

**Supplementary information for: Vibration-rotation-tunneling states of the benzene dimer: an *ab initio* study**

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The geometry definition below (consistent with that of JPCA, 110, 10345 (2006)) differs from the one used in the present paper by the interchange of the monomer x and y axes. This amounts to adding 90 degrees to the Euler angles \gamma\_A and \gamma\_B.

# ----- Fit parameters -----

The following parameters are not changed from pot1 of JPCA, 110, 10345 (2006):

1. Cartesian coordinates of the benzene molecule and off-atomic sites (in Angstrom)

Site	X	Y	Z
C1	0.000000000000000	1.396500000000000	0.0
C2	-1.209404476384990	0.698250000000000	0.0
C3	-1.209404476384990	-0.698250000000000	0.0
C4	0.000000000000000	-1.396500000000000	0.0
C5	1.209404476384990	-0.698250000000000	0.0
C6	1.209404476384990	0.698250000000000	0.0
H1	0.000000000000000	2.481500000000000	0.0
H2	-2.149042039491110	1.240750000000000	0.0
H3	-2.149042039491110	-1.240750000000000	0.0
H4	0.000000000000000	-2.481500000000000	0.0
H5	2.149042039491110	-1.240750000000000	0.0
H6	2.149042039491110	1.240750000000000	0.0
D1	0.000000000000000	1.794554300727060	0.0
D2	-1.554129613367140	0.897277150363530	0.0
D3	-1.554129613367140	-0.897277150363530	0.0
D4	0.000000000000000	-1.794554300727060	0.0
D5	1.554129613367140	-0.897277150363530	0.0
D6	1.554129613367140	0.897277150363530	0.0
P1	-0.725642684858874	1.256850000663900	0.0
P2	-1.451285369717750	0.000000000000000	0.0
P3	-0.725642684858874	-1.256850000663900	0.0
P4	0.725642684858874	-1.256850000663900	0.0
P5	1.451285369717750	0.000000000000000	0.0
P6	0.725642684858874	1.256850000663900	0.0
M	0.000000000000000	0.000000000000000	0.0

2. Site charges q (in atomic units)

Site	q
C	-0.193357181
H	0.278869361
D	-0.522242923
P	0.436730743
M	0.0

3. Asymptotic constants C\_6, C\_10, C\_12

Unit of C\_n: kcal/mol \* (Angstrom)^n

ab	C_6	C_8	C_10
CC	1.65682607E+03	-3.04924411E+04	3.02203727E+05
CH	-7.78366044E+02	1.76849531E+04	-1.31856847E+05
HH	5.60668174E+02	-1.26112754E+04	8.13927374E+04

Below we list only the parameters that are different from pot1 of JPCA, 110, 10345 (2006):

----- pot2 begin -----

Parameters of the exponential term

Units: beta 1/Angstrom  
exp(alpha) kcal/mol  
a\_1 1/Angstrom  
a\_2 1/Angstrom^2

ab	beta	alpha	a_1	a_2
CC	3.56852953E+00	1.42549400E+01	-8.58978323E-01	2.28965059E-01
CH	4.32106867E+00	1.14351275E+01	-1.14008352E+00	3.78455883E-01
HH	2.36344832E+00	6.66101313E+00	-3.16919968E-01	1.93176364E-01
CD	2.48467609E+00	9.93096967E+00	-5.15870900E-01	8.28940494E-06
HD	2.02913482E+00	1.55504520E-08	-2.75419047E+02	1.39225237E+01
DD	2.81842319E+00	9.87920782E+00	-1.25466713E+00	4.98737888E-01
CP	2.51163386E+00	1.07784199E+01	-7.88772336E-01	1.49046241E-01
HP	1.77640258E+00	2.06533477E-09	4.81618704E+01	1.58003320E+01
DP	2.71818560E+00	2.54558471E+00	-2.55426641E+02	7.29726701E+01
PP	2.00257219E+00	3.38080686E-02	1.37516171E+03	-5.42734570E+02
CM	2.19575417E+00	9.98095561E+00	-8.77101928E-01	1.06765442E-01
HM	2.41066829E+00	4.68076322E+00	-4.62747777E+00	-2.76092004E-01
DM	2.62545827E+00	1.03519024E+01	-1.03903878E+00	3.49580177E-01
PM	3.79992577E+00	1.51432340E+01	-7.53893273E-01	1.54411151E-01
MM	1.45787659E+00	8.33045333E+00	-3.45021639E-02	-2.56539253E-02

Damping parameters (in 1/Angstrom)

ab	delta1	delta6	delta8	delta10
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CC 18.663053000 4.16877500 1.05840640 7.47648064
CH 1.786020630 3.29890314 2.22081722 1.33762128
HH 1.340746170 2.66006720 1.57962426 2.89892649
CD 1.146180580
HD 1.202172490
DD 1.202645810
CP 1.072787920
HP 1.051286110
DP 1.007863240
PP 0.949040398

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#----- pot2 end -----

#----- pot3 begin -----

Parameters of the exponential term

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Units: beta      1/Angstrom
      exp(alpha)  kcal/mol
      a_1         1/Angstrom
      a_2         1/Angstrom^2

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ab	beta	alpha	a_1	a_2
CC	3.60378961E+00	1.43264870E+01	-9.04405445E-01	2.43760520E-01
CH	4.10403506E+00	9.94293052E+00	-1.43432939E+00	5.29072306E-01
HH	2.16694450E+00	6.62625341E+00	-3.59376992E-01	1.60204673E-01
CD	2.63881856E+00	1.05467481E+01	-4.87027626E-01	-3.87240175E-04
HD	1.87784424E+00	2.00183627E+00	-3.65253802E+01	2.20603874E+00
DD	2.77522924E+00	8.96220775E+00	-2.09279617E+00	1.09578069E+00
CP	2.54791816E+00	1.06271525E+01	-7.80487851E-01	1.41233025E-01
HP	1.59688943E+00	1.50035229E-09	7.65405713E+01	-1.04085767E+00
DP	2.54560361E+00	2.63504496E-05	-2.01303748E+03	3.74081129E+02
PP	1.93941130E+00	1.11048440E-04	1.19004006E+03	-4.22675632E+02
CM	2.20162936E+00	1.00597948E+01	-8.77418308E-01	1.10224705E-01
HM	2.04864769E+00	1.57406718E-03	-3.16797038E+02	4.07717125E-01
DM	2.62466570E+00	1.03564632E+01	-1.09712124E+00	3.83785143E-01
PM	3.81872124E+00	1.48705037E+01	-7.47657445E-01	1.54846000E-01
MM	1.44959912E+00	8.35709667E+00	-4.33560069E-02	-1.91996193E-02

Damping parameters (in 1/Angstrom)

ab	delta1	delta6	delta8	delta10
CC	19.255681000	2.22142019	1.03087212	7.85356007
CH	1.961588570	3.69026169	1.92624728	0.07343285
HH	1.281376060	2.43288971	1.26179207	3.00421324
CD	1.139464400			
HD	1.199509480			
DD	1.202805750			
CP	1.078882400			
HP	1.054482000			
DP	1.005422520			
PP	0.948741111			

#----- pot2 end -----

#----- Fit parameters end -----

#-----Points used for fitting begin-----

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# SAPT(DFT) results used for the fitting
# Aug-cc-pVTZ MC+BS basis set with midbond, described in text, was used.
# All energies in kcal/mol
# Geometric parameters are described in JPCA, 110, 10345 (2006)
# and can be converted to Cartesian coordinates with programs
# available at http://www.physics.udel.edu/~szalewic/sapt/benzene
# SAPT(DFT) terms:
# elst --- electrostatics E^(1)_{elst}(KS)
# exch --- first-order exchange E^(1)_{exch}(KS)
# ind --- induction E^(2)_{ind}(CKS)
# ex-ind --- exchange-induction \tilde{E}^(2)_{ex-ind}(CKS)
# disp --- dispersion E^(2)_{disp}(CKS)
# ex-disp --- exchange-dispersion \tilde{E}^(2)_{ex-disp}(CKS)
# ind3 --- third-order induction E^(3)_{ind}(KS)
# ex-ind3 --- scaled third-order exchange-induction \tilde{E}^(3)_{ex-ind}(KS)
# exch(S2) --- first-order exchange is the S^2 approximation (used in the above scaling) E^(1)_{exch}(KS)(S^2)
# total2 --- elst + exch + ind + ex-ind + disp + ex-disp
# total3 --- total2 + ind3 + ex-ind3

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# The following geometries and energies (after correcting minor error in unit conversion)
# are taken from JPCA, 110, 10345 (2006). Third-order energies are calculated in this work.
# The points are used in fitting of both 'pot2' and 'pot3'

