

Supporting Information
for
**Functional Relationships between Kinetic, Flow, and Geometrical
Parameters in a High Temperature Chemical Micro-Reactor**

M. V. Zagidullin^{1,2}, R. I. Kaiser^{1,3}, D. P. Porfiriev^{1,2}, I. P. Zavershinskiy¹,
M. Ahmed⁴, V. N. Azyazov*^{1,2} and A. M. Mebel*^{1,5}

¹*Samara University, Samara 443086, Russia*

²*Lebedev Physical Institute of RAS, Samara 443011, Russia*

³*University of Hawaii at Manoa, Honolulu, Hawaii, 96822, USA*

⁴*Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California
94720, USA*

⁵*Florida International University, Miami, Florida 33199, USA*

Content

Table S1. Modified Arrhenius expressions for rate constants	S2
Geometries and frequencies employed for rate constant calculations	S4
Optimized geometries along the MEP for 1-bromonaphthalene	S8
Optimized geometries along the MEP for 2-bromonaphthalene	S15

Table S1. Modified Arrhenius expressions for rate constants

Pressure [atm]	Temperature interval	Modified Arrhenius expressions
1-bromonaphthalene -> 1-naphtyle + Br		
0.01	500 – 2000	$0.40881E+141 * T^{(-35.238)} \exp(-87603/T) + 0.30916E+59 * T^{(-13.034)} \exp(-49175/T)$
0.0394737	500 – 2250	$0.20182E+112 * T^{(-26.899)} \exp(-77372/T) + 0.79938E+70 * T^{(-16.473)} \exp(-51627/T)$
0.1	500 – 2250	$0.41271E+102 * T^{(-24.083)} \exp(-74861/T) + 0.91502E+61 * T^{(-13.762)} \exp(-49757/T)$
0.3	500 – 2500	$0.27169E+97 * T^{(-22.496)} \exp(-74798/T) + 0.34736E+48 * T^{(-9.6986)} \exp(-46933/T)$
1	500 – 2500	$0.69969E+74 * T^{(-16.249)} \exp(-65610/T) + 0.96226E+41 * T^{(-7.7348)} \exp(-45486/T)$
1-naphtyel + Br -> 1-bromonaphthalene		
0.01	500 – 2000	$0.10061E+78 * 6.02E+23 * T^{(-24.828)} \exp(-30335/T) + 0.21311E+17 * 6.02E+23 * T^{(-8.2289)} \exp(-4893.9/T)$
	500 – 1800	$0.92978E+59 * 6.02E+23 * T^{(-19.784)} \exp(-23539/T) + 0.38671E+12 * 6.02E+23 * T^{(-6.7948)} \exp(-3872.4/T)$
	500 – 1650	$0.20355E+47 * 6.02E+23 * T^{(-16.224)} \exp(-19076/T) + 0.24889E+07 * 6.02E+23 * T^{(-5.2016)} \exp(-2835.3/T)$
0.0394737	500 – 2000	$0.71315E+56 * 6.02E+23 * T^{(-18.747)} \exp(-23907/T) + 0.32259E+10 * 6.02E+23 * T^{(-6.1251)} \exp(-3567.2/T)$
	500 – 1800	$0.14399E+31 * 6.02E+23 * T^{(-11.560)} \exp(-14032/T) + 0.99856E+07 * 6.02E+23 * T^{(-5.4021)} \exp(-2906.4/T)$
	500 – 1650	$0.25397E+22 * 6.02E+23 * T^{(-9.1095)} \exp(-10972/T) + 121.68 * 6.02E+23 * T^{(-3.8860)} \exp(-1954.6/T)$
0.1	500 – 2000	$0.58642E+34 * 6.02E+23 * T^{(-12.515)} \exp(-15983/T) + 0.35028E+07 * 6.02E+23 * T^{(-5.2344)} \exp(-2909.4/T)$
	500 – 1800	$0.17217E+21 * 6.02E+23 * T^{(-8.7454)} \exp(-10835/T) + 211.51 * 6.02E+23 * T^{(-3.9549)} \exp(-2017.8/T)$
	500 – 1650	$0.52087E+12 * 6.02E+23 * T^{(-6.3557)} \exp(-7644.6/T) + 2.9856 * 6.02E+23 * T^{(-3.4051)} \exp(-1596.9/T)$
0.3	500 – 2000	$0.61592E+19 * 6.02E+23 * T^{(-8.3023)} \exp(-10624/T) + 363.44 * 6.02E+23 * T^{(-4.0211)} \exp(-2084.5/T)$
	500 – 1800	$0.11587E+10 * 6.02E+23 * T^{(-5.6021)} \exp(-6707.9/T) + 0.81626 * 6.02E+23 * T^{(-3.2395)} \exp(-1465.5/T)$
1	500 – 2000	$0.15978E+10 * 6.02E+23 * T^{(-5.6199)} \exp(-6959.8/T) + 2.8999 * 6.02E+23 * T^{(-3.3998)} \exp(-1600.6/T)$

Pressure [atm]	Temperature interval	Modified Arrhenius expressions
2-bromonaphthalene -> 2-naphtyle + Br		
0.01	500 – 2000	$0.31163E+24 * T^{(-2.4840)} \exp(-42009/T) - 0.15229E+99 * T^{(-22.363)} \exp(-84077/T)$
0.0394737	500 – 2000	$0.23669E+119 * T^{(-28.792)} \exp(-81895/T) + 0.21586E+52 * T^{(-10.878)} \exp(-47976/T)$
0.1	500 – 2000	$0.21831E+96 * T^{(-22.339)} \exp(-73308/T) + 0.27782E+45 * T^{(-8.8080)} \exp(-46476/T)$
0.3	500 – 2000	$0.21369E+46 * T^{(-8.6420)} \exp(-50832/T) + 0.99519E+32 * T^{(-5.1663)} \exp(-43469/T)$
1	500 – 2500	$0.81707E+38 * T^{(-6.5715)} \exp(-47968/T) + 0.84877E+30 * T^{(-4.5499)} \exp(-43005/T)$
2-naphtyle + Br -> 2-bromonaphthalene		
0.01	500 – 2000	$0.63354E-12 * 6.02E+23 * T^{(-0.56693)} \exp(664.30/T - 0.30120E+13 * 6.02E+23 * T^{(-5.9407)} \exp(-14185/T)$
0.0394737	500 – 1800	$0.40903E+31 * 6.02E+23 * T^{(-11.684)} \exp(-14461/T) + 9838.8 * 6.02E+23 * T^{(-4.4591)} \exp(-2383/T)$
	500 – 2000	$0.89593E+48 * 6.02E+23 * T^{(-16.519)} \exp(-21048/T) + 0.70694E+09 * 6.02E+23 * T^{(-5.9322)} \exp(-3412.1/T)$
0.1	500 – 1800	$0.92836E+17 * 6.02E+23 * T^{(-7.8220)} \exp(-9687.1/T) + 58.130 * 6.02E+23 * T^{(-3.7889)} \exp(-1896.5/T)$
	500 – 2000	$0.91206E+32 * 6.02E+23 * T^{(-12.002)} \exp(-15504/T) + 53368 * 6.02E+23 * T^{(-4.6712)} \exp(-2574.4/T)$
0.3	500 – 1800	$0.10768E+10 * 6.02E+23 * T^{(-5.5884)} \exp(-6800.8/T) + 0.67614 * 6.02E+23 * T^{(-3.2086)} \exp(-1475.7/T)$
	500 – 2000	$0.70690E+16 * 6.02E+23 * T^{(-7.4783)} \exp(-9530.9/T) + 104.47 * 6.02E+23 * T^{(-3.8621)} \exp(-1963.4/T)$
1	500 – 2000	$0.16567E+09 * 6.02E+23 * T^{(-5.3480)} \exp(-6589.1/T) + 0.96899 * 6.02E+23 * T^{(-3.2567)} \exp(-1506.9/T)$

