

Supplementary Information for

Oxidative addition of C–I bond on aluminum nanoclusters

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Cartesian coordinates for the optimized structures and harmonic frequencies in cm^{-1} .

$\text{Al}_3 \dots \text{C}_2\text{H}_5\text{I}$ (M062X/TZVP, LANL2DZ level of theory)

Reactant optimized geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.519309	0.090764	-1.270445
2	13	0	3.756342	0.846369	-0.484031
3	13	0	2.278066	-0.437632	1.158000
4	6	0	-1.471668	1.319835	1.006452
5	6	0	-1.668765	2.351913	-0.075863
6	1	0	-0.497045	1.394033	1.482564
7	1	0	-1.669732	3.344982	0.380966
8	1	0	-0.857233	2.319722	-0.804300
9	1	0	-2.614936	2.212432	-0.597474
10	1	0	-2.260375	1.321268	1.751620
11	53	0	-1.509694	-0.706199	0.194044

Low frequencies (cm^{-1}): 15.5864 31.2037 32.2296
46.3841 76.2302 92.2754

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.147854	-0.942350	-0.374098
2	13	0	3.319124	0.105899	-1.054777
3	13	0	2.779371	0.154797	1.489428
4	6	0	-1.740387	1.914644	0.183683
5	6	0	-0.514883	2.543475	-0.365042
6	1	0	-1.896564	1.984788	1.253735
7	1	0	-0.473813	3.601926	-0.088313
8	1	0	0.399057	2.081687	0.037725
9	1	0	-0.469826	2.468082	-1.451953
10	1	0	-2.648912	1.973437	-0.402242
11	53	0	-1.426054	-0.565983	0.017963

Low frequencies (cm^{-1}): -362.5345 24.6195 34.2472
44.5154 63.7185 83.4455

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	13	0	0.168081	0.883227	0.033298
2	13	0	-2.482281	0.159843	-0.299708
3	13	0	-1.704179	2.543560	0.079677
4	6	0	-3.660059	-1.408545	-0.511689
5	6	0	-4.712680	-1.500854	0.605514
6	1	0	-3.044297	-2.313328	-0.529404
7	1	0	-5.367345	-2.364893	0.474056
8	1	0	-4.247609	-1.593799	1.589279
9	1	0	-5.349839	-0.614184	0.632612
10	1	0	-4.148642	-1.356675	-1.489716
11	53	0	2.351568	-0.394847	0.022411

Low frequencies (cm⁻¹): 28.5723 45.1573 55.5322
58.0566 94.0193 159.0976

Al₃ C₂H₃I (B3PW91/TZVP, LANL2DZ level of theory)

Reactant optimized geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.612522	-0.249456	-0.860435
2	13	0	3.883740	0.675308	-0.630411
3	13	0	2.868423	-0.522300	1.382519
4	6	0	-1.501207	1.350954	0.889898
5	6	0	-1.847469	2.466364	-0.057386
6	1	0	-0.488529	1.420864	1.282000
7	1	0	-1.829216	3.410060	0.498856
8	1	0	-1.122545	2.546182	-0.868822
9	1	0	-2.843462	2.347910	-0.486134
10	1	0	-2.215736	1.226729	1.699220
11	53	0	-1.512252	-0.615129	-0.107772

Low frequencies (cm⁻¹): 17.9104 24.3624 28.0112
39.7559 50.9824 85.4436

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.218589	-0.756153	-0.316367
2	13	0	3.366903	0.211563	-1.113292
3	13	0	3.026975	0.070088	1.440409
4	6	0	-1.901153	1.761638	0.319450
5	6	0	-0.793199	2.555117	-0.266964

6	1	0	-1.981039	1.772339	1.401815
7	1	0	-0.842677	3.585859	0.103518
8	1	0	0.195644	2.167418	0.024961
9	1	0	-0.835024	2.579977	-1.356955
10	1	0	-2.863965	1.809141	-0.177888
11	53	0	-1.442809	-0.597108	-0.008493

 Low frequencies (cm⁻¹): -232.0238 11.5189 37.0917
 41.3360 63.9515 72.2028

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.196584	0.869450	-0.000272
2	13	0	-2.464417	0.103279	-0.057739
3	13	0	-1.684722	2.513330	0.006181
4	6	0	-3.606825	-1.519844	-0.108116
5	6	0	-5.101702	-1.266768	0.126822
6	1	0	-3.217202	-2.223302	0.638427
7	1	0	-5.678226	-2.195947	0.087203
8	1	0	-5.289790	-0.814031	1.104151
9	1	0	-5.524541	-0.594862	-0.625048
10	1	0	-3.450897	-2.006993	-1.078846
11	53	0	2.392359	-0.391773	0.008220

 Low frequencies (cm⁻¹): 4.8641 35.3897 62.2832
 70.6395 79.0590 154.2336

Al₃ C₂H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	2.064621	0.069160	-1.133321
2	13	0	4.315253	0.650110	-0.175131
3	13	0	2.747608	-0.815231	1.187117
4	6	0	-1.609301	1.300177	0.929280
5	6	0	-1.995706	2.452322	0.042933
6	1	0	-0.597795	1.376569	1.293722
7	1	0	-1.959375	3.370109	0.624478
8	1	0	-1.314307	2.558774	-0.791678
9	1	0	-2.999771	2.339705	-0.346190
10	1	0	-2.286963	1.161665	1.755366

11 53 0 -1.657906 -0.605176 -0.128144

Low frequencies (cm⁻¹): 8.9337 18.9867 21.2675
28.0830 35.4792 63.0301

Coordinate of TS

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

1 13 0 1.016002 -1.214427 -0.110394
2 13 0 3.000425 -0.034909 -1.228729
3 13 0 2.882616 0.097153 1.360797
4 6 0 -1.390562 2.099868 -0.012451
5 6 0 -0.005743 2.539871 -0.144235
6 1 0 -1.876480 2.201710 0.939058
7 1 0 0.286179 3.203444 0.660576
8 1 0 0.717848 1.681869 -0.086464
9 1 0 0.186081 3.012216 -1.098721
10 1 0 -2.045060 2.176503 -0.859084
11 53 0 -1.482609 -0.474260 0.020811

Low frequencies (cm⁻¹): -122.2417 34.6578 43.5606
55.6969 61.3758 134.0113

Optimized geometry after C-I dissociation

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

1 13 0 0.181778 0.866517 0.014330
2 13 0 -2.506031 0.189632 -0.246716
3 13 0 -1.658255 2.548781 0.075967
4 6 0 -3.693077 -1.370194 -0.489355
5 6 0 -4.809138 -1.505532 0.550154
6 1 0 -3.072995 -2.265609 -0.489578
7 1 0 -5.428909 -2.376550 0.360171
8 1 0 -4.412663 -1.608368 1.555399
9 1 0 -5.465249 -0.640685 0.551663
10 1 0 -4.121421 -1.312720 -1.489076
11 53 0 2.363908 -0.403883 0.022266

Low frequencies (cm⁻¹): 17.6379 42.0571 63.2690
68.0642 92.2068 158.5390

Al₃ C₂H₃I (M062X/TZVP, LANL2DZ level of theory)

Reactant optimized geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	2.426670	1.297453	0.012143
2	13	0	1.691839	-1.207514	0.023703
3	13	0	4.093343	-0.616029	-0.012343
4	6	0	-1.094417	1.466142	0.527112
5	6	0	-0.640063	2.351226	-0.343430
6	1	0	-0.609473	2.167251	-1.410214
7	1	0	-0.303035	3.319616	0.010453
8	1	0	-1.136530	1.629280	1.594126
9	53	0	-1.779210	-0.437381	-0.030226

Low frequencies (cm⁻¹): 22.6802 36.9542 39.8806
 44.0451 73.6529 114.0207

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.595522	0.039812	-0.004564
2	13	0	-3.838357	-1.184129	0.263477
3	13	0	-3.869276	1.231608	-0.030152
4	6	0	3.535360	-0.205785	-0.208964
5	6	0	4.253149	0.347811	0.737266
6	1	0	3.805933	0.883679	1.567434
7	1	0	5.339741	0.285467	0.718949
8	1	0	3.859987	-0.762816	-1.077675
9	53	0	1.154798	-0.045156	-0.138725

Low frequencies (cm⁻¹): -253.0738 18.2910 32.8905
 54.2218 73.9196 82.7070

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.085358	0.824867	0.002624
2	13	0	-2.551389	0.009086	-0.037949
3	13	0	-1.833317	2.434392	0.000182
4	6	0	-3.701278	-1.572163	-0.052391
5	6	0	-5.023181	-1.425099	0.071031

6	1	0	-5.492073	-0.449707	0.183399
7	1	0	-5.711032	-2.266806	0.067696
8	1	0	-3.323478	-2.587531	-0.158937
9	53	0	2.316318	-0.362280	0.004771

 Low frequencies (cm⁻¹): 38.1472 43.8860 58.4384
 70.4151 95.3583 152.9613

Al₃ C₂H₃I (B3PW91/TZVP, LANL2DZ level of theory)

Reactant optimized geometry

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	3.022611	-0.322474	1.401899	
2	13	0	3.053118	-0.930044	-1.045717	
3	13	0	3.045152	1.493048	-0.347107	
4	6	0	-3.277613	-0.287667	0.002145	
5	6	0	-4.099533	0.745401	-0.002684	
6	1	0	-3.756301	1.772988	-0.009416	
7	1	0	-5.172795	0.577985	0.000099	
8	1	0	-3.614258	-1.316048	0.008857	
9	53	0	-1.165382	-0.130344	-0.002156	

 Low frequencies (cm⁻¹): 18.6641 10.9623 14.5503
 26.7839 35.0649 35.7510

Coordinate of TS

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	1.606446	0.003781	-0.001064	
2	13	0	3.845388	1.227693	0.100629	
3	13	0	3.844645	-1.217107	0.153198	
4	6	0	-3.551601	-0.030347	-0.260499	
5	6	0	-4.275338	0.054872	0.828588	
6	1	0	-3.842695	0.138530	1.820521	
7	1	0	-5.364339	0.044201	0.770516	
8	1	0	-3.862971	-0.116922	-1.293290	
9	53	0	-1.147596	-0.007542	-0.150796	

 Low frequencies (cm⁻¹): -219.2564 7.3363 10.8490
 23.6434 63.5098 86.5933

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.087197	0.837478	0.000880
2	13	0	-2.560820	0.050456	-0.000958
3	13	0	-1.810653	2.466736	-0.000097
4	6	0	-3.681504	-1.560908	-0.000284
5	6	0	-5.017586	-1.498014	0.000775
6	1	0	-5.559139	-0.553847	0.001120
7	1	0	-5.646522	-2.386726	0.001335
8	1	0	-3.234634	-2.556498	-0.000508
9	53	0	2.308121	-0.372832	-0.000049

Low frequencies (cm⁻¹): 17.6073 36.1267 63.3411
75.5139 84.5415 156.8040

Al₃ C₂H₃I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-2.723164	1.286148	-0.203915
2	13	0	-2.157990	-1.205355	0.019307
3	13	0	-4.554473	-0.437360	0.094316
4	6	0	1.543697	1.526381	-0.395514
5	6	0	1.037251	2.358455	0.481902
6	1	0	0.796352	2.075136	1.490098
7	1	0	0.853902	3.381110	0.197652
8	1	0	1.788714	1.802911	-1.402293
9	53	0	1.957330	-0.489298	0.006981

Low frequencies (cm⁻¹): 5.2281 22.3763 23.6223
27.3595 31.5191 59.9244

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.657892	0.002547	0.022350
2	13	0	3.962030	1.247625	0.038647
3	13	0	3.962127	-1.242282	0.061251
4	6	0	-3.518610	-0.015890	-0.421170

5	6	0	-4.358039	0.028085	0.576649
6	1	0	-4.039843	0.071554	1.604056
7	1	0	-5.423750	0.021989	0.397758
8	1	0	-3.744452	-0.060374	-1.469713
9	53	0	-1.209409	-0.003942	-0.057627

 Low frequencies (cm⁻¹): -286.9154 9.6565 17.4843
 23.8661 72.7740 73.2770

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.088194	0.803125	0.000045
2	13	0	-2.582728	0.043718	-0.000001
3	13	0	-1.794835	2.440106	-0.000026
4	6	0	-3.731206	-1.537067	-0.000036
5	6	0	-5.056666	-1.447397	0.000028
6	1	0	-5.573625	-0.499574	0.000104
7	1	0	-5.699113	-2.315010	0.000007
8	1	0	-3.313087	-2.535395	-0.000110
9	53	0	2.322167	-0.367426	-0.000003

 Low frequencies (cm⁻¹): 22.6896 37.9963 65.8635
 78.7546 91.5416 155.0018

Al₃ C₆H₅I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	2.190142	-1.593684	0.000023
2	13	0	2.326024	0.999896	-0.000018
3	13	0	4.390212	-0.454671	-0.000005
4	6	0	-1.129969	0.696875	-0.000001
5	6	0	-1.003444	1.366834	1.209529
6	6	0	-0.775696	2.738561	1.201504
7	6	0	-0.663680	3.425475	0.000011
8	6	0	-0.775695	2.738572	-1.201489
9	6	0	-1.003446	1.366843	-1.209526
10	1	0	-1.088358	0.831991	2.145925
11	1	0	-0.676341	3.264052	2.142457
12	1	0	-0.482743	4.492207	0.000016
13	1	0	-0.676338	3.264071	-2.142437
14	1	0	-1.088359	0.832007	-2.145927
15	53	0	-1.503004	-1.378365	-0.000004

Low frequencies (cm⁻¹): 16.0116 34.3228 36.0911
 38.1985 60.8072 64.3629

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-2.257699	-0.370295	-0.292727
2	13	0	-2.689511	1.715988	1.459295
3	13	0	-3.479645	1.701592	-1.040680
4	6	0	1.744096	0.122281	-0.032888
5	6	0	1.310419	1.410176	-0.192204
6	6	0	2.270507	2.420073	-0.232843
7	6	0	3.617671	2.101069	-0.111860
8	6	0	4.015958	0.778707	0.048578
9	6	0	3.065210	-0.240407	0.089665
10	1	0	0.248914	1.643616	-0.289843
11	1	0	1.963606	3.451623	-0.359770
12	1	0	4.362037	2.886459	-0.144562
13	1	0	5.067797	0.536087	0.142705
14	1	0	3.365462	-1.274326	0.213635
15	53	0	-0.030224	-1.630369	0.026238

Low frequencies (cm⁻¹): -178.3803 15.0783 29.6036
 36.3005 45.0782 68.9862

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.427025	1.106665	0.008094
2	13	0	1.322700	1.298544	0.018889
3	13	0	-0.223282	3.301288	0.080165
4	6	0	2.892793	0.127631	0.004845
5	6	0	2.758087	-1.259857	0.147636
6	6	0	3.866066	-2.097382	0.142484
7	6	0	5.138731	-1.559815	-0.005672
8	6	0	5.299712	-0.187488	-0.149155
9	6	0	4.187063	0.643608	-0.143639
10	1	0	1.773566	-1.704384	0.266119
11	1	0	3.738294	-3.167179	0.254157
12	1	0	6.004757	-2.210055	-0.009504
13	1	0	6.291098	0.233201	-0.265349
14	1	0	4.339446	1.712993	-0.257755
15	53	0	-3.070622	-0.812249	-0.025653

Low frequencies (cm⁻¹): 15.7963 19.4106 45.0489
 52.1904 62.2680 139.6541

28.3708 43.4648 47.6266

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.437168	1.102069	-0.004451
2	13	0	-1.321253	1.265409	-0.008947
3	13	0	0.209730	3.279481	-0.017667
4	6	0	-2.913731	0.110249	-0.003930
5	6	0	-2.803617	-1.287790	-0.039919
6	6	0	-3.929666	-2.101208	-0.035746
7	6	0	-5.196691	-1.531129	0.004632
8	6	0	-5.333797	-0.148616	0.040778
9	6	0	-4.204045	0.659666	0.036475
10	1	0	-1.824739	-1.759708	-0.071858
11	1	0	-3.820048	-3.180062	-0.063827
12	1	0	-6.077103	-2.164519	0.008004
13	1	0	-6.321639	0.298560	0.072419
14	1	0	-4.338944	1.738101	0.065330
15	53	0	3.102611	-0.802828	0.007170

Low frequencies (cm⁻¹): 8.0226 22.2909 45.7255
61.2105 62.8176 144.2999

Al₃ C₆H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	2.800763	-1.358936	0.001832
2	13	0	2.655527	1.199276	-0.004517
3	13	0	4.900543	0.040187	0.001272
4	6	0	-1.416257	0.577873	0.000406
5	6	0	-1.399312	1.258310	1.201626
6	6	0	-1.371618	2.640757	1.195607
7	6	0	-1.359606	3.334401	0.001394
8	6	0	-1.373050	2.641658	-1.193316
9	6	0	-1.400757	1.259213	-1.200327
10	1	0	-1.409218	0.723671	2.132782
11	1	0	-1.358554	3.171557	2.130607
12	1	0	-1.338276	4.409124	0.001770
13	1	0	-1.361137	3.173156	-2.127926
14	1	0	-1.411818	0.725273	-2.131862
15	53	0	-1.468608	-1.526847	-0.000365

Low frequencies (cm⁻¹): 8.7789 15.1250 19.2197
 19.3653 23.8769 25.9248

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-2.732122	-0.003100	-0.003195
2	13	0	-4.993791	0.171954	-1.212480
3	13	0	-4.985568	-0.167992	1.218505
4	6	0	2.468500	0.000383	0.000035
5	6	0	3.126195	-1.197948	-0.122749
6	6	0	4.511902	-1.189981	-0.121184
7	6	0	5.201159	0.001820	0.001591
8	6	0	4.510492	1.192887	0.123547
9	6	0	3.124767	1.199384	0.123563
10	1	0	2.587191	-2.122796	-0.218448
11	1	0	5.049106	-2.117363	-0.216166
12	1	0	6.276391	0.002382	0.002232
13	1	0	5.046604	2.120851	0.219163
14	1	0	2.584559	2.123653	0.218506
15	53	0	0.114100	-0.001079	-0.001338

Low frequencies (cm⁻¹): -251.2043 11.2847 11.3261
 13.8275 59.3160 80.6975

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.427054	1.073292	-0.001757
2	13	0	-1.344008	1.243105	-0.004167
3	13	0	0.195583	3.241679	-0.007383
4	6	0	-2.937479	0.105443	-0.001851
5	6	0	-2.838591	-1.286339	-0.016929
6	6	0	-3.962782	-2.089388	-0.014926
7	6	0	-5.219792	-1.514745	0.002286
8	6	0	-5.347798	-0.138637	0.017433
9	6	0	-4.218869	0.657792	0.015348
10	1	0	-1.870905	-1.761802	-0.030483
11	1	0	-3.859851	-3.160150	-0.026666
12	1	0	-6.096778	-2.137540	0.003918
13	1	0	-6.324854	0.311393	0.030854
14	1	0	-4.347709	1.728242	0.027425
15	53	0	3.132638	-0.785658	0.003014

Low frequencies (cm⁻¹): 2.1516 21.9165 48.9418

63.6062

65.7025

144.4903

Al₅ ... C₂H₅I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	3.762295	0.880132	-1.087347
2	13	0	4.639210	-1.252023	0.065170
3	13	0	1.608102	1.803435	-0.339675
4	13	0	2.407079	-0.502747	0.887847
5	13	0	0.226379	0.558673	1.600092
6	6	0	-3.446202	0.596253	0.506875
7	6	0	-3.280023	1.978751	-0.076979
8	1	0	-3.247267	0.564657	1.574656
9	1	0	-4.015119	2.648440	0.376632
10	1	0	-2.286447	2.379024	0.129481
11	1	0	-3.435337	1.978664	-1.155226
12	1	0	-4.415406	0.155548	0.297262
13	53	0	-2.011376	-0.802141	-0.347949

Low frequencies (cm⁻¹): 11.2343 22.5803 34.2973
 41.4189 45.8560 72.8031

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	4.174734	0.603186	-1.019996
2	13	0	4.837978	-0.689086	1.051882
3	13	0	1.796337	1.172525	-1.257718
4	13	0	2.363502	-0.527423	0.837431
5	13	0	0.062841	0.272055	0.554849
6	6	0	-3.684180	1.116350	0.512282
7	6	0	-2.808873	2.107597	1.185024
8	1	0	-4.333326	0.519188	1.139952
9	1	0	-3.407120	2.944384	1.560922
10	1	0	-2.283265	1.675159	2.041200
11	1	0	-2.063562	2.526193	0.501990
12	1	0	-4.119074	1.401664	-0.437461
13	53	0	-2.205574	-0.739936	-0.323665

Low frequencies (cm⁻¹): -419.7713 18.2885 27.4023
 35.8857 44.7678 68.3376

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	3.651713	-0.582773	-0.984065
2	13	0	1.744635	-2.337706	-0.576847
3	13	0	2.113996	-0.792441	1.585389
4	13	0	1.794304	1.154549	0.109306
5	13	0	-0.164257	-0.773587	0.719524
6	6	0	1.351004	2.963262	-0.536148
7	6	0	0.210868	3.615547	0.258754
8	1	0	1.080135	2.877861	-1.593561
9	1	0	-0.037146	4.604830	-0.132596
10	1	0	-0.698062	3.010960	0.223899
11	1	0	0.476879	3.736877	1.310533
12	1	0	2.251668	3.582417	-0.506629
13	53	0	-2.476788	-0.263591	-0.164722

Low frequencies (cm⁻¹): 6.7622 35.9549 38.6210
43.8496 75.5636 90.5252

Al₅ C₂H₃I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	4.116497	0.699446	-0.966253
2	13	0	4.770886	-1.327353	0.467421
3	13	0	1.940359	1.799288	-0.548536
4	13	0	2.431020	-0.532727	0.873751
5	13	0	0.320283	0.796881	1.255278
6	6	0	-3.656415	-0.065754	0.888756
7	6	0	-4.213264	1.312345	0.649024
8	1	0	-3.188274	-0.174172	1.863993
9	1	0	-5.007977	1.501748	1.378916
10	1	0	-3.453089	2.084564	0.775415
11	1	0	-4.643063	1.409814	-0.348719
12	1	0	-4.385317	-0.857787	0.739591
13	53	0	-2.049657	-0.568032	-0.522594

Low frequencies (cm⁻¹): 14.1306 19.9839 21.6705
34.2336 47.7104 52.5120

Coordinate of TS

Center	Atomic	Atomic	Coordinates (Angstroms)		
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Number	Number	Type	X	Y	Z
1	13	0	4.171564	0.614040	-0.974379
2	13	0	4.825349	-0.791906	1.017459
3	13	0	1.798739	1.289468	-1.192474
4	13	0	2.341454	-0.534467	0.869993
5	13	0	0.067107	0.389975	0.552868
6	6	0	-3.697085	0.863359	0.817164
7	6	0	-2.956144	2.114035	1.077461
8	1	0	-3.920587	0.234159	1.671629
9	1	0	-3.420815	2.672540	1.898106
10	1	0	-1.917043	1.917103	1.412096
11	1	0	-2.901221	2.758887	0.199727
12	1	0	-4.477422	0.878643	0.066170
13	53	0	-2.171666	-0.733927	-0.380577

Low frequencies (cm⁻¹): -246.3776 19.2051 25.8634
48.8835 71.4887 74.3242

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	3.490025	-1.115249	-1.022140
2	13	0	1.405780	-2.578675	-0.425760
3	13	0	1.895074	-0.939494	1.639162
4	13	0	2.112592	0.965001	0.034278
5	13	0	-0.292505	-0.633124	0.631002
6	6	0	2.067681	2.869161	-0.526138
7	6	0	1.099478	3.770621	0.244837
8	1	0	1.837533	2.882383	-1.598650
9	1	0	1.142941	4.804199	-0.113837
10	1	0	0.064435	3.435322	0.142560
11	1	0	1.326980	3.789589	1.313813
12	1	0	3.095330	3.243189	-0.445896
13	53	0	-2.611561	-0.039120	-0.165005

Low frequencies (cm⁻¹): 20.2245 32.0998 45.3815
55.3671 81.5519 98.7903

Al₅ C₂H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	4.286462	0.611448	-1.101083

2	13	0	4.988837	-1.383098	0.384933
3	13	0	2.147793	1.766432	-0.669427
4	13	0	2.723012	-0.428715	0.948513
5	13	0	0.632924	0.963355	1.309154
6	6	0	-3.785442	0.292712	0.862555
7	6	0	-4.302716	1.565172	0.248281
8	1	0	-3.274217	0.459350	1.796580
9	1	0	-5.037338	2.006931	0.916888
10	1	0	-3.509865	2.286907	0.097617
11	1	0	-4.782764	1.382071	-0.704716
12	1	0	-4.556042	-0.447709	0.999689
13	53	0	-2.310155	-0.692780	-0.398269

 Low frequencies (cm⁻¹): 4.4557 12.6221 13.6534
 22.8792 26.8167 34.6591

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	4.201408	0.553501	-0.914500
2	13	0	4.849139	-0.668653	1.232804
3	13	0	1.862747	1.463185	-1.211951
4	13	0	2.347734	-0.792071	0.591171
5	13	0	0.138317	0.318554	0.309862
6	6	0	-3.673218	1.103226	0.530904
7	6	0	-2.976228	1.768111	1.654298
8	1	0	-4.521973	0.488595	0.768792
9	1	0	-3.500675	2.684339	1.919359
10	1	0	-2.926308	1.138025	2.533529
11	1	0	-1.960423	2.062044	1.386828
12	1	0	-3.791270	1.674220	-0.372804
13	53	0	-2.218758	-0.691395	-0.366848

 Low frequencies (cm⁻¹): -536.2191 21.2063 25.8897
 39.3062 49.2164 60.1022

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	3.418013	-1.239695	-1.069080
2	13	0	1.350696	-2.692153	-0.324890
3	13	0	1.815892	-0.926402	1.666961
4	13	0	2.190907	0.921348	-0.007114
5	13	0	-0.315681	-0.549732	0.606409
6	6	0	2.258830	2.831206	-0.506251
7	6	0	1.307156	3.762098	0.244251

8	1	0	2.080233	2.894858	-1.578584
9	1	0	1.419476	4.793384	-0.078372
10	1	0	0.269553	3.486642	0.086447
11	1	0	1.484569	3.738281	1.314607
12	1	0	3.289554	3.155008	-0.370451
13	53	0	-2.639944	0.013175	-0.172479

 Low frequencies (cm⁻¹): 19.9122 31.8322 42.7904
 56.9281 73.2536 102.2965

Al₅ C₂H₃I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	3.722700	0.710191	-1.222451	
2	13	0	4.657563	-1.329495	0.088787	
3	13	0	1.631281	1.751676	-0.451339	
4	13	0	2.460599	-0.469611	0.919312	
5	13	0	0.376036	0.747832	1.671593	
6	53	0	-2.242200	-0.800604	-0.278561	
7	6	0	-3.367434	0.896409	0.250792	
8	6	0	-3.000295	2.126428	-0.046681	
9	1	0	-2.095876	2.353427	-0.597462	
10	1	0	-3.622552	2.958489	0.263282	
11	1	0	-4.264903	0.645360	0.796507	

 Low frequencies (cm⁻¹): 13.6127 25.6492 27.5400
 33.3376 53.4152 67.3737

Coordinate of TS

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	-4.596671	1.162625	0.132545	
2	13	0	-5.256573	-1.316108	0.028118	
3	13	0	-2.193936	1.669163	0.093282	
4	13	0	-2.775230	-0.992283	-0.017692	
5	13	0	-0.409968	-0.325914	-0.059505	
6	53	0	2.282636	-0.027645	-0.136912	
7	6	0	4.691154	0.211445	-0.172870	
8	6	0	5.406818	-0.337004	0.776292	
9	1	0	4.961541	-0.902540	1.587738	
10	1	0	6.491246	-0.240104	0.780550	
11	1	0	5.000576	0.793902	-1.030211	

 Low frequencies (cm⁻¹): -249.4272 17.4034 27.9253

35.7010 51.8600 77.0572

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-3.269237	-1.234798	1.274713
2	13	0	-3.747288	-1.035183	-1.116520
3	13	0	-1.184186	-1.974320	-0.154979
4	13	0	-1.776051	0.726496	0.152547
5	13	0	0.628796	-0.256899	-0.183324
6	53	0	3.112621	0.091022	0.009200
7	6	0	-2.206657	2.636785	0.045732
8	6	0	-3.462143	3.081990	-0.044230
9	1	0	-4.315332	2.409068	-0.027820
10	1	0	-3.700344	4.139476	-0.136468
11	1	0	-1.416883	3.385766	0.025983

