4.4242345820934744E-03	-1.4417486530450547	+0.4604569699862239	-2.467193302517E-01
0.5500	-1.658927525706E-01	-5.2439886098900797E-03	-1.2478091748712459	+0.4332804361335373	-2.032428741558E-01
0.6000	-1.706432359337E-01	-6.1183825359500013E-03	-1.0918080441327072	+0.4080429958155022	-1.679285085012E-01
0.6500	-1.744574659265E-01	-7.0458993001146162E-03	-0.9646701196535452	+0.3847300840850335	-1.390226811497E-01
0.7000	-1.775176342045E-01	-8.0254307852646452E-03	-0.8598293603227559	+0.3632479575632747	-1.151982103813E-01
0.7500	-1.799725968793E-01	-9.0562214581421559E-03	-0.7724555472866997	+0.3434667506994762	-9.543916392972E-02
0.8000	-1.819441708986E-01	-1.0137821117209153E-02	-0.6989406079992891	+0.3252442299311212	-7.895966187515E-02
0.8500	-1.835324076260E-01	-1.1270045516341756E-02	-0.6365511385332149	+0.3084386108223358	-6.514583611126E-02
0.9000	-1.848199054461E-01	-1.2452943484967688E-02	-0.5831893048350609	+0.2929151562166336	-5.351382132046E-02
0.9500	-1.858752921352E-01	-1.3686769461005269E-02	-0.5372256675379598	+0.2785492465195172	-4.367899254359E-02
1.0000	-1.867560192674E-01	-1.4971960418266637E-02	-0.4973805344402052	+0.2652274702843564	-3.533319123058E-02
1.0500	-1.875105991960E-01	-1.6309116349692494E-02	-0.4626385698274398	+0.2528476303532916	-2.822769210990E-02
1.1000	-1.881803958215E-01	-1.7698983588253275E-02	-0.4321865317996110	+0.2413181836593651	-2.216034109115E-02
1.1500	-1.888010603085E-01	-1.9142440363334287E-02	-0.4053673165438718	+0.2305574130455487	-1.696575508741E-02
1.2000	-1.894036848598E-01	-2.0640484079214943E-02	-0.3816456497181429	+0.2204925006207385	-1.250779152983E-02
1.2500	-1.900157324178E-01	-2.2194219878193803E-02	-0.3605821981916280	+0.2110585963944981	-8.673715841866E-03
1.3000	-1.906617877198E-01	-2.3804850108547983E-02	-0.3418138390824560	+0.2021979314203813	-5.369650254204E-03
1.3200	-1.909347948550E-01	-2.4465318801100942E-02	-0.3348796883272726	+0.1988024418990684	-4.178376123053E-03
1.3400	-1.912181760159E-01	-2.5135182207368601E-02	-0.3282468765021120	+0.1954873279643073	-3.054749730746E-03
1.3600	-1.915132330326E-01	-2.5814528352795195E-02	-0.3218995618615913	+0.1922496836990616	-1.994623698077E-03
1.3800	-1.918212308222E-01	-2.6503447051262069E-02	-0.3158229628533082	+0.1890867303947350	-9.941206365368E-04
1.3900	-1.919804685999E-01	-2.6851524639267690E-02	-0.3128818318253628	+0.1875324276974540	-5.150848036412E-04
1.4000	-1.921434010194E-01	-2.7202029805514132E-02	-0.3100032752574127	+0.1859958101039746	-4.961274233999E-05
1.4011	-1.921615555705E-01	-2.7240734078298710E-02	-0.3096903856355259	+0.1858278482795212	+7.791741573162E-07
1.4050	-1.922262994426E-01	-2.7378196378436092E-02	-0.3085869649672726	+0.1852340347084376	+1.781678832129E-04
1.4100	-1.923101773802E-01	-2.7554974235198952E-02	-0.3071857079574985	+0.1844765632294467	+4.027130889501E-04
1.4200	-1.924809453017E-01	-2.7910369706395362E-02	-0.3044275967594822	+0.1829743794820630	+8.422968804434E-04
1.4400	-1.928350384305E-01	-2.8628561330526840E-02	-0.2990838582085347	+0.1800200039056206	+1.684791328015E-03
1.4490	-1.930000867867E-01	-2.8954987205007221E-02	-0.2967518091250949	+0.1787117867611821	+2.048594325440E-03
1.4600	-1.932068310248E-01	-2.9356700636045771E-02	-0.2939607608965368	+0.1771303518576428	+2.480855580210E-03
1.4800	-1.935974520859E-01	-3.0094884856062869E-02	-0.2890477192621101	+0.1743031895629862	+3.233290888253E-03

$R/\text{a.u.}$	$\mu_n^2 \mathcal{W}_{\parallel}(R)$	$\mu_n^2 \mathcal{W}_{\perp}(R)$	$\mu_n^2 \mathcal{U}(R)$	$\mu_n^2 \mathcal{V}(R)$	$\mu_n^2 \delta\mathcal{V}(R)$
1.5000	-1.940080112855E-01	-3.0843212389469842E-02	-0.2843348084975869	+0.1715363758663627	+3.944727983279E-03
1.5500	-1.951287700598E-01	-3.2759063155468501E-02	-0.2733683838687937	+0.1648700943574749	+5.559818512695E-03
1.6000	-1.963976076790E-01	-3.4740510898124114E-02	-0.2634653818713912	+0.1585384800500235	+6.968528938599E-03
1.6500	-1.978307433601E-01	-3.6789157304213333E-02	-0.2545136677951841	+0.1525144544594352	+8.200835389009E-03
1.7000	-1.994440384471E-01	-3.8906615578517013E-02	-0.2464167008240547	+0.1467733830460108	+9.282652378133E-03
1.8000	-2.032730900609E-01	-4.3354390827349641E-02	-0.2324644608091538	+0.1360517352084104	+1.108182461642E-02
1.9000	-2.080058278722E-01	-4.8096391512233133E-02	-0.2210648766701048	+0.1262128827262711	+1.251328761798E-02
2.0000	-2.137573953284E-01	-5.3144277834276459E-02	-0.2118048136563521	+0.1171158208657790	+1.368916307100E-02
2.1000	-2.206332722353E-01	-5.8508112778829479E-02	-0.2043672408866304	+0.1086313455223317	+1.469453942556E-02
2.2000	-2.287229251727E-01	-6.4195533807134011E-02	-0.1985069037527584	+0.1006352118511253	+1.559258381869E-02
2.3000	-2.380908524864E-01	-7.0210801844895081E-02	-0.1940330235295072	+0.0930023963816758	+1.642757713715E-02
2.3500	-2.432647487276E-01	-7.3341528771298659E-02	-0.1922681753758715	+0.0892818681369003	+1.683052709895E-02
2.4000	-2.487652506550E-01	-7.6553746624409423E-02	-0.1907969965084283	+0.0856028686610798	+1.722656052036E-02
2.5000	-2.607249214354E-01	-8.3218648232806634E-02	-0.1886837495844010	+0.0782995758304263	+1.800019546461E-02
2.6000	-2.738855870640E-01	-9.0193119473731039E-02	-0.1876057503746764	+0.0709495553589774	+1.874342320447E-02
2.7000	-2.880874206679E-01	-9.7457080038175871E-02	-0.1874987449712592	+0.0634091042484912	+1.943650922232E-02
2.8000	-3.030861976136E-01	-0.1049819373795777	-0.1883181824375924	+0.0555436151827546	+2.004701872022E-02
2.9000	-3.185508256389E-01	-0.1127301047667728	-0.1900351065473541	+0.0472419418369859	+2.053313396177E-02
3.0000	-3.340698730484E-01	-0.1206549874567411	-0.1926302445014918	+0.0384339888114092	+2.084845929309E-02
3.1000	-3.491688784280E-01	-0.1287015470985213	-0.1960853272626429	+0.0291088381274306	+2.094807264743E-02
3.2000	-3.633386334643E-01	-0.1368075089953142	-0.2003714977102158	+0.0193295402091519	+2.079514378664E-02
3.3000	-3.760724739229E-01	-0.1449052084880645	-0.2054359515870473	+0.0092402576984528	+2.036707806608E-02
3.4000	-3.869083651422E-01	-0.1529239898048574	-0.2111893543734452	-0.0009377842078941	+1.966000884372E-02
3.5000	-3.954698855547E-01	-0.1607929876143385	-0.2174974781386254	-0.0109230122048226	+1.869065445129E-02
3.6000	-4.014997158832E-01	-0.1684440557276951	-0.2241803127706764	-0.0204014007965075	+1.749506926496E-02
3.7000	-4.048802482464E-01	-0.1758145747389496	-0.2310204068715578	-0.0290611319680148	+1.612451358653E-02
3.8000	-4.056382690310E-01	-0.1828498799518113	-0.2377797699217065	-0.0366277154654745	+1.463931834768E-02
3.9000	-4.039337104797E-01	-0.1895051017556745	-0.2442222061827609	-0.0428931225385492	+1.310201267140E-02
4.0000	-4.000353485246E-01	-0.1957462917262979	-0.2501364208582736	-0.0477341110693796	+1.157100476621E-02
4.2000	-3.870787797027E-01	-0.2069069701128773	-0.2597673190678501	-0.0530945078658974	+8.714199854117E-03
4.4000	-3.698309831185E-01	-0.2162768644177894	-0.2660192539633600	-0.0533511418380881	+6.321608755328E-03
4.6000	-3.511092717858E-01	-0.2239399720074151	-0.2690762922244614	-0.0499030564202015	+4.467861486532E-03
4.8000	-3.329801769227E-01	-0.2300712226129345	-0.2696398888133680	-0.0442994637109042	+3.108514649072E-03
5.0000	-3.166680349644E-01	-0.2348895411866478	-0.2685577712346111	-0.0378350713516577	+2.147349215773E-03
5.2000	-3.027077719941E-01	-0.2386217121118294	-0.2665763191384057	-0.0314021176647210	+1.482256613720E-03
5.4000	-2.911721373612E-01	-0.2414794357310323	-0.2642421042627645	-0.0255151337606325	+1.026785171938E-03
5.6000	-2.818744295051E-01	-0.2436476709798277	-0.2619025075783368	-0.0204068834111579	+7.155993014908E-04
5.8000	-2.745128383694E-01	-0.2452808856701420	-0.2597489665522595	-0.0161300699931595	+5.023663081102E-04
6.0000	-2.687585646519E-01	-0.2465040289512991	-0.2578670676038669	-0.0126373790165028	+3.553678796352E-04
6.5000	-2.594754494420E-01	-0.2483627445978654	-0.2544076596627404	-0.0066917774066081	+1.543911098554E-04
7.0000	-2.547333876287E-01	-0.2492383120740458	-0.2523807208982149	-0.0034687907790286	+6.987250589677E-05
7.5000	-2.523553543458E-01	-0.2496458534343501	-0.2512627711823145	-0.0017816053826490	+3.286542323471E-05
8.0000	-2.511741053626E-01	-0.2498344033683995	-0.2506657044226683	-0.0009145547765344	+1.611705376190E-05
8.5000	-2.505897620596E-01	-0.2499215511165790	-0.2503524153866256	-0.0004730574970651	+8.294895697208E-06
9.0000	-2.503005639261E-01	-0.2499620099698131	-0.2501893228461237	-0.0002487363191292	+4.510544399413E-06