Geometries and frequencies employed for rate constant calculations

1-bromonaphthalene

Geometry[angstrom]			
C	0.000000	0.590803	0.000000
C	1.114778	1.502009	0.000000
C	2.444614	0.995536	0.000000
C	2.678907	-0.364772	0.000000
C	1.595243	-1.280154	0.000000
C	0.297911	-0.805881	0.000000
C	-1.320657	1.121643	0.000000
C	-1.532291	2.487704	0.000000
C	-0.436071	3.388604	0.000000
C	0.856820	2.902865	0.000000
Br	-1.123561	-2.091236	0.000000
H	3.275852	1.701364	0.000000
H	3.698441	-0.750328	0.000000
H	1.783286	-2.352195	0.000000
H	-2.165590	0.436337	0.000000
H	-2.550885	2.876091	0.000000
H	-0.617440	4.463512	0.000000
H	1.705461	3.588326	0.000000

Frequencies[1/cm]		
103.7530	174.8704	176.2353
227.3542	300.2334	416.9154
420.0139	477.4506	515.4632
533.2080	547.3816	620.3348
659.2340	742.8542	772.6202
797.4585	803.5007	819.2667
867.1792	910.6957	954.6210
965.5856	976.1055	984.5203
1047.5040	1083.6055	1153.5109
1165.3900	1176.1264	1214.3270
1242.0655	1270.0253	1379.1034
1406.6170	1414.2732	1457.2938
1472.8903	1535.9606	1604.9420
1629.7383	1667.2350	3190.2433
3194.6059	3203.2867	3213.0031
3217.5347	3229.0057	3233.4919

1-naphthyl

Geometry[angstrom]

C	1.304416	-1.348095	0.000000
C	2.495246	-0.691106	0.000000
C	2.443751	0.740348	0.000000
C	1.231298	1.397019	0.000000
C	0.000000	0.679043	0.000000
C	0.025790	-0.762025	0.000000
C	-1.198362	-1.490115	0.000000
C	-2.403687	-0.819274	0.000000
C	-2.437764	0.602275	0.000000
C	-1.266483	1.331729	0.000000
H	3.376679	1.305837	0.000000
H	1.200012	2.487265	0.000000
H	-1.162473	-2.579143	0.000000
H	-3.338566	-1.380067	0.000000
H	-3.399213	1.116379	0.000000
H	-1.294612	2.422557	0.000000
H	3.452939	-1.211622	0.000000

Frequencies[1/cm]

172.7702	188.0329	361.4140
404.6562	466.0282	502.6159
510.7959	524.0239	610.3298
626.5319	734.6587	773.8339
782.3074	794.4222	799.7338
867.3656	901.5662	925.9449
968.1683	979.7308	988.3784
1037.6142	1052.3222	1141.0359
1165.5678	1170.6558	1195.6038
1241.6945	1266.4567	1372.7817
1402.0999	1413.1781	1455.1516
1483.8922	1532.2003	1638.6269
1649.8364	1694.2844	3187.7689
3189.3016	3199.6334	3203.1583
3211.5617	3214.1872	3222.2916

2-bromonaphthalene

Geometry[angstrom]			
C	1.331004	0.367283	0.000000
C	1.542158	-1.052025	0.000000
C	0.409130	-1.914463	0.000000
C	-0.876197	-1.408050	0.000000
C	-1.064024	-0.001639	0.000000
C	0.000000	0.875442	0.000000
C	2.461793	1.233472	0.000000
C	3.743816	0.716854	0.000000
C	3.952998	-0.688446	0.000000
C	2.874493	-1.553087	0.000000
Br	-2.851823	0.676388	0.000000
H	0.565931	-2.994036	0.000000
H	-1.740185	-2.069999	0.000000
H	-0.165375	1.952152	0.000000
H	2.299877	2.312251	0.000000
H	4.602125	1.389122	0.000000
H	4.969493	-1.082317	0.000000
H	3.030929	-2.632802	0.000000

Frequencies[1/cm]		
88.4172	175.9388	182.6547
261.5037	272.4004	405.1154
405.3055	483.0491	513.3495
519.8554	585.9649	618.3436
638.7974	750.9577	765.1821
778.8309	824.0888	840.1044
864.1132	891.9084	939.7365
960.8411	974.7124	982.8325
1042.6307	1085.5953	1151.2927
1166.2748	1171.4536	1229.1506
1249.5548	1282.3755	1364.6455
1412.6658	1427.6320	1454.1817
1475.4458	1535.1370	1614.5909
1623.8699	1668.1465	3188.6631
3192.5034	3194.8767	3207.0567
3212.2657	3219.6685	3229.9254

2-naphthyl

Geometry[angstrom]			
C	-2.437444	0.911945	0.000000
C	-1.179473	1.493353	0.000000
C	0.000000	0.693282	0.000000
C	-0.111997	-0.737847	0.000000
C	-1.417650	-1.331681	0.000000
C	-2.485643	-0.490157	0.000000
H	1.384587	2.367353	0.000000
H	-3.341248	1.520615	0.000000
H	-1.079984	2.580653	0.000000
C	1.299311	1.279567	0.000000
C	1.073833	-1.525815	0.000000
H	-1.520050	-2.417678	0.000000
C	2.316855	-0.925464	0.000000
C	2.431410	0.490986	0.000000
H	0.984312	-2.613073	0.000000
H	3.218078	-1.539322	0.000000
H	3.419096	0.952446	0.000000