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#	R	beta_A	gamma_A	alpha_B	beta_B	gamma_B	total3	elst	exch	ind	ex-ind	disp	ex-disp	total2	ind3	ex-ind3	exch(S2)
3.250000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	1.4098	-5.0587	18.8535	-7.8525	7.5711	-14.4227	2.2026	1.2933	-16.1366	16.2531	18.7780
3.600000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	-1.5173	-0.8872	6.7804	-2.4957	2.2450	-8.1500	0.9015	-1.6059	-4.8571	4.9457	6.7824
3.848457	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	-1.7808	0.1577	3.2676	-1.1537	0.9447	-5.5225	0.4658	-1.9405	-2.0966	2.1563	3.2712
4.600000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	-0.8789	0.6586	0.3480	-0.1552	0.0682	-1.8723	0.0579	-0.8948	-0.1661	0.1820	0.3478
5.100000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	-0.4091	0.5311	0.0747	-0.0551	0.0104	-0.9910	0.0138	-0.4162	-0.0227	0.0298	0.0747
3.300000	0.000000	0.000000	0.000000	0.000000	30.000000	0.000000	8.9955	-15.1047	43.2286	-22.1723	20.8324	-21.3235	4.0763	9.5367	-45.9859	45.4447	42.1990
4.000000	0.000000	0.000000	0.000000	0.000000	30.000000	0.000000	-1.4939	-1.0112	5.6030	-2.2902	2.0448	-6.6674	0.7443	-1.5769	-4.4546	4.5375	5.5845
5.500000	0.000000	0.000000	0.000000	0.000000	30.000000	0.000000	-0.4290	0.3502	0.0603	-0.0479	0.0112	-0.8189	0.0121	-0.4330	-0.0290	0.0329	0.0604
3.300000	0.000000	0.000000	0.000000	0.000000	30.000000	8.6091	-15.0046	42.6979	-22.1660	20.7814	-21.1828	4.0406	9.1665	-46.1044	45.5471	41.5598	
3.600000	0.000000	0.000000	0.000000	0.000000	30.000000	1.4402	-5.5131	18.0778	-8.3429	7.8864	-12.7799	2.0240	1.3523	-16.9821	17.0701	17.8579	
4.000000	0.000000	0.000000	0.000000	0.000000	30.000000	-1.4634	-1.0338	5.6465	-2.3144	2.0694	-6.6627	0.7477	-1.5473	-4.5024	4.5862	5.6255	
5.500000	0.000000	0.000000	0.000000	0.000000	30.000000	-0.4304	0.3488	0.0613	-0.0481	0.0113	-0.8198	0.0123	-0.4343	-0.0291	0.0330	0.0615	
4.000000	0.000000	0.000000	0.000000	0.000000	60.000000	6.2547	-10.1729	30.3411	-11.1117	10.0289	-15.4249	2.6270	6.2875	-19.2055	19.1727	29.9248	
5.000000	0.000000	0.000000	0.000000	0.000000	60.000000	-1.9332	-0.4514	1.4706	-0.4433	0.2962	-2.9997	0.1907	-1.9370	-0.6159	0.6197	1.4716	
6.000000	0.000000	0.000000	0.000000	0.000000	60.000000	-0.7371	-0.0167	0.0634	-0.0408	0.0079	-0.7610	0.0106	-0.7365	-0.0210	0.0204	0.0635	
4.000000	0.000000	0.000000	0.000000	0.000000	60.000000	7.7625	-12.3366	36.3453	-14.7760	12.4898	-16.2880	2.8240	8.2584	-25.0135	24.5176	35.2012	
4.400000	0.000000	0.000000	0.000000	0.000000	60.000000	-0.3725	-3.7719	11.1832	-3.8124	3.1980	-8.2562	1.1053	-0.3540	-6.1652	6.1467	11.0670	
5.000000	0.000000	0.000000	0.000000	0.000000	60.000000	-1.9190	-0.6202	1.8063	-0.5591	0.3777	-3.1449	0.2259	-1.9143	-0.7795	0.7748	1.8049	
6.500000	0.000000	0.000000	0.000000	0.000000	60.000000	-0.4535	-0.0176	0.0154	-0.0204	0.0017	-0.4350	0.0030	-0.4529	-0.0052	0.0046	0.0155	
4.300000	0.000000	0.000000	0.000000	90.000000	0.000000	5.1734	-9.2061	27.3416	-8.3482	7.2122	-13.8522	2.2165	5.3638	-12.9163	12.7259	27.0381	

5.000000	0.000000	0.000000	0.000000	90.000000	0.000000	-2.4342	-1.4872	3.2198	-0.7752	0.5585	-4.2777	0.3519	-2.4099	-1.0243	1.0001	3.2212
7.000000	0.000000	0.000000	0.000000	90.000000	0.000000	-0.4540	-0.1389	0.0052	-0.0115	0.0004	-0.3092	0.0009	-0.4531	-0.0016	0.0008	0.0052
4.100000	0.000000	0.000000	0.000000	90.000000	30.000000	8.4381	-14.5582	41.7594	-16.4353	14.0001	-19.0315	3.5072	9.2418	-28.4671	27.6635	40.3040
5.100000	0.000000	0.000000	0.000000	90.000000	30.000000	-2.6435	-1.2974	2.3969	-0.6768	0.4673	-3.8121	0.3092	-2.6128	-0.9676	0.9369	2.3916
7.000000	0.000000	0.000000	0.000000	90.000000	30.000000	-0.4859	-0.1601	0.0055	-0.0138	0.0005	-0.3183	0.0012	-0.4849	-0.0024	0.0014	0.0055
3.250000	0.000000	0.000000	30.000000	30.000000	0.000000	10.2266	-17.2376	48.2613	-25.5335	23.9473	-22.9295	4.4839	10.9899	-53.4810	52.7116	46.9276
3.600000	0.000000	0.000000	30.000000	30.000000	0.000000	1.2667	-5.3865	17.6966	-8.1722	7.7407	-12.7126	2.0049	1.1710	-16.6876	16.7833	17.5017
4.000000	0.000000	0.000000	30.000000	30.000000	0.000000	-1.5255	-0.9935	5.5203	-2.2712	2.0296	-6.6335	0.7386	-1.6097	-4.4312	4.5154	5.5014
5.500000	0.000000	0.000000	30.000000	30.000000	0.000000	-0.4292	-0.3497	0.0601	-0.0478	0.0112	-0.8184	0.0121	-0.4331	-0.0289	0.0329	0.0620
3.300000	0.000000	0.000000	30.000000	30.000000	30.000000	9.1862	-15.4522	44.1884	-22.7426	21.2180	-21.4758	4.1018	9.8378	-46.9537	46.3022	43.0244
4.000000	0.000000	0.000000	30.000000	30.000000	30.000000	-1.4309	-1.0532	5.7354	-2.3343	2.0845	-6.6999	0.7539	-1.5134	-4.5235	4.6060	5.7146
5.500000	0.000000	0.000000	30.000000	30.000000	30.000000	-0.4304	-0.3492	0.0615	-0.0481	0.0113	-0.8205	0.0123	-0.4343	-0.0292	0.0331	0.0618
6.000000	0.000000	0.000000	30.000000	30.000000	30.000000	-0.2052	0.2618	0.0128	-0.0216	0.0020	-0.4648	0.0030	-0.2068	-0.0044	0.0060	0.0129
4.000000	0.000000	0.000000	30.000000	60.000000	0.000000	6.3702	-10.2045	30.5886	-11.2491	10.1300	-15.4741	2.6334	6.4242	-19.3874	19.3334	30.1753
4.190000	0.000000	0.000000	30.000000	60.000000	0.000000	1.5592	-5.7230	17.3815	-5.8931	5.2568	-11.1603	1.6627	1.5246	-9.9596	9.9942	17.2571
5.000000	0.000000	0.000000	30.000000	60.000000	0.000000	-1.9308	-2.4508	1.4751	-0.4445	0.2968	-3.0021	0.1910	-1.9345	-0.6168	0.6204	1.4762
6.000000	0.000000	0.000000	30.000000	60.000000	0.000000	-0.7368	-0.0163	0.0635	-0.0408	0.0079	-0.7611	0.0106	-0.7362	-0.0209	0.0203	0.0636
4.000000	0.000000	0.000000	30.000000	60.000000	30.000000	7.8914	-12.2211	36.6059	-15.0697	12.6498	-16.3420	2.8159	8.4388	-25.3855	24.8381	35.4459
5.000000	0.000000	0.000000	30.000000	60.000000	30.000000	-1.9177	-0.6191	1.8095	-0.5607	0.3785	-3.1468	0.2260	-1.9127	-0.7810	0.7760	1.8080