$R/\text{a.u.}$	$\mu_n^2 \mathcal{W}_{\parallel}(R)$	$\mu_n^2 \mathcal{W}_{\perp}(R)$	$\mu_n^2 \mathcal{U}(R)$	$\mu_n^2 \mathcal{V}(R)$	$\mu_n^2 \delta\mathcal{V}(R)$
9.5000	-2.501566412005E-01	-0.2499809996394286	-0.2501043575180603	-0.0001342168794170	+2.600750188926E-06
10.0000	-2.500841792642E-01	-0.2499900824481149	-0.2500596596432196	-0.0000750204330201	+1.588027832583E-06
10.5000	-2.500470050444E-01	-0.2499945510217251	-0.2500356799119903	-0.0000437703464213	+1.020975606753E-06
11.0000	-2.500274200365E-01	-0.2499968347603128	-0.2500224258724516	-0.0000267711223206	+6.855215509278E-07
11.5000	-2.500167429928E-01	-0.2499980578130779	-0.2500148081451065	-0.0000171652615110	+4.766671859955E-07
12.0000	-2.500106833629E-01	-0.2499987479979165	-0.2500102255298846	-0.0000114947132987	+3.407447419534E-07

II. FORTRAN'90 ROUTINES EVALUATING THE NONADIABATIC POTENTIALS AT ARBITRARY INTERNUCLEAR DISTANCE

```

    real*16 function WTint(R)
! Evaluates  $\mu_n^2 * (W_T(R) - W_T(infty))$ 
    implicit none
    real*16 :: R,W1,W2,a,b,c,R0y,iR,iRs
    real*16, dimension(:) :: P(0:16),Q(20),Ay(8:16)
    data
& R0y/11.700Q0/,
& a/1.10466168412365114082230970833773Q0/,
& b/1.161434318812792614926969387240357Q0/,
& c/1.046019881236837656855107076466617Q0/,
& P(0)/0.250000000000000000000000000000000000Q0/,
& P(1)/6.788368024999779419913194963008291Q2/,
& P(2)/-1.362735040680007543440906343074785Q3/,
& P(3)/1.248183035099494960499932556222404Q3/,
& P(4)/-6.944060098081972034423390892296834Q2/,
& P(5)/2.635915587620845286961548226369195Q2/,
& P(6)/-7.255938965457191816126997779995122Q1/,
& P(7)/1.499768830086866823227587156124188Q1/,
& P(8)/-2.373924273015117946724345451665213Q0/,
& P(9)/2.904265411458847153936538485775932Q-1/,
& P(10)/-2.748163855210913108514732051877217Q-2/,
& P(11)/1.995898365262805614718070205201716Q-3/,
& P(12)/-1.092949629575136576748615003661843Q-4/,
& P(13)/4.369218104334472485569100615549883Q-6/,
& P(14)/-1.203970910005450287181067618972663Q-7/,
& P(15)/2.045074739418371464155512607549481Q-9/,
& P(16)/-1.614352339135951222268726319239260Q-11/,
& Q(1)/-6.785606351132608284173242273496553Q2/,
& Q(2)/1.324342492554007557452444310749662Q3/,

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& Q(3)/-1.881657496129101928959697388905893Q3/ ,
 & Q(4)/2.011052281533817927014938952760115Q3/ ,
 & Q(5)/-1.823196186854297679958098517952106Q3/ ,
 & Q(6)/1.437634373727193894011885147447552Q3/ ,
 & Q(7)/-1.017709137778967053385131828632438Q3/ ,
 & Q(8)/6.559309168188208408363840776134244Q2/ ,
 & Q(9)/-3.887830008008903443213694021396870Q2/ ,
 & Q(10)/2.122975068482467459591181482029274Q2/ ,
 & Q(11)/-1.061259419258636204725815501953624Q2/ ,
 & Q(12)/4.787640235732326507937109216579178Q1/ ,
 & Q(13)/-1.907668662497768357006933804047277Q1/ ,
 & Q(14)/6.540681471331710194291223023450490Q0/ ,
 & Q(15)/-1.871857575215398239010331068557770Q0/ ,
 & Q(16)/4.316507935982159667864806144908653Q-1/ ,
 & Q(17)/-7.664370022485299008451025592197587Q-2/ ,
 & Q(18)/9.812363927280630019869065080607696Q-3/ ,
 & Q(19)/-8.060701137136874317641474179597920Q-4/ ,
 & Q(20)/3.216689269783762022735043976067475Q-5/

data

& Ay(8)/4.435688079888515819759877021567017Q2/ ,
 & Ay(9)/5.843631859649975894130889399942992Q2/ ,
 & Ay(10)/2.855935720592942981839687294786613Q3/ ,
 & Ay(11)/1.034785873697323483958482380157638Q4/ ,
 & Ay(12)/1.347512954099471093223216915047132Q4/ ,
 & Ay(13)/1.366010523117704542445979550539646Q4/ ,
 & Ay(14)/-5.457728060433510988770682809103463Q9/ ,
 & Ay(15)/1.020758850358781126515006597867726Q11/ ,
 & Ay(16)/-4.305280665734900196739551711572737Q11/

if (R<=R0y) then

Wl=P(0)+R*(P(1)+R*(P(2)+R*(P(3)+R*(P(4)+R*(P(5)+R*(P(6)+
 & R*(P(7)+R*(P(8)+R*(P(9)+R*(P(10)+R*(P(11)+R*(P(12)+

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&      R*(P(13)+R*(P(14)+R*(P(15)+R*P(16)))))))))
W2=R*(Q(1)+R*(Q(2)+R*(Q(3)+R*(Q(4)+R*(Q(5)+
&      R*(Q(6)+R*(Q(7)+R*(Q(8)+R*(Q(9)+R*(Q(10)+R*(Q(11)+
&      R*(Q(12)+R*(Q(13)+R*(Q(14)+R*(Q(15)+R*(Q(16)+R*(Q(17)+
&      R*(Q(18)+R*(Q(19)+R*Q(20)))))))))
WTint=EXP(-a*R)*W1+EXP(-(b+c*R)*R)*W2
else
  iR=1.Q0/R
  iRs=iR*iR
  WTint=+iRs*iRs*iRs*iRs*(Ay(8)+iR*(Ay(9)+iR*(Ay(10)+iR*(Ay(11)+
&      iR*(Ay(12)+iR*(Ay(13)+iR*(Ay(14)+iR*(Ay(15)+iR*Ay(16)))))))))
endif
return
end function WTint

```

```

subroutine WIIint(R,WII,DWII)

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! Evaluates  $\mu_n^2 * (W_{II}(R) - W_{II}(infty))$ 

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! and  $\mu_n^2 * d/dR W_{II}(R)$ 

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implicit none

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real*16 :: R,W1,W2,a,b,c,R0x,iR,iRs,WII,DWII

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real*16, dimension(:) :: P(0:14),Q(16),Ax(8:16)

```

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data

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& R0x/10.735Q0/,
& a/1.027993101600837737184971037577331Q0/,
& b/1.320414476926467805709407411384579Q0/,
& c/1.029005093533914595830502921046611Q0/,
& P(0)/+0.250000000000000000000000000000000000Q0/,
& P(1)/-6.976823128243076583850090191393916Q3/,
& P(2)/1.241480671208678824828299918643230Q4/,
& P(3)/-1.001751495262024425392304467319746Q4/,

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& P(4)/4.867064368980094428678084044858411Q3/
 & P(5)/-1.592489422549091326324630926192373Q3/
 & P(6)/3.712095393409728282013822295451242Q2/
 & P(7)/-6.349792893773727584013276012820269Q1/
 & P(8)/8.077184560768227216832903374994982Q0/
 & P(9)/-7.644986831010505426138229926574211Q-1/
 & P(10)/5.319812137594396302595713165027699Q-2/
 & P(11)/-2.646159974926613391981967790859699Q-3/
 & P(12)/8.911882451263913749641066169101843Q-5/
 & P(13)/-1.821723698506568722000371744995044Q-6/
 & P(14)/1.707271641467195828769878041215292Q-8/
 & Q(1)/6.977081281595911959289723020813841Q3/
 & Q(2)/-1.038053012823322092759820669980730Q4/
 & Q(3)/1.389481919759480026346938674264039Q4/
 & Q(4)/-1.321628679624986197978310233015459Q4/
 & Q(5)/1.137027664267665553883759599472471Q4/
 & Q(6)/-8.546490000464176257553253450687466Q3/
 & Q(7)/6.054218225082539541960429281229023Q3/
 & Q(8)/-4.009144503562168745107926746173330Q3/
 & Q(9)/2.472328460627753527743876759176205Q3/
 & Q(10)/-1.354667138256088687480506101755758Q3/
 & Q(11)/6.283112901110511363001303558533226Q2/
 & Q(12)/-2.338932767455568399739974166698976Q2/
 & Q(13)/6.629522652927474404413079489175476Q1/
 & Q(14)/-1.336480474379359139272781358684217Q1/
 & Q(15)/1.711285558088694318564815232677170Q0/
 & Q(16)/-1.062557417129759015766001501312952Q-1/

data

& Ax(8)/-2.775446458388230741646178819172860Q3/
 & Ax(9)/-7.951892799385567386177310989166826Q2/
 & Ax(10)/-4.137230766688273651002871019225784Q3/

& Ax(11)/ -1.213398391622305653582555414444572Q4/
 & Ax(12)/ -1.522888373549849834787939207748314Q4/
 & Ax(13)/ -1.543890538400735949471433035921675Q4/
 & Ax(14)/1.501821349134892445485788447189599Q10/
 & Ax(15)/ -4.048413796310053899858315044534921Q11/
 & Ax(16)/1.996992470864601350253850629744593Q12/

if (R<=R0x) then

W1=P(0)+R*(P(1)+R*(P(2)+R*(P(3)+R*(P(4)+R*(P(5)+R*(P(6)+
 & R*(P(7)+R*(P(8)+R*(P(9)+R*(P(10)+R*(P(11)+R*(P(12)+
 & R*(P(13)+R*(P(14))))))))))

W2=R*(Q(1)+R*(Q(2)+R*(Q(3)+R*(Q(4)+R*(Q(5)+
 & R*(Q(6)+R*(Q(7)+R*(Q(8)+R*(Q(9)+R*(Q(10)+R*(Q(11)+
 & R*(Q(12)+R*(Q(13)+R*(Q(14)+R*(Q(15)+R*(Q(16)
 &))))))))

WII=EXP(-a*R)*W1+EXP(-(b+c*R)*R)*W2

W1=-a*P(0)+P(1)+R*(-a*P(1)+2*P(2)+R*(-a*P(2)+3*P(3)+
 & R*(-a*P(3)+4*P(4)+R*(-a*P(4)+5*P(5)+R*(-a*P(5)+6*P(6)+
 & R*(-a*P(6)+7*P(7)+R*(-a*P(7)+8*P(8)+R*(-a*P(8)+9*P(9)+
 & R*(-a*P(9)+10*P(10)+R*(-a*P(10)+11*P(11)+
 & R*(-a*P(11)+12*P(12)+R*(-a*P(12)+13*P(13)+
 & R*(-a*P(13)+14*P(14)-a*R*P(14))))))))