Frequencies[1/cm]		
178.4359	192.2387	371.6369
395.4065	471.3350	493.4419
509.9461	520.9877	605.3611
622.5114	745.5533	756.8513
773.4201	791.6762	812.7380
850.2766	891.8861	928.5183
961.0646	977.3582	986.3471
1043.5227	1057.9390	1141.9557
1159.1642	1169.4136	1211.5394
1243.7522	1276.9829	1337.2448
1404.0851	1439.4654	1455.5107
1468.0479	1539.7509	1615.8351
1661.6515	1681.1789	3184.1589
3187.3931	3191.4201	3193.5469
3205.7919	3214.5539	3218.5407

Optimized geometries along the MEP for 1-bromonaphthalene

Dihedral angles were fixed

1-bromonaphthalene

C

C, 1, r2

C, 2, r3, 1, a3

C, 3, r4, 2, a4, 1, d4

C, 4, r5, 3, a5, 2, d5

C, 5, r6, 4, a6, 3, d6

C, 1, r7, 2, a7, 3, d7

C, 7, r8, 1, a8, 2, d8

C, 8, r9, 7, a9, 1, d9

C, 9, r10, 8, a10, 7, d10

Br, 6, rsc(i), 5, a11, 4, d11

H, 3, r12, 2, a12, 1, d12

H, 4, r13, 3, a13, 2, d13

H, 5, r14, 4, a14, 3, d14

H, 7, r15, 1, a15, 2, d15

H, 8, r16, 7, a16, 1, d16

H, 9, r17, 8, a17, 7, d17

H, 10, r18, 9, a18, 8, d18

Distance C-Br	2.0	2.1	2.2	2.3	2.4
R2 / ANG	1.44538702	1.44611166	1.44693804	1.44762787	1.44837464
R3 / ANG	1.42572939	1.42621697	1.42657768	1.42686451	1.42714282
A3 / DEGREE	120.00056282	119.93818567	119.90935312	119.87760894	119.83521353
R4 / ANG	1.38696124	1.38743409	1.38780098	1.38813087	1.38841803
A4 / DEGREE	120.71345734	120.90880494	121.06758190	121.20464711	121.32374222
R5 / ANG	1.42109363	1.42279446	1.42438900	1.42585811	1.42732644
A5 / DEGREE	120.39688400	120.45218531	120.49712154	120.54584451	120.59413193
R6 / ANG	1.38515709	1.38156567	1.37822028	1.37534137	1.37283762
A6 / DEGREE	119.12973527	118.25034324	117.46951312	116.76939599	116.15326432
R7 / ANG	1.42559507	1.42494037	1.42431272	1.42383742	1.42344021
A7 / DEGREE	118.99783523	119.26152615	119.52194803	119.77371290	119.98642040
R8 / ANG	1.38835435	1.38815818	1.38800262	1.38786077	1.38777121
A8 / DEGREE	120.51785421	120.34987932	120.18699659	120.02744736	119.89138732
R9 / ANG	1.42112064	1.42147476	1.42179098	1.42208457	1.42231507
A9 / DEGREE	120.69543606	120.69439766	120.69437115	120.69276580	120.69284392
R10 / ANG	1.38715114	1.38734374	1.38749650	1.38761504	1.38775611
A10 / DEGREE	120.02396887	120.12810667	120.22654336	120.32209746	120.40425573
A11 / DEGREE	117.11964070	116.39399232	115.80358517	115.31364965	114.96941229
R12 / ANG	1.09557200	1.09556742	1.09553329	1.09548894	1.09545536
A12 / DEGREE	118.78026404	118.71296360	118.65330041	118.60916130	118.57270529
R13 / ANG	1.09473095	1.09474505	1.09477450	1.09480919	1.09485219
A13 / DEGREE	120.39429009	120.35084889	120.35039466	120.34863999	120.34928600
R14 / ANG	1.09282347	1.09231741	1.09194635	1.09170390	1.09154987
A14 / DEGREE	120.66762429	121.07445820	121.42252860	121.75755817	122.02586579
R15 / ANG	1.09286309	1.09286151	1.09292244	1.09297657	1.09312769
A15 / DEGREE	119.14020845	118.96564884	118.81651669	118.66629239	118.55933044
R16 / ANG	1.09478032	1.09474000	1.09470006	1.09466027	1.09462877
A16 / DEGREE	119.53017172	119.54174262	119.55442214	119.57783517	119.59185186
R17 / ANG	1.09476495	1.09476392	1.09475802	1.09474896	1.09474251
A17 / DEGREE	119.91948463	119.87001689	119.82253744	119.77288660	119.73278222
R18 / ANG	1.09591108	1.09589103	1.09588052	1.09586913	1.09586417
A18 / DEGREE	120.50496619	120.50707325	120.50867576	120.51255407	120.51373950

Distance C-Br	2.5	2.6	2.7	2.8	2.9
R2 / ANG	1.44909662	1.44976798	1.45028422	1.45071857	1.45135901
R3 / ANG	1.42737797	1.42756200	1.42779403	1.42784655	1.42788916
A3 / DEGREE	119.79252819	119.75056015	119.66553885	119.63641056	119.60654840
R4 / ANG	1.38865613	1.38884754	1.38905208	1.38915168	1.38921732
A4 / DEGREE	121.42315082	121.50501821	121.57724300	121.62309947	121.65617075
R5 / ANG	1.42869548	1.42990639	1.43106324	1.43185389	1.43233286
A5 / DEGREE	120.63350769	120.66077734	120.70259953	120.69989257	120.66210475
R6 / ANG	1.37071114	1.36897779	1.36764167	1.36664043	1.36595618
A6 / DEGREE	115.63940925	115.23491985	114.90350584	114.72551592	114.70235783
R7 / ANG	1.42312182	1.42289879	1.42274033	1.42268338	1.42281636
A7 / DEGREE	120.16737331	120.31084926	120.40418730	120.48007091	120.47050274
R8 / ANG	1.38771027	1.38767968	1.38768044	1.38769010	1.38769244
A8 / DEGREE	119.77760938	119.68687564	119.62642418	119.58177439	119.57939904
R9 / ANG	1.42250774	1.42266154	1.42274686	1.42286083	1.42291782
A9 / DEGREE	120.69059845	120.68902243	120.68582151	120.68165402	120.68756104
R10 / ANG	1.38789991	1.38803080	1.38820329	1.38827926	1.38828009
A10 / DEGREE	120.47602536	120.53468623	120.57875105	120.61208431	120.62222935
A11 / DEGREE	114.76925876	114.73124892	114.87958754	115.17809654	115.66045769
R12 / ANG	1.09542916	1.09541115	1.09541033	1.09540394	1.09542887
A12 / DEGREE	118.54321120	118.51897489	118.50588959	118.48899597	118.46984534
R13 / ANG	1.09490276	1.09495780	1.09501970	1.09508015	1.09511926
A13 / DEGREE	120.35640301	120.36871254	120.35791026	120.38466495	120.42968605
R14 / ANG	1.09148414	1.09149889	1.09152330	1.09167507	1.09192102
A14 / DEGREE	122.22602977	122.35897073	122.43022523	122.41477328	122.35068601
R15 / ANG	1.09332017	1.09353957	1.09374849	1.09393979	1.09409777
A15 / DEGREE	118.47467348	118.42319781	118.38153493	118.39282269	118.39700001
R16 / ANG	1.09460344	1.09458539	1.09457862	1.09457314	1.09456422
A16 / DEGREE	119.60384127	119.61275904	119.61755664	119.62426307	119.63042266
R17 / ANG	1.09473768	1.09473389	1.09473395	1.09473151	1.09472799
A17 / DEGREE	119.69858780	119.67083278	119.65278349	119.63689135	119.62634579
R18 / ANG	1.09586665	1.09587629	1.09588617	1.09591165	1.09594123
A18 / DEGREE	120.51218009	120.50904880	120.50387080	120.49823931	120.49529347