6.000000	0.000000	0.000000	30.000000	60.000000	30.000000	-0.7705	-0.0401	0.0776	-0.0466	0.0097	-0.7829	0.0129	-0.7693	-0.0255	0.0243	0.0777
4.600000	0.000000	24.691700	354.691500	90.000000	120.000000	-0.7923	-4.0401	11.0101	-2.9069	2.4249	-8.2700	1.0423	-0.7397	-4.2867	4.2340	10.9719
5.650000	0.000000	24.691700	354.691500	90.000000	120.000000	-1.6672	-0.4562	0.4153	-0.1191	0.0484	-1.6016	0.0538	-1.6594	-0.1035	0.0957	0.4162
5.039048	0.000000	24.691701	354.691508	90.000000	120.000000	-2.4438	-1.3636	2.8455	-0.6815	0.4814	-4.0190	0.3157	-2.4216	-0.8884	0.8661	2.8476
6.350000	0.000000	24.691701	354.691508	90.000000	120.000000	-0.8387	-0.2209	0.0437	-0.0285	0.0035	-0.6406	0.0066	-0.8364	-0.0098	0.0074	0.0438
4.100000	9.303764	0.000000	90.000000	90.000000	40.514430	15.5827	-21.1159	62.3203	-28.6446	21.3348	-21.6850	3.9995	18.0091	-45.1804	42.7540	58.8669
4.974934	9.303764	0.000000	90.000000	90.000000	40.514430	-1.9508	-0.4610	5.2506	-1.5098	1.1679	-5.1045	0.5484	-1.9053	-2.2100	2.1646	5.2198
6.400000	9.303764	0.000000	90.000000	90.000000	40.514430	-0.8662	-0.2505	0.0650	-0.0355	0.0064	-0.6586	0.0098	-0.8633	-0.0171	0.0141	0.0651
4.100000	9.303764	0.000000	270.000000	90.000000	100.514430	8.6246	-14.3600	41.0854	-15.3112	13.3807	-19.2477	3.5326	9.0797	-26.3906	25.9355	40.0547
4.400000	9.303764	0.000000	270.000000	90.000000	100.514430	-4.4094	-6.4696	17.6776	-5.7909	5.0277	-11.7298	1.7805	0.4954	-9.6633	9.5773	17.4704
4.974934	9.303764	0.000000	270.000000	90.000000	100.514430	-2.7847	-1.5850	3.2779	-0.9247	0.6907	-4.6316	0.4127	-2.7600	-1.3877	1.3630	3.2720
5.700000	9.303764	0.000000	270.000000	90.000000	100.514430	-1.7034	-0.4610	0.3555	-0.1240	0.0508	-1.5712	0.0547	-1.6951	-0.1214	0.1131	0.3557
6.400000	9.303764	0.000000	270.000000	90.000000	100.514430	-0.8494	-0.2332	0.0388	-0.0310	0.0041	-0.6326	0.0071	-0.8468	-0.0127	0.0101	0.0388
4.974934	9.303764	360.000000	90.000000	90.000000	40.514430	-1.9507	-2.2579	5.2506	-1.5098	1.1679	-5.1045	0.5484	-1.9053	-2.2100	2.1646	5.2198
4.400000	9.303764	0.000000	90.000000	90.000000	40.514440	4.7719	-9.6512	27.5378	-10.0807	8.3796	-13.1733	2.1838	5.1970	-16.2721	15.8469	26.7788
5.700000	9.303800	0.000000	90.000000	90.000000	40.514440	-1.6767	-0.5566	0.5817	-0.1716	0.0840	-1.6784	0.0751	-1.6658	-0.1794	0.1684	0.5821
3.150000	29.397393	270.000000	0.000000	29.397393	270.000000	5.7520	-18.7808	48.8433	-25.7860	24.6021	-25.8548	5.1635	8.1873	-55.0072	54.3429	48.0259
3.550000	29.397393	270.000000	0.000000	29.397393	270.000000	-1.0991	-5.7498	16.6940	-7.8591	7.3620	-13.7192	2.1411	-1.1310	-16.3824	16.4143	16.5962
4.016410	29.397393	270.000000	0.000000	29.397393	270.000000	-2.6690	-1.1112	4.6851	-2.0390	1.7280	-6.7045	0.7136	-2.7279	-4.0191	4.0781	4.6790
4.700000	29.397393	270.000000	0.000000	29.397393	270.000000	-1.6306	-0.1677	0.7045	-0.3397	0.1984	-2.5113	0.1293	-1.6510	-0.5174	0.5379	0.7046
5.500000	29.397400	270.000000	0.000000	29.397400	270.000000	-0.6589	0.2011	0.0725	-0.0634	0.0145	-0.9045	0.0161	-0.6638	-0.0410	0.0459	0.0728
3.250000	30.000000	0.000000	0.000000	30.000000	0.000000	4.8301	-15.0199	39.4508	-20.3661	19.4119	-22.5749	4.3318	5.2336	-43.2624	42.8589	38.8924
3.600000	30.000000	0.000000	0.000000	30.000000	0.000000	-1.2610	-5.3207	15.5404	-7.2828	6.7912	-13.0170	2.0000	-1.2888	-15.1513	15.1791	15.4531
4.000000	30.000000	0.000000	0.000000	30.000000	0.000000	-2.6102	-1.3591	5.2847	-2.3041	1.9791	-7.0540	0.7847	-2.6686	-4.5756	4.6340	5.2751
5.500000	30.000000	0.000000	0.000000	30.000000	0.000000	-0.6810	0.1890	0.0807	-0.0662	0.0162	-0.9230	0.0173	-0.6859	-0.0460	0.0509	0.0809
3.200000	30.000000	0.000000	0.000000	30.000000	30.000000	6.3337	-17.2105	44.8376	-23.4253	22.3354	-24.4563	4.8113	6.8922	-49.8788	49.3203	44.1431
4.100000	30.000000	0.000000	0.000000	30.000000	30.000000	-2.6015	-0.8801	3.9653	-1.7213	1.4292	-6.0600	0.6117	-2.6552	-3.3544	3.4080	3.9602
6.000000	30.000000	0.000000	0.000000	30.000000	30.000000	-0.3855	0.1376	0.0186	-0.0295	0.0031	-0.5219	0.0046	-0.3876	-0.0083	0.0104	0.0187
4.000000	30.000000	0.000000	0.000000	60.000000	0.000000	4.6124	-11.0211	29.6718	-13.0973	12.2288	-15.8110	2.8888	4.8599	-26.2583	26.1008	29.2369
5.000000	30.000000	0.000000	0.000000	60.000000	0.000000	-2.1027	-0.8457	2.0238	-0.7228	0.5661	-3.4255	0.2812	-2.1229	-1.2743	1.2946	2.0216
6.500000	30.000000	0.000000	0.000000	60.000000	0.000000	-0.5910	-0.1109	0.0279	-0.0229	0.0043	-0.4952	0.0053	-0.5914	-0.0121	0.0125	0.0280
3.750000	30.000000	0.000000	0.000000	60.000000	30.000000	7.4663	-18.4032	46.8273	-23.7379	21.7975	-22.3360	4.4858	8.6336	-49.3441	48.1768	45.6243
4.050000	30.000000	0.000000	0.000000	60.000000	30.000000	0.7499	-8.5654	21.9069	-10.1973	9.4209	-14.0574	2.4290	0.9366	-20.8875	20.7008	21.5898
5.000000	30.000000	0.000000	0.000000	60.000000	30.000000	-2.2423	-0.8137	1.8305	-0.7105	0.5478	-3.3860	0.2732	-2.2588	-1.2729	1.2894	1.8275
6.500000	30.000000	0.000000	0.000000	60.000000	30.000000	-0.6023	-0.1194	0.0283	-0.0245	0.0046	-0.4971	0.0055	-0.6026	-0.0128	0.0131	0.0284
4.400000	30.000000	0.000000	0.000000	90.000000	0.000000	12.5949	-16.3857	46.2439	-17.9294	15.8605	-18.1435	3.3971	13.0429	-30.6880	30.2400	45.0640
5.500000	30.000000	0.000000	0.000000	90.000000	0.000000	-1.9816	-1.0384	1.9391	-0.5348	0.4171	-2.9930	0.2244	-1.9856	-0.7799	0.7938	1.9838
7.000000	30.000000	0.000000	0.000000	90.000000	0.000000	-0.5330	-0.1372	0.0201	-0.0136	0.0025	-0.4071	0.0031	-0.5322	-0.0064	0.0056	0.0201
4.550000	30.000000	0.000000	0.000000	90.000000	30.000000	9.3300	-14.0796	39.3234	-16.5213	13.8666	-15.2182	2.7672	10.1382	-28.0876	27.2794	37.6516
5.000000	30.000000	0.000000	0.000000	90.000000	30.000000</											