W2=Q(1)+R*(-(b*Q(1))+2*Q(2)+R*(-2*c*Q(1)-b*Q(2)+3*Q(3)+
 & R*(-2*c*Q(2)-b*Q(3)+4*Q(4)+R*(-2*c*Q(3)-b*Q(4)+5*Q(5)+
 & R*(-2*c*Q(4)-b*Q(5)+6*Q(6)+R*(-2*c*Q(5)-b*Q(6)+7*Q(7)+
 & R*(-2*c*Q(6)-b*Q(7)+8*Q(8)+R*(-2*c*Q(7)-b*Q(8)+9*Q(9)+
 & R*(-2*c*Q(8)-b*Q(9)+10*Q(10)+
 & R*(-2*c*Q(9)-b*Q(10)+11*Q(11)+
 & R*(-2*c*Q(10)-b*Q(11)+12*Q(12)+
 & R*(-2*c*Q(11)-b*Q(12)+13*Q(13)+
 & R*(-2*c*Q(12)-b*Q(13)+14*Q(14)+
 & R*(-2*c*Q(13)-b*Q(14)+15*Q(15)+

```

&      R*(-2*c*Q(14)-b*Q(15)+16*Q(16)+
&      R*(-2*c*Q(15)-b*Q(16)-2*c*R*Q(16))))))))))))))
      DWII=EXP(-a*R)*W1+EXP(-(b+c*R)*R)*W2
else
      iR=1.Q0/R
      iRs=iR*iR
      WII=+iRs*iRs*iRs*iRs*(Ax(8)+iR*(Ax(9)+iR*(Ax(10)+iR*(Ax(11)+
&      iR*(Ax(12)+iR*(Ax(13)+iR*(Ax(14)+iR*(Ax(15)+iR*Ax(16))))))))))
      DWII=-iR*iRs*iRs*iRs*iRs*(8*Ax(8)+iR*(9*Ax(9)+iR*(10*Ax(10)+
&      iR*(11*Ax(11)+iR*(12*Ax(12)+iR*(13*Ax(13)+iR*(14*Ax(14)+
&      iR*(15*Ax(15)+16*iR*Ax(16))))))))))
endif
return
end subroutine WIIint

```

```

real*16 function PV(R)
! Evaluates - ( 2/R + d/dR ) V(R) * mu_n^2
implicit none
real*16 :: R,W1,W2,a,b,c,R0v,iR,iRs
real*16, dimension (:) :: P(1:10),Q(25),Nv(7:17)
data
&      R0v/11.400Q0/,
&      a/1.535295394622434407038306511976158Q0/,
&      b/1.939237383802406686420696985749654Q0/,
&      c/0.8765393769779657938146244104976943Q0/,
&      P(1)/-2.229105452174879771241506337820855Q3/,
&      P(2)/2.177146119178830017743827126096766Q3/,
&      P(3)/-9.553625796629805738288009697781634Q2/,
&      P(4)/2.488551882374273402792672675763945Q2/,
&      P(5)/-4.232811667591062236865870158214063Q1/,

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& P(6)/4.872680670285068219259963723867540Q0/,
 & P(7)/-3.797083023260985267226591352529952Q-1/,
 & P(8)/1.932814893547585415394859049900694Q-2/,
 & P(9)/-5.838657305905051339619769130204564Q-4/,
 & P(10)/8.000104493106888440207458111537249Q-6/,
 & Q(1)/2.219102058527390719662559787486936Q3/,
 & Q(2)/-1.228539933244788338817382389580025Q3/,
 & Q(3)/2.053905309659658279392363272818492Q3/,
 & Q(4)/-8.501959698562834560392697480990884Q2/,
 & Q(5)/1.153047462822826022754661313791882Q3/,
 & Q(6)/-3.092369329038301498789937667040995Q3/,
 & Q(7)/1.086160657133622959283237749539419Q4/,
 & Q(8)/-2.758516425114171499650163126240050Q4/,
 & Q(9)/5.379803897113368729628287616917377Q4/,
 & Q(10)/-8.314259075666691684305936699578876Q4/,
 & Q(11)/1.041051864492128472324934609409652Q5/,
 & Q(12)/-1.068921623669476791887299902472509Q5/,
 & Q(13)/9.062650328618885514558201100716409Q4/,
 & Q(14)/-6.365478117340681595919020702430721Q4/,
 & Q(15)/3.706026323568496089043516437663041Q4/,
 & Q(16)/-1.784948209119919478692012813994252Q4/,
 & Q(17)/7.079275921760616833130636323525926Q3/,
 & Q(18)/-2.294518160014745361230687143552960Q3/,
 & Q(19)/6.008479675458337701008171870551978Q2/,
 & Q(20)/-1.250123861564588553044152330523974Q2/,
 & Q(21)/2.016489726821822964271732069575560Q1/,
 & Q(22)/-2.429165614277015414482755756046675Q0/,
 & Q(23)/2.055799061974127223523851288183537Q-1/,
 & Q(24)/-1.090315952423371576760645347202482Q-2/,
 & Q(25)/2.729046893210881872639213654058394Q-4/

data

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& Nv(7)/ -7.472182936228868864176663693155737Q1/ ,
& Nv(8)/ -1.086187434856962296669472219455426Q2/ ,
& Nv(9)/ -8.564184097290760947811608186492616Q2/ ,
& Nv(10)/ -2.275930304347636438104799467151248Q3/ ,
& Nv(11)/ -7.002167474330146679697575802381397Q3/ ,
& Nv(12)/ -1.245772796290107692168423911595466Q4/ ,
& Nv(13)/ -1.445995915679935958849996775372432Q4/ ,
& Nv(14)/ -1.596433835564711100482213306910872Q4/ ,
& Nv(15)/4.619370774540983723296448403315812Q10/ ,
& Nv(16)/ -2.790882334099268464659061917676744Q12/ ,
& Nv(17)/1.736331993213003454861657041548325Q13/

```

if(R<=R0v) **then**

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W1=3*P(1)+R*(-a*P(1)+4*P(2)+R*(-a*P(2)+5*P(3)+R*(-a*P(3)+6*P(4)+
& R*(-a*P(4)+7*P(5)+R*(-a*P(5)+8*P(6)+R*(-a*P(6)+9*P(7)+
& R*(-a*P(7)+10*P(8)+R*(-a*P(8)+11*P(9)+R*(-a*P(9)+12*P(10)-
& a*R*P(10))))))))))

```

```

W2=3*Q(1)+R*(-(b*Q(1))+4*Q(2)+R*(-2*c*Q(1)-b*Q(2)+5*Q(3)+
& R*(-2*c*Q(2)-b*Q(3)+6*Q(4)+R*(-2*c*Q(3)-b*Q(4)+7*Q(5)+
& R*(-2*c*Q(4)-b*Q(5)+8*Q(6)+R*(-2*c*Q(5)-b*Q(6)+9*Q(7)+
& R*(-2*c*Q(6)-b*Q(7)+10*Q(8)+R*(-2*c*Q(7)-b*Q(8)+11*Q(9)+
& R*(-2*c*Q(8)-b*Q(9)+12*Q(10)+R*(-2*c*Q(9)-b*Q(10)+13*Q(11)+
& R*(-2*c*Q(10)-b*Q(11)+14*Q(12)+R*(-2*c*Q(11)-b*Q(12)+15*Q(13)+
& R*(-2*c*Q(12)-b*Q(13)+16*Q(14)+R*(-2*c*Q(13)-b*Q(14)+17*Q(15)+
& R*(-2*c*Q(14)-b*Q(15)+18*Q(16)+R*(-2*c*Q(15)-b*Q(16)+19*Q(17)+
& R*(-2*c*Q(16)-b*Q(17)+20*Q(18)+R*(-2*c*Q(17)-b*Q(18)+21*Q(19)+
& R*(-2*c*Q(18)-b*Q(19)+22*Q(20)+R*(-2*c*Q(19)-b*Q(20)+23*Q(21)+
& R*(-2*c*Q(20)-b*Q(21)+24*Q(22)+R*(-2*c*Q(21)-b*Q(22)+25*Q(23)+
& R*(-2*c*Q(22)-b*Q(23)+26*Q(24)+R*(-2*c*Q(23)-b*Q(24)+27*Q(25)+
& R*(-2*c*Q(24)-b*Q(25)-2*c*R*Q(25))))))))))))))))))

```

PV=EXP(-a*R)*W1+EXP(-(b+c*R)*R)*W2

else

```

iR=1.Q0/R
iRs=iR*iR
PV=iR*iRs*iRs*iRs*(Nv(7)+iR*(Nv(8)+iR*(Nv(9)+iR*(Nv(10)+
&      iR*(Nv(11)+iR*(Nv(12)+iR*(Nv(13)+iR*(Nv(14)+iR*(Nv(15)+
&      iR*(Nv(16)+iR*Nv(17))))))))))
endif
return
end function PV