Distance C-Br	3.0	3.1	3.2	3.3	3.4
R2 / ANG	1.45133864	1.45134147	1.45111995	1.45078997	1.45036006
R3 / ANG	1.42780359	1.42789578	1.42791977	1.42783763	1.42782922
A3 / DEGREE	119.57773065	119.50457465	119.44407563	119.40883369	119.35966788
R4 / ANG	1.38920191	1.38932591	1.38935586	1.38924275	1.38921407
A4 / DEGREE	121.67433407	121.69518230	121.69048436	121.66130995	121.63113138
R5 / ANG	1.43276879	1.43304348	1.43313323	1.43302716	1.43292044
A5 / DEGREE	120.65181731	120.62215153	120.59507476	120.57601104	120.55686892
R6 / ANG	1.36587946	1.36599362	1.36643226	1.36710432	1.36784840
A6 / DEGREE	114.71746346	114.81834298	115.00643063	115.24979502	115.49914274
R7 / ANG	1.42284982	1.42322415	1.42356753	1.42390885	1.42426220
A7 / DEGREE	120.46699121	120.43772487	120.37341160	120.27546608	120.19663343
R8 / ANG	1.38766534	1.38770185	1.38772171	1.38774172	1.38774192
A8 / DEGREE	119.59938115	119.60935103	119.65455945	119.72200415	119.78652266
R9 / ANG	1.42297876	1.42305058	1.42308490	1.42305822	1.42308095
A9 / DEGREE	120.66707664	120.66064875	120.64354437	120.63102855	120.60310984
R10 / ANG	1.38833942	1.38840486	1.38844311	1.38840289	1.38842457
A10 / DEGREE	120.63094922	120.64055630	120.63638711	120.61248732	120.60318367
A11 / DEGREE	116.29390292	116.97852388	117.82447880	118.71909635	119.71466557
R12 / ANG	1.09543166	1.09548510	1.09553027	1.09555381	1.09559441
A12 / DEGREE	118.47093790	118.46667189	118.47242200	118.48441309	118.49988520
R13 / ANG	1.09517257	1.09522050	1.09526907	1.09530947	1.09535005
A13 / DEGREE	120.41861100	120.39217826	120.36461721	120.35106615	120.31964962
R14 / ANG	1.09211414	1.09242744	1.09272880	1.09296765	1.09325200
A14 / DEGREE	122.26865315	122.16343406	122.01219985	121.81480822	121.64092878
R15 / ANG	1.09426275	1.09445719	1.09457834	1.09461958	1.09466753
A15 / DEGREE	118.37377030	118.41762921	118.45267384	118.51851029	118.53490373
R16 / ANG	1.09457662	1.09459424	1.09461759	1.09463764	1.09466043
A16 / DEGREE	119.63665226	119.66149738	119.68280740	119.68955778	119.71527004
R17 / ANG	1.09473043	1.09474668	1.09476504	1.09477536	1.09479818
A17 / DEGREE	119.62243042	119.61091436	119.60857437	119.61858511	119.62098007
R18 / ANG	1.09597182	1.09600497	1.09603831	1.09606866	1.09609903
A18 / DEGREE	120.48555896	120.47151988	120.45872393	120.45418688	120.44070144

Distance C-Br	3.5	3.75	4.0	4.25	4.5
R2 / ANG	1.45005139	1.44931025	1.44895001	1.44850129	1.44832749
R3 / ANG	1.42774645	1.42771772	1.42768890	1.42770478	1.42775210
A3 / DEGREE	119.34097255	119.28159164	119.24044467	119.22761730	119.23510801
R4 / ANG	1.38902768	1.38888921	1.38884193	1.38878363	1.38872928
A4 / DEGREE	121.59300319	121.51913352	121.47554087	121.43870058	121.41865418
R5 / ANG	1.43282898	1.43246927	1.43244539	1.43223898	1.43196059
A5 / DEGREE	120.53810802	120.49928514	120.47305095	120.46415668	120.44230646
R6 / ANG	1.36853134	1.37007882	1.37088090	1.37154475	1.37203651
A6 / DEGREE	115.75137925	116.24639151	116.52967387	116.72002803	116.85660511
R7 / ANG	1.42459169	1.42533129	1.42607938	1.42633927	1.42645885
A7 / DEGREE	120.08744981	119.90956539	119.81867168	119.76057699	119.71825573
R8 / ANG	1.38777964	1.38783291	1.38762490	1.38764829	1.38786184
A8 / DEGREE	119.85637943	119.98140777	120.05080833	120.09613024	120.09615451
R9 / ANG	1.42300847	1.42295861	1.42298941	1.42298718	1.42291168
A9 / DEGREE	120.59836502	120.56621465	120.53330236	120.51868979	120.54912310
R10 / ANG	1.38834683	1.38831472	1.38834811	1.38833768	1.38827725
A10 / DEGREE	120.57147333	120.53411920	120.53552247	120.51784168	120.48688421
A11 / DEGREE	120.81724526	123.88359498	127.43717981	131.62862639	135.95317668
R12 / ANG	1.09561306	1.09568116	1.09573016	1.09575291	1.09577363
A12 / DEGREE	118.51101556	118.54017450	118.56857832	118.58474955	118.58043094
R13 / ANG	1.09538282	1.09544232	1.09550117	1.09551778	1.09551523
A13 / DEGREE	120.31161179	120.25704176	120.20911006	120.19049166	120.18569790
R14 / ANG	1.09345095	1.09394987	1.09420480	1.09438866	1.09453429
A14 / DEGREE	121.44149996	121.12694736	120.94878550	120.83886970	120.78243191
R15 / ANG	1.09469636	1.09477606	1.09472219	1.09441531	1.09451393
A15 / DEGREE	118.63301981	118.76403692	118.73921106	118.79466451	118.96990351
R16 / ANG	1.09468306	1.09473290	1.09475223	1.09476064	1.09480586
A16 / DEGREE	119.71330029	119.74062445	119.79383159	119.80039094	119.76671121
R17 / ANG	1.09480673	1.09484680	1.09489241	1.09491055	1.09491413
A17 / DEGREE	119.63366699	119.64731829	119.64393802	119.65600862	119.66799679
R18 / ANG	1.09612635	1.09617647	1.09620647	1.09622529	1.09624012
A18 / DEGREE	120.44169463	120.42419399	120.38586883	120.37807403	120.39539939