4.900000	30.000000	0.000000	30.000000	150.000000	0.000000	-0.9709	0.1520	1.7354	-0.6461	0.5532	-3.0469	0.2437	-1.0087	-1.2062	1.2440	1.7309
6.000000	30.000000	0.000000	30.000000	150.000000	0.000000	-0.3066	0.3140	0.0652	-0.0339	0.0132	-0.6797	0.0118	-0.3093	-0.0325	0.0352	0.0653
4.000000	30.000000	0.000000	30.000000	150.000000	30.000000	8.3819	-8.7468	29.8362	-13.0269	12.0177	-14.1272	2.5602	8.5132	-25.1702	25.0390	29.1734
4.500000	30.000000	0.000000	30.000000	150.000000	30.000000	0.1168	-1.1763	6.6200	-2.4796	2.2857	-5.9765	0.7531	0.0264	-4.7236	4.8140	6.5812
5.000000	30.000000	0.000000	30.000000	150.000000	30.000000	-0.8601	0.2316	1.4583	-0.5118	0.4244	-2.6913	0.1992	-0.8896	-0.9152	0.9446	1.4559
6.000000	30.000000	0.000000	30.000000	150.000000	30.000000	-0.3056	0.3163	0.0704	-0.0347	0.0137	-0.6864	0.0123	-0.3084	-0.0333	0.0361	0.0705
3.400000	30.000000	0.000000	60.000000	30.000000	0.000000	8.8387	-18.8684	50.2614	-28.6857	26.1624	-22.9226	4.5144	10.4614	-60.5310	58.9082	48.3769
5.000000	30.000000	0.000000	60.000000	30.000000	0.000000	-1.1661	0.2047	0.5739	-0.2582	0.1599	-1.9577	0.0958	-1.1815	-0.3961	0.4116	0.5739
6.000000	30.000000	0.000000	60.000000	30.000000	0.000000	-0.3702	0.1795	0.0311	-0.0310	0.0056	-0.5639	0.0065	-0.3723	-0.0151	0.0171	0.0312
3.500000	30.000000	0.000000	60.000000	30.000000	30.000000	7.0392	-14.3738	39.6187	-21.1143	19.5590	-19.6376	3.7338	7.7858	-44.0083	43.2617	38.5144
5.000000	30.000000	0.000000	60.000000	30.000000	30.000000	-1.1698	0.2058	0.5720	-0.2510	0.1583	-1.9599	0.0956	-1.1852	-0.3926	0.4081	0.5719
6.000000	30.000000	0.000000	60.000000	30.000000	30.000000	-0.3709	0.1791	0.0309	-0.0310	0.0055	-0.5640	0.0065	-0.3730	-0.0149	0.0170	0.0311
4.200000	30.000000	0.000000	60.000000	60.000000	0.000000	7.6131	-11.7109	33.7883	-14.6776	13.0208	-15.0932	2.6986	8.0261	-26.8976	26.4846	32.7430
4.600000	30.000000	0.000000	60.000000	60.000000	0.000000	6.2148	-3.6846	11.0127	-4.6058	3.6279	-7.7937	1.1010	0.2125	-7.1923	7.2547	10.8890
5.100000	30.000000	0.000000	60.000000	60.000000	0.000000	-1.6016	-0.8578	2.5962	-0.8521	0.6937	-3.5232	0.3142	-1.6291	-1.4178	1.4453	2.5892
6.500000	30.000000	0.000000	60.000000	60.000000	0.000000	-0.5581	-0.0522	0.0395	-0.0250	0.0059	-0.5334	0.0067	-0.5584	-0.0156	0.0159	0.0395
4.150000	30.000000	0.000000	60.000000	60.000000	30.000000	7.1227	-12.1054	34.0595	-14.8254	13.2981	-15.8793	2.9256	7.4730	-27.9092	27.5589	33.2234
5.000000	30.000000	0.000000	60.000000	60.000000	30.000000	-1.7596	-1.1799	3.2825	-1.1306	0.9316	-4.0937	0.4052	-1.7849	-1.9404	1.9657	3.2724
6.500000	30.000000	0.000000	60.000000	60.000000	30.000000	-0.5824	-0.0724	0.0434	-0.0274	0.0065	-0.5401	0.0074	-0.5826	-0.0169	0.0170	0.0434
4.500000	30.000000	0.000000	60.000000	90.000000	0.000000	13.0966	-15.0287	46.3624	-18.7520	15.3236	-16.8600	2.9519	13.9973	-29.8357	28.9350	44.4353
6.000000	30.000000	0.000000	60.000000	90.000000	0.000000	-1.3376	-0.3691	0.4844	-0.1383	0.0831	-1.4576	0.0602	-1.3373	-0.1621	0.1617	0.4846
7.000000	30.000000	0.000000	60.000000	90.000000	0.000000	-0.5167	-0.1212	0.0212	-0.0142	0.0025	-0.4076	0.0032	-0.5160	-0.0064	0.0057	0.0212
4.500000	30.000000	0.000000	60.000000	90.000000	30.000000	11.6446	-15.7903	45.4515	-19.0474	15.8110	-16.7755	3.0901	12.7394	-32.3198	31.2249	43.4159
4.800000	30.000000	0.000000	60.000000	90.000000	30.000000	3.4076	-7.4846	20.7127	-7.5375	6.4293	-10.2884	1.6846	3.5691	-12.9927	12.1082	20.2462
5.500000	30.000000	0.000000	60.000000	90.000000	30.000000	-1.6709	-1.4055	2.9579	-0.8475	0.6562	-3.3399	0.3167	-1.6620	-1.2202	1.2113	2.9474
7.000000	30.000000	0.000000	60.000000	90.000000	30.000000	-0.5694	-0.1627	0.0342	-0.0188	0.0040	-0.4299	0.0049	-0.5682	-0.0096	0.0085	0.0343
4.400000	30.000000	0.000000	60.000000	120.000000	0.000000	8.6962	-10.3788	32.4066	-12.6195	11.2393	-14.4580	2.5666	8.7564	-21.9768	21.9167	31.5538
5.000000	30.000000	0.000000	60.000000	120.000000	0.000000	-0.7924	-1.4957	5.4551	-1.7270	1.1514	-5.1956	0.5889	-0.8589	-2.8682	2.9346	5.4271
5.500000	30.000000	0.000000	60.000000	120.000000	0.000000	-1.2838	-0.2107	1.1966	-0.3613	0.2753	-2.3499	0.1516	-1.2984	-0.5484	0.5631	1.1953
6.500000	30.000000	0.000000	60.000000	120.000000	0.000000	-0.5011	0.0548	0.0554	-0.0267	0.0086	-0.6022	0.0088	-0.5015	-0.0206	0.0209	0.0554
4.500000	30.000000	0.000000	60.000000	120.000000	30.000000	9.4311	-10.8058	34.3138	-14.1067	11.8301	-13.6627	2.3859	9.9545	-23.4005	22.8771	33.1138
5.500000	30.000000	0.000000	60.000000	120.000000	30.000000	-1.1464	-0.4510	1.7905	-0.5142	0.3940	-2.5771	0.2028	-1.1551	-0.7536	0.7623	1.7869
6.500000	30.000000	0.000000	60.000000	120.000000	30.000000	-0.5319	0.0276	0.0839	-0.0329	0.0118	-0.6344	0.0120	-0.5319	-0.0269	0.0268	0.0840
3.950000	30.000000	0.000000	60.000000	150.000000	0.000000	5.6040	-7.6843	25.1249	-11.5246	10.7435	-13.3754	2.3617	5.6457	-22.9244	22.8827	24.6173
4.900000	30.000000	0.000000	60.000000	150.000000	0.000000	-1.0482	0.1481	1.5107	-0.5702	0.4672	-2.8504	0.2142	-1.0803	-1.0325	1.0646	1.5078
6.000000	30.000000	0.000000	60.000000	150.000000	0.000000	-0.3268	0.2755	0.0562	-0.0335	0.0110	-0.6489	0.0104	-0.3293	-0.0279	0.0304	0.0563
4.000000	30.000000	0.000000	60.000000	150.000000	30.000000	4.3638	-6.6869	21.8505	-10.0152	9.3778	-12.2670	2.1124	4.3716	-20.0173	20.0095	21.4261
5.000000	30.000000	0.000000	60.000000	150.000000	30.000000	-0.9863	0.2118	1.1727	-0.4358	0.3454	-2.4734	0.1681	-1.0112	-0.7688	0.7937	1.1709
6.000000	30.000000	0.000000	60.000000	150.000000	30.000000	-0.3282	0.2742	0.0591	-0.0338	0.0113	-0.6521	0.0107	-0.3307	-0.0284	0.0309	0.0592
3.750000	30.000000	0.000000	90.000000	30.000000	0.000000	7.0657	-10.9807	32.8238	-16.2696	15.0003	-16.0561	2.9458	7.4634	-32.8474	32.4492	31.9227
4.000000	30.000000	0.000000	90.000000	30.000000	0.000000	1.9693	-4.8183	16.0878	-7.2734	6.7874	-10.5501	1.6765	1.9097	-14.5888	14.5684	15.8646
5.500000	30.000000	0.000000	90.000000	30.000000	0.000000	-0.6508	0.2813	0.1972	-0.0935	0.0453	-1.1213	0.0338	-0.6572	-0.1136	0.1199	0.1974
6.000000	30.000000	0.000000	90.000000	30.000000	0.000000	-0.3507	0.2259	0.0444	-0.0324	0.0082	-0.6075	0.0085	-0.3529	-0.0217	0.0239	0.0445
3.750000	30.000000	0.000000	90.000000	30.000000	30.000000	5.5190	-10.0668	29.5996	-15.0596	14.0587	-15.6278	2.8597	5.7638	-31.0538	30.8090	28.8728
4.700000	30.000000	0.000000	90.000000	30.000000	30.000000	-1.3296	-0.0752	1.9690	-0.7991	0.6600	-3.4073	0.2830	-1.3697	-1.4864	1.5265	1.9632
6.000000	30.000000	0.000000	90.000000	30.000000	30.000000	-0.3521	0.2238	0.0437	-0.0324	0.0082	-0.6061	0.0085	-0.3544	-0.0216	0.0238	0.0438
4.400000	30.000000	0.000000	60.000000	60.000000	0.000000	8.3510	-9.7143	31.0023	-12.0311	10.3719	-13.3848	2.2934	8.5373	-19.9958	19.8095	30.1353
5.600000	30.000000	0.000000	90.000000	60.000000	0.000000	-1.2273	-0.1761	0.7996	-0.2485	0.1701	-1.8837	0.1029	-1.2357	-0.3505	0.3590	0.7992
7.000000	30.000000	0.000000	90.000000	60.000000	0.000000	-0.3182	0.0040	0.0105	-0.0111	0.0014	-0.3249	0.0019	-0.3182	-0.0040	0.0040	0.0105
4.400000	30.000000	0.000000	90.000000	60.000000	30.000000	5.9106	-9.3977	27.6164	-11.3736	9.9771	-12.9547	2.2593	6.1268	-20.1398	19.9236	26.8797
5.500000	30.000000	0.000000	90.000000	60.000000	30.000000	-1.3652	-0.3853	1.2023	-0.3751	0.2716	-2.2365	0.1509	-1.3721	-0.5560	0.5629	1.2011
6.500000	30.000000	0.000000	90.000000	60.000000	30.000000	-0.5607	-0.0258	0.0615	-0.0301	0.0089	-0.5846	0.0095	-0.5607	-0.0216	0.0216	0.0615
4.600000	30.000000	0.000000	90.000000	90.000000	0.000000	8.6557	-11.1510	33.5481	-12.7378	10.8384	-13.9841	2.4030	8.9165	-20.5773	20.3165	32.4387
5.000000	30.000000	0.000000	90.000000	90.000000	0.000000	0.2251	-3.5934	10.2920	-3.2272	2.7904	-7.0259	0.9374	0.1734	-4.7970	5.0307	10.1763
5.500000	30.000000	0.000000	90.000000	90.000000	0.000000	-1.6826	-0.9771	2.2580	-0.6210	0.4878	-3.0911	0.2488	-1.6946	-0.8846	0.8966	2.2528
6.500000	30.000000	0.000000	90.000000	90.000000	0.000000	-0.8335	-0.1831	0.1017	-0.0383	0.0141	-0.7409	0.0141	-0.8325	-0.0310	0.0300	0.1017
4.600000	30.000000	0.000000	90.000000	90.000000	30.000000	8.1249	-12.2155	34.7790	-13.9057	11.6943	-14.1782	2.5261	8.7000	-23.2624	22.6873	33.5071
5.500000	30.000000	0.000000	90.000000	90.000000	30.000000	-1.6679	-1.3976	2.9460	-0.8424	0.6509	-3.3316	0.3156	-1.6590	-1.2116	1.2027	2.9354
7.000000	30.000000	0.000000	90.													