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```

real*16 function RpdV(R)
! Evaluates  $R * ( 2/R + d/dR ) dV(R) * \mu_n^2$ 
implicit none
real*16 :: R,W1,W2,a,b,c,R0dv,iR,iRs
real*16, dimension(:) :: P(0:7),Q(30),Ndv(7:17)
data
&      R0dv/10.478Q0/,
&      a/1.476341944091356128570472825054749Q0/,
&      b/5.228765110685560964176093401049546Q0/,
&      c/0.5489643581419930074834090988043598Q0/,
&      P(0)/-2.612046016128400967420886395954259Q0/,
&      P(1)/3.123320575839294037926093781973416Q1/,
&      P(2)/-1.999049672593699107695428947612856Q1/,
&      P(3)/5.643790806049411464753215415109306Q0/,
&      P(4)/-8.718918597597365722585784215420987Q-1/,
&      P(5)/7.710079330866428678492988175720208Q-2/,
&      P(6)/-3.692609173333851500954795390310001Q-3/,
&      P(7)/7.510836080860432964711403436419208Q-5/,
&      Q(1)/-2.050781379319505444765981229948498Q1/,
&      Q(2)/-6.245671638845641302554561532124580Q1/,
&      Q(3)/-4.673492671334046348301460641020805Q2/,

```

& Q(4)/2.775290571132609056357502107874890Q3/,
 & Q(5)/-1.929611381985240594373174137423261Q4/,
 & Q(6)/9.486435593226647135886894233406023Q4/,
 & Q(7)/-3.743283541467850201595778911678327Q5/,
 & Q(8)/1.192110467673869169198529282979016Q6/,
 & Q(9)/-3.117442537011975429900210219940664Q6/,
 & Q(10)/6.765755566331404374767101448795065Q6/,
 & Q(11)/-1.229273067258218857100837283326112Q7/,
 & Q(12)/1.882178777092897955834911185577372Q7/,
 & Q(13)/-2.440844475331365804283130356550500Q7/,
 & Q(14)/2.690778129358984706352418985140552Q7/,
 & Q(15)/-2.527792976959836632812732205008668Q7/,
 & Q(16)/2.026317978111770857846935806661185Q7/,
 & Q(17)/-1.386351609952432355012821151514896Q7/,
 & Q(18)/8.088045741672726308556742880177882Q6/,
 & Q(19)/-4.015064577478505698283630839568315Q6/,
 & Q(20)/1.690035658952137274946405742927352Q6/,
 & Q(21)/-6.000983869268033953974372291990401Q5/,
 & Q(22)/1.784714274210052388475871565082275Q5/,
 & Q(23)/-4.402551318121617125468514761250021Q4/,
 & Q(24)/8.889420042304083810330753020786004Q3/,
 & Q(25)/-1.442571663028314522021450798848065Q3/,
 & Q(26)/1.833277807348720030744375749325572Q2/,
 & Q(27)/-1.755306480182845490937931075564161Q1/,
 & Q(28)/1.189626720930838570495404118347148Q0/,
 & Q(29)/-5.083904033446884557571579460238142Q-2/,
 & Q(30)/1.029858651727620803709825502407178Q-3/

data

& Ndv(7)/-2.946715853536231413299547859031183Q0/,
 & Ndv(8)/-4.735124517844690869537095092186823Q0/,
 & Ndv(9)/-1.070917239073512330236213151105970Q1/,

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&     Ndv(10)/ -2.861091089433546100552926773334360Q1/ ,
&     Ndv(11)/ -3.796613028303815163230470934784121Q1/ ,
&     Ndv(12)/ -4.313266654091046099132698746351802Q1/ ,
&     Ndv(13)/ -4.794930562796385162865826637084648Q1/ ,
&     Ndv(14)/ -5.274532584373873393769437025323082Q1/ ,
&     Ndv(15)/ -2.059203927162487259336871298791335Q9/ ,
&     Ndv(16)/ 1.576760752900018996256365461658068Q10/ ,
&     Ndv(17)/ -3.221663640419939369495553795255815Q10/

```

```

if (R<=R0dv) then

```

```

    W1=2*P(0)+R*(-a*P(0)+3*P(1)+R*(-a*P(1)+4*P(2)+R*(-a*P(2)+5*P(3)+
&     R*(-a*P(3)+6*P(4)+R*(-a*P(4)+7*P(5)+R*(-a*P(5)+8*P(6)+
&     R*(-a*P(6)+9*P(7)-a*R*P(7))))))

```

```

    W2=3*Q(1)+R*(-(b*Q(1))+4*Q(2)+R*(-2*c*Q(1)-b*Q(2)+5*Q(3)+
& R*(-2*c*Q(2)-b*Q(3)+6*Q(4)+R*(-2*c*Q(3)-b*Q(4)+7*Q(5)+
& R*(-2*c*Q(4)-b*Q(5)+8*Q(6)+R*(-2*c*Q(5)-b*Q(6)+9*Q(7)+
& R*(-2*c*Q(6)-b*Q(7)+10*Q(8)+R*(-2*c*Q(7)-b*Q(8)+11*Q(9)+
& R*(-2*c*Q(8)-b*Q(9)+12*Q(10)+R*(-2*c*Q(9)-b*Q(10)+13*Q(11)+
& R*(-2*c*Q(10)-b*Q(11)+14*Q(12)+R*(-2*c*Q(11)-b*Q(12)+15*Q(13)+
& R*(-2*c*Q(12)-b*Q(13)+16*Q(14)+R*(-2*c*Q(13)-b*Q(14)+17*Q(15)+
& R*(-2*c*Q(14)-b*Q(15)+18*Q(16)+R*(-2*c*Q(15)-b*Q(16)+19*Q(17)+
& R*(-2*c*Q(16)-b*Q(17)+20*Q(18)+R*(-2*c*Q(17)-b*Q(18)+21*Q(19)+
& R*(-2*c*Q(18)-b*Q(19)+22*Q(20)+R*(-2*c*Q(19)-b*Q(20)+23*Q(21)+
& R*(-2*c*Q(20)-b*Q(21)+24*Q(22)+R*(-2*c*Q(21)-b*Q(22)+25*Q(23)+
& R*(-2*c*Q(22)-b*Q(23)+26*Q(24)+R*(-2*c*Q(23)-b*Q(24)+27*Q(25)+
& R*(-2*c*Q(24)-b*Q(25)+28*Q(26)+R*(-2*c*Q(25)-b*Q(26)+29*Q(27)+
& R*(-2*c*Q(26)-b*Q(27)+30*Q(28)+R*(-2*c*Q(27)-b*Q(28)+31*Q(29)+
& R*(-2*c*Q(28)-b*Q(29)+32*Q(30)+R*(-2*c*Q(29)-b*Q(30)-2*c*R*Q(30)
& )))))))

```

```

    RpdV=EXP(-a*R)*W1+EXP(-(b+c*R)*R)*W2*R

```

```

else

```

```

    iR=1.Q0/R

```

```

    iRs=iR*iR
    RpdV=iRs*iRs*iRs*(Ndv(7)+iR*(Ndv(8)+iR*(Ndv(9)+iR*(Ndv(10)+
&      iR*(Ndv(11)+iR*(Ndv(12)+iR*(Ndv(13)+iR*(Ndv(14)+iR*(Ndv(15)+
&      iR*(Ndv(16)+iR*Ndv(17))))))))))
endif
return
end function RpdV

```

```

real*16 function RU(R)
! Evaluates R * U(R) * mu_n^2
implicit none
real*16 :: R,W1,W2,a,b,c,R0u,iR,iRs
real*16, dimension(:) :: P(0:16),Q(20),Au(6:16)
data
&    R0u/10.943Q0/,
&    a/1.533800221775688781423963317520503Q0/,
&    b/4.358275759106648506920343788268704Q0/,
&    c/0.8430742511875004421673637531811377Q0/,
&    P(0)/-16.11474950423569226444606367034071Q0/,
&    P(1)/-1.597801610512121516538297241006934Q6/,
&    P(2)/3.309012953430007557625476187883853Q6/,
&    P(3)/-3.186989368644250627770718958819695Q6/,
&    P(4)/1.892777934852434839652472277637295Q6/,
&    P(5)/-7.749059899799896754519771985968581Q5/,
&    P(6)/2.315609965877670146726200877641217Q5/,
&    P(7)/-5.215879404994756797445257052756161Q4/,
&    P(8)/9.015263509093277075687292841973858Q3/,
&    P(9)/-1.205227644354326886525074626539829Q3/,
&    P(10)/1.245967969466150826562658384007904Q2/,
&    P(11)/-9.877655544992889918315509694081757Q0/,

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& P(12)/5.896243426613885281163906552063623Q-1/,
 & P(13)/-2.565037087203693575718160691933129Q-2/,
 & P(14)/7.676512564757049232588616283788814Q-4/,
 & P(15)/-1.413119042316880145424605800258526Q-5/,
 & P(16)/1.206138706042188809267317191945814Q-7/,
 & Q(1)/1.597886117345573340487559855836458Q6/,
 & Q(2)/1.204063360571316145382772926775498Q6/,
 & Q(3)/1.559408593864920082212296511612249Q6/,
 & Q(4)/9.392169665840891928994615239509150Q5/,
 & Q(5)/6.333320911242088238148796847173335Q5/,
 & Q(6)/5.782063193337288858669644698516552Q5/,
 & Q(7)/-4.207052275513858945306180567653897Q5/,
 & Q(8)/1.373472841002073724121895488788441Q6/,
 & Q(9)/-2.097108778311422269267227613178391Q6/,
 & Q(10)/2.849102195158770217263932197958446Q6/,
 & Q(11)/-3.014545597394349568799170214719517Q6/,
 & Q(12)/2.590490510938653350371546092256476Q6/,
 & Q(13)/-1.777208095412428484541316917535973Q6/,
 & Q(14)/9.722842708641441123371307057449953Q5/,
 & Q(15)/-4.177041267621820444207912981135484Q5/,
 & Q(16)/1.383787560571193898326691726404061Q5/,
 & Q(17)/-3.417703171462872442682541553547207Q4/,
 & Q(18)/5.966348409998999196726430114135514Q3/,
 & Q(19)/-6.611919925753985709910374848840511Q2/,
 & Q(20)/3.589295330696601412111845975144198Q1/

data

& Au(6)/1.764271521315327216535667311817119Q1/,
 & Au(7)/2.732210499170234560680035149724180Q1/,
 & Au(8)/2.381553452943955964430713997354216Q2/,
 & Au(9)/8.550513524988028753383410779231207Q2/,
 & Au(10)/3.723555774552514856004914957924202Q3/,