Distance C-Br	4.75	5.0	5.5	6.0	7.0
R2 / ANG	1.44813723	1.44800041	1.44820250	1.44811147	1.44810606
R3 / ANG	1.42777373	1.42781768	1.42777065	1.42773381	1.42773487
A3 / DEGREE	119.23497321	119.23726442	119.22745866	119.20968527	119.20839253
R4 / ANG	1.38870545	1.38870187	1.38875280	1.38875264	1.38875637
A4 / DEGREE	121.40293797	121.39641317	121.38756514	121.38217090	121.38102135
R5 / ANG	1.43192248	1.43181207	1.43172474	1.43178389	1.43178414
A5 / DEGREE	120.43837433	120.42702889	120.44295322	120.45126853	120.45199404
R6 / ANG	1.37224895	1.37236917	1.37248800	1.37242906	1.37242474
A6 / DEGREE	116.92185741	116.95966519	116.97519750	116.97294929	116.97504391
R7 / ANG	1.42660774	1.42686413	1.42628651	1.42632118	1.42631991
A7 / DEGREE	119.72399415	119.71545786	119.71824430	119.66485084	119.66513393
R8 / ANG	1.38787491	1.38781952	1.38806349	1.38797765	1.38798117
A8 / DEGREE	120.08136187	120.05878440	120.07553337	120.16115638	120.16070015
R9 / ANG	1.42292457	1.42305951	1.42279590	1.42290833	1.42291118
A9 / DEGREE	120.55791687	120.59015987	120.57915599	120.51051989	120.51082570
R10 / ANG	1.38828257	1.38811908	1.38836755	1.38827788	1.38827970
A10 / DEGREE	120.48555765	120.46981724	120.46495658	120.48262965	120.48244500
A11 / DEGREE	140.49473666	145.38236129	156.45072498	109.67470415	109.67051494
R12 / ANG	1.09578644	1.09579695	1.09581147	1.09577993	1.09578169
A12 / DEGREE	118.58806032	118.57847561	118.59162724	118.59621307	118.59653977
R13 / ANG	1.09553335	1.09552961	1.09554069	1.09553376	1.09553723
A13 / DEGREE	120.17857953	120.17988522	120.16753064	120.16063177	120.15895320
R14 / ANG	1.09458880	1.09463319	1.09465923	1.09460932	1.09460595
A14 / DEGREE	120.74597664	120.74629464	120.74857587	120.74136178	120.74465213
R15 / ANG	1.09437403	1.09437094	1.09410047	1.09459941	1.09459686
A15 / DEGREE	118.96783297	119.05418375	119.13760770	118.90065292	118.89595987
R16 / ANG	1.09483337	1.09489681	1.09493591	1.09485140	1.09485425
A16 / DEGREE	119.76850022	119.75384016	119.72443106	119.81824870	119.81888750
R17 / ANG	1.09493536	1.09493545	1.09495129	1.09490656	1.09490870
A17 / DEGREE	119.67133422	119.66306215	119.69449671	119.66481180	119.66507416
R18 / ANG	1.09625236	1.09625452	1.09628069	1.09624689	1.09624895
A18 / DEGREE	120.39323720	120.41699793	120.40111727	120.39056592	120.39031519

Distance C-Br	8.0	10.0	12.5	15.0	20.0
R2 / ANG	1.44810312	1.44810078	1.44809730	1.44809005	1.44806757
R3 / ANG	1.42773581	1.42773719	1.42773937	1.42774254	1.42774638
A3 / DEGREE	119.20742540	119.20706019	119.20698379	119.20715045	119.20799882
R4 / ANG	1.38875926	1.38876005	1.38875962	1.38875988	1.38875968
A4 / DEGREE	121.37999957	121.37959396	121.37944333	121.37933426	121.38044334
R5 / ANG	1.43178624	1.43178890	1.43179359	1.43180302	1.43181563
A5 / DEGREE	120.45277977	120.45315089	120.45322704	120.45311983	120.45021333
R6 / ANG	1.37241921	1.37241565	1.37241240	1.37240825	1.37239800
A6 / DEGREE	116.97625970	116.97650560	116.97653379	116.97637314	116.97823366
R7 / ANG	1.42631882	1.42631823	1.42631696	1.42631322	1.42629797
A7 / DEGREE	119.66572194	119.66623931	119.66661018	119.66693415	119.66763066
R8 / ANG	1.38798456	1.38798600	1.38798680	1.38798819	1.38799291
A8 / DEGREE	120.15960029	120.15890689	120.15862002	120.15862524	120.16021254
R9 / ANG	1.42291369	1.42291437	1.42291332	1.42291022	1.42289580
A9 / DEGREE	120.51165668	120.51205710	120.51210013	120.51179074	120.50937477
R10 / ANG	1.38828084	1.38828212	1.38828431	1.38828931	1.38830484
A10 / DEGREE	120.48222353	120.48219719	120.48226409	120.48250573	120.48366313
A11 / DEGREE	109.66794506	109.66676865	109.66596086	109.66473087	109.66263217
R12 / ANG	1.09578362	1.09578476	1.09578568	1.09578792	1.09579121
A12 / DEGREE	118.59670835	118.59670534	118.59661429	118.59630193	118.59598236
R13 / ANG	1.09554007	1.09554111	1.09554080	1.09553785	1.09553173
A13 / DEGREE	120.15759708	120.15715876	120.15719670	120.15758563	120.15787782
R14 / ANG	1.09460344	1.09460286	1.09460374	1.09460898	1.09462625
A14 / DEGREE	120.74772488	120.74905071	120.74928029	120.74878300	120.74597922
R15 / ANG	1.09459542	1.09459510	1.09459439	1.09459353	1.09459087
A15 / DEGREE	118.89338513	118.89249053	118.89187254	118.89062069	118.88679951
R16 / ANG	1.09485610	1.09485658	1.09485639	1.09485543	1.09485426
A16 / DEGREE	119.81880431	119.81856518	119.81851950	119.81890427	119.82188582
R17 / ANG	1.09491103	1.09491238	1.09491334	1.09491491	1.09491863
A17 / DEGREE	119.66551752	119.66575287	119.66591539	119.66618314	119.66604280
R18 / ANG	1.09625094	1.09625186	1.09625192	1.09625109	1.09624802
A18 / DEGREE	120.39020129	120.39017401	120.39012818	120.39020157	120.39027665