6.500000	30.000000	30.000000	30.000000	120.000000	0.000000	-0.4782	0.0980	0.0662	-0.0275	0.0100	-0.6352	0.0100	-0.4786	-0.0229	0.0232	0.0663
4.600000	30.000000	30.000000	30.000000	120.000000	30.000000	9.6286	-10.2247	33.1005	-13.1958	11.0705	-12.9548	2.2555	10.0513	-21.4903	21.0677	31.8931
4.900000	30.000000	30.000000	30.000000	120.000000	30.000000	2.5761	-4.0622	13.8133	-4.7000	4.0482	-7.6857	1.1488	2.5624	-7.4179	7.4316	13.5816
5.600000	30.000000	30.000000	30.000000	120.000000	30.000000	-0.9727	-0.3278	1.6793	-0.4593	0.3549	-2.4149	0.1854	-0.9825	-0.6580	0.6677	1.6756
6.500000	30.000000	30.000000	30.000000	120.000000	30.000000	-0.5041	0.0713	0.1037	-0.0351	0.0144	-0.6727	0.0142	-0.5042	-0.0310	0.0311	0.1038
4.000000	30.000000	30.000000	30.000000	150.000000	30.000000	6.2949	-8.2863	26.7362	-12.5088	11.6322	-13.6099	2.4443	6.4077	-24.9639	24.8541	26.0541
5.000000	30.000000	30.000000	30.000000	150.000000	30.000000	-0.8741	0.2160	1.4406	-0.5157	0.4307	-2.6745	0.1989	-0.9041	-0.9313	0.9613	1.4376
6.000000	30.000000	30.000000	30.000000	150.000000	30.000000	-0.3065	0.3136	0.0722	-0.0350	0.0141	-0.6866	0.0125	-0.3093	-0.0340	0.0369	0.0722
3.500000	30.000000	30.000000	60.000000	30.000000	30.000000	5.9994	-13.4718	36.9032	-19.8446	18.5396	-19.2157	3.6401	6.5509	-41.7965	41.2450	35.9404
4.700000	30.000000	30.000000	60.000000	30.000000	30.000000	-1.5375	0.0316	1.3104	-0.5638	0.4187	-2.9699	0.2040	-1.5670	-0.9946	1.0241	1.3080
5.500000	30.000000	30.000000	60.000000	30.000000	30.000000	-0.6739	0.2298	0.1321	-0.0791	0.0291	-1.0163	0.0269	-0.6794	-0.0779	0.0834	0.1324
4.250000	30.000000	30.000000	60.000000	60.000000	0.000000	5.6131	-9.6491	28.0062	-11.8665	10.6257	-13.7328	2.3969	5.7803	-21.7665	21.5993	27.3256
4.550000	30.000000	30.000000	60.000000	60.000000	0.000000	0.3621	-4.0380	11.9251	-4.5129	4.0574	-8.3439	1.2097	0.2974	-8.1379	8.2026	11.7916
5.000000	30.000000	30.000000	60.000000	60.000000	0.000000	-1.6545	-1.0946	3.3259	-1.1081	0.9262	-4.0613	0.3950	-1.6888	-1.9013	1.9356	3.2439
6.500000	30.000000	30.000000	60.000000	60.000000	0.000000	-0.5602	-0.0546	0.0382	-0.0248	0.0059	-0.5318	0.0066	-0.5605	-0.0155	0.0158	0.0383
4.100000	30.000000	30.000000	60.000000	60.000000	30.000000	7.6806	-13.5794	37.3699	-16.9850	15.1658	-16.9460	3.1699	8.1953	-32.3104	31.7957	36.2891
5.000000	30.000000	30.000000	60.000000	60.000000	30.000000	-1.7875	-1.1956	3.2552	-1.1313	0.9321	-4.0744	0.4032	-1.8109	-1.9489	1.9722	3.2453
6.000000	30.000000	30.000000	60.000000	60.000000	30.000000	-0.9546	-0.1347	0.1874	-0.0778	0.0345	-0.9942	0.0291	-0.9557	-0.0828	0.0839	0.1876
4.600000	30.000000	30.000000	60.000000	90.000000	0.000000	9.1101	-11.5502	34.8930	-13.2344	11.1389	-14.1696	2.4194	9.4970	-21.0439	20.6569	33.7501
5.600000	30.000000	30.000000	60.000000	90.000000	0.000000	-1.6618	-0.8234	1.7522	-0.4701	0.3550	-2.6753	0.1936	-1.6679	-0.6438	0.6498	1.7495
6.500000	30.000000	30.000000	60.000000	90.000000	0.000000	-0.8421	-0.1910	0.1069	-0.0391	0.0146	-0.7468	0.0145	-0.8410	-0.0317	0.0306	0.1070
4.550000	30.000000	30.000000	60.000000	90.000000	30.000000	9.8283	-13.9971	40.1465	-16.7048	13.9247	-15.4774	2.8046	10.6964	-28.1677	27.2996	38.4972
5.050000	30.000000	30.000000	60.000000	90.000000	30.000000	0.0754	-4.0395	10.6087	-3.5084	2.9589	-6.8688	0.9657	0.1166	-5.5103	5.4690	10.4714
5.700000	30.000000	30.000000	60.000000	90.000000	30.000000	-1.6640	-1.9381	1.6880	-0.4730	0.3420	-2.4653	0.1895	-1.6567	-1.9430	1.6376	1.6847
7.000000	30.000000	30.000000	60.000000	90.000000	30.000000	-0.5699	-0.1627	0.0349	-0.0189	0.0040	-0.4310	0.0050	-0.5687	-0.0097	0.0086	0.0349
4.600000	30.000000	30.000000	60.000000	120.000000	0.000000	6.2720	-6.8402	23.4731	-8.1659	7.0792	-11.0755	1.7942	6.2649	-12.9458	12.9529	22.9926
5.800000	30.000000	30.000000	60.000000	120.000000	0.000000	-0.9977	-0.0250	0.5668	-0.1657	0.1082	-1.5593	0.0720	-1.0030	-0.2181	0.2234	0.5670
6.500000	30.000000	30.000000	60.000000	120.000000	0.000000	0.4984	0.0593	0.0630	-0.0278	0.0092	-0.6118	0.0095	-0.4987	-0.0215	0.0218	0.0630
4.500000	30.000000	30.000000	60.000000	120.000000	30.000000	8.3197	-10.1687	31.4862	-12.6715	10.9261	-13.3306	2.3643	8.6058	-21.6540	21.3679	30.4946
5.000000	30.000000	30.000000	60.000000	120.000000	30.000000	-0.0660	-2.2227	7.3928	-2.4074	2.0846	-5.6851	0.7303	-0.1075	-3.9233	3.9647	7.3279
5.500000	30.000000	30.000000	60.000000	120.000000	30.000000	-1.1859	-0.4191	1.6818	-0.4909	0.3800	-2.5454	0.1966	-1.1971	-0.7354	0.7466	1.6783
3.900000	30.000000	30.000000	60.000000	150.000000	30.000000	6.7000	-9.2237	28.9210	-13.7342	12.8251	-14.6034	2.6749	6.8598	-27.7001	27.5404	28.2660
5.000000	30.000000	30.000000	60.000000	150.000000	30.000000	-0.9995	0.2182	1.1504	-0.4335	0.3436	-2.4711	0.1676	-1.0247	-0.7682	0.7935	1.1484
6.000000	30.000000	30.000000	60.000000	150.000000	30.000000	-0.3287	0.2738	0.0591	-0.0339	0.0113	-0.6523	0.0107	-0.3312	-0.0286	0.0312	0.0592
3.850000	30.000000	30.000000	90.000000	30.000000	30.000000	3.8863	-7.6236	23.2748	-11.2154	10.5328	-13.3593	2.3320	3.9412	-22.8888	22.8339	22.8409
5.000000	30.000000	30.000000	90.000000	30.000000	30.000000	-1.1042	0.2023	0.8512	-0.3417	0.2457	-2.2123	0.1308	-1.1240	-0.5799	0.5936	0.8501
6.000000	30.000000	30.000000	90.000000	30.000000	30.000000	-0.3537	0.2230	0.0449	-0.0326	0.0082	-0.6081	0.0086	-0.3559	-0.0217	0.0239	0.0449
4.400000	30.000000	30.000000	90.000000	60.000000	0.000000	5.8649	-8.6699	26.1780	-10.4633	9.3951	-12.7038	2.1812	5.9173	-18.6585	18.6062	25.5214
5.500000	30.000000	30.000000	90.000000	60.000000	0.000000	-1.3247	-0.2600	1.0382	-0.3233	0.2369	-2.1621	0.1335	-1.3367	-0.4780	0.4991	1.0373
6.500000	30.000000	30.000000	90.000000	60.000000	0.000000	-0.5297	0.0011	0.0497	-0.0263	0.0074	-0.5700	0.0080	-0.5301	-0.0186	0.0189	0.0497
4.400000	30.000000	30.000000	90.000000	60.000000	30.000000	6.6632	-9.5679	28.7834	-11.6744	10.2281	-13.2116	2.3225	6.8800	-20.5405	20.3237	28.0696
5.500000	30.000000	30.000000	90.000000	60.000000	30.000000	-1.3649	-0.3801	1.2067	-0.3742	0.2716	-2.2484	0.1521	-1.3724	-0.5572	0.5646	1.2056
6.500000	30.000000	30.000000	90.000000	60.000000	30.000000	-0.5612	-0.0248	0.0612	-0.0300	0.0089	-0.5859	0.0095	-0.5611	-0.0217	0.0217	0.0613
4.600000	30.000000	30.000000	90.000000	90.000000	0.000000	12.3222	-13.1766	42.3046	-16.5906	13.2256	-15.1339	2.5370	13.1660	-25.0191	24.1752	40.5133
5.050000	30.000000	30.000000	90.000000	90.000000	0.000000	0.8124	-3.6004	10.9214	-3.3529	2.7885	-6.8660	0.9096	0.8002	-4.8077	4.8200	10.9778
5.600000	30.000000	30.000000	90.000000	90.000000	0.000000	-1.5160	-0.8294	1.9829	-0.5244	0.3922	-2.7518	0.2082	-1.5223	-0.6921	0.6983	1.7883
6.500000	30.000000	30.000000	90.000000	90.000000	0.000000	-0.8285	-0.1783	0.1154	-0.0409	0.0153	-0.7541	0.0152	-0.8275	-0.0325	0.0315	0.1155
4.600000	30.000000	30.000000	90.000000	90.000000	30.000000	8.8137	-12.3486	36.0227	-14.3645	12.0345	-14.4833	2.5886	9.4494	-23.8973	23.2617	34.7426
5.500000	30.000000	30.000000	90.000000	90.000000	30.000000	-1.6319	-1.3868	0.3012	-0.8644	0.6671	-3.3714	0.3207	-1.6226	-1.2396	1.2304	3.0006
6.500000	30.000000	30.000000	90.000000	90.000000	30.000000	-0.9186	-0.2640	0.1577	-0.0544	0.0215	-0.7977	0.0208	-0.9160	-0.0457	0.0431	0.1580
5.450000	58.926699	353.807950	260.921001	98.533032	47.987449	-0.7004	-2.8958	8.0204	-2.1129	1.8190	-6.3671	0.7699	-0.7665	-3.1363	3.2025	7.9822
5.872856	58.926699	353.807950	260.921007	98.533032	47.987449	-1.7336	-0.9960	2.3372	-0.5626	0.4474	-3.2370	0.2567	-1.7542	-0.7733	0.7939	2.3355
7.050000	58.926699	353.807950	260.921007	98.533032	47.987449	-0.6686	-0.1116	0.0659	-0.0216	0.0081	-0.6190	0.0091	-0.6690	-0.0159	0.0164	0.0660
6.550000	58.926700	353.808000	260.921000	98.533000	47.987400	-1.1165	-0.2408	0.3058	-0.0769	0.0453	-1.1911	0.0389	-1.1188	-0.0825	0.0849	0.3062
4.500000	60.000000	0.000000	0.000000	60.000000	0.000000	8.7223	-15.1535	38.8983	-17.8201	16.5804	-16.7199	3.2859	9.0711	-34.8704	34.5217	37.8701
5.500000	60.000000	0.000000	0.000000	60.000000	0.000000	-1.9191	-1.4271	2.7883	-0.8699	0.7776	-3.5650	0.3373	-1.9588	-1.5726	1.5524	2.7819
7.000000	60.000000	0.000000	0.000000	60.000000	0.000000	-0.6278	-0.1776	0.0357	-0.0144	0.0057	-0.4831	0.0057	-0.6280	-0.0126	0.0128	0.0357
4.500000	60.000000	0.000000	0.000000	60.000000	30.000000	7.9556	-14.7763	37.6182	-17.6908	16.4180	-16.4177	3.2188	8.3701	-34.9651	34.5506	36.52