Low frequencies (cm⁻¹): 17.8666 30.9329 39.1562
67.6210 79.0849 98.6370

Al₅ C₂H₃I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	4.005041	0.707001	-0.858466
2	13	0	4.448180	-1.721677	-0.099929
3	13	0	2.047224	1.910996	0.053826
4	13	0	2.332158	-0.742157	0.821652
5	13	0	0.434834	0.668544	1.705008
6	53	0	-2.045524	-0.136503	-0.622680
7	6	0	-3.919130	0.195513	0.302026
8	6	0	-4.460028	-0.634110	1.172598
9	1	0	-3.988777	-1.557182	1.486920
10	1	0	-5.426856	-0.392745	1.604310
11	1	0	-4.373328	1.120979	-0.024094

Low frequencies (cm⁻¹): 11.4071 13.8089 20.5735
29.4298 39.3115 45.3728

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-4.665158	1.023501	0.082225
2	13	0	-5.204750	-1.474575	-0.028083
3	13	0	-2.297784	1.731139	0.088503
4	13	0	-2.734861	-1.023015	-0.037226
5	13	0	-0.432783	-0.101246	-0.020258
6	53	0	2.300456	0.064166	-0.057909
7	6	0	4.713552	0.165009	-0.104305
8	6	0	5.434520	-0.833855	0.341581
9	1	0	4.999048	-1.741897	0.746591
10	1	0	6.523711	-0.782824	0.319266
11	1	0	5.024023	1.111524	-0.527434

Low frequencies (cm⁻¹): -182.6383 12.4962 21.2484
29.7281 37.9117 52.9171

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-3.297741	-1.196873	1.246501
2	13	0	-3.790638	-1.063536	-1.139227
3	13	0	-1.215496	-2.014296	-0.087109
4	13	0	-1.799334	0.739341	0.146002
5	13	0	0.630119	-0.301327	-0.152060
6	53	0	3.117503	0.082430	-0.001164
7	6	0	-2.135993	2.675611	0.039444
8	6	0	-3.362105	3.202860	-0.038674
9	1	0	-4.259634	2.589024	-0.020839
10	1	0	-3.531503	4.275872	-0.123337
11	1	0	-1.297784	3.372493	0.017869

Low frequencies (cm⁻¹): 28.0287 36.0104 37.7670
70.9390 81.9523 95.5533

Al₅ C₂H₃I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	4.168097	0.335647	-1.252615
2	13	0	4.794461	-1.566944	0.396486

3	13	0	2.217717	1.772200	-0.776177
4	13	0	2.734239	-0.263623	1.053532
5	13	0	0.817321	1.360589	1.391970
6	53	0	-2.341089	-0.606383	-0.306666
7	6	0	-4.073741	0.160158	0.595496
8	6	0	-4.755733	1.174452	0.124435
9	1	0	-4.480217	1.701825	-0.770332
10	1	0	-5.637320	1.508584	0.645370
11	1	0	-4.341758	-0.372084	1.487143

 Low frequencies (cm⁻¹): 8.0325 12.1599 16.4580
 17.3550 24.2000 37.2995

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-4.690276	0.980594	0.083117
2	13	0	-5.241641	-1.521399	-0.024406
3	13	0	-2.351462	1.783035	0.087574
4	13	0	-2.757455	-1.007640	-0.037205
5	13	0	-0.474937	-0.000706	-0.023284
6	53	0	2.347967	0.048029	-0.061676
7	6	0	4.700489	0.152394	-0.084776
8	6	0	5.422821	-0.843064	0.347140
9	1	0	4.992875	-1.751933	0.731130
10	1	0	6.501790	-0.783509	0.331607
11	1	0	5.028245	1.093406	-0.483431

 Low frequencies (cm⁻¹): -262.6463 12.7404 19.5323
 26.0887 41.0760 59.0175

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	3.324563	-1.164512	-1.201624
2	13	0	3.755699	-1.156236	1.208608
3	13	0	1.207454	-2.007092	-0.012137
4	13	0	1.794710	0.775588	-0.162672
5	13	0	-0.636024	-0.283753	0.040614
6	53	0	-3.123136	0.081528	0.024507
7	6	0	2.176625	2.691648	-0.017347
8	6	0	3.404090	3.194666	0.046706
9	1	0	4.284113	2.572680	0.003444
10	1	0	3.591815	4.254090	0.144210
11	1	0	1.362758	3.402439	0.031050

Low frequencies (cm⁻¹): 29.2386 38.9461 41.0028
 67.0757 86.1724 91.7303

Al₅ C₆H₅I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-3.099418	0.765918	1.707937
2	13	0	-2.628560	2.501474	-0.216821
3	13	0	-3.075027	-1.612801	0.973927
4	13	0	-3.515625	0.284743	-0.985721
5	13	0	-2.553930	-1.955673	-1.588202
6	6	0	2.628736	0.002065	0.015011
7	6	0	3.312407	0.786551	-0.902051
8	6	0	4.701990	0.780875	-0.898765
9	6	0	5.398053	-0.002899	0.011402
10	6	0	4.701587	-0.784178	0.923407
11	6	0	3.312018	-0.784964	0.930189
12	1	0	2.771270	1.395970	-1.613951
13	1	0	5.238636	1.392124	-1.613420
14	1	0	6.480295	-0.004871	0.009965
15	1	0	5.237909	-1.397433	1.636592
16	1	0	2.770550	-1.392549	1.643391
17	53	0	0.500299	0.004424	0.016561

Low frequencies (cm⁻¹): 19.6756 26.7440 28.2780
 36.9770 42.2153 47.6542

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-5.598796	1.300321	0.265476
2	13	0	-6.412692	-1.100446	-0.150405
3	13	0	-3.168504	1.647941	0.292815
4	13	0	-3.916288	-0.929317	-0.171174
5	13	0	-1.512988	-0.426796	-0.106689
6	6	0	3.593122	0.007541	0.003957
7	6	0	4.144779	1.209339	-0.381108
8	6	0	5.532239	1.333728	-0.338275
9	6	0	6.317156	0.268332	0.084825
10	6	0	5.724969	-0.928498	0.468189
11	6	0	4.338934	-1.068810	0.430502
12	1	0	3.526062	2.036031	-0.707887
13	1	0	5.995825	2.266414	-0.636641

14	1	0	7.394302	0.371395	0.115763
15	1	0	6.338431	-1.758455	0.797678
16	1	0	3.868641	-1.997868	0.727858
17	53	0	1.186604	-0.230933	-0.067842

 Low frequencies (cm⁻¹): -172.2662 5.0511 10.1157
 21.8960 25.4086 51.6032

Optimized geometry after C-I dissociation

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	-0.273528	3.282685	0.405043	
2	13	0	-0.232237	1.460275	2.185707	
3	13	0	0.034583	2.037137	-1.777530	
4	13	0	1.262701	0.500350	0.136838	
5	13	0	-1.220109	0.381710	-0.061052	
6	6	0	3.012494	-0.370476	0.053943	
7	6	0	3.236984	-1.654042	0.568157	
8	6	0	4.486910	-2.254026	0.488531	
9	6	0	5.543773	-1.578310	-0.109506	
10	6	0	5.347688	-0.303643	-0.625430	
11	6	0	4.094741	0.290242	-0.541523	
12	1	0	2.425331	-2.200679	1.038400	
13	1	0	4.637718	-3.248144	0.891375	
14	1	0	6.519194	-2.044615	-0.173827	
15	1	0	6.170047	0.225812	-1.091052	
16	1	0	3.966088	1.288492	-0.951374	
17	53	0	-3.252295	-1.044964	-0.481350	

 Low frequencies (cm⁻¹): 27.0171 32.6676 54.3337
 55.0853 94.6787 121.4927

Al₅ C₆H₅I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	-4.928618	0.907708	-0.605926	
2	13	0	-5.484607	-1.492825	0.156844	
3	13	0	-2.815864	1.945626	0.152626	
4	13	0	-3.227825	-0.694876	0.898814	
5	13	0	-1.158629	0.551842	1.633640	
6	6	0	2.965934	-0.093084	-0.103683	

7	6	0	3.588574	-1.139741	0.559348
8	6	0	4.878062	-0.954612	1.045043
9	6	0	5.529000	0.258993	0.866936
10	6	0	4.888979	1.295074	0.199652
11	6	0	3.599549	1.125932	-0.292047
12	1	0	3.082642	-2.086568	0.699069
13	1	0	5.370841	-1.768506	1.564873
14	1	0	6.534296	0.397292	1.247624
15	1	0	5.390737	2.245473	0.056483
16	1	0	3.102559	1.934908	-0.812331
17	53	0	0.996611	-0.368021	-0.858023

 Low frequencies (cm⁻¹): 6.0590 7.6021 10.7369
 20.7935 31.3843 42.1151

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	5.687282	1.184624	0.096794
2	13	0	6.391936	-1.265498	-0.121121
3	13	0	3.277290	1.725179	0.155667
4	13	0	3.897652	-0.981167	-0.089228
5	13	0	1.535942	-0.225018	-0.010659
6	6	0	-3.613346	-0.022341	-0.006124
7	6	0	-4.197912	1.210976	-0.193498
8	6	0	-5.590503	1.281040	-0.192314
9	6	0	-6.348899	0.131555	-0.006145
10	6	0	-5.724239	-1.095724	0.179752
11	6	0	-4.332488	-1.182330	0.181090
12	1	0	-3.601868	2.104618	-0.338132
13	1	0	-6.078274	2.239273	-0.337638
14	1	0	-7.431317	0.192365	-0.006132
15	1	0	-6.316127	-1.993405	0.324817
16	1	0	-3.840414	-2.137067	0.325791
17	53	0	-1.210547	-0.151706	-0.002909

 Low frequencies (cm⁻¹): -128.5324 6.5284 8.2538
 13.8929 32.2110 46.6585

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.277768	3.422327	0.000918
2	13	0	0.114800	1.838491	-1.989212
3	13	0	0.115715	1.837270	1.990092
4	13	0	-1.263934	0.530015	0.000569

5	13	0	1.241151	0.395062	0.000220
6	6	0	-3.002737	-0.384910	0.000187
7	6	0	-3.116674	-1.782841	0.002019
8	6	0	-4.358464	-2.404656	0.001716
9	6	0	-5.519323	-1.639349	-0.000408
10	6	0	-5.433979	-0.252722	-0.002243
11	6	0	-4.188650	0.364072	-0.001933
12	1	0	-2.224888	-2.403549	0.003752
13	1	0	-4.422455	-3.487597	0.003151
14	1	0	-6.489498	-2.124211	-0.000637
15	1	0	-6.337534	0.347675	-0.003910
16	1	0	-4.148856	1.450733	-0.003387
17	53	0	3.226994	-1.160033	-0.000540

 Low frequencies (cm⁻¹): 12.0124 22.8492 32.5859
 54.7408 59.1896 86.7048

Al₅ C₆H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	5.175590	0.534125	-1.037958
2	13	0	5.817986	-1.146122	0.829527
3	13	0	3.038848	1.762609	-0.894995
4	13	0	3.563432	-0.056717	1.147912
5	13	0	1.460449	1.360968	1.150392
6	6	0	-3.121685	-0.095495	-0.020547
7	6	0	-3.683141	-0.374497	1.208784
8	6	0	-4.877872	0.227171	1.558115
9	6	0	-5.502765	1.097738	0.686961
10	6	0	-4.929842	1.367584	-0.540369
11	6	0	-3.735335	0.772156	-0.900901
12	1	0	-3.200814	-1.050932	1.889102
13	1	0	-5.316872	0.011009	2.515641
14	1	0	-6.431587	1.563261	0.962958
15	1	0	-5.409693	2.043925	-1.224942
16	1	0	-3.293682	0.984823	-1.856311
17	53	0	-1.301424	-1.008175	-0.561738

 Low frequencies (cm⁻¹): 1.6687 5.5421 10.5134
 12.9911 18.6148 24.8233

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	13	0	-5.731240	1.022396	-0.435098
2	13	0	-6.403625	-1.243149	0.561049
3	13	0	-3.355652	1.654410	-0.697847
4	13	0	-3.897467	-0.877373	0.420449
5	13	0	-1.566414	-0.057236	0.074547
6	6	0	3.611834	0.062680	0.073615
7	6	0	4.206087	1.282755	-0.130323
8	6	0	5.590274	1.345049	-0.145198
9	6	0	6.340754	0.199440	0.041386
10	6	0	5.713192	-1.015217	0.244213
11	6	0	4.329704	-1.091779	0.261530
12	1	0	3.619700	2.171687	-0.275148
13	1	0	6.078376	2.290782	-0.303080
14	1	0	7.414551	0.253181	0.028889
15	1	0	6.296729	-1.907342	0.389674
16	1	0	3.838490	-2.034541	0.419016
17	53	0	1.266505	-0.055824	0.099368

Low frequencies (cm⁻¹): -200.5059 7.5229 10.2585
12.1125 35.3181 49.6193

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.462671	3.453258	0.502456
2	13	0	-0.204009	1.519900	2.184956
3	13	0	-0.107319	2.179784	-1.686690
4	13	0	1.309621	0.603214	0.051026
5	13	0	-1.192371	0.321697	-0.074460
6	6	0	3.043558	-0.304595	-0.010131
7	6	0	3.283001	-1.476942	0.707532
8	6	0	4.507247	-2.115667	0.658419
9	6	0	5.528161	-1.592182	-0.112353
10	6	0	5.319870	-0.430851	-0.831805
11	6	0	4.092181	0.201321	-0.778541
12	1	0	2.504850	-1.905792	1.317357
13	1	0	4.665384	-3.019638	1.219892
14	1	0	6.482301	-2.087244	-0.151958
15	1	0	6.111813	-0.019821	-1.432942
16	1	0	3.957348	1.104970	-1.351097
17	53	0	-2.998159	-1.420368	-0.300705

Low frequencies (cm⁻¹): 14.6645 23.2099 29.7131
52.3532 60.1420 84.5540

Al₆ C₂H₅I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	3.156980	-0.290996	1.489440
2	13	0	0.884359	0.873943	1.401180
3	13	0	1.465472	-1.772002	0.251653
4	13	0	3.124133	-0.612093	-1.354907
5	13	0	0.789171	0.462993	-1.491420
6	13	0	2.556925	1.905611	-0.276212
7	6	0	-2.936883	1.155282	0.632284
8	6	0	-2.692147	2.275890	-0.346287
9	1	0	-2.476930	1.329689	1.600978
10	1	0	-3.143259	3.191722	0.044054
11	1	0	-1.624553	2.458790	-0.478618
12	1	0	-3.134902	2.062886	-1.319085
13	1	0	-3.986705	0.907502	0.753551
14	53	0	-2.029453	-0.715369	-0.048555

Low frequencies (cm⁻¹): 20.8381 29.0251 42.9295
50.6311 63.2304 72.5669

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.631749	-1.855813	0.000266
2	13	0	-0.445696	0.254222	-1.430829
3	13	0	-0.445906	0.254942	1.431098
4	13	0	-2.957260	-0.130610	1.497558
5	13	0	-1.923180	1.976843	-0.000527
6	13	0	-2.957139	-0.130845	-1.497574
7	6	0	2.877170	1.773983	-0.000040
8	6	0	1.742180	2.636231	0.000080
9	1	0	3.405890	1.557586	-0.917326
10	1	0	1.616442	3.233557	0.900574
11	1	0	1.616648	3.234065	-0.900111
12	1	0	0.728937	1.992414	-0.000276
13	1	0	3.406073	1.557518	0.917122
14	53	0	1.815132	-0.808114	-0.000003

Low frequencies (cm⁻¹): -131.9149 41.2227 42.1908
68.2282 77.6346 98.4333

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	13	0	-1.094323	0.348288	1.272631
2	13	0	-3.589207	-0.152739	0.064622
3	13	0	1.111049	0.360699	0.021181
4	13	0	-0.115168	2.539988	-0.004402
5	13	0	-1.411729	0.093723	-1.200119
6	13	0	-2.773420	2.236842	-0.242109
7	6	0	-5.151515	-1.344610	0.209088
8	6	0	-4.795960	-2.817718	-0.039952
9	1	0	-5.905561	-1.008030	-0.508297
10	1	0	-5.674519	-3.462181	0.035457
11	1	0	-4.368356	-2.963795	-1.033910
12	1	0	-4.062523	-3.182209	0.682402
13	1	0	-5.597683	-1.222484	1.200130
14	53	0	3.347010	-0.795243	0.035047

Low frequencies (cm⁻¹): 31.1868 32.7548 55.8820
62.9285 88.7531 102.6903

Al₆ C₂H₅I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	3.195975	-0.357481	1.446821
2	13	0	0.953920	0.861808	1.493918
3	13	0	1.494632	-1.773932	0.161156
4	13	0	3.056039	-0.504701	-1.463551
5	13	0	0.711515	0.566524	-1.404170
6	13	0	2.575249	1.931451	-0.227131
7	6	0	-3.100704	1.059209	0.612928
8	6	0	-2.933750	2.214175	-0.333102
9	1	0	-2.703025	1.252964	1.605907
10	1	0	-3.487227	3.073795	0.060403
11	1	0	-1.886432	2.511145	-0.426073
12	1	0	-3.323376	1.988371	-1.326810
13	1	0	-4.120224	0.687609	0.678375
14	53	0	-1.964307	-0.727582	-0.044572

Low frequencies (cm⁻¹): 18.7914 26.3833 36.4133
40.2529 59.4073 68.8871

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-2.825833	-1.061471	1.236123

2	13	0	-1.424875	-1.514559	-0.919261
3	13	0	-0.450959	-0.023460	1.288778
4	13	0	-2.509122	1.571676	1.132046
5	13	0	-1.018013	1.508796	-1.042293
6	13	0	-3.172640	0.256869	-1.494896
7	6	0	3.385646	1.290592	0.238057
8	6	0	2.587467	2.464963	-0.151527
9	1	0	4.169119	0.942446	-0.424303
10	1	0	3.016872	3.374800	0.288467
11	1	0	2.536007	2.594295	-1.232993
12	1	0	1.554262	2.412668	0.236372
13	1	0	3.584988	1.136599	1.292647
14	53	0	1.839978	-0.803513	-0.061997

Low frequencies (cm⁻¹): -84.3360 31.9001 41.7371
 44.9275 81.4325 86.2236

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.011019	0.296278	1.270253
2	13	0	-3.546560	-0.198252	0.029419
3	13	0	1.192614	0.435280	0.017155
4	13	0	-0.106678	2.580891	0.074987
5	13	0	-1.355689	0.059079	-1.207456
6	13	0	-2.740086	2.209343	-0.201864
7	6	0	-5.149834	-1.357304	0.172931
8	6	0	-4.891570	-2.855463	-0.019543
9	1	0	-5.874987	-0.996024	-0.565808
10	1	0	-5.814681	-3.436364	0.072836
11	1	0	-4.471068	-3.071174	-1.005144
12	1	0	-4.189509	-3.246653	0.721672
13	1	0	-5.605493	-1.170681	1.152497
14	53	0	3.482653	-0.618425	-0.020166

Low frequencies (cm⁻¹): 18.6634 32.0345 50.3523
 63.4168 83.4248 89.0621

Al₆ C₂H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	13	0	3.321593	-0.307090	1.532685
2	13	0	1.099380	0.975032	1.397552
3	13	0	1.607359	-1.765076	0.283425
4	13	0	3.286821	-0.698195	-1.367828
5	13	0	1.004182	0.504528	-1.533286
6	13	0	2.799975	1.919213	-0.311593
7	6	0	-3.145287	1.119007	0.671886
8	6	0	-3.160320	2.200190	-0.372697
9	1	0	-2.573794	1.387294	1.545147
10	1	0	-3.643560	3.081263	0.041894
11	1	0	-2.157956	2.479401	-0.672152
12	1	0	-3.711974	1.897410	-1.253714
13	1	0	-4.132614	0.801419	0.964327
14	53	0	-2.198066	-0.711912	-0.045907

 Low frequencies (cm⁻¹): 7.5913 28.0395 31.0424
 37.2093 40.2571 50.3173

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.905486	-1.558858	-1.061082
2	13	0	0.255438	-0.459822	0.895350
3	13	0	1.146756	1.433589	-0.977941
4	13	0	3.451965	0.466279	-1.386277
5	13	0	2.166780	1.399423	1.444505
6	13	0	2.676194	-1.152603	1.441247
7	6	0	-2.976223	2.008595	0.071071
8	6	0	-1.801669	2.798091	0.018300
9	1	0	-3.414550	1.722819	1.006719
10	1	0	-1.720709	3.417143	-0.863905
11	1	0	-1.593287	3.356454	0.920883
12	1	0	-0.836385	2.116877	-0.055746
13	1	0	-3.551499	1.806356	-0.810935
14	53	0	-2.095288	-0.809884	-0.101107

 Low frequencies (cm⁻¹): -111.4255 21.2878 42.1379
 53.8026 70.7575 78.6084

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.017311	0.231434	1.262439
2	13	0	-3.519073	-0.188603	0.013578
3	13	0	1.180880	0.442308	0.031728
4	13	0	-0.116743	2.569210	0.050962

5	13	0	-1.327860	0.031920	-1.211779
6	13	0	-2.730675	2.224599	-0.157659
7	6	0	-5.117812	-1.335825	0.152742
8	6	0	-4.865170	-2.834377	-0.016689
9	1	0	-5.832024	-0.991235	-0.592462
10	1	0	-5.784156	-3.406322	0.073185
11	1	0	-4.438227	-3.061304	-0.988196
12	1	0	-4.176688	-3.213830	0.731803
13	1	0	-5.583406	-1.142878	1.117188
14	53	0	3.464388	-0.607632	-0.019214

 Low frequencies (cm⁻¹): 21.1415 35.4164 54.4932
 62.6889 89.3295 93.1549

Al₆ C₂H₃I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-2.597721	1.961298	0.156181
2	13	0	-0.916889	0.560343	1.524229
3	13	0	-0.900620	0.815138	-1.415997
4	13	0	-3.209378	-0.288974	-1.485026
5	13	0	-1.557545	-1.746498	-0.156703
6	13	0	-3.231022	-0.528918	1.373845
7	53	0	2.072576	-0.644433	-0.000830
8	6	0	2.742884	1.358398	0.050707
9	6	0	4.010905	1.698686	-0.037353
10	1	0	4.810024	0.976837	-0.142985
11	1	0	4.279070	2.748658	-0.003650
12	1	0	1.912930	2.045917	0.155622

 Low frequencies (cm⁻¹): 9.8717 39.7028 41.6846
 46.0126 62.5104 70.0066

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-2.430867	1.892268	-0.635412
2	13	0	-0.791325	1.179867	1.268764
3	13	0	-0.625452	0.233276	-1.491337
4	13	0	-3.023028	-0.678178	-1.281082
5	13	0	-1.423500	-1.599116	0.552896
6	13	0	-3.075051	0.096099	1.524726
7	53	0	1.753546	-0.746992	0.017464
8	6	0	2.950216	1.560545	-0.039579

9	6	0	4.244083	1.658445	0.021147
10	1	0	4.898840	0.798529	0.088897
11	1	0	4.706301	2.644979	0.002900
12	1	0	2.090991	2.218299	-0.108043

 Low frequencies (cm⁻¹): -115.7572 34.0661 43.1453
 50.5046 82.2359 89.7710

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.103704	-0.291707	1.368842
2	13	0	-1.629955	-1.065648	-0.353757
3	13	0	0.256916	0.315321	-1.405358
4	13	0	-0.430446	2.302209	0.427115
5	13	0	-1.939371	1.603020	-1.536319
6	13	0	-2.117003	0.883771	1.772128
7	53	0	2.555031	-0.411018	-0.008817
8	6	0	-3.481703	-1.638564	-0.696148
9	6	0	-4.388609	-1.886009	0.250774
10	1	0	-4.166950	-1.781599	1.309206
11	1	0	-5.399001	-2.210343	0.013496
12	1	0	-3.798777	-1.787220	-1.727604

 Low frequencies (cm⁻¹): 18.3254 45.7245 59.8876
 69.6600 77.4382 90.9271

Al₆ C₂H₃I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-2.657898	1.945515	0.116844
2	13	0	-0.904293	0.649900	1.516246
3	13	0	-0.898957	0.839946	-1.430579
4	13	0	-3.171735	-0.338517	-1.495546
5	13	0	-1.528975	-1.752693	-0.116129
6	13	0	-3.184932	-0.516144	1.413617
7	53	0	1.987129	-0.607591	-0.001384
8	6	0	2.955565	1.286407	0.013566
9	6	0	4.264269	1.432442	-0.010965
10	1	0	4.957825	0.600896	-0.039796
11	1	0	4.683650	2.434145	-0.002323
12	1	0	2.229948	2.090102	0.041961

Low frequencies (cm⁻¹): 12.4934 34.0605 36.1143
 50.3110 52.8575 63.3918

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	2.696463	1.022871	1.401079
2	13	0	1.036416	1.816386	-0.429001
3	13	0	0.508644	-0.257906	1.558034
4	13	0	2.476433	-1.600851	0.413237
5	13	0	0.602917	-0.886675	-1.331603
6	13	0	2.878243	0.254666	-1.520857
7	53	0	-1.855679	-0.790040	0.034771
8	6	0	-2.056448	1.941472	-0.605155
9	6	0	-2.529118	2.893367	0.150642
10	1	0	-3.495394	2.782959	0.639630
11	1	0	-2.002864	3.828059	0.347612
12	1	0	-1.225884	1.721684	-1.284574

Low frequencies (cm⁻¹): -134.1297 22.6819 36.5193
 52.6555 68.6254 81.9091

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.121766	-0.048582	-1.392732
2	13	0	-1.901643	0.757060	-0.000297
3	13	0	0.121673	-0.048112	1.392554
4	13	0	-0.400593	-2.494191	0.000340
5	13	0	-1.918893	-1.514561	1.815534
6	13	0	-1.918836	-1.515088	-1.815229
7	53	0	2.508573	0.503001	-0.000011
8	6	0	-3.632459	1.688708	-0.000305
9	6	0	-3.731759	3.019606	0.000070
10	1	0	-2.861653	3.672154	0.000461
11	1	0	-4.693775	3.529806	0.000019
12	1	0	-4.558812	1.114269	-0.000691

Low frequencies (cm⁻¹): 23.4554 46.2049 57.9063
 64.3769 72.6553 91.0538

AL₆ C₂H₃I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center	Atomic	Atomic	Coordinates (Angstroms)		
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Number	Number	Type	X	Y	Z
1	13	0	-2.830888	1.960364	0.147344
2	13	0	-1.102989	0.627068	1.544871
3	13	0	-1.085940	0.870284	-1.428036
4	13	0	-3.346159	-0.357236	-1.521946
5	13	0	-1.682464	-1.767168	-0.149156
6	13	0	-3.368122	-0.591077	1.406969
7	53	0	2.232982	-0.616032	-0.000508
8	6	0	3.032629	1.328708	0.030237
9	6	0	4.314770	1.586393	-0.025716
10	1	0	5.066888	0.821838	-0.092187
11	1	0	4.648598	2.610238	-0.005141
12	1	0	2.267379	2.077941	0.096522

 Low frequencies (cm⁻¹): 8.8953 22.9455 29.5930
 34.5288 41.2436 46.0014

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	2.710876	-1.710767	0.588399
2	13	0	2.097046	0.438521	1.955418
3	13	0	0.251340	-1.009445	0.574858
4	13	0	1.773805	-0.750237	-1.732154
5	13	0	1.162634	1.734407	-0.098018
6	13	0	3.441139	1.058429	-1.015542
7	53	0	-2.214781	-0.672528	-0.125086
8	6	0	-1.834670	2.017649	0.541672
9	6	0	-2.353101	3.018823	-0.086594
10	1	0	-3.361575	2.961023	-0.466325
11	1	0	-1.821627	3.941614	-0.271296
12	1	0	-0.985710	1.630710	1.088224

 Low frequencies (cm⁻¹): -218.1910 23.3759 31.5344
 60.8332 64.2373 72.0173

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.687269	-0.656357	-1.504060
2	13	0	-1.869561	1.226580	0.216241
3	13	0	0.398200	-0.231489	-0.096451
4	13	0	-1.238468	-2.044073	0.962114
5	13	0	-0.963735	-0.024947	2.473885
6	13	0	-2.978623	-2.856063	-0.831074