Optimized geometries along the MEP for 2-bromonaphthalene

Dihedral angles were fixed

2-bromonaphthalene

C
C, 1, r2
C, 2, r3, 1, a3
C, 3, r4, 2, a4, 1, d4
C, 4, r5, 3, a5, 2, d5
C, 5, r6, 4, a6, 3, d6
C, 1, r7, 2, a7, 3, d7
C, 7, r8, 1, a8, 2, d8
C, 8, r9, 7, a9, 1, d9
C, 9, r10, 8, a10, 7, d10
Br, 5, rsc(i), 4, a11, 3, d11
H, 3, r12, 2, a12, 1, d12
H, 4, r13, 3, a13, 2, d13
H, 6, r14, 5, a14, 4, d14
H, 7, r15, 1, a15, 2, d15
H, 8, r16, 7, a16, 1, d16
H, 9, r17, 8, a17, 7, d17
H, 10, r18, 9, a18, 8, d18

Distance C-Br	2.0	2.1	2.2	2.3	2.4
R2 / ANG	1.44037479	1.44098366	1.44147056	1.44191228	1.44227513
R3 / ANG	1.42641648	1.42680553	1.42709381	1.42741112	1.42767376
A3 / DEGREE	119.00642296	119.21038844	119.39803208	119.53786903	119.65320105
R4 / ANG	1.38861534	1.38965143	1.39052305	1.39151994	1.39244465
A4 / DEGREE	121.18750318	121.21486540	121.25076280	121.28198169	121.30716459
R5 / ANG	1.41744289	1.41350644	1.41022504	1.40731608	1.40487757
A5 / DEGREE	118.54446786	117.76044811	117.04573919	116.42438003	115.90085335
R6 / ANG	1.38327617	1.37970753	1.37661950	1.37390691	1.37160460
A6 / DEGREE	122.88959972	124.23722304	125.44635061	126.51587893	127.42316806
R7 / ANG	1.42656340	1.42641382	1.42623083	1.42612953	1.42604401
A7 / DEGREE	119.05071181	119.09889469	119.15430221	119.18946832	119.22124109
R8 / ANG	1.38821289	1.38820811	1.38823341	1.38824477	1.38826182
A8 / DEGREE	120.57056222	120.55074270	120.52251794	120.50262294	120.48355555
R9 / ANG	1.42247604	1.42239659	1.42231478	1.42224269	1.42217879
A9 / DEGREE	120.40497575	120.40663364	120.41211920	120.41794244	120.42329727
R10 / ANG	1.38829165	1.38822692	1.38818118	1.38814320	1.38811634
A10 / DEGREE	120.27828769	120.29168564	120.30352679	120.31312568	120.32224705
A11 / DEGREE	118.05389263	117.40645101	116.84221059	116.35713731	115.94763171
R12 / ANG	1.09605378	1.09608657	1.09611010	1.09615965	1.09621453
A12 / DEGREE	119.05793053	119.04888576	119.04369177	119.05163742	119.06466589
R13 / ANG	1.09281466	1.09233184	1.09198764	1.09172404	1.09156081
A13 / DEGREE	121.19390557	121.55150967	121.89649114	122.17283227	122.39491370
R14 / ANG	1.09394889	1.09344878	1.09310847	1.09282762	1.09265309
A14 / DEGREE	121.04028706	121.45838928	121.80364962	122.15761450	122.46925554
R15 / ANG	1.09579532	1.09573405	1.09565961	1.09560693	1.09556197
A15 / DEGREE	118.93973186	118.93903353	118.94788784	118.95222435	118.95730091
R16 / ANG	1.09487424	1.09485646	1.09484611	1.09483304	1.09482245
A16 / DEGREE	119.86463030	119.85871969	119.84701963	119.83711688	119.82789442
R17 / ANG	1.09477747	1.09475151	1.09471884	1.09469426	1.09467289
A17 / DEGREE	119.75728293	119.75492235	119.75143476	119.75018713	119.74866980
R18 / ANG	1.09592859	1.09589376	1.09586696	1.09583494	1.09580632
A18 / DEGREE	120.45594874	120.44513134	120.43674437	120.43115417	120.42670082

Distance C-Br	2.5	2.6	2.7	2.8	2.9
R2 / ANG	1.44256235	1.44279072	1.44293052	1.44299574	1.44299620
R3 / ANG	1.42788232	1.42801939	1.42811899	1.42818542	1.42822050
A3 / DEGREE	119.74631719	119.83279741	119.88491430	119.91566673	119.92755454
R4 / ANG	1.39327221	1.39394548	1.39453084	1.39497284	1.39527723
A4 / DEGREE	121.32400886	121.33201203	121.33243328	121.32203148	121.30556614
R5 / ANG	1.40290623	1.40149964	1.40040095	1.39967813	1.39943813
A5 / DEGREE	115.48233496	115.16018470	114.95132196	114.85544009	114.85506165
R6 / ANG	1.36972187	1.36839179	1.36731487	1.36656526	1.36624068
A6 / DEGREE	128.15571685	128.72083707	129.10008919	129.29012184	129.31134963
R7 / ANG	1.42597499	1.42589803	1.42585565	1.42583696	1.42585184
A7 / DEGREE	119.24907507	119.26647951	119.28502877	119.30544150	119.31368058
R8 / ANG	1.38828147	1.38829877	1.38831786	1.38833581	1.38834505
A8 / DEGREE	120.46697579	120.45990760	120.45194639	120.44412064	120.44539627
R9 / ANG	1.42212550	1.42207033	1.42204181	1.42203624	1.42204130
A9 / DEGREE	120.42690583	120.42807620	120.42510911	120.41891945	120.40957605
R10 / ANG	1.38809858	1.38808118	1.38807754	1.38808158	1.38808256
A10 / DEGREE	120.33106013	120.33541689	120.34477403	120.35589021	120.36465196
A11 / DEGREE	115.61928164	115.37266172	115.20609690	115.12354132	115.11613786
R12 / ANG	1.09627231	1.09631394	1.09636846	1.09642388	1.09648055
A12 / DEGREE	119.07985054	119.07750885	119.09082099	119.11235937	119.12332034
R13 / ANG	1.09148877	1.09145811	1.09150090	1.09164066	1.09181309
A13 / DEGREE	122.55744219	122.67533782	122.70997304	122.67850299	122.61526204
R14 / ANG	1.09257597	1.09254227	1.09258988	1.09274637	1.09293882
A14 / DEGREE	122.73591435	122.94956308	123.13392284	123.26778962	123.33342991
R15 / ANG	1.09552682	1.09549474	1.09548280	1.09548761	1.09550225
A15 / DEGREE	118.96231502	118.96794221	118.97033157	118.97119832	118.96942474
R16 / ANG	1.09481425	1.09480655	1.09480449	1.09480398	1.09480520
A16 / DEGREE	119.82045371	119.81314759	119.81240488	119.81613238	119.82257943
R17 / ANG	1.09465584	1.09464350	1.09463569	1.09463511	1.09463981
A17 / DEGREE	119.74681221	119.74731626	119.74387723	119.73849335	119.73454808
R18 / ANG	1.09578221	1.09576555	1.09575307	1.09574496	1.09574262
A18 / DEGREE	120.42301893	120.41996432	120.41773227	120.41455106	120.41263847