6.500000	60.000000	0.000000	60.000000	90.000000	30.000000	-1.1226	-0.3794	0.8377	-0.1844	0.1269	-1.6192	0.0911	-1.1274	-0.2109	0.2157	0.8377
7.300000	60.000000	0.000000	60.000000	90.000000	30.000000	-0.5364	-0.0661	0.0679	-0.0185	0.0070	-0.5357	0.0086	-0.5368	-0.0128	0.0132	0.0680
5.000000	60.000000	0.000000	60.000000	120.000000	0.000000	5.8441	-6.9461	23.3462	-7.1019	6.1989	-11.6748	1.8641	5.6865	-10.9312	11.0888	22.9476
6.000000	60.000000	0.000000	60.000000	120.000000	0.000000	-1.1764	-0.1491	1.1324	-0.2744	0.2073	-2.2412	0.1330	-1.1921	-0.3684	0.3841	1.1324
7.000000	60.000000	0.000000	60.000000	120.000000	0.000000	-0.4486	0.0707	0.0479	-0.0676	0.0063	-0.5639	0.0071	-0.4495	-0.0130	0.0139	0.0480
5.400000	60.000000	0.000000	60.000000	120.000000	30.000000	5.8591	-3.7501	17.3898	-4.8693	3.7492	-7.8091	1.1229	5.8333	-5.5967	5.6226	17.0818
5.850000	60.000000	0.000000	60.000000	120.000000	30.000000	0.0600	-0.6811	4.1130	-0.9637	0.7283	-3.5129	0.3472	0.0308	-1.0867	1.1159	4.0977
6.400000	60.000000	0.000000	60.000000	120.000000	30.000000	-0.7110	0.0241	0.6780	-0.1487	0.0960	-1.4370	0.0705	-0.7171	-0.1546	0.1607	0.6786
7.200000	60.000000	0.000000	60.000000	120.000000	30.000000	-0.3561	0.0782	0.0485	-0.0153	0.0051	-0.4795	0.0062	-0.3568	-0.0095	0.0102	0.0486
5.100000	60.000000	0.000000	90.000000	60.000000	0.000000	7.6391	-5.3150	22.8258	-6.9277	5.4737	-10.0120	1.5038	7.5486	-8.6175	8.7080	22.3783
6.000000	60.000000	0.000000	90.000000	60.000000	0.000000	-1.0864	-0.2461	1.2663	-0.3133	0.2233	-2.1667	0.1354	-1.1011	-0.3779	0.3926	1.2665
7.000000	60.000000	0.000000	90.000000	60.000000	0.000000	-0.5017	-0.0054	0.0491	-0.0194	0.0064	-0.5401	0.0070	-0.5023	-0.0130	0.0137	0.0493
5.050000	60.000000	0.000000	90.000000	60.000000	30.000000	9.2673	-8.8290	29.4126	-9.6979	8.0240	-11.4459	1.9082	9.3721	-14.0318	13.9270	28.5207
5.350000	60.000000	0.000000	90.000000	60.000000	30.000000	2.4574	-3.6238	12.4666	-3.5559	2.9814	-6.8483	0.9693	2.3892	-4.9242	4.9924	12.2978
6.000000	60.000000	0.000000	90.000000	60.000000	30.000000	-0.9828	-0.4792	1.7487	-0.4124	0.3129	-2.3455	0.1770	-0.9985	-0.5224	0.5381	1.7469
6.900000	60.000000	0.000000	90.000000	60.000000	30.000000	-0.5771	-0.0302	0.1025	-0.0289	0.0127	-0.6471	0.0130	-0.5781	-0.0243	0.0252	0.1027
5.150000	60.000000	0.000000	90.000000	90.000000	0.000000	7.7243	-8.7558	28.0000	-8.2242	6.9291	-12.3983	2.0103	7.5610	-11.5804	11.7437	27.3917
5.370000	60.000000	0.000000	90.000000	90.000000	0.000000	2.3969	-4.5989	14.7633	-3.9236	3.3167	-8.5050	1.1936	2.2460	-5.3202	5.4770	14.5999
6.000000	60.000000	0.000000	90.000000	90.000000	0.000000	-1.4075	-0.8893	2.4620	-0.4792	0.3669	-2.9799	0.2223	-1.4335	-0.5805	0.6064	2.4599
7.000000	60.000000	0.000000	90.000000	90.000000	0.000000	-0.6335	-0.0694	0.0884	-0.0258	0.0103	-0.6997	0.0115	-0.6847	-0.0185	0.0196	0.0885
5.400000	60.000000	0.000000	90.000000	90.000000	30.000000	5.2018	-7.3500	21.9669	-7.1051	5.8562	-9.6951	1.5851	5.2580	-10.3744	10.3181	21.4371
6.000000	60.000000	0.000000	90.000000	90.000000	30.000000	-0.9545	-1.4504	3.8445	-0.9399	0.7469	-3.5414	0.3639	-0.9764	-1.2309	1.2528	3.8283
7.400000	60.000000	0.000000	90.000000	90.000000	30.000000	-0.4929	-0.0686	0.0496	-0.0145	0.0048	-0.4709	0.0064	-0.4932	-0.0091	0.0094	0.0496
4.000000	60.000000	30.000000	0.000000	60.000000	30.000000	16.6201	-46.5294	115.7606	-71.9982	58.9666	-34.0236	7.1491	29.3250	-151.2051	138.5001	106.4102
4.750000	60.000000	30.000000	0.000000	60.000000	30.000000	2.8992	-8.5996	21.5360	-9.4235	8.7605	-11.2851	1.9844	2.9727	-18.1182	18.0448	21.0565
5.500000	60.000000	30.000000	0.000000	60.000000	30.000000	-1.7059	-1.6455	3.3110	-1.0667	0.9506	-3.6738	0.3842	-1.7402	-1.8462	1.8805	3.2988
7.000000	60.000000	30.000000	0.000000	60.000000	30.000000	-0.6569	-0.2063	0.0514	-0.0185	0.0076	-0.4989	0.0076	-0.6570	-0.0160	0.0161	0.0515
5.100000	60.000000	30.000000	0.000000	90.000000	0.000000	8.8961	-11.1477	33.1693	-10.7801	9.3702	-14.2051	2.4699	8.8766	-16.8740	16.8935	32.3576
6.000000	60.000000	30.000000	0.000000	90.000000	0.000000	-1.4087	-0.8893	2.4847	-0.5726	0.4698	-3.1883	0.2603	-1.4354	-0.7685	0.7952	2.4801
7.000000	60.000000	30.000000	0.000000	90.000000	0.000000	-0.6753	-0.0454	0.1141	-0.0280	0.0142	-0.7459	0.0146	-0.6764	-0.0250	0.0261	0.1141
5.500000	60.000000	30.000000	0.000000	90.000000	30.000000	8.8406	-8.6192	27.9262	-8.7931	6.8716	-9.9301	1.6264	9.0818	-11.4549	11.2137	27.0105
6.500000	60.000000	30.000000	0.000000	90.000000	30.000000	-0.8096	-0.4878	1.5014	-0.3062	0.2154	-1.8742	0.1368	-0.8147	-0.3159	0.3210	1.5000
7.250000	60.000000	30.000000	0.000000	90.000000	30.000000	-0.5332	-0.0452	0.1403	-0.0296	0.0138	-0.6283	0.0152	-0.5337	-0.0217	0.0222	0.1404
6.050000	60.000000	30.000000	0.000000	120.000000	30.000000	1.3241	-0.3213	4.9999	-1.1337	0.7973	-3.3977	0.3579	1.3025	-1.0238	1.0454	4.9728
6.700000	60.000000	30.000000	0.000000	120.000000	30.000000	-0.3281	0.2424	0.5627	-0.1113	0.0657	-1.1448	0.0529	-0.3324	-0.0916	0.0959	0.5630
7.700000	60.000000	30.000000	0.000000	120.000000	30.000000	-0.1421	0.1436	0.0192	-0.0067	0.0016	-0.3025	0.0023	-0.1425	-0.0026	0.0030	0.0192
4.600000	60.000000	30.000000	30.000000	60.000000	30.000000	7.6774	-13.8301	36.0021	-16.4185	14.8636	-15.2590	2.9045	8.2625	-31.4204	30.8353	34.8414
4.900000	60.000000	30.000000	30.000000	60.000000	30.000000	2.0106	-6.7935	17.3577	-6.8936	6.3570	-9.6390	1.6088	1.9973	-12.7231	12.7364	17.0481
6.000000	60.000000	30.000000	30.000000	60.000000	30.000000	-1.5013	-0.6663	0.9583	-0.2711	0.2128	-1.8633	0.1198	-1.5099	-0.4106	0.4192	0.9583
7.000000	60.000000	30.000000	30.000000	60.000000	30.000000	-0.6462	-0.1888	0.0552	-0.0192	0.0079	-0.5095	0.0080	-0.6464	-0.0167	0.0168	0.0553
5.300000	60.000000	30.000000	30.000000	90.000000	0.000000	6.2839	-7.5305	23.8903	-7.0237	5.9169	-10.7705	1.7104	6.1929	-9.7844	9.8754	23.3736
5.500000	60.000000	30.000000	30.000000	90.000000	30.000000	8.7515	-8.5699	27.7530	-8.7570	6.8471	-9.9202	1.6266	8.9796	-11.4178	11.1897	26.8472
6.500000	60.000000	30.000000	30.000000	90.000000	30.000000	-0.8203	-0.4907	1.4902	-0.3055	0.2139	-1.8698	0.1362	-0.8257	-0.3145	0.3199	1.4888
7.200000	60.000000	30.000000	30.000000	90.000000	30.000000	-0.5664	-0.0604	0.1636	-0.0343	0.0164	-0.6700	0.0176	-0.5670	-0.0257	0.0263	0.1636
5.500000	60.000000	30.000000	30.000000	120.000000	30.000000	9.2273	-4.2849	22.1935	-6.3300	4.7348	-8.2926	1.2406	9.2615	-6.7618	6.7276	21.6320
6.500000	60.000000	30.000000	30.000000	120.000000	30.000000	-0.4003	0.1363	0.9098	-0.1825	0.1197	-1.4758	0.0848	-0.4076	-0.1720	0.1793	0.9098
7.300000	60.000000	30.000000	30.000000	120.000000	30.000000	-0.2596	0.1536	0.0643	-0.0161	0.0060	-0.4756	0.0074	-0.2604	-0.0098	0.0107	0.0644
4.850000	60.000000	30.000000	60.000000	60.000000	30.000000	6.6264	-10.4012	28.7262	-11.2067	9.9871	-12.5714	2.2793	6.8134	-19.7623	19.5753	28.0045
5.300000	60.000000	30.000000	60.000000	60.000000	30.000000	-0.0839	-3.3002	8.7060	-2.7939	2.4961	-6.0990	0.8474	-0.1436	-4.6664	4.7262	8.6290
6.000000	60.000000	30.000000	60.000000	60.000000	30.000000	-1.3867	-0.6455	1.2440	-0.3285	0.2590	-2.0736	0.1466	-1.3981	-0.4838	0.4952	1.2430
7.000000	60.000000	30.000000	60.000000	60.000000	30.000000	-0.6112	-0.1347	0.0666	-0.0211	0.0088	-0.5406	0.0093	-0.6116	-0.0184	0.0187	0.0667
5.500000	60.000000	30.000000	60.000000	90.000000	0.000000	8.0986	-5.2600	22.7019	-6.3873	4.7425	-9.0039	1.3105	8.1037	-6.6670	6.6619	22.1761
5.800000	60.000000	30.000000	60.000000	90.000000	0.000000	1.7407	-2.0337	8.9212	-2.1827	1.6276	-5.2672	0.6299	1.6951	-2.2004	2.2461	8.8396
6.500000	60.000000	30.000000	60.000000	90.000000	0.000000	-0.8760	-0.1848	0.9164	-0.1913	0.1209	-1.6314	0.0872	-0.8831	-0.1717	0.1788	0.9169
7.500000	60.000000	30.000000	60.000000	90.000000	0.000000	-0.3892	-0.0045	0.0325	-0.0115	0.0029	-0.4130	0.0040	-0.3896	-0.0050	0.0054	0.0325
5.500000	60.000000	30.000000	60.000000	90.000000	30.000000	8.6364	-8.4264	27.4745	-8.7025	6.8116	-9.9570	1.6362	8.8365	-11.3756	11.1756	26.9100
6.500000	60.000000	30.000000	60.000000	90.000000	30.000000	-0.8355	-0.4860	1.4687	-0.3046	0.2110	-1.8660	0.1352	-0.8417	-0.3114	0.3176	1.4674
7.400000	60.000000	30.000000	60.000000	90.000000	30.000000	-0.4733	-0.0423	0.0845	-0.0203	0.0077	-0.5129	0.0095	-0.4738	-0.0125	0.0130	0.0846
5.350000	60.000000	30.000000	60.000000	120.000000	30.000000	5.5866	-5.1304	18.6268	-5.5348	4.6813	-8.4792</					