```

& Au(11)/1.115987288837899988434482477118217Q4/,
& Au(12)/1.361082970183686725988365038417660Q4/,
& Au(13)/1.375959814875091325759964558591339Q4/,
& Au(14)/-8.613110080358075747651036003325528Q9/,
& Au(15)/2.550607210203041871442573986328024Q11/,
& Au(16)/-1.332077797360706174112478754799057Q12/
if(R<=R0u) then
    W1=P(0)+R*(P(1)+R*(P(2)+R*(P(3)+R*(P(4)+R*(P(5)+R*(P(6)+
& R*(P(7)+R*(P(8)+R*(P(9)+R*(P(10)+R*(P(11)+R*(P(12)+R*(P(13)+
& R*(P(14)+R*(P(15)+R*(P(16))))))))))))))
    W2=R*(Q(1)+R*(Q(2)+R*(Q(3)+R*(Q(4)+R*(Q(5)+R*(Q(6)+R*(Q(7)+
& R*(Q(8)+R*(Q(9)+R*(Q(10)+R*(Q(11)+R*(Q(12)+R*(Q(13)+R*(Q(14)+
& R*(Q(15)+R*(Q(16)+R*(Q(17)+R*(Q(18)+R*(Q(19)+R*(Q(20)
& ))))))))))))
    RU=EXP(-a*R)*W1+EXP(-(b+c*R)*R)*W2
    RU=RU*R
else
    iR=1.Q0/R
    iRs=iR*iR
    RU=-iR*iRs*iRs*(Au(6)+iR*(Au(7)+iR*(Au(8)+iR*(Au(9)+iR*(Au(10)+
& iR*(Au(11)+iR*(Au(12)+iR*(Au(13)+iR*(Au(14)+iR*(Au(15)+
& iR*(Au(16))))))))))
endif
return
end function RU

```

III. NUMERICAL VALUES OF THE LEADING NONADIABATIC CORRECTION TO ROVIBRATIONAL LEVELS

The following tables collect the nonadiabatic dissociation energy and the leading nonadiabatic correction for all rovibrational levels of H₂, D₂, and T₂. The abbreviations used within the table:

v – vibrational quantum number

J – rotational quantum number

D0 – nonadiabatic dissociation energy

Delta D0 – leading nonadiabatic correction to dissociation energy

icm – inverse centimeter

A. H₂

Molecule: H2

Proton-electron mass ratio = 1836.15267377

2 Ry = 219474.63137078

v	J	D0/hartree	D0/icm	Delta D0/icm
0	0	-0.1645693511338747	36118.797675036	0.433961787
0	1	-0.1640294925582100	36000.312413149	0.440635439
0	2	-0.1629547293619702	35764.429156844	0.453975401
0	3	-0.1613548122596836	35413.287940595	0.473967490
0	4	-0.1592439861300503	34950.015153906	0.500591645
0	5	-0.1566405640143075	34378.630044751	0.533823242
0	6	-0.1535664070417083	33703.930576414	0.573634666
0	7	-0.1500463434181767	32931.365910238	0.619997007
0	8	-0.1461075598475617	32066.902838028	0.672881765
0	9	-0.1417789959442039	31116.892870973	0.732262478
0	10	-0.1370907672205699	30087.945600072	0.798116208
0	11	-0.1320736360941529	28986.812595563	0.870424847
0	12	-0.1267585439728971	27820.284711548	0.949176226
0	13	-0.1211762115593269	26595.104362891	1.034365036
0	14	-0.1153568095150405	25317.893244423	1.125993577
0	15	-0.1093296977613950	23995.095114061	1.224072339
0	16	-0.1031232289798301	22632.932666113	1.328620456
0	17	-0.0967646102098110	21237.377155535	1.439666022
0	18	-0.0902798156501029	19814.129260028	1.557246288
0	19	-0.0836935436564426	18368.609642112	1.681407724
0	20	-0.0770292113143616	16905.957758001	1.812205931
0	21	-0.0703089807001349	15431.037621217	1.949705377
0	22	-0.0635538119154962	13948.449442361	2.093978759

0	23	-0.0567835391330315	12462.546319150	2.245106193
0	24	-0.0500169671963421	10977.455437702	2.403173683
0	25	-0.0432719878370207	9497.103579211	2.568270881
0	26	-0.0365657164078576	8025.247129423	2.740487648
0	27	-0.0299146524344628	6565.507315639	2.919908769
0	28	-0.0233348707012576	5121.412145243	3.106605769
0	29	-0.0168422548672997	3696.447678453	3.300623966
0	30	-0.0104527944561861	2294.123210066	3.501961353
0	31	-0.0041829821132203	918.058457330	3.710532722
1	0	-0.1456096921371894	31957.633505822	1.270465977
1	1	-0.1450967715347537	31845.060445680	1.276134116
1	2	-0.1440757191222526	31620.965343836	1.287471879
1	3	-0.1425559580423031	31287.416341043	1.304482628
1	4	-0.1405512488846822	30847.433537668	1.327172317
1	5	-0.1380792725981685	30304.897453428	1.355550429
1	6	-0.1351611227898522	29664.437599964	1.389630990
1	7	-0.1318207406015882	28931.308450557	1.429433523
1	8	-0.1280843253074358	28111.260081225	1.474983841
1	9	-0.1239797506674479	27210.410075179	1.526314590
1	10	-0.1195360118561729	26235.122137667	1.583465509
1	11	-0.1147827215098224	25191.895491103	1.646483412
1	12	-0.1097496670426916	24087.267717261	1.715421896
1	13	-0.1044664355721624	22927.732437820	1.790340817
1	14	-0.0989621079881128	21719.672170366	1.871305561
1	15	-0.0932650200834782	20469.305902610	1.958386114
1	16	-0.0874025862172374	19182.650390881	2.051655923
1	17	-0.0814011795814499	17865.493881785	2.151190513
1	18	-0.0752860626083533	16523.380838326	2.257065780
1	19	-0.0690813611940554	15161.606282657	2.369355806
1	20	-0.0628100770705774	13785.218511435	2.488130024
1	21	-0.0564941337137676	12399.029171441	2.613449413
1	22	-0.0501544525794101	11007.629991469	2.745361276

1	23	-0.0438110582423989	9615.415857714	2.883891942
1	24	-0.0374832133141460	8226.614424715	3.029036371
1	25	-0.0311895871452231	6845.323141305	3.180742940
1	26	-0.0249484669093070	5475.555578186	3.338890859
1	27	-0.0187780269357867	4121.300539602	3.503255357
1	28	-0.0126966846356624	2786.600180043	3.673452230
1	29	-0.0067235945520877	1475.658435806	3.848845007
1	30	-0.0008793791098262	193.001405964	4.028379383
2	0	-0.1277222559253297	28031.795037056	2.027046508
2	1	-0.1272356828588893	27925.004592664	2.031818053
2	2	-0.1262671693251019	27712.440441859	2.041370331
2	3	-0.1248258291723991	27396.102843164	2.055721947
2	4	-0.1229249669055347	26978.911797858	2.074901338
2	5	-0.1205816703021040	26464.617639627	2.098947207
2	6	-0.1178163159226284	25857.692506582	2.127908865
2	7	-0.1146520206364587	25163.209965102	2.161846310
2	8	-0.1111140719931665	24386.719990807	2.200829956
2	9	-0.1072293669134234	23534.125775446	2.244939924
2	10	-0.1030258827727029	22611.567643188	2.294264896
2	11	-0.0985321985983659	21625.317965529	2.348900528
2	12	-0.0937770777469469	20581.689569540	2.408947458
2	13	-0.0887891177625757	19486.958890678	2.474508912
2	14	-0.0835964685384937	18347.304116385	2.545687921
2	15	-0.0782266165590609	17168.757832683	2.622584070
2	16	-0.0727062308565468	15957.173215599	2.705289677
2	17	-0.0670610652387887	14718.202572615	2.793885185
2	18	-0.0613159111573256	13457.286998418	2.888433442
2	19	-0.0554945961328489	12179.656029327	2.988972379
2	20	-0.0496200238322417	10890.336439191	3.095505365
2	21	-0.0437142536853597	9594.169713243	3.207988124
2	22	-0.0377986204616327	8295.838292141	3.326310539
2	23	-0.0318938978340804	6999.901470112	3.450270661

2	24	-0.0260205153593298	5710.843016567	3.579536462
2	25	-0.0201988469579246	4433.134490205	3.713587820
2	26	-0.0144496039291828	3171.321495811	3.851624712
2	27	-0.0087943935092659	1930.146273576	3.992414618
2	28	-0.0032565611898930	714.732566688	4.134021386
3	0	-0.1108847996479062	24336.400527347	2.708775571
3	1	-0.1104241729559617	24235.304653933	2.712729937
3	2	-0.1095074057095361	24034.097500471	2.720653998
3	3	-0.1081433222770312	23734.715791963	2.732578450
3	4	-0.1063448016222750	23339.986134248	2.748549333
3	5	-0.1041283804747285	22853.537919927	2.768627834
3	6	-0.1015137729888029	22279.697905775	2.792889754
3	7	-0.0985233398453310	21623.373693972	2.821424474
3	8	-0.0951815392441913	20889.933238922	2.854333323
3	9	-0.0915143886870497	20085.086722213	2.891727272
3	10	-0.0875489609258594	19214.775926098	2.933723923
3	11	-0.0833129310827149	18285.074837798	2.980443784
3	12	-0.0788341856893231	17302.103843580	3.032005805
3	13	-0.0741404989269395	16271.958671636	3.088522111
3	14	-0.0692592770485650	15200.654299241	3.150091793
3	15	-0.0642173689642323	14094.083381026	3.216793498
3	16	-0.0590409392298200	12957.988373249	3.288676400
3	17	-0.0537553990810470	11797.946397502	3.365748897
3	18	-0.0483853915738442	10619.365979400	3.447964047
3	19	-0.0429548282708727	9427.495100345	3.535200238
3	20	-0.0374869773278645	8227.440530238	3.627234778
3	21	-0.0320046065968598	7024.199235013	3.723706725
3	22	-0.0265301912173701	5822.703937629	3.824062937
3	23	-0.0210862046809621	4627.886999363	3.927476957
3	24	-0.0156955288582742	3444.770410339	4.032721855
3	25	-0.0103820493897524	2278.596462689	4.137960320
3	26	-0.0051715661150485	1135.027566710	4.240373777

3	27	-0.0000932925937037	20.475357613	4.335443816
4	0	-0.0950834942351519	20868.414846706	3.318782488
4	1	-0.0946486226149120	20772.971558160	3.321957826
4	2	-0.0937832300080400	20583.039834776	3.328327653
4	3	-0.0924958736049583	20300.497762766	3.337930013
4	4	-0.0907990411997833	19928.086096143	3.350821242
4	5	-0.0887087658948152	19469.323694121	3.367074875
4	6	-0.0862441610515783	18928.405454677	3.386779900
4	7	-0.0834269081946489	18310.089922424	3.410038174
4	8	-0.0802807299003122	17619.583601048	3.436960868
4	9	-0.0768308760175247	16862.428191840	3.467663845
4	10	-0.0731036459933637	16044.395756253	3.502261859
4	11	-0.0691259637639344	15171.395415239	3.540861477
4	12	-0.0649250155917632	14249.393863744	3.583552546
4	13	-0.0605279560539601	13284.350842570	3.630397902
4	14	-0.0559616834843775	12282.169853622	3.681420840
4	15	-0.0512526836853618	11248.663858608	3.736589553
4	16	-0.0464269396508106	10189.535465535	3.795797356
4	17	-0.0415099053520362	9110.371175374	3.858836832
4	18	-0.0365265433835072	8016.649644344	3.925365029
4	19	-0.0315014297192303	6913.764675281	3.994855180
4	20	-0.0264589347043615	5807.064940703	4.066527440
4	21	-0.0214234992860903	4701.914608487	4.139245850
4	22	-0.0164200428119061	3603.782843236	4.211358245
4	23	-0.0114745712268692	2518.377290155	4.280433929
4	24	-0.0066151209571687	1451.851233548	4.342803207
4	25	-0.0018733251547884	411.147347785	4.392670162