Distance C-Br	3.0	3.1	3.2	3.3	3.4
R2 / ANG	1.44298675	1.44286177	1.44273410	1.44259363	1.44245449
R3 / ANG	1.42829362	1.42820368	1.42816678	1.42812923	1.42809743
A3 / DEGREE	119.94422487	119.94107410	119.92645783	119.90509232	119.88085286
R4 / ANG	1.39552807	1.39556188	1.39555847	1.39549310	1.39539131
A4 / DEGREE	121.26949562	121.24189868	121.20526484	121.16751012	121.13125632
R5 / ANG	1.39952224	1.39996310	1.40059891	1.40136274	1.40215864
A5 / DEGREE	114.93013771	115.08160470	115.28864555	115.52246799	115.75763458
R6 / ANG	1.36620337	1.36654869	1.36705878	1.36769637	1.36837271
A6 / DEGREE	129.21395109	128.96870358	128.63563418	128.25654185	127.87436854
R7 / ANG	1.42587891	1.42589470	1.42593063	1.42597254	1.42601478
A7 / DEGREE	119.30978819	119.30766036	119.29584419	119.27953537	119.26108642
R8 / ANG	1.38834538	1.38834728	1.38834572	1.38834299	1.38833951
A8 / DEGREE	120.46003365	120.47235095	120.49142118	120.51270353	120.53418718
R9 / ANG	1.42204885	1.42206893	1.42209470	1.42212215	1.42214813
A9 / DEGREE	120.39550096	120.38246891	120.36914004	120.35713258	120.34693021
R10 / ANG	1.38807381	1.38806704	1.38805764	1.38804658	1.38803443
A10 / DEGREE	120.36917079	120.37168702	120.37059903	120.36642307	120.36023960
A11 / DEGREE	115.16828950	115.27945083	115.44271208	115.62931013	115.81818122
R12 / ANG	1.09653155	1.09656016	1.09659203	1.09661843	1.09663922
A12 / DEGREE	119.11474784	119.11314614	119.10186826	119.08720220	119.07097640
R13 / ANG	1.09205375	1.09225661	1.09251135	1.09277612	1.09303556
A13 / DEGREE	122.52433426	122.37303895	122.20462095	122.03015342	121.86386663
R14 / ANG	1.09319760	1.09343328	1.09371472	1.09400372	1.09428382
A14 / DEGREE	123.36557763	123.34662341	123.30199065	123.23580614	123.16024121
R15 / ANG	1.09553070	1.09555390	1.09559441	1.09563891	1.09568335
A15 / DEGREE	118.96323371	118.95958203	118.95182258	118.94315976	118.93444384
R16 / ANG	1.09480811	1.09481679	1.09482950	1.09484541	1.09486269
A16 / DEGREE	119.83148294	119.84140138	119.85202081	119.86198664	119.87073379
R17 / ANG	1.09465310	1.09466672	1.09468607	1.09470724	1.09472833
A17 / DEGREE	119.73330575	119.73124099	119.73113956	119.73240158	119.73456871
R18 / ANG	1.09574979	1.09576392	1.09578613	1.09581334	1.09584257
A18 / DEGREE	120.40886371	120.40576696	120.40174432	120.39737630	120.39305216

Distance C-Br	3.5	3.75	4.0	4.25	4.5
R2 / ANG	1.44227446	1.44214315	1.44190191	1.44182192	1.44176391
R3 / ANG	1.42801679	1.42811401	1.42800229	1.42800454	1.42800548
A3 / DEGREE	119.85109895	119.81037484	119.76645834	119.74848742	119.73342322
R4 / ANG	1.39528080	1.39498129	1.39478028	1.39470688	1.39463714
A4 / DEGREE	121.10433884	121.03153311	120.99721545	120.97622669	120.96403325
R5 / ANG	1.40293407	1.40441710	1.40546416	1.40592556	1.40625092
A5 / DEGREE	115.97376687	116.40132801	116.66754137	116.81187128	116.90734429
R6 / ANG	1.36902481	1.37031314	1.37108992	1.37153973	1.37185187
A6 / DEGREE	127.51673389	126.83358149	126.40368086	126.16939108	126.01395961
R7 / ANG	1.42607486	1.42609622	1.42619407	1.42622286	1.42623569
A7 / DEGREE	119.24374302	119.20141678	119.17648952	119.16058068	119.15269643
R8 / ANG	1.38833092	1.38834812	1.38832324	1.38832168	1.38831799
A8 / DEGREE	120.55240574	120.59630873	120.62081905	120.63573970	120.64220450
R9 / ANG	1.42217786	1.42218636	1.42223366	1.42224833	1.42226456
A9 / DEGREE	120.33837194	120.32479808	120.31539261	120.31128904	120.31036119
R10 / ANG	1.38802086	1.38801322	1.38797974	1.38796775	1.38795979
A10 / DEGREE	120.35413849	120.33577034	120.32520870	120.31834577	120.31427235
A11 / DEGREE	115.99538271	116.40656904	113.59239860	113.67525120	113.73783807
R12 / ANG	1.09665825	1.09667773	1.09668479	1.09669777	1.09669967
A12 / DEGREE	119.06247469	119.01236653	119.00719959	118.99209897	118.98456889
R13 / ANG	1.09324102	1.09378411	1.09403160	1.09420302	1.09431743
A13 / DEGREE	121.70481399	121.44690678	121.26828335	121.17421259	121.10949370
R14 / ANG	1.09450897	1.09507583	1.09535816	1.09552244	1.09563431
A14 / DEGREE	123.09609585	122.91587809	122.85037567	122.78791454	122.74957161
R15 / ANG	1.09571890	1.09581195	1.09585548	1.09588807	1.09591415
A15 / DEGREE	118.92698119	118.91089911	118.90111842	118.89534863	118.89418691
R16 / ANG	1.09487882	1.09491623	1.09493940	1.09495260	1.09495917
A16 / DEGREE	119.87959176	119.88838369	119.89952227	119.90331632	119.90350084
R17 / ANG	1.09474718	1.09478694	1.09480955	1.09482437	1.09483422
A17 / DEGREE	119.73632142	119.74522836	119.74723073	119.75064045	119.75315106
R18 / ANG	1.09586574	1.09593503	1.09596538	1.09598843	1.09600557
A18 / DEGREE	120.38990861	120.37954880	120.37671858	120.37398248	120.37312916