6.700000	90.000000	0.000000	270.000000	90.000000	60.000000	-1.2047	-0.2333	0.3947	-0.0691	0.0388	-1.3865	0.0454	-1.2101	-0.0578	0.0632	0.3949
7.400000	90.000000	0.000000	270.000000	90.000000	60.000000	-0.5492	-0.0417	0.0404	-0.0112	0.0027	-0.5459	0.0053	-0.5504	-0.0040	0.0052	0.0404
6.400000	90.000000	30.000000	0.000000	90.000000	30.000000	4.8248	-0.8276	10.9611	-2.8151	1.7333	-4.7914	0.5884	4.8487	-1.8788	1.8548	10.8231
7.500000	90.000000	30.000000	0.000000	90.000000	30.000000	-0.2613	0.2090	0.2600	-0.0537	0.0213	-0.7235	0.0233	-0.2636	-0.0243	0.0266	0.2603
8.300000	90.000000	30.000000	0.000000	90.000000	30.000000	-0.1258	0.1161	0.0160	-0.0066	0.0009	-0.2545	0.0017	-0.1263	-0.0010	0.0015	0.0161
6.400000	90.000000	30.000000	30.000000	90.000000	30.000000	4.7517	-0.9067	10.9559	-2.8203	1.7357	-4.7787	0.5886	4.7746	-1.8806	1.8577	10.8177
6.900000	90.000000	30.000000	30.000000	90.000000	30.000000	0.1830	0.0904	2.0278	-0.4223	0.2356	-1.9048	0.1490	0.1758	-0.2528	0.2600	2.0247
7.500000	90.000000	30.000000	30.000000	90.000000	30.000000	-0.2878	0.1799	0.2599	-0.0540	0.0214	-0.7206	0.0233	-0.2901	-0.0244	0.0267	0.2602
8.100000	90.000000	30.000000	30.000000	90.000000	30.000000	-0.1748	0.1181	0.0323	-0.0104	0.0020	-0.3208	0.0033	-0.1755	-0.0023	0.0030	0.0324
6.350000	90.000000	30.000000	60.000000	90.000000	30.000000	5.7332	-1.2580	12.9229	-3.4370	2.1148	-5.2373	0.6655	5.7709	-2.3049	2.2672	12.7278
7.500000	90.000000	30.000000	60.000000	90.000000	30.000000	-0.3365	0.1263	0.2598	-0.0546	0.0216	-0.7152	0.0233	-0.3389	-0.0244	0.0268	0.2601
8.150000	90.000000	30.000000	60.000000	90.000000	30.000000	-0.1965	0.0799	0.0271	-0.0095	0.0017	-0.2992	0.0028	-0.1972	-0.0019	0.0025	0.0272
6.300000	90.000000	30.000000	90.000000	90.000000	30.000000	6.9883	-1.5570	15.2261	-4.1805	2.5673	-5.7549	0.7484	7.0494	-2.8197	2.7585	14.9550
6.700000	90.000000	30.000000	90.000000	90.000000	30.000000	9.9377	-0.2643	3.9999	-0.8977	0.5299	-2.7046	0.2660	0.9288	-0.5641	0.5730	3.9836
7.500000	90.000000	30.000000	90.000000	90.000000	30.000000	-0.3590	0.1015	0.2597	-0.0549	0.0216	-0.7127	0.0233	-0.3614	-0.0245	0.0268	0.2600
8.500000	90.000000	30.000000	90.000000	90.000000	30.000000	-0.1481	0.0465	0.0080	-0.0047	0.0005	-0.1996	0.0009	-0.1485	-0.0004	0.0008	0.0080
3.600000	125.593400	30.000000	180.000000	23.438600	240.000800	8.0748	-17.2833	45.8215	-21.5443	19.8588	-22.4365	4.4074	8.8237	-43.5116	42.7627	44.9333
4.000000	125.593400	30.000000	180.000000	23.438600	240.000800	-0.8681	-5.7350	15.5731	-6.5804	5.9734	-11.8963	1.8435	-0.8217	-13.0546	13.0081	15.4588
5.200000	125.593400	30.000000	180.000000	23.438600	240.000800	-1.6621	-0.1965	0.5540	-0.2426	0.1349	-2.0140	0.0958	-1.6684	-0.3489	0.3552	0.5542
4.505428	125.593420	30.000000	180.000000	23.438603	240.000769	-2.6471	-1.3639	3.8849	-1.5201	1.2382	-5.4618	0.5568	-2.6660	-2.8433	2.8622	3.8782
5.900000	125.593420	30.000000	180.000000	23.438603	240.000769	-0.8259	-0.0547	0.0738	-0.0535	0.0135	-0.8215	0.0150	-0.8273	-0.0388	0.0402	0.0740
3.300000	152.736759	0.000000	0.000000	148.777353	90.000000	3.1195	-12.3260	33.1041	-16.5900	15.8189	-20.4432	3.7660	3.3299	-35.0298	34.8195	32.7306
4.016997	152.736759	0.000000	0.000000	148.777353	90.000000	-2.6561	-1.1183	4.7116	-2.0381	1.7260	-6.7095	0.7144	-2.7139	-4.0074	4.0652	4.7057
5.300000	152.736759	0.000000	0.000000	148.777353	90.000000	-0.8307	0.2213	0.1289	-0.0916	0.0280	-1.1513	0.0271	-0.8376	-0.0789	0.0857	0.1293
3.650000	152.736800	0.000000	0.000000	148.777400	90.000000	-1.8165	-4.2072	12.8453	-5.8721	5.4250	-11.7705	1.7087	-1.8709	-12.1192	12.1736	12.7920
4.600000	152.736800	0.000000	0.000000	148.777400	90.000000	-1.7998	0.1149	0.9380	-0.4338	0.2734	-2.8836	0.1671	-1.8240	-0.6989	0.7231	0.9377
4.600000	171.783200	329.999800	90.000000	90.000000	200.424200	0.3931	-5.4050	14.6724	-4.8162	3.9945	-9.2506	1.3382	0.5333	-7.5751	7.4348	14.4466
5.600000	171.783200	329.999800	90.000000	90.000000	200.424200	-1.8263	-0.6320	0.7393	-0.2136	0.1116	-1.9135	0.0952	-1.8131	-0.2365	0.2232	0.7395
4.200000	171.783237	329.999823	90.000000	90.000000	200.424164	10.2968	-15.3054	44.7454	-17.9888	14.7366	-17.9697	3.2215	11.4395	-29.9008	28.7581	42.9060
4.980308	171.783237	329.999823	90.000000	90.000000	200.424164	-2.0992	-2.1205	4.8401	-1.3848	1.0609	-4.9694	0.5184	-2.0552	-2.0247	1.9808	4.8146
6.200000	171.783237	329.999823	90.000000	90.000000	200.424164	-1.0520	-0.3007	0.1135	-0.0510	0.0122	-0.8386	0.1668	-1.0477	-0.0308	0.0265	0.1137
4.600000	171.783237	330.000000	270.000000	90.000000	200.424164	-1.7681	-3.8823	10.0161	-3.0623	2.5685	-8.4494	1.0944	-1.7150	-4.9570	4.9038	9.9454
4.980308	171.783237	330.000000	270.000000	90.000000	200.424164	-2.7701	-1.5755	3.2499	-0.9160	0.6787	-4.5883	0.4081	-2.7430	-0.1369	1.3388	3.2436
6.200000	171.783237	330.000000	270.000000	90.000000	200.424164	-1.0370	-0.2772	0.0734	-0.0438	0.0082	-0.8067	0.1028	-1.0333	-0.2633	0.0196	0.0734
3.840185	180.000000	160.478555	0.000000	180.000000	130.478555	-1.7886	0.1391	3.3306	-1.1793	0.9690	-5.5835	0.4750	-1.8491	-2.1497	2.2102	3.3344
3.840185	180.000000	160.478555	0.000000	180.000000	130.478555	-1.0042	0.6710	0.4696	-0.1967	0.0977	-2.1414	0.0767	-1.0231	-0.2362	0.2552	0.4695
3.500000	180.000000	160.478600	0.000000	180.000000	130.478600	-1.1490	-1.6260	9.0135	-3.4261	3.1643	-9.5406	1.1640	-1.2508	-6.8021	6.9040	9.0095
5.000000	180.000000	160.478600	0.000000	180.000000	130.478600	-0.4822	0.5592	0.1018	-0.0663	0.0153	-1.1188	0.0184	-0.4905	-0.0355	0.0437	0.1017
4.250000	180.000000	274.934400	115.066100	90.000000	330.000000	3.7898	-9.8861	27.8388	-10.2188	8.7726	-14.9084	2.5441	4.1421	-17.3986	17.0463	27.1482
4.500000	180.000000	274.934400	115.066100	90.000000	330.000000	-0.6367	-5.2116	13.8908	-4.5626	3.8567	-9.9275	1.4336	-0.5205	-7.5213	7.4052	13.7041
5.500000	180.000000	274.934400	115.066100	90.000000	330.000000	-2.0504	-0.6460	0.7023	-0.2141	0.1067	-2.0861	0.1020	-2.0353	-0.2437	0.2285	0.7024
5.000127	180.000000	274.934400	115.066123	90.000000	330.000000	-2.6985	-1.5972	3.2343	-0.9199	0.6703	-4.4535	0.4040	-2.6620	-1.3630	1.3265	3.2239
6.000000	180.000000	274.934400	115.066123	90.000000	330.000000	-1.2796	-0.3525	0.1452	-0.0660	0.0164	-1.0408	0.0241	-1.2736	-0.0442	0.0381	0.1455
# The following points are used in fitting of both 'pot2' and 'pot3' and were not used in 'pot1'																
3.806669	0.000000	0.000000	0.000000	0.000000	0.000000	-1.7856	0.0412	3.6936	-1.3086	1.0920	-5.8886	0.5209	-1.8496	-2.4115	2.4755	3.6974
4.350000	0.000000	0.000000	0.000000	90.000000	30.000000	1.6014	-7.6428	21.1699	-7.4186	6.3545	-12.6819	2.0354	1.8165	-12.4725	12.2575	20.7570
4.350000	0.000000	24.691700	354.691500	90.000000	120.000000	3.6111	-8.0348	23.4278	-6.9145	5.9823	-12.6780	1.9633	3.7460	-10.6485	10.5136	23.2077
3.792801	0.000000	30.000000	0.000000	0.000000	0.000000	-1.7914	0.0020	3.8273	-1.3611	1.1422	-6.0066	0.5393	-1.8569	-2.5197	2.5852	3.8315
3.973084	26.836784	120.000000	0.000000	31.123042	270.000000	-2.6647	-1.2911	5.2190	-2.2589	1.9353	-7.1111	0.7821	-2.7249	-4.4673	4.5275	5.2120
3.991842	27.091851	120.000000	0.000000	32.025903	270.000000	-2.6522	-1.3074	5.1930	-2.2542	1.9310	-7.0566	0.7776	-2.7165	-4.4637	4.5281	5.1797
5.650000	60.000000	30.000000	30.000000	90.000000	0.000000	0.5076	-2.7287	8.7253	-2.1974	1.8371	-5.9411	0.7349	0.4302	-2.8679	2.9453	8.6531
6.200000	60.000000	30.000000	30.000000	90.000000	0.000000	-1.1977	-0.5278	1.6503	-0.3567	0.2705	-2.4163	0.1665	-1.2135	-0.4199	0.4357	1.6488
7.000000	60.000000	30.000000	30.000000	90.000000	0.000000	-0.6678	-0.0435	0.1312	-0.0315	0.0155	-0.7566	0.0159	-0.6691	-0.0261	0.0273	0.1313
5.800000	60.000000	30.000000	30.000000	120.000000	30.000000	2.6861	-1.3733	8.7618	-2.1505	1.6253	-4.8198	0.6028	2.6462	-2.2266	2.2664	8.6728
5.907655	60.173287	300.000000	90.000000	90.000000	70.912901	-1.7393	-0.9953	2.3706	-0.5462	0.4296	-3.2749	0.2563	-1.7599	-0.7251	0.7456	2.3694
4.974668	60.000000	90.000000	180.000000	0.000000	90.000000	-2.6986	-1.6868	3.4893	-0.9958	0.7345	-4.6348	0.4322	-2.6613	-1.4873	1.4501	3.4750
4.959671	90.000000	100.900344	90.000000	8.594202	150.000000	-2.7812	-1.6260	3.4142	-0.9566	0.7147	-4.7264	0.4255	-2.7547	-1.4293	1.4027	3.4083
4.950043	90.000000	101.284462	90.000000	9.140574	180.000000	-2.7931	-1.6572	3.4914	-0.9805	0.7384	-4.7968	0.4356	-2.7691	-1.4752	1.4512	3.4816
6.103850	90.000000	120.000000	90.000000	90.000000	240.000000	-1.7902	-1.0747	2.5552	-0.4593	0.3443	-3.4393	0.2574	-1.			