7	53	0	2.886947	0.166267	-0.202051
8	6	0	-2.672216	3.007292	0.235291
9	6	0	-3.175641	3.586009	-0.847976
10	1	0	-3.175090	3.105168	-1.813515
11	1	0	-3.612793	4.573285	-0.826143
12	1	0	-2.720246	3.572130	1.155976

 Low frequencies (cm⁻¹): 26.7786 34.3017 47.2387
 60.1413 70.3541 88.6181

Al₆ C₆H₅I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	3.886149	0.160513	-1.430343
2	13	0	2.601500	-1.540808	0.008882
3	13	0	1.379445	0.681411	-1.477776
4	13	0	2.739169	2.316061	-0.005298
5	13	0	1.369203	0.691622	1.469679
6	13	0	3.876182	0.171679	1.443943
7	6	0	-2.611755	0.052792	-0.000271
8	6	0	-3.919926	-0.404094	0.009362
9	6	0	-4.951458	0.526388	0.010533
10	6	0	-4.671031	1.886726	0.001990
11	6	0	-3.353266	2.320627	-0.007662
12	6	0	-2.309453	1.402095	-0.008973
13	1	0	-4.137464	-1.463840	0.016115
14	1	0	-5.977289	0.180439	0.018124
15	1	0	-5.479511	2.606153	0.002950
16	1	0	-3.126036	3.379169	-0.014293
17	1	0	-1.280777	1.743694	-0.016151
18	53	0	-1.040925	-1.384887	-0.002920

 Low frequencies (cm⁻¹): 10.5960 10.7142 28.1399
 36.0051 51.4584 60.1787

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.204130	-1.157022	0.000132
2	13	0	2.243074	-1.806401	1.497328
3	13	0	2.000977	0.717531	1.394441
4	13	0	2.000982	0.717655	-1.394292
5	13	0	4.161121	-0.484079	-0.000100
6	13	0	2.242906	-1.806280	-1.497326

7	6	0	-2.122394	-0.214732	-0.000019
8	6	0	-2.729145	-0.511626	-1.213569
9	6	0	-3.937631	-1.196785	-1.207180
10	6	0	-4.537227	-1.540536	0.000006
11	6	0	-3.937803	-1.196431	1.207176
12	6	0	-2.729316	-0.511274	1.213534
13	1	0	-2.249628	-0.244488	-2.149300
14	1	0	-4.411256	-1.462001	-2.144337
15	1	0	-5.480905	-2.070867	0.000017
16	1	0	-4.411566	-1.461359	2.144345
17	1	0	-2.249937	-0.243851	2.149254
18	53	0	-0.534473	1.625521	-0.000038

 Low frequencies (cm⁻¹): -335.7710 26.6987 49.1629
 49.8966 72.8247 77.5660

Optimized geometry after C-I dissociation

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	-1.655556	2.022306	0.463363	
2	13	0	-2.220086	0.146927	2.228424	
3	13	0	-0.403604	-0.341140	0.423145	
4	13	0	-1.915467	-1.228982	-1.720726	
5	13	0	-3.241946	-1.103604	0.403973	
6	13	0	-3.030444	1.096033	-1.466975	
7	6	0	0.394954	1.692439	0.080735	
8	6	0	0.916349	1.861475	-1.220281	
9	6	0	2.227270	2.250865	-1.433107	
10	6	0	3.062471	2.497427	-0.348008	
11	6	0	2.580439	2.365071	0.947227	
12	6	0	1.267674	1.968558	1.153831	
13	1	0	0.280299	1.662305	-2.075618	
14	1	0	2.605151	2.355731	-2.442229	
15	1	0	4.091399	2.791174	-0.515002	
16	1	0	3.229959	2.557287	1.791757	
17	1	0	0.911618	1.848128	2.172627	
18	53	0	1.665264	-1.787163	0.031706	

 Low frequencies (cm⁻¹): 29.5386 36.0431 44.7590
 68.9027 78.1892 94.2723

Al₆ C₆H₅I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	3.849283	0.145588	-1.458867
2	13	0	2.587185	-1.551903	0.000005
3	13	0	1.354995	0.722308	-1.474807
4	13	0	2.784480	2.309208	0.000328
5	13	0	1.354159	0.721936	1.474207
6	13	0	3.848685	0.145547	1.459494
7	6	0	-2.628559	0.041293	-0.000024
8	6	0	-3.913759	-0.475744	0.000232
9	6	0	-4.985688	0.409910	0.000248
10	6	0	-4.764515	1.781503	0.000059
11	6	0	-3.466291	2.273532	-0.000161
12	6	0	-2.382826	1.400737	-0.000191
13	1	0	-4.087339	-1.544721	0.000397
14	1	0	-5.996995	0.018910	0.000434
15	1	0	-5.604666	2.466266	0.000082
16	1	0	-3.285545	3.342651	-0.000296
17	1	0	-1.366496	1.783859	-0.000365
18	53	0	-0.979875	-1.340741	-0.000111

Low frequencies (cm⁻¹): 14.4804 21.4178 29.5447
37.7012 54.2675 62.1928

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.170774	-1.139416	0.006581
2	13	0	-2.207917	-1.791439	-1.491794
3	13	0	-2.162960	0.752875	-1.414316
4	13	0	-2.151278	0.781665	1.383495
5	13	0	-4.168629	-0.669459	0.007773
6	13	0	-2.207147	-1.762491	1.518286
7	6	0	2.156000	-0.224875	0.001501
8	6	0	2.771378	-0.512415	1.216066
9	6	0	3.975439	-1.205725	1.207405
10	6	0	4.569112	-1.560057	-0.000593
11	6	0	3.967894	-1.215757	-1.207705
12	6	0	2.763700	-0.522583	-1.214486
13	1	0	2.303568	-0.232461	2.154081
14	1	0	4.452013	-1.466890	2.146140
15	1	0	5.512807	-2.093522	-0.001323
16	1	0	4.438567	-1.484639	-2.147236
17	1	0	2.289729	-0.250802	-2.151849
18	53	0	0.559912	1.636684	-0.002703

Low frequencies (cm⁻¹): -285.0504 19.9710 31.6774
43.6317 57.7318 71.8831

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.565886	2.055959	0.471324
2	13	0	-2.159748	0.187137	2.223867
3	13	0	-0.360411	-0.350590	0.400412
4	13	0	-2.029585	-1.137514	-1.708137
5	13	0	-3.297674	-1.049571	0.444872
6	13	0	-3.051262	1.218045	-1.429377
7	6	0	0.484840	1.681542	0.080674
8	6	0	1.003532	1.895380	-1.216997
9	6	0	2.289900	2.367592	-1.417063
10	6	0	3.103816	2.653050	-0.324958
11	6	0	2.627041	2.467668	0.966886
12	6	0	1.341244	1.987784	1.163287
13	1	0	0.383065	1.675016	-2.079068
14	1	0	2.664142	2.510834	-2.424692
15	1	0	4.112676	3.018257	-0.482743
16	1	0	3.261036	2.688021	1.818304
17	1	0	0.987626	1.836201	2.179343
18	53	0	1.613747	-1.925499	0.004517

Low frequencies (cm⁻¹): 31.7465 35.8232 51.4638
 69.6590 73.0823 94.0954

Al₆ C₆H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	4.093138	0.028114	-1.469645
2	13	0	2.732883	-1.592892	0.000490
3	13	0	1.625687	0.760551	-1.491631
4	13	0	3.081647	2.302194	0.000040
5	13	0	1.624957	0.761206	1.491490
6	13	0	4.092315	0.028353	1.470874
7	6	0	-2.791419	0.081975	-0.000101
8	6	0	-4.107725	-0.331163	0.001857
9	6	0	-5.110698	0.620149	0.002093
10	6	0	-4.797779	1.965586	0.000402
11	6	0	-3.475088	2.361527	-0.001534
12	6	0	-2.461879	1.420124	-0.001815
13	1	0	-4.355323	-1.376036	0.003202
14	1	0	-6.138075	0.302720	0.003615
15	1	0	-5.581366	2.701480	0.000596
16	1	0	-3.221910	3.406587	-0.002857
17	1	0	-1.434804	1.735567	-0.003318
18	53	0	-1.265267	-1.381460	-0.000522

 Low frequencies (cm⁻¹): 11.7308 23.9261 24.8069
 32.8527 39.5012 45.5366

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.207787	-1.182518	0.000084
2	13	0	2.227920	-1.654490	1.574399
3	13	0	2.174796	0.908800	1.375404
4	13	0	2.174820	0.908639	-1.375406
5	13	0	4.283717	-0.879546	0.000128
6	13	0	2.227974	-1.654682	-1.574102
7	6	0	-2.086765	-0.327817	-0.000015
8	6	0	-2.713141	-0.604615	-1.206557
9	6	0	-3.927620	-1.260230	-1.199953
10	6	0	-4.531571	-1.594292	0.000040
11	6	0	-3.927656	-1.260054	1.200003
12	6	0	-2.713177	-0.604439	1.206548
13	1	0	-2.244064	-0.341810	-2.137771
14	1	0	-4.403361	-1.509555	-2.131756
15	1	0	-5.480506	-2.099508	0.000063
16	1	0	-4.403426	-1.509243	2.131828
17	1	0	-2.244129	-0.341499	2.137737
18	53	0	-0.654455	1.620937	-0.000134

Low frequencies (cm⁻¹): -383.7791 6.1978 35.0091
 45.4650 67.4749 77.9367

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.587374	2.016795	0.529088
2	13	0	-2.159677	0.087644	2.202737
3	13	0	-0.336104	-0.380821	0.408294
4	13	0	-2.105695	-1.140094	-1.738107
5	13	0	-3.333997	-1.126717	0.433772
6	13	0	-3.107022	1.229054	-1.368779
7	6	0	0.446053	1.703948	0.106140
8	6	0	0.938458	1.931185	-1.191250
9	6	0	2.219829	2.383100	-1.414778
10	6	0	3.057864	2.637415	-0.343279
11	6	0	2.609762	2.442099	0.948985
12	6	0	1.327819	1.982047	1.164828
13	1	0	0.304198	1.738802	-2.038282
14	1	0	2.570044	2.534294	-2.420108

15	1	0	4.060590	2.985439	-0.517176
16	1	0	3.260552	2.637828	1.782212
17	1	0	1.001684	1.822744	2.179068
18	53	0	1.686651	-1.870077	-0.012842

Low frequencies (cm⁻¹): 32.0063 36.8154 56.9590
 73.0275 75.4077 96.6384

Al₇ C₂H₅I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	13	0	2.452148	-1.739435	-0.564668
2	13	0	4.139557	-0.665295	1.220279
3	13	0	3.795269	0.219406	-1.355640
4	13	0	1.538959	-0.284909	1.561365
5	13	0	2.727865	1.728512	0.680174
6	13	0	1.379834	1.100075	-1.420050
7	13	0	0.040783	-0.800526	-0.488773
8	6	0	-2.804505	1.555884	-0.469639
9	6	0	-2.246795	2.329796	0.698770
10	1	0	-3.779061	1.902598	-0.796831
11	1	0	-2.920520	2.308728	1.554419
12	1	0	-1.274367	1.941484	1.003705
13	1	0	-2.109303	3.370397	0.393091
14	1	0	-2.116742	1.509576	-1.310333
15	53	0	-3.140747	-0.539597	0.048231

Low frequencies (cm⁻¹): 12.2850 22.8722 28.1772
 34.4798 72.4008 80.5517

Coordinate of TS

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	13	0	-2.011621	-0.967095	1.398214
2	13	0	-4.219836	-1.087447	-0.000711
3	13	0	-3.385450	1.173528	1.349711
4	13	0	-2.011952	-0.964209	-1.400112
5	13	0	-3.386822	1.175736	-1.347088
6	13	0	-1.240637	1.606050	0.000554
7	13	0	0.115213	-0.523344	-0.000691
8	6	0	2.970561	1.708441	-0.000088
9	6	0	4.404860	2.123186	0.000165
10	1	0	2.400227	1.890287	0.904597

11	1	0	4.927047	1.765540	0.887531
12	1	0	4.927589	1.764568	-0.886497
13	1	0	4.466436	3.217413	-0.000441
14	1	0	2.400639	1.890143	-0.905060
15	53	0	2.763395	-0.733765	0.000019

 Low frequencies (cm⁻¹): -630.0453 3.0485 23.8996
 27.1708 42.2941 50.3940

Optimized geometry after C-I dissociation

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	1.089980	-2.437947	0.032879	
2	13	0	3.388449	-1.869631	-0.974332	
3	13	0	1.431715	-0.273447	-1.640495	
4	13	0	0.971116	-0.789714	1.995050	
5	13	0	3.217936	-0.249812	0.943720	
6	13	0	1.208767	1.377696	0.346451	
7	13	0	-0.685746	-0.543977	-0.232913	
8	6	0	1.161527	3.354723	0.339889	
9	6	0	2.188731	3.975619	-0.614937	
10	1	0	1.329697	3.699038	1.363795	
11	1	0	2.146401	5.066949	-0.593336	
12	1	0	3.207509	3.682288	-0.353014	
13	1	0	2.015334	3.660723	-1.645862	
14	1	0	0.147954	3.660699	0.066222	
15	53	0	-3.151647	-0.028735	-0.062305	

 Low frequencies (cm⁻¹): 24.4288 29.0798 47.2854
 59.2843 68.4504 85.0074

Al₇ C₂H₅I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	2.215463	-1.764424	-0.507429	
2	13	0	4.297250	-0.844741	0.934289	
3	13	0	3.558946	0.077494	-1.579274	
4	13	0	1.853257	-0.080453	1.753213	
5	13	0	3.200017	1.684212	0.564817	
6	13	0	1.369310	1.439500	-1.265098	
7	13	0	0.084455	-0.392487	-0.090665	
8	6	0	-3.191829	1.495038	-0.435436	
9	6	0	-3.139033	2.312913	0.825316	
10	1	0	-4.128739	1.583684	-0.978343	

11	1	0	-3.958251	2.074561	1.504743
12	1	0	-2.193970	2.181739	1.354298
13	1	0	-3.223225	3.370495	0.552010
14	1	0	-2.348900	1.675779	-1.099841
15	53	0	-3.050657	-0.665703	-0.022646

 Low frequencies (cm⁻¹): 18.6330 20.4529 24.1010
 31.3396 41.4892 52.9386

Coordinate of TS

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	2.005183	-0.945316	-1.423686	
2	13	0	4.201543	-1.198309	-0.000057	
3	13	0	3.508521	1.121276	-1.350820	
4	13	0	2.004710	-0.946045	1.422992	
5	13	0	3.508090	1.120551	1.351696	
6	13	0	1.399898	1.759785	0.000239	
7	13	0	-0.065937	-0.292783	-0.000484	
8	6	0	-3.332904	1.627608	-0.000380	
9	6	0	-4.814959	1.788075	0.000236	
10	1	0	-2.811450	1.928011	-0.903851	
11	1	0	-5.276768	1.352158	-0.887216	
12	1	0	-5.275928	1.353011	0.888542	
13	1	0	-5.054740	2.859657	-0.000176	
14	1	0	-2.810640	1.928509	0.902458	
15	53	0	-2.739423	-0.716312	0.000050	

 Low frequencies (cm⁻¹): -336.7763 10.1621 26.0001
 31.7408 40.6389 56.9481

Optimized geometry after C-I dissociation

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	0.918651	-2.513735	0.215125	
2	13	0	3.204660	-2.123600	-0.907887	
3	13	0	1.326599	-0.492403	-1.728323	
4	13	0	1.034895	-0.644958	1.999319	
5	13	0	3.291102	-0.305688	0.847087	
6	13	0	1.345661	1.360082	0.113440	
7	13	0	-0.727229	-0.491867	-0.157913	
8	6	0	1.299058	3.351352	0.017542	
9	6	0	2.629762	4.019112	-0.335299	
10	1	0	0.943083	3.695292	0.995879	
11	1	0	2.536088	5.109850	-0.353027	
12	1	0	3.412104	3.773242	0.387623	

13	1	0	2.990793	3.710009	-1.319538
14	1	0	0.522997	3.626089	-0.704204
15	53	0	-3.190649	0.068320	-0.038703

 Low frequencies (cm⁻¹): 21.9069 31.0044 47.6784
 63.3540 73.8844 79.1496

Al₇ C₂H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	2.552822	-1.818820	-0.869832
2	13	0	4.558309	-0.595863	0.454063
3	13	0	3.267851	0.522298	-1.582401
4	13	0	2.276786	-0.730024	1.875194
5	13	0	3.005491	1.515005	0.912563
6	13	0	1.162782	1.971080	-0.921700
7	13	0	0.570861	-0.439669	-0.015748
8	6	0	-3.370360	1.438817	-0.359820
9	6	0	-3.452636	2.185787	0.943142
10	1	0	-4.259345	1.541573	-0.959669
11	1	0	-4.306309	1.873091	1.531111
12	1	0	-2.558513	2.049191	1.538014
13	1	0	-3.557090	3.247286	0.733101
14	1	0	-2.504718	1.711452	-0.941517
15	53	0	-3.169996	-0.710987	-0.065637

 Low frequencies (cm⁻¹): 9.9543 13.3669 17.3507
 22.4708 27.2476 54.2600

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	2.003856	-0.962306	-1.446339
2	13	0	4.195184	-1.153738	-0.000586
3	13	0	3.432099	1.159156	-1.346075
4	13	0	2.003881	-0.963901	1.445336
5	13	0	3.431637	1.157979	1.347340
6	13	0	1.301373	1.730785	0.000489
7	13	0	-0.070471	-0.393360	-0.000175
8	6	0	-3.181471	1.688589	0.000007
9	6	0	-4.644985	1.943093	-0.000070
10	1	0	-2.639015	1.922561	-0.898729
11	1	0	-5.126163	1.537752	-0.881530
12	1	0	-5.126248	1.537792	0.881363

13	1	0	-4.815691	3.019639	-0.000104
14	1	0	-2.639108	1.922535	0.898806
15	53	0	-2.727610	-0.739629	0.000013

 Low frequencies (cm⁻¹): -1314.1805 14.2387 19.6942
 29.2758 42.4615 59.6322

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.966716	-2.529593	0.190903
2	13	0	3.208179	-2.075379	-0.973963
3	13	0	1.378295	-0.327057	-1.718297
4	13	0	1.117513	-0.700152	2.022377
5	13	0	3.349074	-0.261345	0.801390
6	13	0	1.319919	1.410623	0.221034
7	13	0	-0.682022	-0.496718	-0.197376
8	6	0	1.200970	3.383187	0.352748
9	6	0	2.144528	4.155632	-0.569183
10	1	0	1.382944	3.658944	1.388863
11	1	0	2.028217	5.228963	-0.449150
12	1	0	3.185081	3.921296	-0.367514
13	1	0	1.960609	3.927168	-1.614028
14	1	0	0.169296	3.660050	0.146473
15	53	0	-3.157526	-0.016873	-0.043489

Low frequencies (cm⁻¹): 13.2126 31.9980 39.3039
 57.0321 75.1781 85.4673

Al₇ C₂H₃I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-2.474178	-1.194959	-1.183518
2	13	0	-4.398278	0.477559	-1.512912
3	13	0	-4.503723	-1.467765	0.369658
4	13	0	-2.347379	1.550781	-0.392645
5	13	0	-4.394329	1.131385	1.107391
6	13	0	-2.462878	-0.495595	1.594372
7	13	0	-0.379837	-0.148983	0.021526
8	53	0	3.427983	0.070900	0.001347
9	6	0	5.514277	0.383840	-0.008068
10	6	0	6.395884	-0.595314	-0.007544
11	1	0	5.778262	1.431673	-0.013256

12	1	0	7.455125	-0.362629	-0.012516
13	1	0	6.110356	-1.639423	-0.002302

 Low frequencies (cm⁻¹): 6.1679 13.3761 22.2879
 33.0228 36.7963 62.8742

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	2.004649	-1.153454	-1.177132
2	13	0	4.005751	-1.471953	0.403029
3	13	0	3.992748	0.440036	-1.507543
4	13	0	2.000224	-0.407629	1.606343
5	13	0	3.992050	1.135174	1.102784
6	13	0	1.988556	1.630561	-0.427493
7	13	0	-0.022818	0.012081	0.000316
8	53	0	-2.817741	-0.114420	-0.000253
9	6	0	-5.137100	-0.315874	0.001725
10	6	0	-5.901203	0.750249	-0.000440
11	1	0	-5.441992	-1.354029	0.004519
12	1	0	-6.984751	0.652656	0.000454
13	1	0	-5.498245	1.756772	-0.003186

 Low frequencies (cm⁻¹): -149.0877 10.4271 21.4970
 43.3288 48.4419 60.8946

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.941795	-2.032322	-0.794798
2	13	0	3.018846	-1.688861	1.047330
3	13	0	3.227119	-0.941407	-1.389338
4	13	0	1.043773	-0.264409	1.654941
5	13	0	3.219950	1.097011	0.816762
6	13	0	1.232784	0.648120	-0.940542
7	13	0	-0.928282	-0.535826	-0.052806
8	53	0	-3.374964	0.037098	0.014638
9	6	0	2.062386	2.498482	-0.704297
10	6	0	1.428153	3.463518	-0.017451
11	1	0	0.678149	3.233445	0.734223
12	1	0	1.640812	4.518122	-0.173980
13	1	0	2.783112	2.840250	-1.445730

 Low frequencies (cm⁻¹): 33.8269 48.6653 61.4320
 84.9865 90.2886 128.0257

Al₇ C₂H₃I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	2.573224	0.985785	-1.430759
2	13	0	4.551083	-0.665231	-1.296737
3	13	0	4.443613	1.577305	0.244625
4	13	0	2.448218	-1.650624	-0.170580
5	13	0	4.351741	-0.874316	1.395078
6	13	0	2.337608	0.740944	1.478509
7	13	0	0.423140	0.048582	-0.208146
8	53	0	-3.462860	-0.108218	-0.056384
9	6	0	-5.557420	-0.287559	0.210268
10	6	0	-6.398788	0.726975	0.151602
11	1	0	-5.858080	-1.309013	0.401279
12	1	0	-7.460201	0.550352	0.300184
13	1	0	-6.085041	1.745906	-0.040207

Low frequencies (cm⁻¹): 10.6193 11.8758 15.9207
19.8453 27.5972 32.5636

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.980510	1.191755	-1.205011
2	13	0	4.019593	-0.357222	-1.538767
3	13	0	4.003864	1.581390	0.346160
4	13	0	2.069418	-1.623704	-0.416262
5	13	0	4.087030	-1.033534	1.078323
6	13	0	2.073387	0.473291	1.648665
7	13	0	0.028955	-0.032639	0.067730
8	53	0	-2.885634	-0.137162	0.029791
9	6	0	-5.157533	-0.250658	-0.114461
10	6	0	-5.919966	0.818548	-0.057111
11	1	0	-5.486636	-1.275289	-0.233589
12	1	0	-7.002570	0.725125	-0.129709
13	1	0	-5.523030	1.821041	0.062870

Low frequencies (cm⁻¹): -80.4665 10.6353 15.1166
18.7387 35.1319 36.5414

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	13	0	0.918651	-2.513735	0.215125
2	13	0	3.204660	-2.123600	-0.907887
3	13	0	1.326599	-0.492403	-1.728323
4	13	0	1.034895	-0.644958	1.999319
5	13	0	3.291102	-0.305688	0.847087
6	13	0	1.345661	1.360082	0.113440
7	13	0	-0.727229	-0.491867	-0.157913
8	6	0	1.299058	3.351352	0.017542
9	6	0	2.629762	4.019112	-0.335299
10	1	0	0.943083	3.695292	0.995879
11	1	0	2.536088	5.109850	-0.353027
12	1	0	3.412104	3.773242	0.387623
13	1	0	2.990793	3.710009	-1.319538
14	1	0	0.522997	3.626089	-0.704204
15	53	0	-3.190649	0.068320	-0.038703

 Low frequencies (cm⁻¹): 21.9069 31.0044 47.6784
 63.3540 73.8844 79.1496

Al₇ C₂H₃I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-2.340911	0.821680	1.517805
2	13	0	-4.248497	-0.889337	1.551941
3	13	0	-4.308518	1.777656	0.182356
4	13	0	-2.789818	-1.686863	-0.392571
5	13	0	-5.100640	-0.509929	-0.956031
6	13	0	-2.843087	0.714124	-1.624700
7	13	0	-0.676746	-0.092482	-0.334015
8	53	0	3.690773	-0.101378	0.014020
9	6	0	5.777324	-0.252866	0.178597
10	6	0	6.612594	0.693119	-0.173910
11	1	0	6.091389	-1.194497	0.585249
12	1	0	7.672250	0.538067	-0.057762
13	1	0	6.292724	1.634907	-0.580895

 Low frequencies (cm⁻¹): 10.7029 6.5226 9.2898

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	2.072437	-1.184680	-1.227595
2	13	0	4.077049	-1.445336	0.378829

3	13	0	4.016865	0.489451	-1.508118
4	13	0	2.061076	-0.455839	1.653219
5	13	0	4.006300	1.154022	1.117818
6	13	0	2.002006	1.680611	-0.420672
7	13	0	0.046458	-0.035702	0.005999
8	53	0	-2.888880	-0.140636	0.001571
9	6	0	-5.173062	-0.243974	-0.008381
10	6	0	-5.917265	0.829097	-0.001595
11	1	0	-5.515927	-1.261463	-0.019154
12	1	0	-6.994284	0.748183	-0.006707
13	1	0	-5.505665	1.823386	0.009198

Low frequencies (cm⁻¹): -181.8346 -13.1149 7.6223
 11.6027 16.6007 17.6246

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.889607	-2.010569	-0.897172
2	13	0	3.021566	-1.776924	0.957776
3	13	0	3.208552	-0.950503	-1.433427
4	13	0	1.048045	-0.370467	1.707957
5	13	0	3.209645	1.087399	1.018640
6	13	0	1.259146	0.717352	-0.925009
7	13	0	-0.912487	-0.496426	-0.043501
8	53	0	-3.367880	0.033656	0.024060
9	6	0	2.005161	2.572094	-0.796706
10	6	0	1.468048	3.558211	-0.077812
11	1	0	0.688832	3.384118	0.646591
12	1	0	1.785016	4.584834	-0.183094
13	1	0	2.771589	2.867270	-1.500030

Low frequencies (cm⁻¹): 33.3409 45.5520 50.6540
 61.3285 78.0575 101.5393

Al₇ C₆H₅I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-3.085993	0.607962	-1.684777
2	13	0	-4.705239	0.499613	0.320208
3	13	0	-3.609164	-1.723944	-0.728353
4	13	0	-2.380323	1.423138	0.947935

5	13	0	-2.888833	-0.957041	1.745148
6	13	0	-1.214649	-0.931658	-0.203866
7	13	0	-0.678475	1.509608	-1.066812
8	53	0	2.595366	-1.602866	-0.005353
9	6	0	1.988040	1.103099	1.242561
10	6	0	2.573055	0.499779	0.138165
11	6	0	3.112519	1.258383	-0.891273
12	6	0	3.075585	2.644880	-0.803403
13	6	0	2.495179	3.263277	0.296373
14	6	0	1.954465	2.491335	1.315972
15	1	0	1.555297	0.504325	2.033510
16	1	0	3.560405	0.776564	-1.749685
17	1	0	3.495541	3.238769	-1.605137
18	1	0	2.462871	4.343251	0.357787
19	1	0	1.493219	2.964653	2.173583

 Low frequencies (cm⁻¹): 10.0397 16.6349 23.9952
 34.6324 50.0824 64.4715

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-3.102358	-1.381661	-0.935201
2	13	0	-5.007848	0.233609	-1.541308
3	13	0	-5.085931	-1.280014	0.693904
4	13	0	-2.914377	1.481933	-0.729431
5	13	0	-4.909374	1.411061	0.887486
6	13	0	-3.001942	-0.127763	1.658227
7	13	0	-0.988414	-0.140866	-0.015672
8	53	0	1.835134	-0.146780	-0.011915
9	6	0	4.888181	-1.136109	0.010690
10	6	0	4.138591	0.022987	0.001257
11	6	0	4.710169	1.279177	-0.000032
12	6	0	6.099135	1.374331	0.008019
13	6	0	6.879159	0.224814	0.017375
14	6	0	6.276271	-1.026377	0.018715
15	1	0	4.413497	-2.109401	0.011779
16	1	0	4.097497	2.172193	-0.006985
17	1	0	6.568678	2.350560	0.007031
18	1	0	7.958659	0.304523	0.023628
19	1	0	6.883682	-1.923368	0.025851