Distance C-Br	4.75	5.0	5.5	6.0	7.0
R2 / ANG	1.44174228	1.44173530	1.44173733	1.44174076	1.44174539
R3 / ANG	1.42800946	1.42802299	1.42802712	1.42803008	1.42802951
A3 / DEGREE	119.72747494	119.72299087	119.72183655	119.72050008	119.71992413
R4 / ANG	1.39461150	1.39459519	1.39459146	1.39459186	1.39459409
A4 / DEGREE	120.95814366	120.95009400	120.94797739	120.94619401	120.94528535
R5 / ANG	1.40637086	1.40645282	1.40646201	1.40645937	1.40645405
A5 / DEGREE	116.94802941	116.98708768	116.99514514	117.00165436	117.00446596
R6 / ANG	1.37196729	1.37204688	1.37205518	1.37205394	1.37205366
A6 / DEGREE	125.94893469	125.89050241	125.87957285	125.87129201	125.86795394
R7 / ANG	1.42624848	1.42626502	1.42627020	1.42627577	1.42627919
A7 / DEGREE	119.14656986	119.13869560	119.13665530	119.13422303	119.13304450
R8 / ANG	1.38831963	1.38832342	1.38832440	1.38832594	1.38832619
A8 / DEGREE	120.64829391	120.65646943	120.65868713	120.66137539	120.66274900
R9 / ANG	1.42226589	1.42226523	1.42226571	1.42226565	1.42226659
A9 / DEGREE	120.30817386	120.30513567	120.30425763	120.30320542	120.30267316
R10 / ANG	1.38795789	1.38795712	1.38795763	1.38795836	1.38795837
A10 / DEGREE	120.31212928	120.30959039	120.30896043	120.30817223	120.30777197
A11 / DEGREE	113.76752486	113.79626477	113.80191179	113.80612794	113.80774009
R12 / ANG	1.09670488	1.09671671	1.09672061	1.09672501	1.09672746
A12 / DEGREE	118.97969302	118.97248992	118.97083687	118.96899878	118.96825099
R13 / ANG	1.09435828	1.09438676	1.09438757	1.09438440	1.09438261
A13 / DEGREE	121.08443192	121.06565832	121.06446501	121.06579220	121.06731770
R14 / ANG	1.09567442	1.09570338	1.09570452	1.09570205	1.09570066
A14 / DEGREE	122.73151832	122.70981915	122.70301258	122.69572647	122.69149896
R15 / ANG	1.09592304	1.09593421	1.09593747	1.09593993	1.09594146
A15 / DEGREE	118.89170255	118.88800202	118.88682031	118.88512073	118.88411672
R16 / ANG	1.09496424	1.09497058	1.09497249	1.09497486	1.09497627
A16 / DEGREE	119.90559622	119.90822403	119.90888576	119.90983536	119.91029124
R17 / ANG	1.09483876	1.09484453	1.09484636	1.09484846	1.09484979
A17 / DEGREE	119.75399845	119.75529864	119.75567391	119.75600111	119.75618667
R18 / ANG	1.09601262	1.09602155	1.09602461	1.09602756	1.09602960
A18 / DEGREE	120.37207198	120.37051544	120.37003944	120.36939472	120.36906118

Distance C-Br	8.0	10.0	12.5	15.0	20.0
R2 / ANG	1.44175279	1.44176554	1.44179099	1.44184818	1.44199800
R3 / ANG	1.42802488	1.42801267	1.42798762	1.42793901	1.42778574
A3 / DEGREE	119.71933587	119.71918200	119.71929025	119.72154603	119.71474032
R4 / ANG	1.39460097	1.39461458	1.39464373	1.39471513	1.39489497
A4 / DEGREE	120.94476112	120.94461941	120.94465409	120.94265781	120.94506856
R5 / ANG	1.40644430	1.40643003	1.40640498	1.40635618	1.40627185
A5 / DEGREE	117.00626694	117.00669936	117.00668939	117.00854887	117.01612420
R6 / ANG	1.37205415	1.37205987	1.37207330	1.37209682	1.37209015
A6 / DEGREE	125.86591005	125.86550062	125.86559451	125.86447148	125.84712383
R7 / ANG	1.42628234	1.42628411	1.42628454	1.42628653	1.42633893
A7 / DEGREE	119.13189334	119.13140824	119.13129757	119.13282887	119.13032863
R8 / ANG	1.38832623	1.38832478	1.38832214	1.38831673	1.38830507
A8 / DEGREE	120.66409420	120.66477346	120.66515851	120.66454526	120.66749612
R9 / ANG	1.42226794	1.42227084	1.42227625	1.42228995	1.42228935
A9 / DEGREE	120.30221544	120.30202214	120.30205027	120.30204807	120.30223213
R10 / ANG	1.38795770	1.38795527	1.38794999	1.38794124	1.38794855
A10 / DEGREE	120.30736094	120.30729806	120.30745352	120.30879313	120.30674498
A11 / DEGREE	113.80867267	113.80869993	113.80831863	113.80831490	113.81414367
R12 / ANG	1.09672961	1.09673084	1.09673244	1.09674295	1.09678151
A12 / DEGREE	118.96777290	118.96819168	118.96949154	118.97272326	118.98148204
R13 / ANG	1.09438078	1.09437995	1.09437925	1.09437231	1.09432084
A13 / DEGREE	121.06872602	121.06878565	121.06749892	121.06446287	121.05018013
R14 / ANG	1.09569953	1.09570050	1.09570585	1.09572230	1.09574880
A14 / DEGREE	122.68783177	122.68556323	122.68285696	122.67595799	122.65838291
R15 / ANG	1.09594250	1.09594305	1.09594382	1.09594819	1.09596373
A15 / DEGREE	118.88298665	118.88221540	118.88128265	118.88023096	118.87703661
R16 / ANG	1.09497765	1.09497832	1.09497833	1.09497730	1.09497744
A16 / DEGREE	119.91079742	119.91112492	119.91152593	119.91189783	119.91261060
R17 / ANG	1.09485114	1.09485192	1.09485235	1.09485165	1.09485323
A17 / DEGREE	119.75630496	119.75622642	119.75599557	119.75541306	119.75615594
R18 / ANG	1.09603148	1.09603289	1.09603467	1.09603888	1.09603371
A18 / DEGREE	120.36873246	120.36864386	120.36862277	120.36961384	120.36752433