5	0	-0.0803137692068459	17626.834890670	3.857563353
5	1	-0.0799047016362688	17537.054936412	3.859936283
5	2	-0.0790907944941068	17358.422966416	3.864701443
5	3	-0.0778803639893361	17092.764177582	3.871896747
5	4	-0.0762855471462436	16742.742338840	3.881577257

5	5	-0.0743219292710337	16311.778029525	3.893812771
5	6	-0.0720080957059680	15803.950260779	3.908684261
5	7	-0.0693651402888487	15223.888594878	3.926278931
5	8	-0.0664161621453531	14576.662703913	3.946683704
5	9	-0.0631857786995897	13867.675487968	3.969976887
5	10	-0.0596996772566548	13102.564658859	3.996217773
5	11	-0.0559842213731723	12287.116348457	4.025433792
5	12	-0.0520661224713005	11427.193036295	4.057604653
5	13	-0.0479721824561632	10528.677060618	4.092642595
5	14	-0.0437291098726458	9597.430269471	4.130367374
5	15	-0.0393634106015170	8639.270031265	4.170473864
5	16	-0.0349013544116482	7659.961893837	4.212488946
5	17	-0.0303690211484767	6665.229721653	4.255712385
5	18	-0.0257924356351983	5660.785303190	4.299132987
5	19	-0.0211978100447393	4652.381545437	4.341305102
5	20	-0.0166119300038065	3645.897213943	4.380158405
5	21	-0.0120627538312624	2647.468450433	4.412688475
5	22	-0.0075803621423724	1663.697186854	4.434417014
5	23	-0.0031985493412773	702.000437598	4.438357037
6	0	-0.0665815599998031	14612.963337048	4.321854880
6	1	-0.0661986296458075	14528.919838764	4.323307356
6	2	-0.0654368901252369	14361.737338287	4.326225830
6	3	-0.0643044489001766	14113.195217867	4.330635994
6	4	-0.0628131420204878	13785.891190187	4.336572903
6	5	-0.0609781760226091	13383.162704225	4.344076485
6	6	-0.0588176986516041	12908.992729638	4.353185095
6	7	-0.0563523305569691	12367.906975875	4.363926762
6	8	-0.0536046892883244	11764.869421300	4.376307746
6	9	-0.0505989332348663	11105.182219477	4.390297883
6	10	-0.0473603478220322	10394.394879832	4.405812054
6	11	-0.0439149905268544	9638.226357533	4.422686751
6	12	-0.0402894061337574	8842.502559354	4.440650246

6	13	-0.0365104198949851	8013.110947644	4.459283991
6	14	-0.0326050144492328	7155.973527084	4.477971552
6	15	-0.0286002970181972	6277.039645164	4.495829169
6	16	-0.0245235673323603	5382.300900166	4.511608168
6	17	-0.0204025055019447	4477.832374080	4.523552449
6	18	-0.0162655160597666	3569.868141273	4.529180649
6	19	-0.0121422974636145	2664.926259821	4.524933983
6	20	-0.0080647745818639	1770.013428443	4.505564734
6	21	-0.0040686872428162	892.973632780	4.462967496
6	22	-0.0001965373550731	43.134963555	4.383614686
7	0	-0.0539050881012241	11830.799340026	4.702901027
7	1	-0.0535489753452080	11752.641624173	4.703168202
7	2	-0.0528407846263059	11597.211727201	4.703700666
7	3	-0.0517884563167919	11366.252359390	4.704492227
7	4	-0.0504035900289850	11062.309341375	4.705527391
7	5	-0.0487011034118332	10688.656718662	4.706773464
7	6	-0.0466988251867805	10249.207443317	4.708169295
7	7	-0.0444170544527078	9748.416652584	4.709610036
7	8	-0.0418781175786340	9191.184418073	4.710927094
7	9	-0.0391059505985245	8582.764092015	4.711862098
7	10	-0.0361257302118122	7928.681321238	4.712033201
7	11	-0.0329635716067865	7234.667727064	4.710891135
7	12	-0.0296463075650357	6506.612424341	4.707660980
7	13	-0.0262013617574728	5750.534213134	4.701263216
7	14	-0.0226567309898270	4972.577682059	4.690203335
7	15	-0.0190410981983651	4179.038007981	4.672411575
7	16	-0.0153841137628937	3376.422697077	4.644999216
7	17	-0.0117169150750838	2571.565616907	4.603866090
7	18	-0.0080730226084192	1771.823661031	4.543020180
7	19	-0.0044899080203463	985.420907654	4.453275835
7	20	-0.0010119469384914	222.096681292	4.319382993
8	0	-0.0423173659970005	9287.588302774	4.983902674

8	1	-0.0419891895558653	9215.561899331	4.982493559
8	2	-0.0413368127766036	9072.381746188	4.979642448
8	3	-0.0403680656033381	8859.766317444	4.975279378
8	4	-0.0390943993782732	8580.228892209	4.969288613
8	5	-0.0375305664890162	8237.007245313	4.961494935
8	6	-0.0356942413059080	7833.980452674	4.951644021
8	7	-0.0336056147482158	7375.579908853	4.939375631
8	8	-0.0312869945359440	6866.701592476	4.924187747
8	9	-0.0287624405510056	6312.626037256	4.905388822
8	10	-0.0260574612286287	5718.951697612	4.882033800
8	11	-0.0231987941924864	5091.546803643	4.852836916
8	12	-0.0202142942739090	4436.524784187	4.816049647
8	13	-0.0171329569949026	3760.249420748	4.769283679
8	14	-0.0139851195324683	3069.378954065	4.709241953
8	15	-0.0108029124287686	2370.965223035	4.631285293
8	16	-0.0076211039684803	1672.638984121	4.528678661
8	17	-0.0044786407636532	982.948030645	4.391137983
8	18	-0.0014216247883767	312.010576377	4.201577968
9	0	-0.0318697142578724	6994.593788639	5.136468906
9	1	-0.0315711653792571	6929.069883558	5.132549939
9	2	-0.0309780246910242	6798.890549657	5.124623011
9	3	-0.0300980931129323	6605.767890924	5.112502816
9	4	-0.0289428012024198	6352.210624739	5.095892565
9	5	-0.0275269165809846	6041.459869386	5.074359845
9	6	-0.0258682029576070	5677.414308345	5.047301603
9	7	-0.0239870645560351	5264.552151103	5.013895306
9	8	-0.0219062107137411	4807.857521129	4.973031567
9	9	-0.0196503749323374	4312.758794572	4.923220679
9	10	-0.0172461228852932	3785.086462825	4.862460388
9	11	-0.0147217878648606	3231.058964759	4.788042716
9	12	-0.0121075846864926	2657.307685858	4.696258665
9	13	-0.0094359835206368	2070.959004813	4.581918791

9	14	-0.0067424955242968	1479.806719714	4.437509884
9	15	-0.0040671939129624	892.645884761	4.251539485
9	16	-0.0014577748841121	319.944605312	4.004716777
10	0	-0.0226367300970863	4968.187993498	5.116038240
10	1	-0.0223702764493345	4909.708177380	5.108267754
10	2	-0.0218413674890967	4793.626078303	5.092540829
10	3	-0.0210578995844794	4621.674748747	5.068472430
10	4	-0.0200314793412545	4396.401544233	5.035450965
10	5	-0.0187771723323240	4121.112975822	4.992593772
10	6	-0.0173132209722919	3799.812790735	4.938680765
10	7	-0.0156607701977148	3437.141766126	4.872058130
10	8	-0.0138436444456223	3038.328761531	4.790498038
10	9	-0.0118882260170729	2609.164022750	4.690989377
10	10	-0.0098234987666812	2156.008770589	4.569412073
10	11	-0.0076813531686163	1685.862155111	4.419998147
10	12	-0.0054973251364334	1206.523407844	4.234360353
10	13	-0.0033121355875841	726.929737135	3.999517170
10	14	-0.0011749754517599	257.877304145	3.693068373
11	0	-0.0147233976215368	3231.412265512	4.856599734
11	1	-0.0144926086808731	3180.759947836	4.842893924
11	2	-0.0140351693149751	3080.363611631	4.815129691
11	3	-0.0133592773611448	2932.022474217	4.772576283
11	4	-0.0124770463798466	2738.395154813	4.714070279
11	5	-0.0114043263269846	2502.960316647	4.637923976
11	6	-0.0101605301729178	2229.978614233	4.541781181
11	7	-0.0087685221858945	1924.468174416	4.422391034
11	8	-0.0072546441381830	1592.210347954	4.275241850
11	9	-0.0056489957480855	1239.811259426	4.093931136
11	10	-0.0039861786783675	874.865096013	3.868975817
11	11	-0.0023069619782691	506.319629767	3.585228099
11	12	-0.0006621416050315	145.323284680	3.214823933
12	0	-0.0082754520474183	1816.251787534	4.265733795

12	1	-0.0080855614634320	1774.575621613	4.242902658
12	2	-0.0077102401353951	1692.202111496	4.196583206
12	3	-0.0071583708376512	1571.080800809	4.125401154
12	4	-0.0064432077771104	1414.120651727	4.027131242
12	5	-0.0055823577357235	1225.185906228	3.898454036
12	6	-0.0045978748928305	1009.116897193	3.734524715
12	7	-0.0035166101921635	771.806725600	3.528170342
12	8	-0.0023710931721506	520.394799904	3.268228691
12	9	-0.0012016228632326	263.725734955	2.935424737
12	10	-0.0000618587126331	13.576418152	2.487819781
13	0	-0.0034947351958056	767.005718838	3.222119410
13	1	-0.0033537610184289	736.065463225	3.185055143
13	2	-0.0030769976234815	675.322919142	3.109570845
13	3	-0.0026748997756056	587.072642205	2.992733985
13	4	-0.0021634299143649	474.817982952	2.829478095
13	5	-0.0015646300194517	343.396596751	2.611339086
13	6	-0.0009079937174704	199.281586429	2.323215232
13	7	-0.0002342082407986	51.402767313	1.931766017
14	0	-0.0006602771187855	144.914077248	1.584729731
14	1	-0.0005820661980672	127.748764254	1.522632233
14	2	-0.0004330747494117	95.048920983	1.393374332
14	3	-0.0002293084512748	50.327387814	1.182529524
14	4	-0.0000004042248912	0.088717109	0.088717109

B. D₂

Molecule: D2

Deuteron-electron mass ratio = 3670.4829652

2 Ry = 219474.63137078

v	J	D0/hartree	D0/icm	Delta D0/icm
0	0	-0.1674411787281583	36749.090977651	0.156315991
0	1	-0.1671688018028114	36689.311152367	0.158025424
0	2	-0.1666252997296355	36570.026235207	0.161443173
0	3	-0.1658131560648963	36391.781303769	0.166567032
0	4	-0.1647360469055438	36155.383168074	0.173393776
0	5	-0.1633987838782217	35861.887858106	0.181919251
0	6	-0.1618072414292533	35512.584665808	0.192138492
0	7	-0.1599682709615124	35108.977300299	0.204045861
0	8	-0.1578896046783359	34652.762784056	0.217635196
0	9	-0.1555797521438618	34145.808750531	0.232899969
0	10	-0.1530478925607604	33590.129801848	0.249833520
0	11	-0.1503037656166462	32987.863552354	0.268429017
0	12	-0.1473575634952456	32341.246927815	0.288679864
0	13	-0.1442198263008646	31652.593213740	0.310579712
0	14	-0.1409013427621399	30924.270262369	0.334122628
0	15	-0.1374130576701374	30158.680177685	0.359303233
0	16	-0.1337659871064082	29358.240710127	0.386116814
0	17	-0.1299711421426892	28525.368510606	0.414559434
0	18	-0.1260394613607549	27662.464320323	0.444628025