 Low frequencies (cm⁻¹): -106.5954 10.2511 13.2924
 16.6006 43.0802 45.6123

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	13	0	-0.551667	-2.135196	1.488864
2	13	0	-2.183375	-3.603279	0.000208
3	13	0	-2.968777	-1.404339	1.322724
4	13	0	-0.551960	-2.135349	-1.488954
5	13	0	-2.969011	-1.404364	-1.322350
6	13	0	-1.329870	0.198263	-0.000063
7	13	0	1.103407	-0.884950	-0.000194
8	6	0	-1.422537	2.166511	-0.000125
9	6	0	-0.251191	2.932994	0.000545
10	6	0	-0.297592	4.322077	0.000652
11	6	0	-1.523043	4.974498	0.000173
12	6	0	-2.699103	4.234649	-0.000500
13	6	0	-2.645907	2.846645	-0.000670
14	1	0	0.721269	2.448630	0.000955
15	1	0	0.622422	4.893760	0.001135
16	1	0	-1.562128	6.056755	0.000295
17	1	0	-3.657281	4.740105	-0.000893
18	1	0	-3.576682	2.288695	-0.001224
19	53	0	3.459527	-0.028159	-0.000071

 Low frequencies (cm⁻¹): 18.4477 26.1191 38.7273
 49.9300 56.3588 97.2314

Al₇ C₆H₅I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-2.911548	-0.013085	-1.586981
2	13	0	-5.296150	0.762316	-1.002377
3	13	0	-4.349483	-1.657585	-0.198434
4	13	0	-3.579543	2.037462	0.430817
5	13	0	-4.916454	0.195912	1.651752
6	13	0	-2.480060	-0.540130	1.203306
7	13	0	-1.102407	1.274775	-0.142412
8	53	0	2.240282	-1.298013	-0.192715
9	6	0	4.749515	-0.071469	1.033854
10	6	0	3.833678	0.085509	0.003518
11	6	0	3.941861	1.132050	-0.900880
12	6	0	4.989570	2.035854	-0.766249
13	6	0	5.915093	1.893053	0.259050
14	6	0	5.792427	0.839725	1.155626
15	1	0	4.656175	-0.891398	1.734709
16	1	0	3.222526	1.246315	-1.701901
17	1	0	5.076678	2.855447	-1.470797
18	1	0	6.730007	2.600626	0.359148
19	1	0	6.510192	0.719708	1.959471

Low frequencies (cm⁻¹): 6.8374 9.4913 11.0629
 14.1858 17.4716 21.5092

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	2.759437	-0.809731	-1.435176
2	13	0	4.932228	-0.705183	0.008284
3	13	0	3.906266	1.488693	-1.352138
4	13	0	2.755932	-0.789886	1.448479
5	13	0	3.906561	1.505593	1.338186
6	13	0	1.710472	1.699193	-0.007821
7	13	0	0.601746	-0.568255	0.001901
8	53	0	-1.879936	-1.562817	-0.000635
9	6	0	-4.610868	0.103871	0.002774
10	6	0	-3.250627	0.316997	0.000123
11	6	0	-2.665009	1.555111	-0.002472
12	6	0	-3.502665	2.668622	-0.002233
13	6	0	-4.882111	2.502892	0.000487
14	6	0	-5.435237	1.227692	0.002954
15	1	0	-5.036099	-0.893502	0.004718
16	1	0	-1.580130	1.672372	-0.004692
17	1	0	-3.069674	3.663387	-0.004213
18	1	0	-5.530454	3.371568	0.000665
19	1	0	-6.512291	1.098832	0.005048

Low frequencies (cm⁻¹): -222.1687 2.2308 26.2426
 26.3414 35.3059 43.6324

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.056668	-2.227308	-1.519222
2	13	0	1.281869	-3.985899	0.069571
3	13	0	2.584738	-2.036029	-1.279351
4	13	0	0.027238	-2.175894	1.558566
5	13	0	2.561513	-1.984345	1.360110
6	13	0	1.352105	-0.034169	-0.018421
7	13	0	-1.269200	-0.616292	-0.021658
8	6	0	1.930299	1.860987	-0.001797
9	6	0	1.027387	2.878070	0.334141
10	6	0	1.415797	4.212774	0.351443
11	6	0	2.721794	4.560309	0.030771
12	6	0	3.635621	3.568933	-0.306077
13	6	0	3.242343	2.236292	-0.320617
14	1	0	-0.000763	2.635721	0.587654
15	1	0	0.696643	4.981275	0.614300
16	1	0	3.026882	5.601039	0.042698

17	1	0	4.656997	3.834248	-0.558061
18	1	0	3.975505	1.480301	-0.586021
19	53	0	-3.432619	0.666838	-0.048538

 Low frequencies (cm⁻¹): 6.0898 22.9866 34.8784
 46.8295 55.6904 83.9707

Al₇ C₆H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	4.277310	0.078433	1.505757
2	13	0	4.812008	0.900167	-0.860797
3	13	0	3.608873	-1.783015	-0.119898
4	13	0	2.460838	1.833713	-0.435282
5	13	0	2.732800	-0.213403	-2.108224
6	13	0	1.388149	-0.556016	0.164396
7	13	0	1.946484	1.202249	2.073491
8	53	0	-2.426988	-1.655675	0.081739
9	6	0	-3.178274	0.934679	-1.309986
10	6	0	-3.122493	0.327907	-0.072103
11	6	0	-3.513045	1.000014	1.067768
12	6	0	-3.966469	2.301732	0.961885
13	6	0	-4.027319	2.922162	-0.270420
14	6	0	-3.633268	2.237003	-1.402913
15	1	0	-2.873070	0.405617	-2.193170
16	1	0	-3.467098	0.521384	2.027749
17	1	0	-4.271293	2.827634	1.848956
18	1	0	-4.379888	3.934738	-0.347597
19	1	0	-3.677083	2.712733	-2.366254

 Low frequencies (cm⁻¹): 4.1784 6.6708 14.0182
 17.0611 18.3752 20.6285

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-3.115379	-1.481173	-0.940825
2	13	0	-4.982405	0.164725	-1.585456
3	13	0	-5.007372	-1.346305	0.793230
4	13	0	-3.004466	1.555390	-0.697673
5	13	0	-5.112046	1.322310	0.811545
6	13	0	-3.038498	0.034098	1.713616
7	13	0	-1.062813	-0.081035	-0.019844

8	53	0	1.889958	-0.124921	-0.046886
9	6	0	4.906206	-1.138562	0.065770
10	6	0	4.167151	0.018984	0.004093
11	6	0	4.757422	1.260143	-0.025766
12	6	0	6.139576	1.341173	0.005697
13	6	0	6.903338	0.191051	0.067005
14	6	0	6.287681	-1.045832	0.096842
15	1	0	4.427416	-2.100467	0.088794
16	1	0	4.163291	2.154536	-0.073609
17	1	0	6.616240	2.305448	-0.017708
18	1	0	7.976191	0.258462	0.091306
19	1	0	6.879577	-1.943030	0.144618

Low frequencies (cm⁻¹): -153.3197 8.2878 10.0858
 10.9189 23.5624 34.2228

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.023238	-2.214438	-1.563350
2	13	0	1.202057	-4.016749	0.000376
3	13	0	2.512393	-2.053031	-1.317856
4	13	0	-0.023626	-2.214257	1.563592
5	13	0	2.512066	-2.052888	1.318711
6	13	0	1.345340	-0.039485	0.000174
7	13	0	-1.277220	-0.607703	-0.000125
8	6	0	1.965323	1.830669	0.000144
9	6	0	1.053856	2.885634	-0.000029
10	6	0	1.471968	4.203695	-0.000052
11	6	0	2.820967	4.499928	0.000098
12	6	0	3.746691	3.473516	0.000271
13	6	0	3.320912	2.158970	0.000293
14	1	0	-0.005335	2.688390	-0.000150
15	1	0	0.745040	4.996873	-0.000187
16	1	0	3.149614	5.524203	0.000081
17	1	0	4.799226	3.697292	0.000389
18	1	0	4.064283	1.379556	0.000429
19	53	0	-3.400984	0.735479	-0.000466

Low frequencies (cm⁻¹): 16.7738 23.1378 26.0381
 41.8361 55.5021 78.2433

Al₈ C₂H₅I (M062X/TZVP, LANL2DZ level of theory)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.592735	-0.606659	0.313927
2	13	0	-1.359375	-0.215710	-1.554278
3	13	0	-0.383121	1.979001	-0.190673
4	13	0	-1.166073	0.499417	1.742176
5	13	0	-3.497772	-0.527544	1.462048
6	13	0	-2.899119	1.268965	-0.218858
7	13	0	-4.039372	-1.266913	-1.370788
8	13	0	-1.670165	-1.857131	0.356139
9	6	0	0.834119	3.442435	-0.684679
10	6	0	2.041233	3.576937	0.254563
11	1	0	0.253510	4.370095	-0.699912
12	1	0	2.681023	4.414111	-0.033002
13	1	0	1.728769	3.742302	1.287555
14	1	0	2.657550	2.675731	0.245120
15	1	0	1.167026	3.278586	-1.713960
16	53	0	3.051876	-0.965125	-0.066436

Low frequencies (cm⁻¹): 20.6277 28.5370 45.7432
 61.1800 82.1011 101.9869

Al₈ C₂H₅I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.021128	0.084509	-0.234601
2	13	0	1.613206	-1.427097	1.094504
3	13	0	0.348275	2.608855	-0.374502
4	13	0	2.667073	1.851599	-1.065846
5	13	0	4.162899	0.308151	0.274055
6	13	0	2.011661	1.090253	1.572594
7	13	0	3.885112	-2.215221	0.281131
8	13	0	2.144638	-0.665032	-1.537303
9	53	0	-2.901878	-0.862893	-0.231245
10	6	0	-3.873995	1.587977	1.389110
11	6	0	-3.758370	1.156583	-0.046861
12	1	0	-2.898061	1.637581	1.874214
13	1	0	-4.310780	2.592392	1.413754
14	1	0	-4.520381	0.925944	1.966717
15	1	0	-4.712721	1.074407	-0.560143
16	1	0	-3.066258	1.767414	-0.622463

Low frequencies (cm⁻¹): 20.2398 27.6608 37.3973
 40.4263 47.2212 53.9727

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.435396	-0.157766	0.004427
2	13	0	1.730066	-0.693614	1.347159
3	13	0	0.573128	2.130959	0.033756
4	13	0	2.776480	1.663979	-1.308128
5	13	0	4.200747	-0.168828	0.000756
6	13	0	2.775822	1.626481	1.359856
7	13	0	3.417548	-2.660383	-0.046153
8	13	0	1.724582	-0.653034	-1.361384
9	53	0	-2.933080	-0.905080	0.000151
10	6	0	-3.228960	2.476585	-0.169104
11	6	0	-4.153620	1.386410	0.127795
12	1	0	-3.303261	2.826367	-1.198436
13	1	0	-3.367833	3.312875	0.522143
14	1	0	-2.150047	2.184715	-0.016003
15	1	0	-4.468498	1.240134	1.153805
16	1	0	-4.880372	1.085865	-0.615417

Low frequencies (cm⁻¹): -124.3147 20.9247 33.4922
 45.0341 51.1110 54.0888

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.742026	-0.577837	0.273687
2	13	0	-1.279538	-0.368625	-1.604150
3	13	0	-0.517356	1.914566	-0.190064
4	13	0	-1.104560	0.343906	1.776566
5	13	0	-3.318064	-0.928135	1.477461
6	13	0	-2.952250	0.945462	-0.194939
7	13	0	-3.830929	-1.701652	-1.362545
8	13	0	-1.378992	-2.062461	0.326759
9	6	0	0.466849	3.556377	-0.695698
10	6	0	0.186447	4.766098	0.203689
11	1	0	0.215172	3.787759	-1.737069
12	1	0	0.753926	5.644266	-0.119724
13	1	0	-0.870739	5.045262	0.194421
14	1	0	0.459798	4.570936	1.243983
15	1	0	1.536415	3.317863	-0.690521
16	53	0	3.232100	-0.766959	-0.046700

Low frequencies (cm⁻¹): 6.9139 36.7153 46.3394
 60.8292 80.3981 97.0932

35.4401 41.5555 47.5961

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.623768	-0.596103	0.265087
2	13	0	-1.373451	-0.212200	-1.613171
3	13	0	-0.450177	2.006265	-0.172132
4	13	0	-1.116368	0.473094	1.788335
5	13	0	-3.425793	-0.613075	1.515358
6	13	0	-2.931410	1.211556	-0.167949
7	13	0	-4.053765	-1.354096	-1.376546
8	13	0	-1.605584	-1.889358	0.331012
9	6	0	0.662266	3.548502	-0.687415
10	6	0	1.864482	3.834676	0.213366
11	1	0	0.006136	4.416700	-0.722651
12	1	0	2.414275	4.708594	-0.123644
13	1	0	1.562386	4.019445	1.239216
14	1	0	2.560800	3.002965	0.229686
15	1	0	0.992278	3.392514	-1.712652
16	53	0	3.087354	-0.965630	-0.065577

Low frequencies (cm⁻¹): 28.0673 36.6996 47.4837
64.0390 78.2876 87.6885

Al₈ C₂H₃I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.043794	0.123934	-0.157200
2	13	0	-2.081494	-0.518660	-1.593384
3	13	0	-0.318506	2.651366	-0.006505
4	13	0	-2.054237	0.909376	1.634474
5	13	0	-4.125217	0.275532	0.203998
6	13	0	-2.575176	1.931956	-0.934957
7	13	0	-3.872965	-2.247658	-0.051719
8	13	0	-1.642082	-1.539741	0.946131
9	53	0	3.032737	-0.856038	-0.057462
10	6	0	3.881204	1.061867	-0.263753
11	6	0	3.615544	2.048301	0.566646
12	1	0	2.949344	1.942819	1.413506
13	1	0	4.075691	3.016783	0.404073
14	1	0	4.534559	1.130020	-1.120383

Low frequencies (cm⁻¹): 16.7599 26.7530 33.9522

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.059039	0.209941	-0.090838
2	13	0	-2.043668	-0.436846	-1.650722
3	13	0	-0.462680	2.711606	0.136395
4	13	0	-2.199059	0.854488	1.697728
5	13	0	-4.195877	0.186450	0.131088
6	13	0	-2.680655	1.967397	-0.854044
7	13	0	-3.819626	-2.309682	-0.171738
8	13	0	-1.638458	-1.550524	0.888904
9	53	0	3.032853	-0.843655	0.006361
10	6	0	4.110589	0.919350	-0.455282
11	6	0	4.026047	2.026487	0.253967
12	1	0	3.398308	2.127530	1.130398
13	1	0	4.606569	2.892383	-0.050131
14	1	0	4.721918	0.791986	-1.337555

Low frequencies (cm⁻¹): 13.8767 22.8966 27.6765
 35.3377 47.5275 49.3485

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.526244	-0.422234	-0.000003
2	13	0	1.689740	-0.615024	1.373517
3	13	0	0.494934	1.888020	-0.000491
4	13	0	2.719405	1.710754	-1.325877
5	13	0	4.067709	-0.214107	0.000170
6	13	0	2.719193	1.711025	1.325604
7	13	0	3.317116	-2.746759	0.000057
8	13	0	1.690006	-0.615525	-1.372971
9	53	0	-3.025309	-0.828706	-0.000073
10	6	0	-3.858651	1.874617	0.000344
11	6	0	-2.866050	2.661526	0.000181
12	1	0	-1.777305	2.229641	-0.000069
13	1	0	-2.856627	3.748415	0.000192
14	1	0	-4.910643	1.676555	0.000490

Low frequencies (cm⁻¹): -111.7779 28.4611 41.0411
 47.4812 54.3091 85.8104

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.777905	-0.544188	0.232517

2	13	0	-1.259436	-0.019429	-1.556623
3	13	0	-0.560982	1.944589	0.303786
4	13	0	-1.081794	-0.008858	1.900603
5	13	0	-3.267825	-1.239884	1.352755
6	13	0	-2.963557	0.938812	0.086246
7	13	0	-3.771793	-1.444508	-1.588311
8	13	0	-1.305008	-2.069707	-0.007680
9	53	0	3.269494	-0.614798	-0.107974
10	6	0	0.346694	3.668304	0.108598
11	6	0	-0.199794	4.701232	-0.538994
12	1	0	-1.179737	4.645376	-1.008390
13	1	0	0.303768	5.661807	-0.635113
14	1	0	1.333713	3.821169	0.545711

 Low frequencies (cm⁻¹): 16.9611 35.7519 48.2037
 64.7594 81.8891 94.7918

Al₈ C₂H₃I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.289470	0.269768	0.068928
2	13	0	-2.155896	-0.295293	-1.641329
3	13	0	-0.472888	2.827836	-0.026135
4	13	0	-2.527932	0.564736	1.888927
5	13	0	-4.404971	0.114239	0.097595
6	13	0	-2.828228	1.979652	-0.574518
7	13	0	-3.789744	-2.248810	-0.553553
8	13	0	-1.742785	-1.683979	0.820197
9	53	0	3.260149	-0.823543	0.041967
10	6	0	4.237217	0.935302	-0.560382
11	6	0	4.223576	2.048190	0.129242
12	1	0	3.706778	2.154173	1.065057
13	1	0	4.749296	2.909639	-0.247234
14	1	0	4.746149	0.817071	-1.496664

 Low frequencies (cm⁻¹): 5.8058 16.1928 18.1861
 21.6044 23.1612 39.7907

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.514403	-0.417370	-0.000008
2	13	0	-1.687135	-0.612159	-1.385304
3	13	0	-0.467612	1.901807	0.000042

1	13	0	0.756767	-0.638677	0.627145
2	13	0	3.052831	-1.737322	0.769961
3	13	0	0.165575	1.773605	1.292020
4	13	0	2.050853	2.037687	-0.414221
5	13	0	4.354186	0.947690	-0.264621
6	13	0	2.919428	0.611112	1.850442
7	13	0	4.803350	-1.445757	-1.044334
8	13	0	2.170627	-0.305099	-1.495571
9	6	0	-2.841151	0.382308	-0.270235
10	6	0	-2.140645	0.945969	-1.327080
11	6	0	-2.139045	2.328508	-1.475798
12	6	0	-2.820650	3.133250	-0.572322
13	6	0	-3.513767	2.553093	0.482710
14	6	0	-3.527085	1.171578	0.640767
15	1	0	-1.591172	0.322864	-2.020552
16	1	0	-1.586673	2.771976	-2.294649
17	1	0	-2.808823	4.209162	-0.687954
18	1	0	-4.046370	3.173338	1.192377
19	1	0	-4.060768	0.720292	1.466484
20	53	0	-2.784324	-1.706565	0.005762

 Low frequencies (cm⁻¹): 13.9902 16.5776 20.7895
 30.9550 41.6726 57.4868

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.118927	-2.197095	-0.000012
2	13	0	-2.237430	-0.126651	-1.400113
3	13	0	-0.067062	0.439183	0.000026
4	13	0	-1.444281	2.292574	1.275844
5	13	0	-3.773786	1.491436	0.000003
6	13	0	-1.444255	2.292606	-1.275774
7	13	0	-4.571005	-1.155507	-0.000045
8	13	0	-2.237460	-0.126685	1.400111
9	53	0	1.685849	-1.909490	0.000003
10	6	0	2.786738	0.898525	-1.214586
11	6	0	2.394182	0.346813	0.000004
12	6	0	2.786819	0.898512	1.214572
13	6	0	3.516762	2.079369	1.208315
14	6	0	3.873355	2.668987	-0.000034
15	6	0	3.516681	2.079381	-1.208366
16	1	0	2.488164	0.436888	-2.149452
17	1	0	2.488309	0.436866	2.149454
18	1	0	3.804404	2.540779	2.144701
19	1	0	4.442317	3.589931	-0.000048
20	1	0	3.804260	2.540801	-2.144767

 Low frequencies (cm⁻¹): -301.9048 22.7376 26.1185
 41.1497 49.7929 68.6928

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.392687	1.303928	0.222990
2	13	0	1.604834	-0.425758	-1.512396
3	13	0	-0.160122	-1.441942	0.347112
4	13	0	1.504171	-0.254342	1.869991
5	13	0	3.971247	-0.710877	1.344933
6	13	0	2.322236	-2.202063	0.131222
7	13	0	4.445315	-0.934032	-1.587302
8	13	0	2.958615	1.136402	-0.040652
9	6	0	-1.992599	-2.081163	0.145841
10	6	0	-3.068529	-1.315668	0.613830
11	6	0	-4.379759	-1.745635	0.455724
12	6	0	-4.640620	-2.956598	-0.172519
13	6	0	-3.590034	-3.733877	-0.644097
14	6	0	-2.281155	-3.296472	-0.487770
15	1	0	-2.888367	-0.365280	1.107491
16	1	0	-5.197238	-1.136175	0.820714
17	1	0	-5.662110	-3.294605	-0.295807
18	1	0	-3.791244	-4.678299	-1.134782
19	1	0	-1.475937	-3.917691	-0.868198
20	53	0	-1.561806	2.830970	-0.173248

Low frequencies (cm⁻¹): 21.0610 33.5463 38.0918
 49.4042 52.1808 101.0765

Al₈ C₆H₅I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.789283	0.157736	-0.070349
2	13	0	2.571762	-1.448953	0.834563
3	13	0	0.952888	2.680590	0.214820
4	13	0	3.218413	2.192503	-0.829792
5	13	0	4.931022	0.562963	0.085754
6	13	0	2.898510	0.977441	1.696399
7	13	0	4.792591	-1.944700	-0.297752
8	13	0	2.804493	-0.240276	-1.678883
9	6	0	-3.606677	-0.020702	-0.022280
10	6	0	-4.884933	-0.499591	-0.260832
11	6	0	-5.936678	0.408122	-0.316548
12	6	0	-5.704529	1.765394	-0.136795
13	6	0	-4.414362	2.220758	0.099780

14	6	0	-3.350487	1.327308	0.160784
15	1	0	-5.067742	-1.557084	-0.403229
16	1	0	-6.940850	0.044245	-0.502654
17	1	0	-6.528742	2.467690	-0.181988
18	1	0	-4.224260	3.278947	0.239731
19	1	0	-2.343153	1.684859	0.341268
20	53	0	-1.999543	-1.420969	0.074535

 Low frequencies (cm⁻¹): 7.0026 7.0691 21.5589
 27.8534 32.4143 46.8598

Coordinate of TS

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	-1.089475	-2.175639	-0.000002	
2	13	0	-2.284679	-0.151112	-1.418013	
3	13	0	-0.113695	0.500563	0.000032	
4	13	0	-1.556555	2.308153	1.283027	
5	13	0	-3.836593	1.444706	0.000011	
6	13	0	-1.556529	2.308160	-1.282984	
7	13	0	-4.646779	-1.182736	-0.000017	
8	13	0	-2.284695	-0.151130	1.418030	
9	53	0	1.720257	-1.906005	-0.000014	
10	6	0	2.890232	0.896657	-1.214987	
11	6	0	2.505574	0.342109	0.000009	
12	6	0	2.890425	0.896566	1.214985	
13	6	0	3.620671	2.079268	1.207830	
14	6	0	3.980132	2.668324	-0.000022	
15	6	0	3.620475	2.079362	-1.207860	
16	1	0	2.603698	0.431585	-2.152071	
17	1	0	2.604038	0.431427	2.152081	
18	1	0	3.909205	2.539912	2.146325	
19	1	0	4.552532	3.588992	-0.000033	
20	1	0	3.908854	2.540078	-2.146367	

 Low frequencies (cm⁻¹): -246.1450 11.2627 17.7029
 35.5003 45.5209 58.0317

Optimized geometry after C-I dissociation

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	0.480986	1.282229	0.191742	
2	13	0	1.559314	-0.573710	-1.542845	
3	13	0	-0.352701	-1.419032	0.310430	
4	13	0	1.385123	-0.386690	1.904373	
5	13	0	3.801285	-1.088141	1.397658	
6	13	0	2.053248	-2.430301	0.137532	
7	13	0	4.340768	-1.355318	-1.526215	

8	13	0	3.032676	0.869771	-0.008761
9	6	0	-2.222231	-1.981699	0.116126
10	6	0	-3.250016	-1.375236	0.852373
11	6	0	-4.571417	-1.781652	0.714786
12	6	0	-4.894051	-2.808313	-0.164275
13	6	0	-3.893286	-3.425870	-0.904920
14	6	0	-2.573676	-3.014525	-0.765121
15	1	0	-3.022591	-0.570109	1.545174
16	1	0	-5.350443	-1.296432	1.293010
17	1	0	-5.925143	-3.126858	-0.272770
18	1	0	-4.141814	-4.227446	-1.592339
19	1	0	-1.809065	-3.511770	-1.356027
20	53	0	-1.193056	3.120224	-0.187580

 Low frequencies (cm⁻¹): 12.3053 20.7924 34.2031
 50.2546 54.2329 90.4693

Al₈ C₆H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.920645	-0.058974	-0.437910
2	13	0	-2.821639	-1.750727	-0.285575
3	13	0	-0.626552	2.378696	-1.179067
4	13	0	-2.932281	2.308285	-0.057460
5	13	0	-4.918773	0.752271	0.174693
6	13	0	-3.410047	0.199963	-1.915566
7	13	0	-4.605334	-1.392694	1.473360
8	13	0	-2.463495	0.358749	1.603106
9	6	0	3.423040	0.089640	0.195588
10	6	0	3.258284	0.712330	1.415407
11	6	0	3.960523	1.874227	1.677565
12	6	0	4.816278	2.402235	0.730949
13	6	0	4.970771	1.766336	-0.485289
14	6	0	4.273236	0.604862	-0.760603
15	1	0	2.594533	0.304917	2.154518
16	1	0	3.834129	2.363540	2.626656
17	1	0	5.360449	3.305413	0.940053
18	1	0	5.634802	2.171134	-1.227845
19	1	0	4.394349	0.114038	-1.707759
20	53	0	2.359489	-1.684891	-0.213394

 Low frequencies (cm⁻¹): 8.6472 10.4900 17.9415
 21.6087 22.9476 31.1658

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.107848	-2.227046	-0.000003
2	13	0	-2.271935	-0.159586	-1.435340
3	13	0	-0.098512	0.454305	0.000004
4	13	0	-1.520988	2.290908	1.277349
5	13	0	-3.824450	1.434745	0.000036
6	13	0	-1.521007	2.290922	-1.277301
7	13	0	-4.786426	-1.108485	0.000029
8	13	0	-2.271914	-0.159601	1.435373
9	53	0	1.754881	-1.883163	-0.000023
10	6	0	2.821353	0.924925	-1.206751
11	6	0	2.386711	0.397131	-0.000016
12	6	0	2.821374	0.924911	1.206718
13	6	0	3.619889	2.050331	1.201420
14	6	0	4.012497	2.614392	-0.000018
15	6	0	3.619867	2.050344	-1.201455
16	1	0	2.515705	0.481271	-2.137600
17	1	0	2.515743	0.481247	2.137567
18	1	0	3.935809	2.487013	2.131960
19	1	0	4.638154	3.488774	-0.000018
20	1	0	3.935770	2.487038	-2.131995

Low frequencies (cm⁻¹): -358.1026 21.1265 38.4276
49.2447 51.8182 68.3415

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.463819	1.295668	0.185748
2	13	0	1.557395	-0.546897	-1.560869
3	13	0	-0.316303	-1.439218	0.319778
4	13	0	1.377989	-0.346223	1.910705
5	13	0	3.807486	-1.003739	1.424452
6	13	0	2.102993	-2.373063	0.148221
7	13	0	4.386688	-1.288277	-1.558853
8	13	0	3.008060	0.913190	-0.009461
9	6	0	-2.171492	-2.018106	0.122187
10	6	0	-3.219298	-1.350977	0.756802
11	6	0	-4.529437	-1.766337	0.613577
12	6	0	-4.823148	-2.865795	-0.170360
13	6	0	-3.804230	-3.545832	-0.810082
14	6	0	-2.496631	-3.123773	-0.664081
15	1	0	-3.018599	-0.490475	1.373146
16	1	0	-5.319684	-1.232851	1.111730
17	1	0	-5.842279	-3.191041	-0.282958
18	1	0	-4.028375	-4.402029	-1.421759
19	1	0	-1.721401	-3.671068	-1.175096