S5 5.008800 90.000000 360.000000 90.000000 180.000000 120.000000 -2.4411 -1.4599 3.1254 -0.7500 0.5385 -4.2170 0.3435 -2.4195 -0.9889 0.9672 3.1215  
 S6 5.906800 90.000000 70.731000 270.000000 60.538700 120.000000 -1.7382 -1.0070 2.4092 -0.5529 0.4351 -3.3046 0.2598 -1.7604 -0.7324 0.7547 2.4043  
 S7 3.802900 0.000000 30.000000 0.000000 0.000000 0.000000 -1.7880 0.0332 3.7156 -1.3200 1.1029 -5.9135 0.5249 -1.8569 -2.4359 2.5047 3.7131  
 S8 3.815900 0.000000 0.000000 0.000000 0.000000 0.000000 -1.7817 0.0687 3.5946 -1.2724 1.0574 -5.8053 0.5082 -1.8488 -2.3378 2.4049 3.5924

# SAPT(DFT), MP2, CCSD, and CCSD(T) results for the characteristic points.

# SAPT --- SAPT(DFT) with third-order (total above)

# SAPT2 --- SAPT(DFT) up to second-order (total2 above)

# pot3 --- value from the pot3 fit

# pot2 --- value from the pot2 fit at the specified geometry (these are not characteristic points on the pot2 surface)

# CCSD(T) --- CCSD(T) interaction energy with aug-cc-pVTZ basis set with midbond. Dimer basis set used.

# MP2, SCF --- MP2, SCF interaction energies with the same basis set as above.

#	R	beta_A	gamma_A	alpha_B	beta_B	gamma_B	SAPT	pot3	pot3-SAPT	SAPT2	pot2	pot2-SAPT2	CCSD(T)	MP2	SCF
M1	3.936900	152.124100	30.000000	0.000000	152.124100	150.000000	-2.6832	-2.6862	0.0031	-2.7511	-2.7462	-0.0049	-2.6190	-4.5022	3.7708
M2	4.943600	9.222600	240.000000	270.000000	90.000000	101.750800	-2.7951	-2.7894	-0.0058	-2.7715	-2.7638	-0.0078	-2.7515	-3.6100	1.2666
M3	6.103400	90.000000	120.000000	90.000000	90.000000	240.000000	-1.7894	-1.7962	0.0068	-1.8165	-1.8218	0.0053	-1.7853	-2.0603	1.1648
S1	4.947900	90.000000	101.120300	270.000000	171.625600	330.000000	-2.7812	-2.7735	-0.0077	-2.7554	-2.7453	-0.0101	-2.7397	-3.5909	1.2444
S2	3.959100	153.914400	300.000000	0.000000	149.554100	330.000000	-2.6657	-2.6662	0.0006	-2.7314	-2.7244	-0.0070	-2.6014	-4.4493	3.7001
S3	4.970500	0.000000	270.000000	180.000000	90.000000	90.000000	-2.6982	-2.7118	0.0136	-2.6607	-2.6741	0.0134	-2.6401	-3.4818	1.1666
S3a	4.842600	13.290200	180.000000	180.000000	105.780600	90.000000	-2.7329	-2.7185	-0.0144	-2.7107	-2.6885	-0.0221	-2.6694	-3.6230	1.4509
S4	4.221000	135.279000	330.000000	180.000000	23.349300	60.000000	-2.5914	-2.6345	0.0430	-2.6362	-2.6767	0.0406	-2.4740	-4.0181	3.1338
S5	5.008800	90.000000	360.000000	90.000000	180.000000	120.000000	-2.4411	-2.4514	0.0103	-2.4195	-2.4286	0.0092	-2.3333	-3.0698	1.3056
S6	5.906800	90.000000	70.731000	270.000000	60.538700	120.000000	-1.7382	-1.7391	0.0009	-1.7604	-1.7633	0.0029	-1.7470	-2.0943	1.1001
S7	3.802900	0.000000	30.000000	0.000000	0.000000	0.000000	-1.7880	-1.8039	0.0159	-1.8569	-1.8670	0.0101	-1.5891	-3.2678	4.2412
S8	3.815900	0.000000	0.000000	0.000000	0.000000	0.000000	-1.7817	-1.7721	-0.0096	-1.8488	-1.8366	-0.0122	-1.5933	-3.2403	4.1394

#pot2 characteristic points and pot2 energy.

#	R	beta_A	gamma_A	alpha_B	beta_B	gamma_B	pot2
M1	3.939444	151.695572	30.000000	0.000000	151.695572	30.000000	-2.7470
M2	4.949811	9.754128	240.000000	270.000000	90.000000	102.148241	-2.7646
M3	6.089739	90.000000	120.000000	90.000000	90.000000	240.000000	-1.8225
S1	4.954779	90.000033	101.480134	270.000000	171.182945	330.000000	-2.7460
S2	3.958399	153.601628	300.000000	0.000000	149.269719	330.000000	-2.7250
S3	4.980625	0.000000	270.000000	180.000000	90.000000	90.000000	-2.6746
S3a	4.745264	17.611967	180.000000	180.000000	111.809229	90.000000	-2.6933
S4	4.342634	50.026295	330.000000	180.000000	156.713304	60.000000	-2.6713
S5	5.014794	90.000000	360.000000	90.000000	180.000000	120.000000	-2.4288
S6	5.890549	90.000000	70.718822	270.000000	60.128612	120.000000	-1.7637
S7	3.791276	0.000000	30.000000	0.000000	0.000000	0.000000	-1.8676
S8	3.803704	0.000000	30.000000	0.000000	0.000000	0.000000	-1.8373

#-----characteristic points end -----