0	19	-0.1219817522569370	26771.900110553	0.476320503
0	20	-0.1178086413629020	25856.008135415	0.509635766
0	21	-0.1135305327363461	24917.071821638	0.544573841
0	22	-0.1091575743413860	23957.318389904	0.581135910

0	23	-0.1046996317525396	22978.913083545	0.619324334
0	24	-0.1001662685660237	21983.954869315	0.659142733
0	25	-0.0955667328828075	20974.473470764	0.700596001
0	26	-0.0909099492354638	19952.427596390	0.743690324
0	27	-0.0862045153575721	18919.704230600	0.788433213
0	28	-0.0814587032362137	17878.118864710	0.834833541
0	29	-0.0766804639408502	16829.416556758	0.882901458
0	30	-0.0718774357861348	15775.273723039	0.932648530
0	31	-0.0670569554502209	14717.300578284	0.984087558
0	32	-0.0622260717495253	13657.044158879	1.037232630
0	33	-0.0573915618466824	12595.991880094	1.092099101
0	34	-0.0525599497562660	11535.575597623	1.148703384
0	35	-0.0477375271118972	10477.176165436	1.207062942
0	36	-0.0429303762656165	9422.128505505	1.267196061
0	37	-0.0381443959256736	8371.727234648	1.329121629
0	38	-0.0333853297017989	7327.232929494	1.392858793
0	39	-0.0286587981409184	6289.879157508	1.458426527
0	40	-0.0239703351236667	5260.880465101	1.525842973
0	41	-0.0193254298969205	4241.441602708	1.595124582
0	42	-0.0147295766053911	3232.768395716	1.666284836
0	43	-0.0101883340749231	2236.080865376	1.739332437
0	44	-0.0057073999942230	1252.629509818	1.814268635
1	0	-0.1538012657265095	33755.476099685	0.460800129
1	1	-0.1535385026716572	33697.806275083	0.462324502
1	2	-0.1530141985735803	33582.734826432	0.465372937
1	3	-0.1522307776886853	33410.793816511	0.469944843
1	4	-0.1511918277539007	33182.770662562	0.476039403
1	5	-0.1499020437090546	32899.695784771	0.483655650
1	6	-0.1483671560011071	32562.826870874	0.492792569
1	7	-0.1465938460360380	32173.630319984	0.503449202
1	8	-0.1445896516518694	31733.760496324	0.515624767
1	9	-0.1423628656246682	31245.037453862	0.529318771

1	10	-0.1399224301970676	30709.423788005	0.544531126
1	11	-0.1372778304566577	30129.001234855	0.561262300
1	12	-0.1344389891167755	29505.947578265	0.579513249
1	13	-0.1314161649046105	28842.514348601	0.599285704
1	14	-0.1282198563595465	28141.005708926	0.620582110
1	15	-0.1248607124394982	27403.758835352	0.643405706
1	16	-0.1213494509305792	26633.126010035	0.667760555
1	17	-0.1176967852873769	25831.458564473	0.693651573
1	18	-0.1139133602056194	25001.092739335	0.721084531
1	19	-0.1100096959546865	24144.337466866	0.750066054
1	20	-0.1059961412766941	23263.464033428	0.780603610
1	21	-0.1018828344907867	22360.697542876	0.812705509
1	22	-0.0976796723210470	21438.210075080	0.846380821
1	23	-0.0933962858914554	20498.115417427	0.881639392
1	24	-0.0890420232904199	19542.465238173	0.918491765
1	25	-0.0846259381004659	18573.246569006	0.956949120
1	26	-0.0801567833048841	17592.380467707	0.997023196
1	27	-0.0756430100199726	16601.721739910	1.038726191
1	28	-0.0710927705545603	15603.059610590	1.082070663
1	29	-0.0665139253633610	14598.119250147	1.127069314
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1	32	-0.0526802252201179	11561.973010715	1.272115759
1	33	-0.0480601594026726	10547.985768522	1.323853798
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1	35	-0.0388468615085044	8525.900609491	1.432470622
1	36	-0.0342663597736028	7520.596679730	1.489360176
1	37	-0.0297115592940163	6520.933523505	1.547971016
1	38	-0.0251885574403326	5528.249358979	1.608296239
1	39	-0.0207034235050824	4543.876241891	1.670320416
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2	3	-0.1391901111723858	30548.698340017	0.752703045
2	4	-0.1381886602972375	30328.905278358	0.758124859
2	5	-0.1369455384769171	30056.071575094	0.764905697
2	6	-0.1354663380000795	29731.424595717	0.773048159
2	7	-0.1337575774689520	29356.395008047	0.782555561
2	8	-0.1318266089733382	28932.596409283	0.793432007
2	9	-0.1296815186071524	28461.803491908	0.805682460
2	10	-0.1273310233013276	27945.929401123	0.819312798
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3	37	-0.0145042140531974	3183.307032648	1.924822625
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4	0	-0.1161016776585975	25481.372905650	1.254072615
4	1	-0.1158668791326528	25429.840585722	1.255122671
4	2	-0.1153984215455625	25327.026029482	1.257224469
4	3	-0.1146985648879247	25173.425247535	1.260381390
4	4	-0.1137706525856673	24969.772037052	1.264598523
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12	3	-0.0376433394911722	8261.758058390	2.525202382
12	4	-0.0370155400363371	8123.972004465	2.522985794
12	5	-0.0362380642249213	7953.335787355	2.520165918
12	6	-0.0353156059873389	7750.879605707	2.516706355
12	7	-0.0342536530570368	7517.807877796	2.512559633
12	8	-0.0330584198174154	7255.484503128	2.507664929
12	9	-0.0317367776723231	6965.417580530	2.501945240
12	10	-0.0302961858635486	6649.244224343	2.495303837
12	11	-0.0287446255288126	6308.716091827	2.487619982
12	12	-0.0270905396097771	5945.686194491	2.478743558
12	13	-0.0253427810419718	5562.097527097	2.468488455
12	14	-0.0235105715442900	5159.974022999	2.456624290
12	15	-0.0216034733461900	4741.414348984	2.442865908
12	16	-0.0196313764293722	4308.589105137	2.426859870
12	17	-0.0176045044355526	3863.742121458	2.408166713
12	18	-0.0155334434877099	3409.196783384	2.386237108
12	19	-0.0134292001060618	2947.368742882	2.360378900
12	20	-0.0113032977557032	2480.787108207	2.329710034
12	21	-0.0091679274813671	2012.127504407	2.293088549
12	22	-0.0070361789455457	1544.262780332	2.249003315
12	23	-0.0049223993473914	1080.341782228	2.195392797
12	24	-0.0028427724621495	623.916438201	2.129319787
12	25	-0.0008163159894481	179.160650866	2.046321561
13	0	-0.0313667095084169	6884.197006674	2.572126609

13	1	-0.0312179227745265	6851.542093101	2.571108452
13	2	-0.0309213438999018	6786.450553920	2.569060672
13	3	-0.0304789476821604	6689.355807111	2.565959870
13	4	-0.0298936611386645	6560.900258731	2.561769764
13	5	-0.0291693234497539	6401.926511470	2.556439720
13	6	-0.0283106359719213	6213.466393810	2.549902714
13	7	-0.0273231049328616	5996.728383045	2.542072639
13	8	-0.0262129797291638	5753.084063188	2.532840861
13	9	-0.0249871899047751	5484.054293342	2.522071839
13	10	-0.0236532839263271	5191.295770439	2.509597683
13	11	-0.0222193728370707	4876.588662706	2.495211267
13	12	-0.0206940818322759	4541.825981696	2.478657561
13	13	-0.0190865128324400	4189.005368053	2.459622569
13	14	-0.0174062213393395	3820.224012010	2.437719029
13	15	-0.0156632113801308	3437.677543737	2.412467551
13	16	-0.0138679533832356	3043.663956653	2.383271184
13	17	-0.0120314317313305	2640.594044096	2.349380109
13	18	-0.0101652321274756	2231.010573976	2.309840947
13	19	-0.0082816850142174	1817.619765624	2.263420881
13	20	-0.0063940926758006	1403.341132972	2.208488177
13	21	-0.0045170902086681	991.386708416	2.142811603
13	22	-0.0026672391551527	585.391330355	2.063194392
13	23	-0.0008640705595322	189.641567532	1.964724858
14	0	-0.0247482566332292	5431.614501647	2.572027850
14	1	-0.0246107268493146	5401.430203020	2.570359519
14	2	-0.0243366675182368	5341.281132358	2.567003321
14	3	-0.0239280658100412	5251.603423075	2.561919484
14	4	-0.0233878700343821	5133.044154344	2.555046567
14	5	-0.0227199529255134	4986.453293089	2.546299242
14	6	-0.0219290662253355	4812.873726111	2.535565180
14	7	-0.0210207892998374	4613.529982705	2.522700910
14	8	-0.0200014748997556	4389.816330496	2.507526404

14	9	-0.0188781954325371	4143.284983502	2.489818167
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14	11	-0.0163513390051931	3588.704100583	2.445633026
14	12	-0.0149651011578961	3284.460060056	2.418397581
14	13	-0.0135095328061952	2964.999732631	2.387076291
14	14	-0.0119947799046369	2632.549897944	2.351025348
14	15	-0.0104316194071697	2289.475823989	2.309436793
14	16	-0.0088315381214963	1938.298573652	2.261283397
14	17	-0.0072068698847295	1581.725111288	2.205235258
14	18	-0.0055710209324639	1222.697765511	2.139526602
14	19	-0.0039388382603759	864.475075225	2.061727996
14	20	-0.0023272310005900	510.768165969	1.968319947
14	21	-0.0007562940312328	165.987353713	1.853786589
15	0	-0.0187753287794241	4120.708362729	2.516904253
15	1	-0.0186498666622366	4093.172610809	2.514352199
15	2	-0.0183999589368486	4038.324204902	2.509216785
15	3	-0.0180276268001544	3956.606746454	2.501434317
15	4	-0.0175358733570011	3848.679340792	2.490906491
15	5	-0.0169286515563901	3715.409559943	2.477496913
15	6	-0.0162108252443351	3557.864894717	2.461026164
15	7	-0.0153881263551082	3377.303359274	2.441265093
15	8	-0.01446711117929379	3175.164027755	2.417925919
15	9	-0.0134551240438051	2953.058389562	2.390650428
15	10	-0.0123602600987755	2712.763528826	2.358994267
15	11	-0.0111913540222496	2456.218298573	2.322405740
15	12	-0.0099579797191351	2185.523928055	2.280196583
15	13	-0.0086704825822521	1902.950968547	2.231500506
15	14	-0.0073400525384631	1610.955325121	2.175212211
15	15	-0.0059788581570251	1312.207690031	2.109893482
15	16	-0.0046002754128196	1009.643750433	2.033619932
15	17	-0.0032192737798121	706.548926106	1.943711420
15	18	-0.0018530894242853	406.706118292	1.836207322

15	19	-0.0005224945843693	114.674306298	1.704683541
16	0	-0.0134931249843174	2961.398631973	2.392301332
16	1	-0.0133807854440666	2936.742952788	2.388550273
16	2	-0.0131571547634783	2887.661691603	2.380999508