20 53 0 -1.261319 3.080446 -0.186221

Low frequencies (cm⁻¹): 14.6622 22.0820 35.7222
51.8707 56.7431 85.0300

Al₁₃ C₂H₅I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.867836	-0.589154	0.124166
2	13	0	0.279948	0.379756	-2.156972
3	13	0	3.047379	-0.598417	-2.217957
4	13	0	3.389203	-2.128034	0.039780
5	13	0	1.039006	-2.024543	1.630321
6	13	0	0.900857	-2.257166	-1.099008
7	13	0	1.762763	-0.005761	0.002824
8	13	0	3.196066	-0.409104	2.176812
9	13	0	0.440409	0.578993	2.218339
10	13	0	0.091756	2.093890	-0.028146
11	13	0	2.436485	2.003904	-1.632105
12	13	0	4.420098	0.549356	-0.114230
13	13	0	2.601602	2.240023	1.097582
14	6	0	-4.002639	1.516841	-0.477162
15	6	0	-3.890542	2.311304	0.801413
16	1	0	-4.852700	1.804562	-1.087327
17	1	0	-3.716875	3.361942	0.552849
18	1	0	-4.801606	2.244510	1.395211
19	1	0	-3.052219	1.967156	1.408654
20	1	0	-3.091468	1.543702	-1.070040
21	53	0	-4.315408	-0.598668	-0.069493

Low frequencies (cm⁻¹): 15.1927 18.2652 28.3726
33.8126 61.6967 70.3884

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.867836	-0.589154	0.124166
2	13	0	0.279948	0.379756	-2.156972

Al₁₃ C₂H₅I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.871158	-0.411885	0.119758
2	13	0	0.228844	1.409313	-1.603703
3	13	0	2.963455	0.412694	-2.341540
4	13	0	3.226686	-2.008156	-1.062679
5	13	0	0.969198	-2.485953	0.624443
6	13	0	0.673621	-1.446679	-1.899929
7	13	0	1.818458	0.014896	0.005489
8	13	0	3.316270	-1.435695	1.625606
9	13	0	0.686088	-0.393499	2.374517
10	13	0	0.325716	1.990187	1.087175
11	13	0	2.546738	2.518933	-0.635388
12	13	0	4.523413	0.410517	-0.064043
13	13	0	2.921072	1.500514	1.894867
14	6	0	-4.392751	1.393140	-0.749798
15	6	0	-4.604142	2.404898	0.344704
16	1	0	-5.210227	1.351276	-1.464352
17	1	0	-4.656190	3.402305	-0.105485
18	1	0	-5.534452	2.230870	0.886999
19	1	0	-3.779896	2.403118	1.059160
20	1	0	-3.448023	1.523649	-1.273124
21	53	0	-4.276586	-0.654280	0.032225

Low frequencies (cm⁻¹): 16.3460 18.1210 20.3875
27.2832 40.6178 41.6290

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.913186	-0.107120	-0.027653
2	13	0	0.502703	1.465932	-1.808109
3	13	0	3.091098	0.135100	-2.314463
4	13	0	3.071686	-2.189421	-0.839902
5	13	0	0.690893	-2.325653	0.752144
6	13	0	0.651405	-1.464378	-1.860074
7	13	0	1.794967	0.030277	0.008511
8	13	0	3.055604	-1.460605	1.804562
9	13	0	0.533334	-0.075505	2.343533
10	13	0	0.460201	2.233570	0.833652
11	13	0	2.840263	2.394774	-0.761799
12	13	0	4.471238	0.162627	0.100918

13	13	0	2.903692	1.578035	1.855428
14	6	0	-6.340327	-0.303058	-0.032830
15	6	0	-6.798333	1.105593	-0.046969
16	1	0	-6.394450	-0.869316	0.889390
17	1	0	-7.899138	1.145432	-0.053309
18	1	0	-6.465957	1.653005	0.837226
19	1	0	-6.456125	1.638313	-0.936351
20	1	0	-6.382654	-0.884080	-0.946370
21	53	0	-3.557932	-0.234109	-0.008293

 Low frequencies (cm⁻¹): -133.3454 17.2765 24.5457
 32.9204 36.1882 41.7965

Optimized geometry after C-I dissociation

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	-1.181375	-0.994724	0.216855	
2	13	0	-0.151436	2.069997	-0.390030	
3	13	0	2.161337	1.740391	-1.775013	
4	13	0	2.798611	-0.975882	-2.060335	
5	13	0	0.627673	-2.491918	-1.094474	
6	13	0	0.210159	-0.133933	-2.471018	
7	13	0	1.235867	-0.073249	-0.013351	
8	13	0	2.856702	-2.133487	0.388653	
9	13	0	0.625169	-1.980020	1.870671	
10	13	0	0.080706	0.732827	2.241712	
11	13	0	2.093786	2.268683	1.055372	
12	13	0	3.876540	0.530991	-0.043300	
13	13	0	2.668538	-0.161784	2.299412	
14	6	0	-1.835722	3.077553	-0.728944	
15	6	0	-2.445706	3.761024	0.494821	
16	1	0	-2.550556	2.389091	-1.187329	
17	1	0	-3.328569	4.345939	0.216344	
18	1	0	-2.762068	3.032142	1.244234	
19	1	0	-1.742290	4.443571	0.978623	
20	1	0	-1.575727	3.812023	-1.499368	
21	53	0	-3.680789	-0.721261	-0.024052	

 Low frequencies (cm⁻¹): 29.3257 29.8836 33.0199
 44.2596 53.5186 56.4820

Al₁₃ C₂H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	0.799870	-0.402316	-0.141267	

2	13	0	-0.179148	1.029651	1.996764
3	13	0	-2.878629	0.134072	2.459144
4	13	0	-3.201447	-2.057190	0.773576
5	13	0	-0.816598	-2.442251	-0.600691
6	13	0	-0.708942	-1.553169	1.964999
7	13	0	-1.802028	0.055226	0.007118
8	13	0	-2.547921	-1.270788	-2.270388
9	13	0	-0.446920	0.387608	-2.354443
10	13	0	-0.170344	2.237285	-0.364521
11	13	0	-2.548442	2.379276	1.100867
12	13	0	-4.349906	-0.000668	-0.730724
13	13	0	-2.634083	1.953648	-1.656867
14	6	0	4.313269	1.280498	0.699153
15	6	0	4.566640	2.275660	-0.396807
16	1	0	5.170976	1.102427	1.326187
17	1	0	4.796506	3.235504	0.058602
18	1	0	5.405807	1.988225	-1.017225
19	1	0	3.696785	2.405593	-1.027606
20	1	0	3.453656	1.522968	1.302605
21	53	0	3.839544	-0.706541	-0.091378

Low frequencies (cm⁻¹): 7.8691 23.1950 29.6406
 30.1774 34.6484 39.7908

Coordinate of TS

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	13	0	-0.820582	-1.199979	0.056542
2	13	0	0.417180	2.496043	-0.137887
3	13	0	2.935384	1.960687	-1.385830
4	13	0	3.021621	-0.565911	-2.256547
5	13	0	0.819184	-1.899050	-1.870097
6	13	0	0.486362	0.886470	-2.286538
7	13	0	1.525946	0.026035	-0.000565
8	13	0	2.713771	-2.401755	0.127774
9	13	0	0.811403	-1.706816	2.047952
10	13	0	0.455755	1.113345	2.170935
11	13	0	2.910815	2.106260	1.185077
12	13	0	4.204319	-0.163700	0.029164
13	13	0	2.992971	-0.313347	2.326222
14	6	0	-5.934247	0.237163	-0.020945
15	6	0	-6.031824	1.723894	-0.028669
16	1	0	-6.258580	-0.259611	0.876535
17	1	0	-7.082200	2.016612	-0.040405
18	1	0	-5.579589	2.160983	0.852826
19	1	0	-5.562134	2.153106	-0.904896
20	1	0	-6.240235	-0.267865	-0.920235
21	53	0	-3.578198	-0.414476	0.006664

Low frequencies (cm⁻¹): -291.7833 8.0577 8.6003
 17.5803 25.9572 28.4224

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.462099	-0.950811	-0.942055
2	13	0	0.043087	2.206738	0.543752
3	13	0	-2.514228	1.941366	1.212723
4	13	0	-3.181748	-0.513738	1.750837
5	13	0	-0.863138	-2.041418	1.932113
6	13	0	-0.701838	0.505656	2.667490
7	13	0	-0.968782	-0.128574	0.027506
8	13	0	-2.938055	-2.327127	-0.166643
9	13	0	-0.401193	-2.710055	-0.696466
10	13	0	0.075538	0.563030	-2.463115
11	13	0	-1.869342	2.025794	-1.487081
12	13	0	-3.596372	0.319065	-0.731714
13	13	0	-2.082539	-0.947135	-2.381436
14	6	0	1.591422	3.423867	0.661182
15	6	0	1.921836	4.239269	-0.586973
16	1	0	2.445114	2.814432	0.948579
17	1	0	2.777487	4.886904	-0.418621
18	1	0	2.162806	3.600255	-1.429710
19	1	0	1.092243	4.870489	-0.888405
20	1	0	1.402257	4.085178	1.504030
21	53	0	3.717268	-0.745139	0.177020

Low frequencies (cm⁻¹): 18.6380 28.2342 36.0057
 41.6349 58.9125 63.1136

Al₁₃ C₂H₃I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.822861	-0.702475	0.040682
2	13	0	0.352185	0.312113	-2.207156
3	13	0	3.151667	-0.555517	-2.188234
4	13	0	3.519291	-2.056671	0.084225
5	13	0	1.115528	-2.061272	1.610734
6	13	0	1.064272	-2.304394	-1.118781
7	13	0	1.780673	-0.016002	-0.001679
8	13	0	3.177118	-0.349023	2.213476

9	13	0	0.377223	0.518067	2.173776
10	13	0	0.023628	2.013762	-0.091195
11	13	0	2.425515	2.022363	-1.621178
12	13	0	4.397201	0.655228	-0.046618
13	13	0	2.485220	2.270608	1.110345
14	53	0	-4.552940	-0.504672	-0.077022
15	6	0	-4.219834	1.567489	-0.188784
16	6	0	-3.612958	2.252890	0.759509
17	1	0	-3.245491	1.799563	1.671442
18	1	0	-3.469295	3.320932	0.635598
19	1	0	-4.589243	1.996615	-1.108375

 Low frequencies (cm⁻¹): 16.0217 8.8711 11.8405
 27.2007 61.9729 69.7295

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.833559	-0.219733	-0.817791
2	13	0	1.146117	-0.419071	-2.606994
3	13	0	3.382737	-1.454610	-1.296905
4	13	0	2.724350	-2.045453	1.304360
5	13	0	0.083762	-1.398454	1.671420
6	13	0	0.851730	-2.414125	-0.766493
7	13	0	1.607228	0.035409	0.016715
8	13	0	1.733300	0.467011	2.682931
9	13	0	-0.066632	1.763499	1.166838
10	13	0	0.618774	2.022463	-1.485314
11	13	0	3.237870	1.206073	-1.736782
12	13	0	3.962653	0.343713	1.158465
13	13	0	2.492744	2.516190	0.560717
14	53	0	-3.359538	-0.246961	0.045854
15	6	0	-5.929052	-0.110334	-0.060519
16	6	0	-6.472919	1.074804	-0.004803
17	1	0	-5.882786	1.982447	0.069157
18	1	0	-7.555957	1.192553	-0.029204
19	1	0	-6.327898	-1.110761	-0.143473

 Low frequencies (cm⁻¹): -284.5976 -22.9351 21.7834
 23.3713 31.5315 36.8676

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.210458	-0.901092	-0.044878
2	13	0	-0.170586	1.973585	-0.580452
3	13	0	2.163571	1.687262	-1.783658
4	13	0	2.705072	-1.018537	-2.035642

5	13	0	0.625801	-2.517045	-1.042560
6	13	0	0.162623	-0.142073	-2.406812
7	13	0	1.240378	-0.091367	0.012109
8	13	0	2.778966	-2.148341	0.503414
9	13	0	0.453576	-1.929661	1.818587
10	13	0	0.046647	0.749197	2.234640
11	13	0	2.061946	2.238248	0.997969
12	13	0	3.848577	0.476076	-0.041214
13	13	0	2.631976	-0.178104	2.329540
14	53	0	-3.709040	-0.590008	0.014953
15	6	0	-1.839979	2.970408	-0.348514
16	6	0	-1.871232	4.158837	0.252826
17	1	0	-0.984692	4.621843	0.676889
18	1	0	-2.792139	4.728136	0.351089
19	1	0	-2.771954	2.569081	-0.739921

 Low frequencies (cm⁻¹): 16.9938 27.7261 31.4142
 44.3833 66.0437 82.7986

Al₁₃ C₂H₃I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.833503	-0.241026	-0.043960
2	13	0	0.635274	-0.016257	-2.348952
3	13	0	3.274884	-1.263551	-1.840475
4	13	0	3.218617	-2.201538	0.739239
5	13	0	0.766340	-1.435748	2.002922
6	13	0	0.817389	-2.357045	-0.587260
7	13	0	1.869644	0.011610	0.004927
8	13	0	3.079915	0.019298	2.359776
9	13	0	0.449684	1.282680	1.849224
10	13	0	0.472088	2.202380	-0.735475
11	13	0	2.931956	1.456411	-2.006402
12	13	0	4.573928	0.265585	0.056846
13	13	0	2.886094	2.386607	0.582555
14	53	0	-4.561696	-0.588401	-0.122461
15	6	0	-4.939795	1.489050	-0.129497
16	6	0	-4.660281	2.287255	0.882382
17	1	0	-4.212672	1.942594	1.806441
18	1	0	-4.883469	3.346714	0.798002
19	1	0	-5.383555	1.815806	-1.059886

 Low frequencies (cm⁻¹): 4.7047 10.4321 11.8441
 18.0715 24.3508 41.4083

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.966520	-0.059701	-0.120730
2	13	0	0.546391	1.196669	-2.043389
3	13	0	3.087543	-0.264060	-2.244684
4	13	0	2.971117	-2.338487	-0.446304
5	13	0	0.554013	-2.176202	1.067895
6	13	0	0.607287	-1.717124	-1.648639
7	13	0	1.735920	0.017458	0.024397
8	13	0	2.899200	-1.223901	2.069185
9	13	0	0.400828	0.298474	2.295372
10	13	0	0.461605	2.360811	0.451647
11	13	0	2.879289	2.208472	-1.065360
12	13	0	4.406605	0.095956	0.198752
13	13	0	2.837158	1.804531	1.657768
14	53	0	-3.542058	-0.110805	-0.087937
15	6	0	-6.495399	-0.208681	-0.261498
16	6	0	-7.181339	0.593850	0.501993
17	1	0	-6.707004	1.290773	1.188476
18	1	0	-8.274325	0.601094	0.485445
19	1	0	-6.694826	-0.967861	-1.003069

Low frequencies (cm⁻¹): -63.9649 12.6703 19.5786
26.8456 34.8192 37.6288

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.255409	-0.977375	-0.108679
2	13	0	-0.093903	2.112290	-0.390049
3	13	0	2.214829	1.817451	-1.642431
4	13	0	2.680940	-0.875175	-2.116590
5	13	0	0.576192	-2.447854	-1.288735
6	13	0	0.145108	0.083087	-2.420089
7	13	0	1.185227	-0.096857	0.020251
8	13	0	2.741901	-2.240006	0.281720
9	13	0	0.438617	-2.084403	1.695570
10	13	0	0.099655	0.567584	2.369046
11	13	0	2.116836	2.109052	1.228314
12	13	0	3.852840	0.405434	-0.004791
13	13	0	2.665857	-0.441351	2.299229
14	53	0	-3.745653	-0.590988	0.021571
15	6	0	-1.744412	3.163588	-0.243096
16	6	0	-1.761550	4.426267	0.186543
17	1	0	-0.866663	4.949203	0.514579
18	1	0	-2.682469	5.005135	0.233465
19	1	0	-2.688462	2.714536	-0.547952

12	13	0	-3.745261	0.723435	1.838776
13	13	0	-1.003423	0.876084	2.565206
14	53	0	3.563645	-0.143206	-0.026972
15	6	0	5.894122	-0.232442	-0.204609
16	6	0	6.646437	0.732972	0.244943
17	1	0	6.244373	1.613191	0.715891
18	1	0	7.721857	0.675116	0.156267
19	1	0	6.196944	-1.142266	-0.686568

Low frequencies (cm⁻¹): -229.6669 15.4837 18.5409
 22.0685 31.5174 43.3793

Optimized geometry after C-I dissociation

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	13	0	1.536382	-0.898626	0.911613
2	13	0	-0.083358	2.293575	-0.471307
3	13	0	-1.931788	1.874252	1.606119
4	13	0	-2.006610	-1.163960	2.325948
5	13	0	-0.249914	-2.721841	0.559586
6	13	0	0.073760	0.449527	2.514258
7	13	0	-0.924899	-0.128141	-0.024701
8	13	0	-2.794887	-2.441175	0.014399
9	13	0	-0.721662	-1.929058	-2.032453
10	13	0	-0.703858	0.660505	-2.620610
11	13	0	-2.623512	1.914382	-1.081193
12	13	0	-3.574726	0.124148	0.754445
13	13	0	-3.117022	-0.532700	-1.783889
14	53	0	3.791299	-0.577737	-0.171093
15	6	0	1.361554	3.602975	-0.422020
16	6	0	1.406405	4.636646	0.406882
17	1	0	0.637080	4.827996	1.138186
18	1	0	2.219734	5.346587	0.398164
19	1	0	2.183801	3.496212	-1.116353

Low frequencies (cm⁻¹): 18.3470 24.8539 30.8830
 39.5252 57.1992 63.9233

Al₁₃ C₆H₅I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	13	0	0.073925	-1.858015	0.305521
2	13	0	-0.186814	0.785670	0.989036

3	13	0	1.473117	2.327069	-0.826546
4	13	0	2.721219	0.552066	-2.509342
5	13	0	2.010445	-2.118294	-1.758634
6	13	0	0.157622	-0.091548	-1.790901
7	13	0	2.091458	-0.107494	0.013805
8	13	0	4.385705	-0.986226	-0.963844
9	13	0	2.686998	-2.539160	0.867414
10	13	0	1.432662	-0.762657	2.539806
11	13	0	2.175549	1.891010	1.804870
12	13	0	4.090314	1.660582	-0.263654
13	13	0	4.012262	-0.153118	1.824916
14	6	0	-3.626817	0.736673	-0.049801
15	6	0	-3.230126	1.306893	-1.251758
16	6	0	-2.807729	2.631630	-1.270898
17	6	0	-2.779199	3.377302	-0.099330
18	6	0	-3.185072	2.797468	1.095802
19	6	0	-3.605611	1.471848	1.128377
20	1	0	-3.248823	0.726899	-2.165502
21	1	0	-2.488130	3.073034	-2.206856
22	1	0	-2.439751	4.404707	-0.117197
23	1	0	-3.165243	3.370353	2.014220
24	1	0	-3.913159	1.019485	2.062149
25	53	0	-4.187841	-1.289130	0.001453

Low frequencies (cm⁻¹): 13.0640 8.2120 18.8566
 25.8991 54.3493 65.7507

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.007848	0.517860	0.483537
2	13	0	-1.193964	1.195625	-1.899668
3	13	0	-3.990343	1.827493	-1.295230
4	13	0	-4.297836	1.539533	1.408622
5	13	0	-1.895449	0.541160	2.555023
6	13	0	-1.854480	2.487060	0.617775
7	13	0	-2.588818	0.013675	0.013753
8	13	0	-3.989964	-1.129432	1.937715
9	13	0	-1.198043	-1.808591	1.336136
10	13	0	-0.827127	-1.478347	-1.367964
11	13	0	-3.239230	-0.514527	-2.535039
12	13	0	-5.193915	-0.503428	-0.454795
13	13	0	-3.270864	-2.468915	-0.596101
14	6	0	5.554775	0.027748	0.007046
15	6	0	6.113574	1.227008	-0.341259
16	6	0	7.507521	1.288955	-0.289146
17	6	0	8.246349	0.178644	0.101531
18	6	0	7.610971	-1.008016	0.444665
19	6	0	6.218112	-1.101373	0.403190
20	1	0	5.519295	2.078708	-0.641457

21	1	0	8.007690	2.212030	-0.555147
22	1	0	9.326338	0.238765	0.138241
23	1	0	8.190721	-1.871475	0.747848
24	1	0	5.702718	-2.014426	0.665743
25	53	0	2.861582	-0.135294	-0.093591

 Low frequencies (cm⁻¹): -92.0672 14.4570 17.1256
 27.5884 34.7910 37.7120

Optimized geometry after C-I dissociation

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	-0.455621	-1.342735	-0.000222	
2	13	0	-0.221829	1.813637	0.000027	
3	13	0	1.953702	2.332601	-1.439331	
4	13	0	3.215420	-0.030759	-2.215524	
5	13	0	1.624659	-2.191708	-1.453388	
6	13	0	0.489843	0.149912	-2.357368	
7	13	0	1.692478	0.088242	0.000046	
8	13	0	3.770857	-1.500307	0.000093	
9	13	0	1.624540	-2.191772	1.453282	
10	13	0	0.489726	0.149758	2.357342	
11	13	0	1.953667	2.332552	1.439470	
12	13	0	4.029441	1.367688	-0.000014	
13	13	0	3.215336	-0.030817	2.215600	
14	6	0	-2.172816	2.005229	0.000073	
15	6	0	-2.893513	2.043363	-1.199569	
16	6	0	-4.281032	2.101329	-1.201765	
17	6	0	-4.976443	2.124331	0.000025	
18	6	0	-4.281090	2.100887	1.201840	
19	6	0	-2.893577	2.042916	1.199712	
20	1	0	-2.371092	2.016495	-2.150041	
21	1	0	-4.819424	2.121494	-2.141246	
22	1	0	-6.058717	2.160494	0.000002	
23	1	0	-4.819541	2.120721	2.141294	
24	1	0	-2.371211	2.015752	2.150205	
25	53	0	-2.915812	-1.834813	-0.000043	

 Low frequencies (cm⁻¹): 10.1940 26.1932 28.6083
 40.0863 53.0415 65.2469

Al₁₃ C₆H₅I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	-0.132381	-0.426754	-0.083464
2	13	0	0.988536	1.001730	1.971710
3	13	0	3.295710	2.499616	0.859496
4	13	0	3.391345	1.910636	-1.821292
5	13	0	1.411974	-0.061274	-2.461002
6	13	0	0.852580	2.034702	-0.772713
7	13	0	2.527972	0.119393	-0.005437
8	13	0	4.036274	-0.759427	-1.995752
9	13	0	1.747826	-2.266169	-0.869415
10	13	0	1.611847	-1.669236	1.802822
11	13	0	3.598709	0.286878	2.460038
12	13	0	5.192236	0.653272	0.071771
13	13	0	4.162975	-1.811926	0.771453
14	6	0	-4.819707	0.275941	0.029093
15	6	0	-5.345149	0.793339	-1.145597
16	6	0	-6.085860	1.968508	-1.090976
17	6	0	-6.293974	2.613200	0.121233
18	6	0	-5.759446	2.080454	1.286889
19	6	0	-5.017079	0.905581	1.249041
20	1	0	-5.183086	0.292798	-2.091790
21	1	0	-6.499328	2.377668	-2.005958
22	1	0	-6.872187	3.529193	0.157564
23	1	0	-5.916886	2.577643	2.237467
24	1	0	-4.601464	0.491997	2.159137
25	53	0	-3.696464	-1.523399	-0.041912

Low frequencies (cm⁻¹): 4.7536 7.8612 12.7524
 15.8931 21.0195 24.5753

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.110329	-0.075907	0.007227
2	13	0	-1.281938	1.069346	2.080610
3	13	0	-3.822314	-0.380190	2.334925
4	13	0	-3.819055	-2.349882	0.419799
5	13	0	-1.489583	-2.114279	-1.214815
6	13	0	-1.390362	-1.809293	1.523487
7	13	0	-2.595955	0.023428	0.012605
8	13	0	-3.874036	-1.100030	-2.033793
9	13	0	-1.387163	0.429357	-2.309511
10	13	0	-1.322044	2.379145	-0.343192
11	13	0	-3.650732	2.154110	1.294124
12	13	0	-5.267414	0.124986	-0.022408
13	13	0	-3.763822	1.918585	-1.445287
14	6	0	5.818444	0.009519	0.036954
15	6	0	6.494696	-1.153437	0.297588
16	6	0	7.887006	-1.062602	0.377954
17	6	0	8.519198	0.163221	0.198776
18	6	0	7.778060	1.310911	-0.062172

19	6	0	6.384706	1.243646	-0.146714
20	1	0	5.985256	-2.100589	0.435143
21	1	0	8.472118	-1.953632	0.581448
22	1	0	9.599794	0.224612	0.262615
23	1	0	8.278845	2.263665	-0.200636
24	1	0	5.791075	2.128178	-0.348571
25	53	0	2.656290	-0.134560	-0.167799

 Low frequencies (cm⁻¹): -19.7412 7.3825 9.0180
 14.2057 34.2019 37.4253

Optimized geometry after C-I dissociation

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	-0.269483	-1.638162	-0.074042	
2	13	0	-0.457745	1.707704	-0.197752	
3	13	0	1.720179	2.394933	-1.548439	
4	13	0	3.222783	0.152556	-2.184709	
5	13	0	1.936468	-2.174508	-1.416058	
6	13	0	0.498521	0.011015	-2.398788	
7	13	0	1.607484	0.156478	0.008462	
8	13	0	3.913488	-1.177821	0.108505	
9	13	0	1.819036	-2.053212	1.573266	
10	13	0	0.422409	0.190313	2.393609	
11	13	0	1.620296	2.488355	1.355428	
12	13	0	3.836966	1.695308	-0.007788	
13	13	0	3.169901	0.324163	2.246226	
14	6	0	-2.393827	2.046677	-0.099289	
15	6	0	-3.205118	1.948832	-1.237284	
16	6	0	-4.563581	2.233766	-1.177401	
17	6	0	-5.139883	2.624945	0.024567	
18	6	0	-4.353476	2.731344	1.164885	
19	6	0	-2.995299	2.445748	1.101947	
20	1	0	-2.777579	1.644046	-2.187387	
21	1	0	-5.173038	2.148372	-2.070685	
22	1	0	-6.200565	2.846183	0.072749	
23	1	0	-4.798397	3.035837	2.106234	
24	1	0	-2.400770	2.536499	2.005730	
25	53	0	-2.684273	-2.328328	0.061431	

 Low frequencies (cm⁻¹): 10.4574 22.9571 24.3979
 28.3258 36.3789 40.6392

Al₁₃ C₆H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	0.085677	-1.064521	0.080725
2	13	0	-0.572693	1.580250	-0.346391
3	13	0	-2.994332	2.652485	-0.389972
4	13	0	-2.902850	1.747145	2.047426
5	13	0	-1.967711	-2.127471	1.725176
6	13	0	-0.761916	0.278174	2.168778
7	13	0	-2.518555	-0.113403	0.042415
8	13	0	-4.169979	-0.736892	2.082436
9	13	0	-2.082755	-2.595301	-0.885079
10	13	0	-0.979577	-0.496074	-2.245375
11	13	0	-3.069382	1.026157	-2.414062
12	13	0	-4.995009	0.814075	-0.041012
13	13	0	-4.273991	-1.346477	-1.595270
14	6	0	4.331317	0.615401	-0.040965
15	6	0	4.630508	1.305072	1.116102
16	6	0	4.658626	2.687043	1.090733
17	6	0	4.389784	3.370112	-0.079073
18	6	0	4.091814	2.667029	-1.229725
19	6	0	4.060537	1.284833	-1.216750
20	1	0	4.839681	0.778008	2.027876
21	1	0	4.890891	3.226336	1.991586
22	1	0	4.411550	4.444757	-0.093669
23	1	0	3.880163	3.190628	-2.144784
24	1	0	3.826540	0.742594	-2.113420
25	53	0	4.279540	-1.490475	-0.009375

Low frequencies (cm⁻¹): 11.1432 10.7630 5.3060
6.0031 11.4991 12.3749

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.028262	0.212484	-0.017085
2	13	0	-1.249209	2.187441	1.086047
3	13	0	-4.566370	0.170210	1.994242
4	13	0	-3.549806	-2.140287	1.254908
5	13	0	-1.121929	-2.071226	0.342603
6	13	0	-1.801984	-0.152745	2.296667
7	13	0	-2.763415	0.127758	-0.115299
8	13	0	-3.273440	-2.121932	-1.507357
9	13	0	-1.329049	-0.611782	-2.289633
10	13	0	-1.623250	2.000128	-1.610141
11	13	0	-3.854987	2.464312	0.862846
12	13	0	-5.292135	-0.627109	-0.522488
13	13	0	-4.322212	1.581228	-1.747558
14	6	0	5.715264	0.060040	0.046023
15	6	0	6.258568	0.066080	1.292216
16	6	0	7.612977	0.370233	1.354850

17	6	0	8.322316	0.646018	0.200754
18	6	0	7.697772	0.623179	-1.032328
19	6	0	6.344508	0.322744	-1.130030
20	1	0	5.687725	-0.150730	2.173859
21	1	0	8.103528	0.389612	2.311934
22	1	0	9.369447	0.880589	0.262775
23	1	0	8.254066	0.838786	-1.927361
24	1	0	5.838693	0.299554	-2.075362
25	53	0	3.063998	-0.528827	-0.103689

Low frequencies (cm⁻¹): -90.5478 12.0381 14.1176
 14.9870 22.5686 31.5373

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.268640	1.892284	0.921479
2	13	0	-0.674079	-1.786604	-0.387809
3	13	0	1.210912	-2.271880	1.716069
4	13	0	2.930614	0.296362	2.226638
5	13	0	2.194321	2.437729	0.404427
6	13	0	0.323192	0.036368	2.572515
7	13	0	1.322295	-0.136537	-0.025677
8	13	0	4.164122	0.822509	-0.189700
9	13	0	2.029958	1.409402	-2.135782
10	13	0	0.623645	-0.797415	-2.566903
11	13	0	1.676541	-2.827342	-0.951841
12	13	0	3.492731	-1.701733	0.729769
13	13	0	3.319463	-1.040970	-1.850918
14	6	0	-2.575794	-2.196404	-0.181577
15	6	0	-3.041208	-3.041862	0.824734
16	6	0	-4.385917	-3.330843	0.957733
17	6	0	-5.301112	-2.774257	0.084604
18	6	0	-4.866174	-1.931171	-0.919677
19	6	0	-3.519522	-1.649581	-1.050093
20	1	0	-2.349451	-3.484704	1.521560
21	1	0	-4.719428	-3.987064	1.742413
22	1	0	-6.348753	-2.995523	0.187553
23	1	0	-5.574308	-1.492080	-1.600096
24	1	0	-3.208618	-0.988133	-1.841167
25	53	0	-2.380133	2.833471	-0.081398

Low frequencies (cm⁻¹): 10.2242 16.6103 24.5625
 34.0611 40.9072 49.9249

Al₂₀ C₂H₅I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.841907	-2.377117	1.344702
2	13	0	-1.100214	0.261240	2.451478
3	13	0	-1.344387	2.119814	0.229828
4	13	0	-1.251637	0.547692	-2.208899
5	13	0	-0.930444	-2.186757	-1.482035
6	13	0	-2.361059	-0.439469	0.117233
7	13	0	0.099304	-0.176967	0.039999
8	13	0	1.448788	-2.489023	-0.166124
9	13	0	1.350449	-1.035092	2.248046
10	13	0	1.054147	1.765591	1.609650
11	13	0	0.956381	1.944183	-1.342950
12	13	0	1.212096	-0.726942	-2.338789
13	13	0	3.862714	-1.885598	-1.560688
14	13	0	3.949323	-2.118963	1.065116
15	13	0	3.850868	0.032592	2.534884
16	13	0	3.705777	2.349665	1.438519
17	13	0	3.593185	2.578778	-1.110933
18	13	0	3.658789	0.496456	-2.622665
19	13	0	2.617618	0.129015	-0.013963
20	13	0	5.133547	0.282900	-0.091106
21	6	0	-5.318311	1.609836	-0.695857
22	6	0	-5.413934	2.567020	0.463862
23	1	0	-6.166062	1.649222	-1.372122
24	1	0	-5.392866	3.586448	0.069461
25	1	0	-6.339056	2.433256	1.023071
26	1	0	-4.568439	2.454841	1.143332
27	1	0	-4.383914	1.695954	-1.246827
28	53	0	-5.309048	-0.468242	-0.001168

Low frequencies (cm⁻¹): 21.3762 2.7087 24.2025
 27.8186 54.4685 59.6277

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.174111	-0.816360	-2.341204
2	13	0	-0.848023	-2.823541	-0.348165
3	13	0	-0.943980	-1.621066	2.212127
4	13	0	-1.359284	1.173864	1.909082
5	13	0	-1.446687	1.665669	-1.015373
6	13	0	-2.465470	-0.621550	0.113395
7	13	0	0.005336	-0.272913	0.056387
8	13	0	0.937693	0.965987	-2.145547
9	13	0	1.291875	-1.804005	-1.711465
10	13	0	1.444089	-2.305563	1.035868

11	13	0	1.156592	0.126052	2.435520
12	13	0	0.771865	2.248395	0.519612
13	13	0	3.404705	2.850252	0.282305
14	13	0	3.513718	1.868651	-2.079269
15	13	0	3.693309	-0.657738	-2.477878
16	13	0	3.869638	-2.256579	-0.431807
17	13	0	3.799615	-1.242880	2.046164
18	13	0	3.640351	1.320513	2.328425
19	13	0	2.541955	0.167310	-0.026140
20	13	0	5.097396	0.385700	-0.070330
21	6	0	-5.406466	2.310095	0.273151
22	6	0	-4.317981	3.098931	-0.186135
23	1	0	-5.515162	2.088366	1.325755
24	1	0	-4.513048	3.655102	-1.099200
25	1	0	-3.845451	3.698808	0.588893
26	1	0	-3.391860	2.415522	-0.497215
27	1	0	-6.277974	2.153610	-0.346245
28	53	0	-5.060516	-0.472040	-0.080873

 Low frequencies (cm⁻¹): -216.6753 20.1148 22.3046
 37.9909 40.9230 73.0395

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.395466	0.410538	2.343291
2	13	0	1.295924	-2.260435	1.424605
3	13	0	1.295816	-2.261527	-1.423170
4	13	0	1.395430	0.408781	-2.343846
5	13	0	1.398402	2.059441	-0.000804
6	13	0	2.738521	-0.347111	-0.000037
7	13	0	0.193036	-0.243328	-0.000014
8	13	0	-0.928772	1.688364	1.502515
9	13	0	-0.937687	-1.012555	2.294864
10	13	0	-1.072298	-2.595936	0.000990
11	13	0	-0.937852	-1.014260	-2.294211
12	13	0	-0.928694	1.687314	-1.503895
13	13	0	-3.639613	2.124203	-1.286751
14	13	0	-3.639790	2.125351	1.284232
15	13	0	-3.489602	-0.023085	2.639675
16	13	0	-3.426249	-2.264711	1.365744
17	13	0	-3.426155	-2.266332	-1.363354
18	13	0	-3.490291	-0.026095	-2.639551
19	13	0	-2.393845	-0.076903	-0.000077
20	13	0	-4.990267	-0.230435	0.000184
21	6	0	2.165185	3.887076	-0.001492
22	6	0	1.116743	5.001157	0.000690
23	1	0	2.811199	3.960009	-0.879588
24	1	0	1.585681	5.988328	-0.000071
25	1	0	0.468947	4.943276	-0.876837

26	1	0	0.472357	4.943010	0.880705
27	1	0	2.814238	3.959461	0.874403
28	53	0	5.260505	-0.444908	0.000021

 Low frequencies (cm⁻¹): -16.1165 22.9539 27.8923
 32.1388 44.1319 47.3750

Al₂₀ C₂H₅I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.289706	1.528162	-1.616878
2	13	0	1.270504	1.806286	1.340980
3	13	0	0.987224	-0.838091	2.427616
4	13	0	0.849334	-2.692822	0.268533
5	13	0	1.004970	-1.289732	-2.201256
6	13	0	2.344202	-0.380231	0.055844
7	13	0	-0.137437	-0.135195	0.017563
8	13	0	-1.142614	0.423603	-2.428721
9	13	0	-0.915062	2.434377	-0.218804
10	13	0	-1.176731	0.865728	2.305604
11	13	0	-1.423666	-1.910691	1.610098
12	13	0	-1.420440	-2.179383	-1.211591
13	13	0	-3.910039	-1.321991	-2.136303
14	13	0	-3.766813	1.256798	-2.403476
15	13	0	-3.624221	2.799849	-0.318374
16	13	0	-3.776393	1.757220	2.056870
17	13	0	-3.887839	-0.817604	2.369805
18	13	0	-3.961526	-2.373507	0.259704
19	13	0	-2.647527	0.156220	-0.024368
20	13	0	-5.166425	0.268041	-0.029886
21	6	0	5.575688	1.553800	-0.705271
22	6	0	5.802580	2.515701	0.426460
23	1	0	4.648287	1.732840	-1.246806
24	1	0	5.913077	3.519492	0.001507
25	1	0	4.956400	2.538499	1.114255
26	1	0	6.708872	2.286489	0.988215
27	1	0	6.409839	1.477534	-1.397285
28	53	0	5.336495	-0.521006	0.011595

 Low frequencies (cm⁻¹): 13.2547 17.4251 25.0723
 27.2592 44.6939 55.3893

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	13	0	-1.241510	0.257347	-2.366523
2	13	0	-0.882116	-2.399773	-1.414625
3	13	0	-0.882185	-2.398757	1.416226
4	13	0	-1.241668	0.259111	2.366165
5	13	0	-1.434633	1.958854	-0.000954
6	13	0	-2.446486	-0.575246	0.000106
7	13	0	0.054584	-0.245651	0.000053
8	13	0	0.846404	1.849658	-1.527888
9	13	0	1.261493	-0.904646	-2.316749
10	13	0	1.470114	-2.552210	0.000909
11	13	0	1.261350	-0.902925	2.317403
12	13	0	0.846192	1.850862	1.526421
13	13	0	3.486069	2.534868	1.295455
14	13	0	3.486195	2.534069	-1.296816
15	13	0	3.761544	0.318605	-2.610255
16	13	0	3.884383	-1.927709	-1.333112
17	13	0	3.884322	-1.926958	1.334382
18	13	0	3.761589	0.320116	2.610113
19	13	0	2.576854	0.197967	-0.000006
20	13	0	5.129491	0.390543	-0.000065
21	6	0	-5.794504	2.142114	0.000497
22	6	0	-4.689868	3.063052	-0.000360
23	1	0	-6.330498	1.938413	0.917301
24	1	0	-4.643165	3.672536	-0.902851
25	1	0	-4.642598	3.673307	0.901594
26	1	0	-3.656301	2.537148	-0.000364
27	1	0	-6.331874	1.938338	-0.915466
28	53	0	-5.095380	-0.514837	-0.000079

 Low frequencies (cm⁻¹): -148.0717 20.8980 24.2605
 36.3700 38.0965 64.3124

 Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.391674	0.377294	-2.367595
2	13	0	-1.252491	-2.285285	-1.431948
3	13	0	-1.253327	-2.287048	1.428384
4	13	0	-1.391135	0.372850	2.369103
5	13	0	-1.420422	2.066515	0.007307
6	13	0	-2.733652	-0.395160	-0.000667
7	13	0	-0.164856	-0.226301	-0.000391
8	13	0	0.896104	1.739211	-1.542673
9	13	0	0.976119	-0.994857	-2.322138
10	13	0	1.104477	-2.611996	-0.001016
11	13	0	0.975738	-0.997584	2.320871
12	13	0	0.898576	1.736461	1.545407
13	13	0	3.625297	2.166369	1.296862
14	13	0	3.622471	2.167639	-1.298102
15	13	0	3.590798	-0.013348	-2.653840

16	13	0	3.458323	-2.232339	-1.362370
17	13	0	3.458479	-2.231274	1.361696
18	13	0	3.588912	-0.012938	2.654413
19	13	0	2.416925	-0.014503	-0.000616
20	13	0	5.019024	-0.196681	0.000345
21	6	0	-2.384252	3.814468	-0.001247
22	6	0	-1.499436	5.059272	-0.001455
23	1	0	-3.043326	3.803448	0.872408
24	1	0	-2.103890	5.972617	-0.006803
25	1	0	-0.855552	5.101208	0.880710
26	1	0	-0.848290	5.095657	-0.878530
27	1	0	-3.036702	3.798389	-0.879750
28	53	0	-5.266378	-0.503115	-0.000212

 Low frequencies (cm⁻¹): 8.9777 26.8909 33.8050
 39.1673 48.0350 56.8045

Al₂₀ C₂H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.296918	1.546194	1.649008
2	13	0	-1.265887	1.833794	-1.365074
3	13	0	-1.006369	-0.819012	-2.433078
4	13	0	-0.874265	-2.683909	-0.285935
5	13	0	-1.002059	-1.325530	2.211345
6	13	0	-2.303635	-0.342217	-0.034619
7	13	0	0.159338	-0.109954	-0.004378
8	13	0	1.117957	0.422356	2.456442
9	13	0	0.889281	2.469697	0.227413
10	13	0	1.181724	0.878450	-2.296287
11	13	0	1.409752	-1.883872	-1.620779
12	13	0	1.424385	-2.181502	1.181736
13	13	0	3.953761	-1.416026	2.070989
14	13	0	3.762337	1.153957	2.446782
15	13	0	3.595017	2.783380	0.418126
16	13	0	3.762135	1.827959	-2.004040
17	13	0	3.859657	-0.736651	-2.419192
18	13	0	3.953855	-2.375121	-0.361747
19	13	0	2.679538	0.151661	0.035223
20	13	0	5.217913	0.280657	0.019135
21	6	0	-5.660234	1.503946	0.713645
22	6	0	-5.892167	2.471199	-0.410762
23	1	0	-4.772605	1.719518	1.286715
24	1	0	-6.061036	3.455474	0.018525
25	1	0	-5.033501	2.537127	-1.066141
26	1	0	-6.761356	2.207115	-0.999328
27	1	0	-6.508230	1.386706	1.367370

28 53 0 -5.308992 -0.534393 -0.019025

Low frequencies (cm⁻¹): 12.1150 14.9334 26.4565
28.8791 39.0464 51.8567

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.197416	-0.280348	-2.460850
2	13	0	-0.892504	-2.659562	-0.906524
3	13	0	-0.935668	-2.038689	1.864480
4	13	0	-1.292781	0.764670	2.237865
5	13	0	-1.443895	1.930779	-0.565097
6	13	0	-2.425521	-0.550232	0.044241
7	13	0	0.046512	-0.210288	0.022245
8	13	0	0.872286	1.492096	-1.923562
9	13	0	1.283198	-1.368683	-2.061816
10	13	0	1.433205	-2.481687	0.529137
11	13	0	1.216329	-0.383243	2.433562
12	13	0	0.762852	2.176960	1.068938
13	13	0	3.409198	2.739364	0.809831
14	13	0	3.494017	2.213374	-1.735821
15	13	0	3.788025	-0.221365	-2.588335
16	13	0	3.850602	-2.168639	-0.885266
17	13	0	3.816569	-1.646480	1.747664
18	13	0	3.743376	0.814986	2.532131
19	13	0	2.595560	0.201434	-0.014410
20	13	0	5.183936	0.380220	-0.028026
21	6	0	-5.732644	2.202555	0.138097
22	6	0	-4.649644	3.097774	-0.096872
23	1	0	-6.039639	1.964118	1.137099
24	1	0	-4.752407	3.667263	-1.009991
25	1	0	-4.425033	3.725726	0.754692
26	1	0	-3.649660	2.537772	-0.251448
27	1	0	-6.423626	1.957592	-0.643830
28	53	0	-5.045629	-0.543681	-0.033942

Low frequencies (cm⁻¹): -184.1381 3.7099 23.0531
38.9226 43.0699 61.2539

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.422638	0.597513	-2.318585
2	13	0	-1.251200	-2.107868	-1.671034

3	13	0	-1.142818	-2.518313	1.172756
4	13	0	-1.389494	0.011114	2.479849
5	13	0	-1.439574	2.066179	0.009347
6	13	0	-2.677112	-0.493095	0.056943
7	13	0	-0.151940	-0.223693	0.028042
8	13	0	0.972341	1.997573	-1.132755
9	13	0	0.975887	-0.497320	-2.406986
10	13	0	1.121705	-2.567780	-0.556691
11	13	0	1.048564	-1.372888	2.134411
12	13	0	0.750118	1.517309	1.895627
13	13	0	3.428463	1.784477	2.046252
14	13	0	3.800008	2.369093	-0.475436
15	13	0	3.373682	0.963359	-2.564501
16	13	0	3.504415	-1.596256	-1.967410
17	13	0	3.412160	-2.531128	0.656946
18	13	0	3.774949	-0.762743	2.460768
19	13	0	2.454136	0.025008	0.065322
20	13	0	5.097831	-0.212061	-0.146542
21	6	0	-2.558509	3.642559	0.440800
22	6	0	-2.026808	4.978855	-0.070239
23	1	0	-2.685361	3.673619	1.518868
24	1	0	-2.693748	5.795217	0.193392
25	1	0	-1.052361	5.210352	0.347738
26	1	0	-1.923154	4.983245	-1.150442
27	1	0	-3.544682	3.446504	0.028552
28	53	0	-5.201926	-0.540899	-0.002333

Low frequencies (cm⁻¹): 13.6985 28.9239 30.7348
 39.9869 43.0998 52.0540

Al₂₀ C₂H₃I (M062X/TZVP, LANL2DZ level of theory)

Center	Atomic	Atomic	Coordinates (Angstroms)		
			Number	Type	X
1	13	0	1.230871	1.595980	-1.673408
2	13	0	1.269718	1.911992	1.235442
3	13	0	1.085034	-0.718720	2.382253
4	13	0	0.957721	-2.607941	0.278009
5	13	0	1.041278	-1.235272	-2.215193
6	13	0	2.387674	-0.259775	-0.013199
7	13	0	-0.082200	-0.111442	-0.002050
8	13	0	-1.178395	0.372999	-2.400329
9	13	0	-1.020565	2.380683	-0.242459
10	13	0	-1.122628	0.886620	2.257721
11	13	0	-1.302382	-1.864850	1.629579
12	13	0	-1.326183	-2.190269	-1.156468
13	13	0	-3.833079	-1.458525	-2.044215
14	13	0	-3.810459	1.096502	-2.399928
15	13	0	-3.719404	2.703126	-0.400079

16	13	0	-3.697906	1.784194	2.001568
17	13	0	-3.745718	-0.775018	2.435366
18	13	0	-3.832213	-2.430274	0.388938
19	13	0	-2.604871	0.090207	-0.010109
20	13	0	-5.114696	0.150414	0.037780
21	53	0	5.451731	-0.448388	-0.038158
22	6	0	5.606593	1.600842	0.455169
23	6	0	5.146461	2.550058	-0.331086
24	1	0	4.671905	2.356240	-1.285031
25	1	0	5.233062	3.583217	-0.013088
26	1	0	6.074236	1.751480	1.416167

 Low frequencies (cm⁻¹): 26.7450 9.6741 22.2692
 25.0620 44.5554 66.0993

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.326625	-0.321805	-2.352638
2	13	0	1.796760	1.570386	-0.243945
3	13	0	1.395631	0.319488	2.256873
4	13	0	0.718843	-2.406574	1.763562
5	13	0	0.665457	-2.815837	-1.099717
6	13	0	2.409756	-1.093750	0.081998
7	13	0	0.019494	-0.412491	0.029098
8	13	0	-1.284221	-1.231595	-2.151042
9	13	0	-0.622645	1.531513	-1.691260
10	13	0	-0.591735	1.923264	1.189225
11	13	0	-1.189622	-0.574232	2.405078
12	13	0	-1.625389	-2.484065	0.374933
13	13	0	-3.980019	-1.921102	-0.960510
14	13	0	-3.658228	0.056800	-2.603685
15	13	0	-3.206340	2.408959	-1.705460
16	13	0	-3.139831	2.861382	0.812782
17	13	0	-3.453481	0.980102	2.520412
18	13	0	-3.905377	-1.444751	1.676376
19	13	0	-2.457604	0.248277	-0.031429
20	13	0	-4.989648	0.626054	-0.011472
21	53	0	5.012346	-0.201451	-0.052400
22	6	0	4.321662	2.069821	-0.462843
23	6	0	4.841831	2.953697	0.380683
24	1	0	4.902243	2.794672	1.449130
25	1	0	5.162780	3.916200	-0.008629
26	1	0	4.330173	2.164661	-1.539664

 Low frequencies (cm⁻¹): -583.9606 9.8440 35.6502
 39.1406 43.1813 73.2957

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.353955	0.434801	-2.344229
2	13	0	1.381155	2.085341	-0.001240
3	13	0	1.354081	0.436899	2.343732
4	13	0	1.190444	-2.231676	1.425367
5	13	0	1.190506	-2.232866	-1.423490
6	13	0	2.676800	-0.350895	0.000126
7	13	0	0.133843	-0.192603	0.000077
8	13	0	-1.011726	-0.934069	-2.295218
9	13	0	-0.940559	1.766040	-1.505754
10	13	0	-0.940377	1.767460	1.504158
11	13	0	-1.011744	-0.932051	2.295983
12	13	0	-1.188190	-2.514763	0.000998
13	13	0	-3.527513	-2.123539	-1.367010
14	13	0	-3.542456	0.115391	-2.642277
15	13	0	-3.643801	2.264659	-1.286327
16	13	0	-3.643555	2.265611	1.284987
17	13	0	-3.542898	0.116930	2.642106
18	13	0	-3.527400	-2.122803	1.368346
19	13	0	-2.446408	0.038805	0.000049
20	13	0	-5.046011	-0.056657	-0.000040
21	53	0	5.197348	-0.516484	-0.000049
22	6	0	2.321321	3.799799	-0.001163
23	6	0	3.651411	3.872122	0.000760
24	1	0	4.284007	2.988311	0.002226
25	1	0	4.177114	4.823796	0.000878
26	1	0	1.757139	4.729850	-0.002615

Low frequencies (cm⁻¹): 6.9541 30.1234 33.6647
38.3279 59.1907 68.8583

Al₂₀ C₂H₃I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.193183	1.000167	-2.133014
2	13	0	1.276633	2.174236	0.592724
3	13	0	1.087724	-0.027105	2.463188
4	13	0	0.926199	-2.444685	0.977718
5	13	0	0.968197	-1.853348	-1.808362
6	13	0	2.355260	-0.279983	0.006857
7	13	0	-0.129695	-0.100720	0.000477
8	13	0	-1.239081	-0.335641	-2.458456
9	13	0	-0.983020	2.259710	-0.994638
10	13	0	-1.105040	1.546760	1.912657

11	13	0	-1.332795	-1.326411	2.102897
12	13	0	-1.399926	-2.444371	-0.501260
13	13	0	-3.923445	-1.918403	-1.586360
14	13	0	-3.870712	0.479532	-2.583757
15	13	0	-3.705494	2.557286	-1.031452
16	13	0	-3.747199	2.240872	1.548142
17	13	0	-3.816015	-0.141252	2.583186
18	13	0	-3.900044	-2.237449	1.012940
19	13	0	-2.637183	0.127268	-0.025665
20	13	0	-5.145141	0.191243	0.016271
21	53	0	5.520951	-0.477911	-0.041393
22	6	0	5.920245	1.546345	0.447991
23	6	0	5.547850	2.555864	-0.311603
24	1	0	5.011906	2.439668	-1.245141
25	1	0	5.779846	3.566741	0.010146
26	1	0	6.447982	1.629434	1.387318

 Low frequencies (cm⁻¹): 5.9371 10.6963 18.2956
 20.3960 33.7943 48.0619

Coordinate of TS

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	13	0	1.325547	-0.280605	-2.350040
2	13	0	1.831042	1.559573	-0.193866
3	13	0	1.371801	0.260203	2.304251
4	13	0	0.692642	-2.457888	1.737055
5	13	0	0.671439	-2.794849	-1.163947
6	13	0	2.393239	-1.091145	0.094597
7	13	0	-0.017876	-0.408036	0.034162
8	13	0	-1.287749	-1.174999	-2.212036
9	13	0	-0.573440	1.601069	-1.681627
10	13	0	-0.529955	1.958315	1.231579
11	13	0	-1.240438	-0.618531	2.418965
12	13	0	-1.646173	-2.528638	0.292182
13	13	0	-3.997157	-1.837757	-1.149466
14	13	0	-3.625957	0.258393	-2.648262
15	13	0	-3.162434	2.545471	-1.534160
16	13	0	-3.139960	2.801027	1.042150
17	13	0	-3.640525	0.764046	2.554643
18	13	0	-3.982417	-1.578356	1.502922
19	13	0	-2.470768	0.282788	-0.020135
20	13	0	-5.000135	0.637648	-0.054533
21	53	0	5.062198	-0.212716	-0.034440
22	6	0	4.352017	2.024125	-0.453511
23	6	0	4.905657	2.939356	0.346939
24	1	0	5.028413	2.810675	1.414976
25	1	0	5.170570	3.906892	-0.074769
26	1	0	4.339028	2.105034	-1.533076

Low frequencies (cm⁻¹): -472.9188 10.2987 27.8786
 31.1404 39.4897 64.7853

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X Y Z		
1	13	0	1.354212	0.432837	-2.373345
2	13	0	1.406667	2.107817	0.009622
3	13	0	1.358726	0.423973	2.367356
4	13	0	1.199970	-2.231052	1.425802
5	13	0	1.193440	-2.228323	-1.440748
6	13	0	2.693662	-0.351315	-0.009191
7	13	0	0.121474	-0.167529	-0.003451
8	13	0	-1.027301	-0.923265	-2.324238
9	13	0	-0.916667	1.811880	-1.543941
10	13	0	-0.920680	1.806404	1.545350
11	13	0	-1.019256	-0.926030	2.321666
12	13	0	-1.169657	-2.538141	0.001200
13	13	0	-3.517182	-2.143211	-1.351738
14	13	0	-3.640220	0.069625	-2.650319
15	13	0	-3.637452	2.260089	-1.307690
16	13	0	-3.644987	2.263559	1.289031
17	13	0	-3.618532	0.093536	2.660563
18	13	0	-3.516927	-2.129417	1.372980
19	13	0	-2.454305	0.069234	-0.000704
20	13	0	-5.058377	-0.086361	0.006594
21	53	0	5.222059	-0.548637	0.001952
22	6	0	2.311645	3.852232	-0.000869
23	6	0	3.635871	4.009774	-0.002938
24	1	0	4.329045	3.172816	0.000954
25	1	0	4.096590	4.996408	-0.008753
26	1	0	1.694232	4.750505	-0.005142

Low frequencies (cm⁻¹): 11.9215 29.9742 35.3539
 38.7809 49.9996 57.3736

Al₂₀ C₂H₃I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X Y Z		
1	13	0	1.028331	-0.609850	-2.448888
2	13	0	1.250251	2.013908	-1.110700
3	13	0	1.184732	1.453676	1.860366
4	13	0	0.982748	-1.395795	2.151411
5	13	0	0.914588	-2.599554	-0.417787
6	13	0	2.291664	-0.237459	-0.005431

7	13	0	-0.174324	-0.075119	-0.005222
8	13	0	-1.390649	-1.774894	-1.729026
9	13	0	-1.123269	1.102072	-2.245188
10	13	0	-0.971320	2.460495	0.473884
11	13	0	-1.247654	0.228611	2.458976
12	13	0	-1.412982	-2.245617	1.050881
13	13	0	-3.943594	-2.438735	-0.300725
14	13	0	-3.946555	-0.880588	-2.395829
15	13	0	-3.801628	1.703423	-2.093056
16	13	0	-3.691529	2.751303	0.294541
17	13	0	-3.843273	1.196105	2.385745
18	13	0	-3.896138	-1.391552	2.111462
19	13	0	-2.685846	0.130911	-0.012456
20	13	0	-5.202279	0.209861	0.008902
21	53	0	5.591670	-0.495819	-0.032522
22	6	0	6.014903	1.495662	0.504725
23	6	0	5.892245	2.502773	-0.321435
24	1	0	5.566260	2.396791	-1.339504
25	1	0	6.122154	3.496423	0.024657
26	1	0	6.333603	1.578935	1.524601