16	3	-0.0128243201166349	2814.612930179	2.369549975
16	4	-0.0123853891782742	2718.278724285	2.354048538
16	5	-0.0118444651294700	2599.559618074	2.334282177
16	6	-0.0112066177762689	2459.568305360	2.309969546
16	7	-0.0104778544991256	2299.623253752	2.280749223
16	8	-0.0096650956813127	2121.243311819	2.246163448
16	9	-0.0087761603903715	1926.144566528	2.205635580
16	10	-0.0078197696816957	1716.241068295	2.158438264
16	11	-0.0068055774636517	1493.651605100	2.103647263
16	12	-0.0057442433781739	1260.715697929	2.040071922
16	13	-0.0046475706104232	1020.023846492	1.966145150
16	14	-0.0035287484751062	774.470770774	1.879737778
16	15	-0.0024027765150529	527.348489908	1.777817383
16	16	-0.0012872373794867	282.515949350	1.655741605
16	17	-0.0002038519740234	44.740336853	1.505499511
17	0	-0.0089585340269992	1966.170953198	2.180230115
17	1	-0.0088607056407212	1944.700104182	2.174855326
17	2	-0.0086661536032908	1902.000867485	2.164030484
17	3	-0.0083770813856714	1838.556849083	2.147601872
17	4	-0.0079967804699995	1755.090445806	2.125330623
17	5	-0.0075296174805899	1652.560020915	2.096881785
17	6	-0.0069810231612266	1532.157484901	2.061807910
17	7	-0.0063574888510167	1395.307522021	2.019524953
17	8	-0.0056665783333199	1243.670190839	1.969276815
17	9	-0.0049169663291277	1079.149372548	1.910081945
17	10	-0.0041185207438041	903.910822039	1.840649837
17	11	-0.0032824568357655	720.416004020	1.759243114
17	12	-0.0024216144987198	531.482949429	1.663432055

17	13	-0.0015509634620262	340.397134098	1.549609609
17	14	-0.0006885872375955	151.127430138	1.411872246
18	0	-0.0052431833155783	1150.745725396	1.859050861
18	1	-0.0051617362269871	1132.870155651	1.851466974
18	2	-0.0050000451930080	1097.383075573	1.836178820
18	3	-0.0047605175319242	1044.812830453	1.812938737
18	4	-0.0044467689838978	975.952983532	1.781356893
18	5	-0.0040636358365569	891.864977253	1.740875826
18	6	-0.0036172028339607	793.884258577	1.690729439
18	7	-0.0031148596718216	683.632678245	1.629876921
18	8	-0.0025654073932025	563.041841939	1.556892473
18	9	-0.0019792528137198	434.395781681	1.469769385
18	10	-0.0013687669607733	300.409624148	1.365536887
18	11	-0.0007489835876413	164.382896800	1.239393015
18	12	-0.0001391510928238	30.540134802	1.082187616
19	0	-0.0024374061607607	534.948818634	1.403862688
19	1	-0.0023749708675468	521.245855671	1.393193125
19	2	-0.0022514872451773	494.144333171	1.371638247
19	3	-0.0020697482141859	454.257226339	1.338745326
19	4	-0.0018339969698214	402.515808887	1.293775827
19	5	-0.0015500116840096	340.188242968	1.235612155
19	6	-0.0012252612474566	268.913760618	1.162579894
19	7	-0.0008691970857554	190.766709985	1.072081411
19	8	-0.0004938395755154	108.385258793	0.959714265
19	9	-0.0001151595339742	25.274596268	0.816422199
20	0	-0.0006542045402464	143.581300312	0.789619751
20	1	-0.0006148436815279	134.942590354	0.774193394
20	2	-0.0005379438172236	118.065020983	0.742773514
20	3	-0.0004272574670691	93.772175085	0.694056974
20	4	-0.0002887515484757	63.373639659	0.625490901
20	5	-0.0001313104019550	28.819302064	0.531550782
21	0	-0.0000076301909978	1.674633357	0.066958148

21 1 -0.0000002468255949 0.054171956 0.030999159

C. T₂

Molecule: T2

Triton-electron mass ratio = 5496.9215267

2 Ry = 219474.63137078

v	J	D0/hartree	D0/icm	Delta D0/icm
0	0	-0.1687175626239232	37029.224862662	0.085966396
0	1	-0.1685350245622163	36989.162388858	0.086736481
0	2	-0.1681705086750429	36909.160398892	0.088276295
0	3	-0.1676251294474173	36789.463493951	0.090585124
0	4	-0.1669005437905200	36630.435324007	0.093661920
0	5	-0.1659989336815167	36432.554777693	0.097505314
0	6	-0.1649229836949625	36196.411051021	0.102113641
0	7	-0.1636758539673357	35922.697713779	0.107484970
0	8	-0.1622611492252235	35612.205912005	0.113617140
0	9	-0.1606828845705901	35265.816858724	0.120507790
0	10	-0.1589454487527724	34884.493773078	0.128154459
0	11	-0.1570535656648159	34469.273429752	0.136554448
0	12	-0.1550122547910752	34021.257478225	0.145705087
0	13	-0.1528267912906122	33541.603682086	0.155603642
0	14	-0.1505026663530591	33031.517218157	0.166247389
0	15	-0.1480455483936479	32492.242159781	0.177633650
0	16	-0.1454612455794174	31925.053252277	0.189759834
0	17	-0.1427556700980432	31331.248070857	0.202623470
0	18	-0.1399348044992434	30712.139633414	0.216222240
0	19	-0.1370046703592967	30069.049523182	0.230554011
0	20	-0.1339712994445635	29403.301559860	0.245616881
0	21	-0.1308407074809594	28716.216042676	0.261409160
0	22	-0.1276188705769596	28009.104575833	0.277929445

0	23	-0.1243117042938241	27283.265474960	0.295176617
0	24	-0.1209250453143811	26539.979743869	0.313149860
0	25	-0.1174646356258693	25780.507603091	0.331848693
0	26	-0.1139361091049484	25006.085545630	0.351272949
0	27	-0.1103449803740057	24217.923891201	0.371422895
0	28	-0.1066966357818252	23417.204806718	0.392299063
0	29	-0.1029963263585995	22605.080760098	0.413902435
0	30	-0.0992491625868467	21782.673372607	0.436234365
0	31	-0.0954601108354181	20951.072636217	0.459296621
0	32	-0.0916339913057913	20111.336462872	0.483091362
0	33	-0.0877754773483690	19264.490534428	0.507621174
0	34	-0.0838890960148094	18411.528423878	0.532889060
0	35	-0.0799792297240811	17553.411961012	0.558898449
0	36	-0.0760501189317272	16691.071818245	0.585653184
0	37	-0.0721058657055877	15825.408295405	0.613157577
0	38	-0.0681504381237958	14957.292284977	0.641416284
0	39	-0.0641876754291714	14087.566403365	0.670434480
0	40	-0.0602212938845620	13217.046275986	0.700217658
0	41	-0.0562548932968446	12346.521969128	0.730771755
0	42	-0.0522919641899369	11476.759564240	0.762103079
0	43	-0.0483358956308983	10608.502875568	0.794218296
0	44	-0.0443899837343104	9742.475316643	0.827124382
0	45	-0.0404574408972172	8879.381927122	0.860828598
0	46	-0.0365414058479921	8019.911578258	0.895338414
0	47	-0.0326449546316677	7164.739383901	0.930661447
0	48	-0.0287711127028579	6314.529354587	0.966805354
0	49	-0.0249228683607825	5469.937346185	1.003777697
0	50	-0.0211031878450073	4631.614373031	1.041585739
0	51	-0.0173150325252237	3800.210380647	1.080236268
0	52	-0.0135613787760829	2976.378607760	1.119735218
0	53	-0.0098452413568010	2160.780717540	1.160087262
0	54	-0.0061697014454134	1354.092950400	1.201295200

1	0	-0.1574884648875758	34564.722776351	0.254209690
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1	2	-0.1569571981294477	34448.123200451	0.256314043
1	3	-0.1564275733691099	34331.884001411	0.258417924
1	4	-0.1557239429387952	34177.454972096	0.261222384
1	5	-0.1548484456726540	33985.305532344	0.264726843
1	6	-0.1538037126519583	33756.013137746	0.268930620
1	7	-0.1525928404750512	33490.257413082	0.273832956
1	8	-0.1512193606640411	33188.813437865	0.279433044
1	9	-0.1496872059048153	32852.544336881	0.285730056
1	10	-0.1480006738511851	32482.393336116	0.292723177
1	11	-0.1461643892316201	32079.375446145	0.300411682
1	12	-0.1441832649784381	31644.568930978	0.308794814
1	13	-0.1420624630643755	31179.106712679	0.317872013
1	14	-0.1398073556701331	30684.167848626	0.327642823
1	15	-0.1374234872428683	30160.969204316	0.338106949
1	16	-0.1349165379256656	29610.757427057	0.349264274
1	17	-0.1322922887575876	29034.801308268	0.361114885
1	18	-0.1295565889620003	28434.384604091	0.373659086
1	19	-0.1267153255617125	27810.799366685	0.386897414
1	20	-0.1237743954854250	27165.339822305	0.400830652
1	21	-0.1207396802628084	26499.296817506	0.415459836
1	22	-0.1176170233464508	25813.952841891	0.430786273
1	23	-0.1144122100481243	25110.577624628	0.446811525
1	24	-0.1111309500355629	24390.424292940	0.463537434
1	25	-0.1077788623018827	23654.726073268	0.480966109
1	26	-0.1043614624950891	22904.693510425	0.499099945
1	27	-0.1008841524763370	22141.512175898	0.517941591
1	28	-0.0973522119647419	21366.340834092	0.537493975
1	29	-0.0937707921195669	20580.310033788	0.557760284
1	30	-0.0901449109100551	19784.521091936	0.578743956
1	31	-0.0864794501256670	18980.045437479	0.600448697

1	32	-0.0827791538851089	18167.924284119	0.622878430
1	33	-0.0790486285121227	17349.168603064	0.646037285
1	34	-0.0752923436563949	16524.759369029	0.669929615
1	35	-0.0715146345504353	15695.648055573	0.694559944
1	36	-0.0677197053084472	14862.757359109	0.719932941
1	37	-0.0639116331884844	14026.982134347	0.746053395
1	38	-0.0600943737565382	13189.190527674	0.772926150
1	39	-0.0562717669105918	12350.225299285	0.800556071
1	40	-0.0524475437432304	11510.905329348	0.828947964
1	41	-0.0486253342455587	10672.027308825	0.858106490
1	42	-0.0448086758823143	9834.367621484	0.888036057
1	43	-0.0410010231004043	8998.684430786	0.918740688
1	44	-0.0372057578722764	8165.719993888	0.950223851
1	45	-0.0334262014241407	7336.203235689	0.982488233
1	46	-0.0296656273617607	6510.852629605	1.015535473
1	47	-0.0259272764881771	5690.379449691	1.049365822
1	48	-0.0222143737178340	4875.491482854	1.083977641
1	49	-0.0185301476443825	4066.897323497	1.119366851
1	50	-0.0148778535328728	3265.311419716	1.155526093
1	51	-0.0112608008195682	2471.460108815	1.192443672
1	52	-0.0076823866643248	1686.088981200	1.230102071
1	53	-0.0041461378101553	909.972067496	1.268475890
2	0	-0.1466237713914864	32180.198176340	0.413070522
2	1	-0.1464516867397126	32142.429960827	0.413708082
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