Low frequencies (cm⁻¹): 15.9140 6.9734 18.1216
 19.7704 22.5028 34.6699

Coordinate of TS

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	1.319490	-0.197522	-2.406451	
2	13	0	1.792964	1.692985	-0.226097	
3	13	0	1.375698	0.422534	2.306752	
4	13	0	0.803645	-2.337184	1.788777	
5	13	0	0.756808	-2.735356	-1.171664	
6	13	0	2.384272	-0.975419	0.072773	
7	13	0	-0.011888	-0.315575	0.016792	
8	13	0	-1.262243	-1.187904	-2.187347	
9	13	0	-0.630204	1.642574	-1.726983	
10	13	0	-0.610594	2.042421	1.177853	
11	13	0	-1.189804	-0.522742	2.413632	
12	13	0	-1.502579	-2.519871	0.368247	
13	13	0	-3.870563	-2.007010	-0.997764	
14	13	0	-3.721274	0.016075	-2.613167	
15	13	0	-3.263353	2.391984	-1.673437	
16	13	0	-3.234669	2.802032	0.884127	
17	13	0	-3.602035	0.856906	2.554078	
18	13	0	-3.821468	-1.569384	1.657835	
19	13	0	-2.526021	0.272474	-0.032492	
20	13	0	-5.129138	0.458379	-0.006399	
21	53	0	4.993404	-0.296687	-0.023677	
22	6	0	4.496987	2.076241	-0.494507	

23	6	0	5.087333	2.921038	0.318313
24	1	0	5.167706	2.779794	1.379931
25	1	0	5.462727	3.847938	-0.091428
26	1	0	4.471701	2.117882	-1.564289

 Low frequencies (cm⁻¹): -612.1698 8.8983 30.3819
 41.3957 43.9580 56.8610

Optimized geometry after C-I dissociation

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	1.502057	0.743043	-2.367448	
2	13	0	1.519238	2.289936	-0.302322	
3	13	0	1.320308	-0.467822	2.559379	
4	13	0	1.072750	-2.621053	0.795970	
5	13	0	1.208457	-1.865998	-1.867835	
6	13	0	2.628272	-0.485700	0.049209	
7	13	0	0.171906	-0.023867	0.081768	
8	13	0	-1.018550	0.034619	-2.383628	
9	13	0	-1.076340	2.323089	-0.673316	
10	13	0	-0.799989	1.084712	2.355516	
11	13	0	-1.146938	-1.731500	1.811860	
12	13	0	-1.178562	-2.312887	-0.967136	
13	13	0	-3.506119	-1.170339	-2.155269	
14	13	0	-3.370730	1.457381	-2.327415	
15	13	0	-3.828378	2.520917	-0.052800	
16	13	0	-3.433555	1.556604	2.311787	
17	13	0	-3.779371	-1.039468	2.310026	
18	13	0	-3.530461	-2.534639	0.210845	
19	13	0	-2.488964	0.111362	0.092840	
20	13	0	-5.147590	-0.079226	-0.229589	
21	53	0	5.148960	-0.505657	0.015185	
22	6	0	2.645842	3.528663	0.703220	
23	6	0	3.921718	3.759359	0.426153	
24	1	0	4.447572	3.246284	-0.363097	
25	1	0	4.511447	4.472545	0.982305	
26	1	0	2.213976	4.093689	1.518010	

 Low frequencies (cm⁻¹): 26.6418 38.4351 44.4189
 46.0046 50.4821 53.5579

Al₂₀ C₆H₅I (M062X/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	0.880481	0.045363	-2.305640
2	13	0	1.287840	1.638336	0.000768
3	13	0	0.879995	0.044167	2.306352
4	13	0	0.180594	-2.628578	1.463562
5	13	0	0.180968	-2.627772	-1.464414
6	13	0	1.899529	-1.084184	0.000204
7	13	0	-0.487680	-0.425327	0.000086
8	13	0	-1.727415	-0.790857	-2.346829
9	13	0	-1.057880	1.796591	-1.399834
10	13	0	-1.058155	1.795955	1.400884
11	13	0	-1.727962	-0.792043	2.346515
12	13	0	-2.170100	-2.506262	-0.000762
13	13	0	-4.841370	-2.001124	-0.000262
14	13	0	-4.456238	-0.779622	-2.223298
15	13	0	-3.696350	1.695005	-2.266695
16	13	0	-3.334306	2.973530	0.000172
17	13	0	-3.696774	1.694712	2.266763
18	13	0	-4.456746	-0.779799	2.222937
19	13	0	-2.947985	0.166140	-0.000002
20	13	0	-5.352264	0.884697	-0.000215
21	6	0	4.962376	0.805861	-0.000039
22	6	0	4.914353	1.472917	1.212637
23	6	0	4.827285	2.860319	1.202868
24	6	0	4.783355	3.552274	-0.000014
25	6	0	4.826740	2.860311	-1.202905
26	6	0	4.913986	1.472947	-1.212701
27	1	0	4.931902	0.930035	2.148207
28	1	0	4.782741	3.394687	2.142981
29	1	0	4.706801	4.631638	0.000001
30	1	0	4.781720	3.394665	-2.143011
31	1	0	4.931252	0.930096	-2.148276
32	53	0	4.992842	-1.312735	-0.000052

Low frequencies (cm⁻¹): 0.5736 11.4521 22.1384
 27.4176 40.5004 50.9777

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.615504	1.081979	0.000126
2	13	0	-0.929930	-0.406662	-2.325767
3	13	0	0.146542	-2.907310	-1.446418
4	13	0	0.143812	-2.905924	1.446239
5	13	0	-0.931219	-0.405863	2.322865
6	13	0	-1.793761	-1.660839	-0.002244
7	13	0	0.461925	-0.609575	-0.001017
8	13	0	0.746378	1.616812	1.454096
9	13	0	0.744834	1.617476	-1.454452

10	13	0	1.781053	-0.909516	-2.300068
11	13	0	2.415581	-2.420908	0.003992
12	13	0	1.776759	-0.907669	2.301480
13	13	0	3.830034	0.881082	2.606179
14	13	0	3.132889	2.944021	1.267565
15	13	0	3.137051	2.933731	-1.291226
16	13	0	3.851582	0.859586	-2.603789
17	13	0	4.584132	-1.284368	-1.329098
18	13	0	4.578142	-1.271931	1.351102
19	13	0	2.808043	0.433667	-0.001153
20	13	0	5.257580	1.194563	0.004259
21	6	0	-4.288490	1.154058	-0.000110
22	6	0	-4.665046	1.704151	1.215783
23	6	0	-5.335858	2.920928	1.202371
24	6	0	-5.664143	3.536921	0.000168
25	6	0	-5.335532	2.921387	-1.202188
26	6	0	-4.664722	1.704621	-1.215893
27	1	0	-4.401223	1.226852	2.150450
28	1	0	-5.600992	3.384648	2.144485
29	1	0	-6.193211	4.480500	0.000279
30	1	0	-5.600407	3.385472	-2.144194
31	1	0	-4.400627	1.227676	-2.150666
32	53	0	-4.485242	-1.315059	-0.000676

Low frequencies (cm⁻¹): -411.2522 8.0884 20.9008
 34.5935 35.0842 58.2672

Optimized geometry after C-I dissociation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.514443	1.337253	0.028846
2	13	0	1.112270	-0.291245	2.337461
3	13	0	0.345308	-2.840206	1.386954
4	13	0	0.344696	-2.797058	-1.464458
5	13	0	1.112013	-0.218910	-2.337394
6	13	0	2.221828	-1.329317	-0.016606
7	13	0	-0.219288	-0.591995	-0.004835
8	13	0	-0.822925	1.590271	-1.468344
9	13	0	-0.820057	1.543867	1.529772
10	13	0	-1.500659	-1.082318	2.284993
11	13	0	-2.031901	-2.549783	-0.037204
12	13	0	-1.499671	-1.010344	-2.309516
13	13	0	-3.723995	0.593625	-2.630242
14	13	0	-3.342756	2.683436	-1.231053
15	13	0	-3.337804	2.640246	1.338097
16	13	0	-3.736033	0.499545	2.654254
17	13	0	-4.220998	-1.663415	1.341598
18	13	0	-4.223730	-1.612895	-1.392897
19	13	0	-2.680425	0.220153	0.008763
20	13	0	-5.234293	0.717435	0.016656

21	6	0	2.785807	2.831174	0.024211
22	6	0	3.096729	3.507586	-1.160428
23	6	0	4.003352	4.560125	-1.169097
24	6	0	4.618291	4.956391	0.011383
25	6	0	4.325124	4.296629	1.197663
26	6	0	3.417760	3.244334	1.201919
27	1	0	2.629123	3.212055	-2.094142
28	1	0	4.230819	5.069890	-2.097336
29	1	0	5.325121	5.776842	0.006537
30	1	0	4.804412	4.600289	2.120373
31	1	0	3.205008	2.741351	2.139614
32	53	0	4.641412	-2.031630	-0.021923

 Low frequencies (cm⁻¹): 13.6700 15.3721 22.1365
 34.5015 38.5625 41.0850

Al₂₀ C₆H₅I (B3PW91/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.714307	0.244448	2.323640
2	13	0	-1.068029	1.849083	-0.003494
3	13	0	-0.713144	0.237126	-2.325237
4	13	0	-0.162733	-2.465030	-1.476847
5	13	0	-0.163385	-2.460618	1.483699
6	13	0	-1.790388	-0.821098	0.000678
7	13	0	0.647930	-0.300866	0.000391
8	13	0	1.854738	-0.745197	2.379062
9	13	0	1.297518	1.918182	1.415374
10	13	0	1.298314	1.913702	-1.421208
11	13	0	1.855968	-0.752332	-2.376425
12	13	0	2.164437	-2.530360	0.003852
13	13	0	4.863223	-2.065367	0.004832
14	13	0	4.605848	-0.779518	2.247288
15	13	0	3.955520	1.735365	2.262918
16	13	0	3.625918	3.004090	-0.004786
17	13	0	3.956626	1.727068	-2.267752
18	13	0	4.607021	-0.787741	-2.242465
19	13	0	3.123969	0.177328	0.000297
20	13	0	5.553176	0.819758	-0.000298
21	6	0	-5.558793	0.558054	-0.000237
22	6	0	-5.787226	1.186876	-1.213102
23	6	0	-6.273869	2.489227	-1.202160
24	6	0	-6.523458	3.136468	0.000675
25	6	0	-6.285438	2.484035	1.203058
26	6	0	-5.798863	1.181653	1.213075
27	1	0	-5.589553	0.682939	-2.150318
28	1	0	-6.454754	2.994640	-2.143863

29	1	0	-6.901452	4.152108	0.001047
30	1	0	-6.475400	2.985399	2.145138
31	1	0	-5.610211	0.673681	2.149975
32	53	0	-4.829804	-1.446055	-0.001049

 Low frequencies (cm⁻¹): 11.7299 4.6816 7.9510
 12.6799 22.5188 30.2721

Coordinate of TS

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	13	0	-1.615202	1.124876	-0.000141	
2	13	0	-0.907919	-0.359976	-2.342134	
3	13	0	0.115776	-2.876542	-1.465614	
4	13	0	0.115594	-2.876292	1.465904	
5	13	0	-0.908052	-0.359628	2.341962	
6	13	0	-1.795494	-1.592374	-0.000058	
7	13	0	0.500802	-0.567862	-0.000028	
8	13	0	0.731483	1.682508	1.466417	
9	13	0	0.731432	1.682327	-1.466710	
10	13	0	1.802892	-0.887929	-2.330124	
11	13	0	2.402021	-2.456752	0.000333	
12	13	0	1.802691	-0.887538	2.330291	
13	13	0	3.951376	0.843614	2.615528	
14	13	0	3.184817	2.927027	1.293716	
15	13	0	3.184978	2.926400	-1.295030	
16	13	0	3.952217	0.842343	-2.615465	
17	13	0	4.603226	-1.318235	-1.333480	
18	13	0	4.602969	-1.317539	1.334631	
19	13	0	2.843052	0.458202	-0.000053	
20	13	0	5.316468	1.148503	0.000108	
21	6	0	-4.405925	1.137116	-0.000047	
22	6	0	-4.783128	1.683378	1.216179	
23	6	0	-5.464482	2.896090	1.203175	
24	6	0	-5.798667	3.507875	0.000019	
25	6	0	-5.464680	2.896047	-1.203171	
26	6	0	-4.783319	1.683341	-1.216237	
27	1	0	-4.520369	1.208738	2.153028	
28	1	0	-5.731981	3.359378	2.146755	
29	1	0	-6.338339	4.447466	0.000047	
30	1	0	-5.732331	3.359301	-2.146725	
31	1	0	-4.520700	1.208669	-2.153113	
32	53	0	-4.508523	-1.361573	-0.000003	

 Low frequencies (cm⁻¹): -322.2668 8.2769 18.5751
 28.5813 36.7027 55.8702

Optimized geometry after C-I dissociation

Center	Atomic	Atomic	Coordinates (Angstroms)			

Number	Number	Type	X	Y	Z
1	13	0	1.527722	1.368985	0.006519
2	13	0	1.109228	-0.277481	2.356371
3	13	0	0.338477	-2.825018	1.410548
4	13	0	0.333898	-2.802181	-1.456985
5	13	0	1.101077	-0.239009	-2.365657
6	13	0	2.225961	-1.330685	-0.014295
7	13	0	-0.235897	-0.558525	-0.004502
8	13	0	-0.807513	1.622971	-1.520542
9	13	0	-0.795192	1.597966	1.556010
10	13	0	-1.515292	-1.048035	2.318720
11	13	0	-2.034836	-2.567476	-0.019691
12	13	0	-1.520800	-1.007226	-2.331237
13	13	0	-3.819389	0.578427	-2.645972
14	13	0	-3.357739	2.684787	-1.254812
15	13	0	-3.344746	2.654497	1.339463
16	13	0	-3.829398	0.511264	2.667764
17	13	0	-4.225778	-1.657888	1.349132
18	13	0	-4.229929	-1.620975	-1.377990
19	13	0	-2.691694	0.262212	0.010144
20	13	0	-5.263696	0.704295	0.014918
21	6	0	2.845440	2.838257	0.014229
22	6	0	3.172560	3.521804	-1.163490
23	6	0	4.104819	4.552568	-1.161128
24	6	0	4.730777	4.921957	0.022787
25	6	0	4.421768	4.255896	1.202014
26	6	0	3.489189	3.225344	1.196053
27	1	0	2.698523	3.250101	-2.101884
28	1	0	4.343462	5.066719	-2.086160
29	1	0	5.459077	5.725594	0.026085
30	1	0	4.908903	4.537368	2.129601
31	1	0	3.266526	2.718802	2.130269
32	53	0	4.645248	-2.072742	-0.023650

Low frequencies (cm⁻¹): 8.0393 18.1768 18.9229
 30.4278 37.7209 40.4050

Al₂₀ C₆H₅I (BHandHLYP/TZVP, LANL2DZ level of theory)

Optimized geometry of reactant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.897713	0.984913	-1.875816
2	13	0	1.050029	1.682237	0.874474
3	13	0	0.527471	-0.614946	2.489971
4	13	0	0.073544	-2.903614	0.632590
5	13	0	0.281416	-1.790449	-2.136550
6	13	0	1.735365	-0.856539	0.016316

7	13	0	-0.678258	-0.319760	0.009704
8	13	0	-1.690465	0.150539	-2.452686
9	13	0	-1.216173	2.260109	-0.617279
10	13	0	-1.445321	1.296292	2.036442
11	13	0	-1.982422	-1.619103	1.982097
12	13	0	-2.133445	-2.375450	-0.956830
13	13	0	-4.830384	-1.967624	-0.704205
14	13	0	-4.449463	-0.138585	-2.525269
15	13	0	-3.796752	2.287533	-1.835938
16	13	0	-3.655962	2.925582	0.712167
17	13	0	-4.176652	1.125778	2.523260
18	13	0	-4.702762	-1.331288	1.821757
19	13	0	-3.150153	0.187663	0.013020
20	13	0	-5.597545	0.810364	-0.012129
21	6	0	5.567350	0.570746	-0.000545
22	6	0	5.783541	1.207418	1.202587
23	6	0	6.239324	2.512591	1.191807
24	6	0	6.472504	3.160751	-0.005136
25	6	0	6.249296	2.504788	-1.199770
26	6	0	5.793625	1.199584	-1.205921
27	1	0	5.600343	0.705727	2.133800
28	1	0	6.408944	3.019042	2.124782
29	1	0	6.825583	4.175953	-0.006961
30	1	0	6.426663	3.005279	-2.134514
31	1	0	5.618526	0.691674	-2.135317
32	53	0	4.881301	-1.431140	0.003469

Low frequencies (cm⁻¹): 10.3096 9.7079 11.4434
 14.9110 23.5746 25.5161

Coordinate of TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.607713	1.206097	0.000195
2	13	0	0.909136	-0.286647	2.372648
3	13	0	-0.074698	-2.836922	1.495727
4	13	0	-0.075486	-2.837449	-1.495446
5	13	0	0.908858	-0.286982	-2.373312
6	13	0	1.764908	-1.534777	-0.000705
7	13	0	-0.503278	-0.502230	-0.000329
8	13	0	-0.761803	1.742493	-1.465175
9	13	0	-0.762765	1.742514	1.464238
10	13	0	-1.785350	-0.851172	2.324908
11	13	0	-2.329397	-2.462668	0.001412
12	13	0	-1.786200	-0.852542	-2.324657
13	13	0	-3.985242	0.813156	-2.619257
14	13	0	-3.238587	2.913532	-1.299197
15	13	0	-3.238192	2.917331	1.290850

26	6	0	4.288568	2.418035	-0.267638
27	1	0	1.540545	4.358497	-0.109677
28	1	0	3.203613	6.001717	0.558526
29	1	0	5.579945	5.375697	0.703312
30	1	0	6.269872	3.073460	0.169672
31	1	0	4.622105	1.419317	-0.491156
32	53	0	4.615857	-1.912450	0.045576

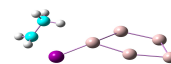
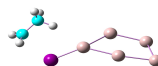
Low frequencies (cm⁻¹): 14.5949 20.2871 35.2431

37.9174	43.6554	44.4774
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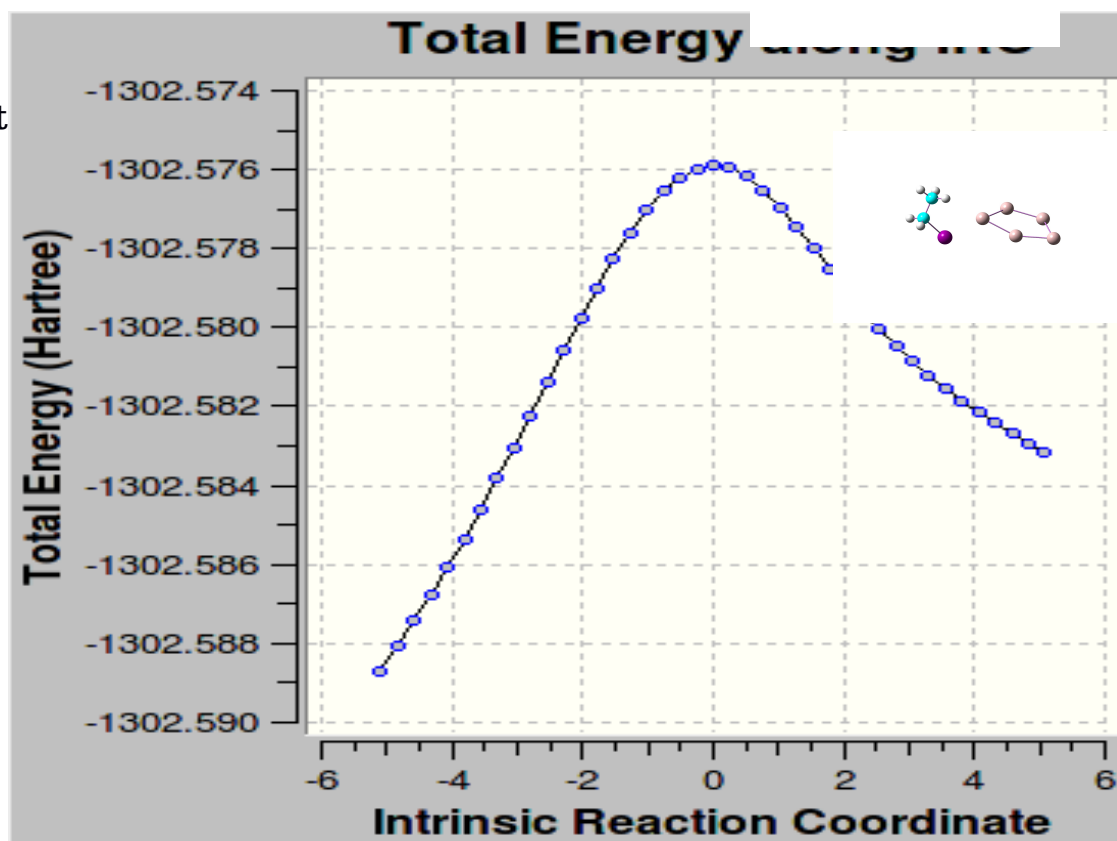
Sample IRC plot (for Al₅ cluster with ethyl iodide)

Total Energy along IRC
X-Axis: Intrinsic Reaction Coordinate
Y-Axis: Total Energy (Hartree)

X	Y
-5.0889700000	-1302.5886851900
-4.8345600000	-1302.5880730200
-4.5801100000	-1302.5874333000
-4.3256600000	-1302.5867657000
-4.0712000000	-1302.5860699800
-3.8167500000	-1302.5853465400
-3.5623000000	-1302.5845964900
-3.3078600000	-1302.5838221500
-3.0534100000	-1302.5830271100
-2.7989600000	-1302.5822167700
-2.5445000000	-1302.5813985200
-2.2900500000	-1302.5805820300
-2.0356000000	-1302.5797793300
-1.7811400000	-1302.5790049200
-1.5266900000	-1302.5782755400
-1.2722300000	-1302.5776097300
-1.0178000000	-1302.5770270800
-0.7633500000	-1302.5765474800
-0.5089000000	-1302.5761892700
-0.2544800000	-1302.5759679300
0.0000000000	-1302.5758928500
0.2545100000	-1302.5759655900
0.5089300000	-1302.5761786000
0.7633500000	-1302.5765147900
1.0177500000	-1302.5769479700
1.2721600000	-1302.5774472500
1.5265400000	-1302.5779808800
1.7808900000	-1302.5785209900
2.0351800000	-1302.5790463700
2.2894500000	-1302.5795448300
2.5432000000	-1302.5800101200
2.7968400000	-1302.5804407100
3.0496300000	-1302.5808380800
3.3026400000	-1302.5812041900
3.5564200000	-1302.5815454900
3.8103000000	-1302.5818607100
4.0643400000	-1302.5821547800
4.3185400000	-1302.5824297400
4.5727900000	-1302.5826868700
4.8266300000	-1302.5829274600
5.0796900000	-1302.5831520700



Sample IRC Plot
(Screenshot
taken from
Gaussview 5.0)



Grid data for Three Dimensional Potential energy surface

DFT Functional: B3PW91
BASIS SET: TZVP(Al,C,H)+LANL2DZ,LANL2(I)
 # 2-Coordinate Scan of Total Energy
 # X-axis = Scan Coordinate 1 = C-I bond
 # Y-axis = Scan Coordinate 2 = C-I-Al angle
 # Z-axis = Energy

#	Node	X	Y	Z
1	1	2.0395485475E+00	8.7000040532E+01	-8.1775600451E+02
1	2	2.0395485475E+00	8.7500040532E+01	-8.1775531412E+02
1	3	2.0395485475E+00	8.8000040532E+01	-8.1775602771E+02
1	4	2.0395485475E+00	8.8500040532E+01	-8.1775582233E+02
1	5	2.0395485475E+00	8.9000040532E+01	-8.1775608467E+02
1	6	2.0395485475E+00	8.9500040532E+01	-8.1775607306E+02

1	7	2.0395485475E+00	9.0000040532E+01	-8.1775610458E+02
1	8	2.0395485475E+00	9.0500040532E+01	-8.1775598775E+02
1	9	2.0395485475E+00	9.1000040532E+01	-8.1775601996E+02
1	10	2.0395485475E+00	9.1500040532E+01	-8.1775611620E+02
1	11	2.0395485475E+00	9.2000040532E+01	-8.1775610572E+02
1	12	2.0395485475E+00	9.2500040532E+01	-8.1775611213E+02
1	13	2.0395485475E+00	9.3000040532E+01	-8.1775610152E+02
1	14	2.0395485475E+00	9.3500040532E+01	-8.1775606157E+02
1	15	2.0395485475E+00	9.4000040532E+01	-8.1775603738E+02
1	16	2.0395485475E+00	9.4500040532E+01	-8.1775606717E+02
1	17	2.0395485475E+00	9.5000040532E+01	-8.1775602862E+02
1	18	2.0395485475E+00	9.5500040532E+01	-8.1775598801E+02
1	19	2.0395485475E+00	9.6000040532E+01	-8.1775596287E+02
1	20	2.0395485475E+00	9.6500040532E+01	-8.1775572735E+02
1	21	2.0395485475E+00	9.7000040532E+01	-8.1775596681E+02
1	22	2.0395485475E+00	9.7500040532E+01	-8.1775584937E+02
1	23	2.0395485475E+00	9.8000040532E+01	-8.1775586331E+02
1	24	2.0395485475E+00	9.8500040532E+01	-8.1775584736E+02
1	25	2.0395485475E+00	9.9000040532E+01	-8.1775581306E+02
1	26	2.0395485475E+00	9.9500040532E+01	-8.1775578389E+02
1	27	2.0395485475E+00	1.0000004053E+02	-8.1775575939E+02
1	28	2.0395485475E+00	1.0050004053E+02	-8.1775541311E+02
1	29	2.0395485475E+00	1.0100004053E+02	-8.1775569547E+02
1	30	2.0395485475E+00	1.0150004053E+02	-8.1775569736E+02
1	31	2.0395485475E+00	1.0200004053E+02	-8.1775566262E+02
1	32	2.0395485475E+00	1.0250004053E+02	-8.1775556685E+02
1	33	2.0395485475E+00	1.0300004053E+02	-8.1775534580E+02
1	34	2.0395485475E+00	1.0350004053E+02	-8.1775479981E+02
1	35	2.0395485475E+00	1.0400004053E+02	-8.1775549892E+02
1	36	2.0395485475E+00	1.0450004053E+02	-8.1775548477E+02
1	37	2.0395485475E+00	1.0500004053E+02	-8.1775544664E+02
1	38	2.0395485475E+00	1.0550004053E+02	-8.1775538524E+02
1	39	2.0395485475E+00	1.0600004053E+02	-8.1775535075E+02
1	40	2.0395485475E+00	1.0650004053E+02	-8.1775534299E+02
1	41	2.0395485475E+00	1.0700004053E+02	-8.1775531081E+02
1	42	2.0395485475E+00	1.0750004053E+02	-8.1775527719E+02
1	43	2.0395485475E+00	1.0800004053E+02	-8.1775524477E+02
1	44	2.0395485475E+00	1.0850004053E+02	-8.1775521450E+02
1	45	2.0395485475E+00	1.0900004053E+02	-8.1775518583E+02
1	46	2.0395485475E+00	1.0950004053E+02	-8.1775515257E+02
1	47	2.0395485475E+00	1.1000004053E+02	-8.1775512130E+02
1	48	2.0395485475E+00	1.1050004053E+02	-8.1775508506E+02
1	49	2.0395485475E+00	1.1100004053E+02	-8.1775505552E+02
1	50	2.0395485475E+00	1.1150004053E+02	-8.1775502563E+02
1	51	2.0395485475E+00	1.1200004053E+02	-8.1775499650E+02
1	52	2.0395485475E+00	1.1250004053E+02	-8.1775496716E+02
1	53	2.0395485475E+00	1.1300004053E+02	-8.1775485930E+02
1	54	2.0395485475E+00	1.1350004053E+02	-8.1775490776E+02
1	55	2.0395485475E+00	1.1400004053E+02	-8.1775482264E+02
1	56	2.0395485475E+00	1.1450004053E+02	-8.1775483099E+02
1	57	2.0395485475E+00	1.1500004053E+02	-8.1775480085E+02
1	58	2.0395485475E+00	1.1550004053E+02	-8.1775468864E+02

1	59	2.0395485475E+00	1.1600004053E+02	-8.1775472290E+02
1	60	2.0395485475E+00	1.1650004053E+02	-8.1775471606E+02
1	61	2.0395485475E+00	1.1700004053E+02	-8.1775468662E+02
2	1	2.0495485475E+00	8.7000040532E+01	-8.1775681471E+02
2	2	2.0495485475E+00	8.7500040532E+01	-8.1775684534E+02
2	3	2.0495485475E+00	8.8000040532E+01	-8.1775686549E+02
2	4	2.0495485475E+00	8.8500040532E+01	-8.1775687802E+02
2	5	2.0495485475E+00	8.9000040532E+01	-8.1775690341E+02
2	6	2.0495485475E+00	8.9500040532E+01	-8.1775691140E+02
2	7	2.0495485475E+00	9.0000040532E+01	-8.1775692012E+02
2	8	2.0495485475E+00	9.0500040532E+01	-8.1775685826E+02
2	9	2.0495485475E+00	9.1000040532E+01	-8.1775693093E+02
2	10	2.0495485475E+00	9.1500040532E+01	-8.1775693011E+02
2	11	2.0495485475E+00	9.2000040532E+01	-8.1775692948E+02
2	12	2.0495485475E+00	9.2500040532E+01	-8.1775692102E+02
2	13	2.0495485475E+00	9.3000040532E+01	-8.1775690993E+02
2	14	2.0495485475E+00	9.3500040532E+01	-8.1775687399E+02
2	15	2.0495485475E+00	9.4000040532E+01	-8.1775685356E+02
2	16	2.0495485475E+00	9.4500040532E+01	-8.1775673114E+02
2	17	2.0495485475E+00	9.5000040532E+01	-8.1775679786E+02
2	18	2.0495485475E+00	9.5500040532E+01	-8.1775680460E+02
2	19	2.0495485475E+00	9.6000040532E+01	-8.1775649956E+02
2	20	2.0495485475E+00	9.6500040532E+01	-8.1775679718E+02
2	21	2.0495485475E+00	9.7000040532E+01	-8.1775646489E+02
2	22	2.0495485475E+00	9.7500040532E+01	-8.1775670305E+02
2	23	2.0495485475E+00	9.8000040532E+01	-8.1775667604E+02
2	24	2.0495485475E+00	9.8500040532E+01	-8.1775665001E+02
2	25	2.0495485475E+00	9.9000040532E+01	-8.1775643273E+02
2	26	2.0495485475E+00	9.9500040532E+01	-8.1775659284E+02
2	27	2.0495485475E+00	1.0000004053E+02	-8.1775657178E+02
2	28	2.0495485475E+00	1.0050004053E+02	-8.1775650499E+02
2	29	2.0495485475E+00	1.0100004053E+02	-8.1775653619E+02
2	30	2.0495485475E+00	1.0150004053E+02	-8.1775650107E+02
2	31	2.0495485475E+00	1.0200004053E+02	-8.1775642062E+02
2	32	2.0495485475E+00	1.0250004053E+02	-8.1775625117E+02
2	33	2.0495485475E+00	1.0300004053E+02	-8.1775637924E+02
2	34	2.0495485475E+00	1.0350004053E+02	-8.1775623275E+02
2	35	2.0495485475E+00	1.0400004053E+02	-8.1775575329E+02
2	36	2.0495485475E+00	1.0450004053E+02	-8.1775629092E+02
2	37	2.0495485475E+00	1.0500004053E+02	-8.1775625211E+02
2	38	2.0495485475E+00	1.0550004053E+02	-8.1775621087E+02
2	39	2.0495485475E+00	1.0600004053E+02	-8.1775617473E+02
2	40	2.0495485475E+00	1.0650004053E+02	-8.1775614846E+02
2	41	2.0495485475E+00	1.0700004053E+02	-8.1775611389E+02
2	42	2.0495485475E+00	1.0750004053E+02	-8.1775608118E+02
2	43	2.0495485475E+00	1.0800004053E+02	-8.1775605055E+02
2	44	2.0495485475E+00	1.0850004053E+02	-8.1775601965E+02
2	45	2.0495485475E+00	1.0900004053E+02	-8.1775598673E+02
2	46	2.0495485475E+00	1.0950004053E+02	-8.1775559652E+02
2	47	2.0495485475E+00	1.1000004053E+02	-8.1775592565E+02
2	48	2.0495485475E+00	1.1050004053E+02	-8.1775589430E+02
2	49	2.0495485475E+00	1.1100004053E+02	-8.1775586324E+02

2	50	2.0495485475E+00	1.1150004053E+02	-8.1775583406E+02
2	51	2.0495485475E+00	1.1200004053E+02	-8.1775580442E+02
2	52	2.0495485475E+00	1.1250004053E+02	-8.1775577454E+02
2	53	2.0495485475E+00	1.1300004053E+02	-8.1775574484E+02
2	54	2.0495485475E+00	1.1350004053E+02	-8.1775571487E+02
2	55	2.0495485475E+00	1.1400004053E+02	-8.1775568648E+02
2	56	2.0495485475E+00	1.1450004053E+02	-8.1775563946E+02
2	57	2.0495485475E+00	1.1500004053E+02	-8.1775558437E+02
2	58	2.0495485475E+00	1.1550004053E+02	-8.1775558268E+02
2	59	2.0495485475E+00	1.1600004053E+02	-8.1775555387E+02
2	60	2.0495485475E+00	1.1650004053E+02	-8.1775521191E+02
2	61	2.0495485475E+00	1.1700004053E+02	-8.1775549546E+02
3	1	2.0595485475E+00	8.7000040532E+01	-8.1775756329E+02
3	2	2.0595485475E+00	8.7500040532E+01	-8.1775755195E+02
3	3	2.0595485475E+00	8.8000040532E+01	-8.1775761164E+02
3	4	2.0595485475E+00	8.8500040532E+01	-8.1775762818E+02
3	5	2.0595485475E+00	8.9000040532E+01	-8.1775763651E+02
3	6	2.0595485475E+00	8.9500040532E+01	-8.1775765620E+02
3	7	2.0595485475E+00	9.0000040532E+01	-8.1775766657E+02
3	8	2.0595485475E+00	9.0500040532E+01	-8.1775767057E+02
3	9	2.0595485475E+00	9.1000040532E+01	-8.1775767111E+02
3	10	2.0595485475E+00	9.1500040532E+01	-8.1775767184E+02
3	11	2.0595485475E+00	9.2000040532E+01	-8.1775766932E+02
3	12	2.0595485475E+00	9.2500040532E+01	-8.1775746633E+02
3	13	2.0595485475E+00	9.3000040532E+01	-8.1775765489E+02
3	14	2.0595485475E+00	9.3500040532E+01	-8.1775761414E+02
3	15	2.0595485475E+00	9.4000040532E+01	-8.1775763171E+02
3	16	2.0595485475E+00	9.4500040532E+01	-8.1775757752E+02
3	17	2.0595485475E+00	9.5000040532E+01	-8.1775759790E+02
3	18	2.0595485475E+00	9.5500040532E+01	-8.1775754639E+02
3	19	2.0595485475E+00	9.6000040532E+01	-8.1775755759E+02
3	20	2.0595485475E+00	9.6500040532E+01	-8.1775745694E+02
3	21	2.0595485475E+00	9.7000040532E+01	-8.1775749710E+02
3	22	2.0595485475E+00	9.7500040532E+01	-8.1775744886E+02
3	23	2.0595485475E+00	9.8000040532E+01	-8.1775738993E+02
3	24	2.0595485475E+00	9.8500040532E+01	-8.1775614146E+02
3	25	2.0595485475E+00	9.9000040532E+01	-8.1775736298E+02
3	26	2.0595485475E+00	9.9500040532E+01	-8.1775733694E+02
3	27	2.0595485475E+00	1.0000004053E+02	-8.1775730705E+02
3	28	2.0595485475E+00	1.0050004053E+02	-8.1775728437E+02
3	29	2.0595485475E+00	1.0100004053E+02	-8.1775727197E+02
3	30	2.0595485475E+00	1.0150004053E+02	-8.1775723648E+02
3	31	2.0595485475E+00	1.0200004053E+02	-8.1775716344E+02
3	32	2.0595485475E+00	1.0250004053E+02	-8.1775716392E+02
3	33	2.0595485475E+00	1.0300004053E+02	-8.1775710539E+02
3	34	2.0595485475E+00	1.0350004053E+02	-8.1775708549E+02
3	35	2.0595485475E+00	1.0400004053E+02	-8.1775698616E+02
3	36	2.0595485475E+00	1.0450004053E+02	-8.1775702617E+02
3	37	2.0595485475E+00	1.0500004053E+02	-8.1775698746E+02
3	38	2.0595485475E+00	1.0550004053E+02	-8.1775694602E+02
3	39	2.0595485475E+00	1.0600004053E+02	-8.1775691693E+02
3	40	2.0595485475E+00	1.0650004053E+02	-8.1775688258E+02

3 41	2.0595485475E+00	1.0700004053E+02	-8.1775684894E+02
3 42	2.0595485475E+00	1.0750004053E+02	-8.1775659675E+02
3 43	2.0595485475E+00	1.0800004053E+02	-8.1775678530E+02
3 44	2.0595485475E+00	1.0850004053E+02	-8.1775675459E+02
3 45	2.0595485475E+00	1.0900004053E+02	-8.1775672340E+02
3 46	2.0595485475E+00	1.0950004053E+02	-8.1775669191E+02
3 47	2.0595485475E+00	1.1000004053E+02	-8.1775666021E+02
3 48	2.0595485475E+00	1.1050004053E+02	-8.1775663377E+02
3 49	2.0595485475E+00	1.1100004053E+02	-8.1775660206E+02
3 50	2.0595485475E+00	1.1150004053E+02	-8.1775657223E+02
3 51	2.0595485475E+00	1.1200004053E+02	-8.1775654180E+02
3 52	2.0595485475E+00	1.1250004053E+02	-8.1775651313E+02
3 53	2.0595485475E+00	1.1300004053E+02	-8.1775648208E+02
3 54	2.0595485475E+00	1.1350004053E+02	-8.1775615589E+02
3 55	2.0595485475E+00	1.1400004053E+02	-8.1775642423E+02
3 56	2.0595485475E+00	1.1450004053E+02	-8.1775637843E+02
3 57	2.0595485475E+00	1.1500004053E+02	-8.1775635016E+02
3 58	2.0595485475E+00	1.1550004053E+02	-8.1775632190E+02
3 59	2.0595485475E+00	1.1600004053E+02	-8.1775629288E+02
3 60	2.0595485475E+00	1.1650004053E+02	-8.1775626371E+02
3 61	2.0595485475E+00	1.1700004053E+02	-8.1775623420E+02
4 1	2.0695485475E+00	8.7000040532E+01	-8.1775823751E+02
4 2	2.0695485475E+00	8.7500040532E+01	-8.1775826236E+02
4 3	2.0695485475E+00	8.8000040532E+01	-8.1775829256E+02
4 4	2.0695485475E+00	8.8500040532E+01	-8.1775830474E+02
4 5	2.0695485475E+00	8.9000040532E+01	-8.1775832408E+02
4 6	2.0695485475E+00	8.9500040532E+01	-8.1775830616E+02
4 7	2.0695485475E+00	9.0000040532E+01	-8.1775823953E+02
4 8	2.0695485475E+00	9.0500040532E+01	-8.1775834629E+02
4 9	2.0695485475E+00	9.1000040532E+01	-8.1775834928E+02
4 10	2.0695485475E+00	9.1500040532E+01	-8.1775834868E+02
4 11	2.0695485475E+00	9.2000040532E+01	-8.1775834531E+02
4 12	2.0695485475E+00	9.2500040532E+01	-8.1775830725E+02
4 13	2.0695485475E+00	9.3000040532E+01	-8.1775799543E+02
4 14	2.0695485475E+00	9.3500040532E+01	-8.1775828812E+02
4 15	2.0695485475E+00	9.4000040532E+01	-8.1775713464E+02
4 16	2.0695485475E+00	9.4500040532E+01	-8.1775825718E+02
4 17	2.0695485475E+00	9.5000040532E+01	-8.1775827039E+02
4 18	2.0695485475E+00	9.5500040532E+01	-8.1775821955E+02
4 19	2.0695485475E+00	9.6000040532E+01	-8.1775794810E+02
4 20	2.0695485475E+00	9.6500040532E+01	-8.1775816908E+02
4 21	2.0695485475E+00	9.7000040532E+01	-8.1775816954E+02
4 22	2.0695485475E+00	9.7500040532E+01	-8.1775812325E+02
4 23	2.0695485475E+00	9.8000040532E+01	-8.1775809239E+02
4 24	2.0695485475E+00	9.8500040532E+01	-8.1775806631E+02
4 25	2.0695485475E+00	9.9000040532E+01	-8.1775796167E+02
4 26	2.0695485475E+00	9.9500040532E+01	-8.1775801430E+02
4 27	2.0695485475E+00	1.0000004053E+02	-8.1775795176E+02
4 28	2.0695485475E+00	1.0050004053E+02	-8.1775795326E+02
4 29	2.0695485475E+00	1.0100004053E+02	-8.1775767062E+02
4 30	2.0695485475E+00	1.0150004053E+02	-8.1775776218E+02
4 31	2.0695485475E+00	1.0200004053E+02	-8.1775787518E+02

4	32	2.0695485475E+00	1.0250004053E+02	-8.1775781816E+02
4	33	2.0695485475E+00	1.0300004053E+02	-8.1775723167E+02
4	34	2.0695485475E+00	1.0350004053E+02	-8.1775775315E+02
4	35	2.0695485475E+00	1.0400004053E+02	-8.1775771458E+02
4	36	2.0695485475E+00	1.0450004053E+02	-8.1775765230E+02
4	37	2.0695485475E+00	1.0500004053E+02	-8.1775765569E+02
4	38	2.0695485475E+00	1.0550004053E+02	-8.1775759887E+02
4	39	2.0695485475E+00	1.0600004053E+02	-8.1775758434E+02
4	40	2.0695485475E+00	1.0650004053E+02	-8.1775754998E+02
4	41	2.0695485475E+00	1.0700004053E+02	-8.1775751738E+02
4	42	2.0695485475E+00	1.0750004053E+02	-8.1775748512E+02
4	43	2.0695485475E+00	1.0800004053E+02	-8.1775745373E+02
4	44	2.0695485475E+00	1.0850004053E+02	-8.1775742288E+02
4	45	2.0695485475E+00	1.0900004053E+02	-8.1775739184E+02
4	46	2.0695485475E+00	1.0950004053E+02	-8.1775735928E+02
4	47	2.0695485475E+00	1.1000004053E+02	-8.1775732758E+02
4	48	2.0695485475E+00	1.1050004053E+02	-8.1775730628E+02
4	49	2.0695485475E+00	1.1100004053E+02	-8.1775727441E+02
4	50	2.0695485475E+00	1.1150004053E+02	-8.1775710026E+02
4	51	2.0695485475E+00	1.1200004053E+02	-8.1775721386E+02
4	52	2.0695485475E+00	1.1250004053E+02	-8.1775718429E+02
4	53	2.0695485475E+00	1.1300004053E+02	-8.1775715384E+02
4	54	2.0695485475E+00	1.1350004053E+02	-8.1775712251E+02
4	55	2.0695485475E+00	1.1400004053E+02	-8.1775709489E+02
4	56	2.0695485475E+00	1.1450004053E+02	-8.1775705163E+02
4	57	2.0695485475E+00	1.1500004053E+02	-8.1775702326E+02
4	58	2.0695485475E+00	1.1550004053E+02	-8.1775699445E+02
4	59	2.0695485475E+00	1.1600004053E+02	-8.1775696549E+02
4	60	2.0695485475E+00	1.1650004053E+02	-8.1775693624E+02
4	61	2.0695485475E+00	1.1700004053E+02	-8.1775690639E+02
5	1	2.0795485475E+00	8.7000040532E+01	-8.1775885604E+02
5	2	2.0795485475E+00	8.7500040532E+01	-8.1775888108E+02
5	3	2.0795485475E+00	8.8000040532E+01	-8.1775890410E+02
5	4	2.0795485475E+00	8.8500040532E+01	-8.1775891803E+02
5	5	2.0795485475E+00	8.9000040532E+01	-8.1775893295E+02
5	6	2.0795485475E+00	8.9500040532E+01	-8.1775894114E+02
5	7	2.0795485475E+00	9.0000040532E+01	-8.1775895039E+02
5	8	2.0795485475E+00	9.0500040532E+01	-8.1775896079E+02
5	9	2.0795485475E+00	9.1000040532E+01	-8.1775896107E+02
5	10	2.0795485475E+00	9.1500040532E+01	-8.1775897982E+02
5	11	2.0795485475E+00	9.2000040532E+01	-8.1775893820E+02
5	12	2.0795485475E+00	9.2500040532E+01	-8.1775890697E+02
5	13	2.0795485475E+00	9.3000040532E+01	-8.1775893795E+02
5	14	2.0795485475E+00	9.3500040532E+01	-8.1775889758E+02
5	15	2.0795485475E+00	9.4000040532E+01	-8.1775891302E+02
5	16	2.0795485475E+00	9.4500040532E+01	-8.1775886511E+02
5	17	2.0795485475E+00	9.5000040532E+01	-8.1775887735E+02
5	18	2.0795485475E+00	9.5500040532E+01	-8.1775833549E+02
5	19	2.0795485475E+00	9.6000040532E+01	-8.1775883674E+02
5	20	2.0795485475E+00	9.6500040532E+01	-8.1775877396E+02
5	21	2.0795485475E+00	9.7000040532E+01	-8.1775878510E+02
5	22	2.0795485475E+00	9.7500040532E+01	-8.1775872832E+02

5	23	2.0795485475E+00	9.8000040532E+01	-8.1775870504E+02
5	24	2.0795485475E+00	9.8500040532E+01	-8.1775866661E+02
5	25	2.0795485475E+00	9.9000040532E+01	-8.1775831232E+02
5	26	2.0795485475E+00	9.9500040532E+01	-8.1775862209E+02
5	27	2.0795485475E+00	1.0000004053E+02	-8.1775855904E+02
5	28	2.0795485475E+00	1.0050004053E+02	-8.1775817907E+02
5	29	2.0795485475E+00	1.0100004053E+02	-8.1775852869E+02
5	30	2.0795485475E+00	1.0150004053E+02	-8.1775841916E+02
5	31	2.0795485475E+00	1.0200004053E+02	-8.1775845749E+02
5	32	2.0795485475E+00	1.0250004053E+02	-8.1775839139E+02
5	33	2.0795485475E+00	1.0300004053E+02	-8.1775810085E+02
5	34	2.0795485475E+00	1.0350004053E+02	-8.1775785224E+02
5	35	2.0795485475E+00	1.0400004053E+02	-8.1775824642E+02
5	36	2.0795485475E+00	1.0450004053E+02	-8.1775824562E+02
5	37	2.0795485475E+00	1.0500004053E+02	-8.1775825816E+02
5	38	2.0795485475E+00	1.0550004053E+02	-8.1775817808E+02
5	39	2.0795485475E+00	1.0600004053E+02	-8.1775818820E+02
5	40	2.0795485475E+00	1.0650004053E+02	-8.1775813020E+02
5	41	2.0795485475E+00	1.0700004053E+02	-8.1775812169E+02
5	42	2.0795485475E+00	1.0750004053E+02	-8.1775808959E+02
5	43	2.0795485475E+00	1.0800004053E+02	-8.1775805833E+02
5	44	2.0795485475E+00	1.0850004053E+02	-8.1775802704E+02
5	45	2.0795485475E+00	1.0900004053E+02	-8.1775799562E+02
5	46	2.0795485475E+00	1.0950004053E+02	-8.1775796356E+02
5	47	2.0795485475E+00	1.1000004053E+02	-8.1775793075E+02
5	48	2.0795485475E+00	1.1050004053E+02	-8.1775791550E+02
5	49	2.0795485475E+00	1.1100004053E+02	-8.1775788186E+02
5	50	2.0795485475E+00	1.1150004053E+02	-8.1775785251E+02
5	51	2.0795485475E+00	1.1200004053E+02	-8.1775782215E+02
5	52	2.0795485475E+00	1.1250004053E+02	-8.1775779195E+02
5	53	2.0795485475E+00	1.1300004053E+02	-8.1775776100E+02
5	54	2.0795485475E+00	1.1350004053E+02	-8.1775770985E+02
5	55	2.0795485475E+00	1.1400004053E+02	-8.1775770163E+02
5	56	2.0795485475E+00	1.1450004053E+02	-8.1775766105E+02
5	57	2.0795485475E+00	1.1500004053E+02	-8.1775763223E+02
5	58	2.0795485475E+00	1.1550004053E+02	-8.1775760345E+02
5	59	2.0795485475E+00	1.1600004053E+02	-8.1775757400E+02
5	60	2.0795485475E+00	1.1650004053E+02	-8.1775754479E+02
5	61	2.0795485475E+00	1.1700004053E+02	-8.1775751475E+02
6	1	2.0895485475E+00	8.7000040532E+01	-8.1775940539E+02
6	2	2.0895485475E+00	8.7500040532E+01	-8.1775943362E+02
6	3	2.0895485475E+00	8.8000040532E+01	-8.1775945301E+02
6	4	2.0895485475E+00	8.8500040532E+01	-8.1775947331E+02
6	5	2.0895485475E+00	8.9000040532E+01	-8.1775948884E+02
6	6	2.0895485475E+00	8.9500040532E+01	-8.1775949428E+02
6	7	2.0895485475E+00	9.0000040532E+01	-8.1775941744E+02
6	8	2.0895485475E+00	9.0500040532E+01	-8.1775950998E+02
6	9	2.0895485475E+00	9.1000040532E+01	-8.1775950833E+02
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6	11	2.0895485475E+00	9.2000040532E+01	-8.1775950308E+02
6	12	2.0895485475E+00	9.2500040532E+01	-8.1775947307E+02
6	13	2.0895485475E+00	9.3000040532E+01	-8.1775948783E+02

6	14	2.0895485475E+00	9.3500040532E+01	-8.1775945100E+02
6	15	2.0895485475E+00	9.4000040532E+01	-8.1775946105E+02
6	16	2.0895485475E+00	9.4500040532E+01	-8.1775941489E+02
6	17	2.0895485475E+00	9.5000040532E+01	-8.1775942571E+02
6	18	2.0895485475E+00	9.5500040532E+01	-8.1775936050E+02
6	19	2.0895485475E+00	9.6000040532E+01	-8.1775938461E+02
6	20	2.0895485475E+00	9.6500040532E+01	-8.1775932989E+02
6	21	2.0895485475E+00	9.7000040532E+01	-8.1775933603E+02
6	22	2.0895485475E+00	9.7500040532E+01	-8.1775927956E+02
6	23	2.0895485475E+00	9.8000040532E+01	-8.1775925041E+02
6	24	2.0895485475E+00	9.8500040532E+01	-8.1775922585E+02
6	25	2.0895485475E+00	9.9000040532E+01	-8.1775919753E+02
6	26	2.0895485475E+00	9.9500040532E+01	-8.1775917448E+02
6	27	2.0895485475E+00	1.0000004053E+02	-8.1775914438E+02
6	28	2.0895485475E+00	1.0050004053E+02	-8.1775877894E+02
6	29	2.0895485475E+00	1.0100004053E+02	-8.1775906397E+02
6	30	2.0895485475E+00	1.0150004053E+02	-8.1775904994E+02
6	31	2.0895485475E+00	1.0200004053E+02	-8.1775902805E+02
6	32	2.0895485475E+00	1.0250004053E+02	-8.1775898913E+02
6	33	2.0895485475E+00	1.0300004053E+02	-8.1775893764E+02
6	34	2.0895485475E+00	1.0350004053E+02	-8.1775891394E+02
6	35	2.0895485475E+00	1.0400004053E+02	-8.1775885192E+02
6	36	2.0895485475E+00	1.0450004053E+02	-8.1775883459E+02
6	37	2.0895485475E+00	1.0500004053E+02	-8.1775880055E+02
6	38	2.0895485475E+00	1.0550004053E+02	-8.1775875173E+02
6	39	2.0895485475E+00	1.0600004053E+02	-8.1775873112E+02
6	40	2.0895485475E+00	1.0650004053E+02	-8.1775867390E+02
6	41	2.0895485475E+00	1.0700004053E+02	-8.1775866492E+02
6	42	2.0895485475E+00	1.0750004053E+02	-8.1775863312E+02
6	43	2.0895485475E+00	1.0800004053E+02	-8.1775860178E+02
6	44	2.0895485475E+00	1.0850004053E+02	-8.1775857045E+02
6	45	2.0895485475E+00	1.0900004053E+02	-8.1775853869E+02
6	46	2.0895485475E+00	1.0950004053E+02	-8.1775850631E+02
6	47	2.0895485475E+00	1.1000004053E+02	-8.1775847311E+02
6	48	2.0895485475E+00	1.1050004053E+02	-8.1775846255E+02
6	49	2.0895485475E+00	1.1100004053E+02	-8.1775843137E+02
6	50	2.0895485475E+00	1.1150004053E+02	-8.1775840018E+02
6	51	2.0895485475E+00	1.1200004053E+02	-8.1775836895E+02
6	52	2.0895485475E+00	1.1250004053E+02	-8.1775833861E+02
6	53	2.0895485475E+00	1.1300004053E+02	-8.1775830799E+02
6	54	2.0895485475E+00	1.1350004053E+02	-8.1775823359E+02
6	55	2.0895485475E+00	1.1400004053E+02	-8.1775824700E+02
6	56	2.0895485475E+00	1.1450004053E+02	-8.1775820935E+02
6	57	2.0895485475E+00	1.1500004053E+02	-8.1775818035E+02
6	58	2.0895485475E+00	1.1550004053E+02	-8.1775815145E+02
6	59	2.0895485475E+00	1.1600004053E+02	-8.1775730988E+02
6	60	2.0895485475E+00	1.1650004053E+02	-8.1775809257E+02
6	61	2.0895485475E+00	1.1700004053E+02	-8.1775806249E+02
7	1	2.0995485475E+00	8.7000040532E+01	-8.1775990602E+02
7	2	2.0995485475E+00	8.7500040532E+01	-8.1775992832E+02
7	3	2.0995485475E+00	8.8000040532E+01	-8.1775995108E+02
7	4	2.0995485475E+00	8.8500040532E+01	-8.1775996390E+02

7 5	2.0995485475E+00	8.9000040532E+01	-8.1775995208E+02
7 6	2.0995485475E+00	8.9500040532E+01	-8.1775999138E+02
7 7	2.0995485475E+00	9.0000040532E+01	-8.1775999843E+02
7 8	2.0995485475E+00	9.0500040532E+01	-8.1776000196E+02
7 9	2.0995485475E+00	9.1000040532E+01	-8.1776000317E+02
7 10	2.0995485475E+00	9.1500040532E+01	-8.1775996630E+02
7 11	2.0995485475E+00	9.2000040532E+01	-8.1775999616E+02
7 12	2.0995485475E+00	9.2500040532E+01	-8.1775973347E+02
7 13	2.0995485475E+00	9.3000040532E+01	-8.1775997864E+02
7 14	2.0995485475E+00	9.3500040532E+01	-8.1775994189E+02
7 15	2.0995485475E+00	9.4000040532E+01	-8.1775995083E+02
7 16	2.0995485475E+00	9.4500040532E+01	-8.1775991145E+02
7 17	2.0995485475E+00	9.5000040532E+01	-8.1775991521E+02
7 18	2.0995485475E+00	9.5500040532E+01	-8.1775983375E+02
7 19	2.0995485475E+00	9.6000040532E+01	-8.1775987258E+02
7 20	2.0995485475E+00	9.6500040532E+01	-8.1775967229E+02
7 21	2.0995485475E+00	9.7000040532E+01	-8.1775982407E+02
7 22	2.0995485475E+00	9.7500040532E+01	-8.1775976957E+02
7 23	2.0995485475E+00	9.8000040532E+01	-8.1775973745E+02
7 24	2.0995485475E+00	9.8500040532E+01	-8.1775971722E+02
7 25	2.0995485475E+00	9.9000040532E+01	-8.1775905088E+02
7 26	2.0995485475E+00	9.9500040532E+01	-8.1775966217E+02
7 27	2.0995485475E+00	1.000004053E+02	-8.1775961345E+02
7 28	2.0995485475E+00	1.0050004053E+02	-8.1775960553E+02
7 29	2.0995485475E+00	1.0100004053E+02	-8.1775958222E+02
7 30	2.0995485475E+00	1.0150004053E+02	-8.1775954415E+02
7 31	2.0995485475E+00	1.0200004053E+02	-8.1775950412E+02
7 32	2.0995485475E+00	1.0250004053E+02	-8.1775947441E+02
7 33	2.0995485475E+00	1.0300004053E+02	-8.1775944160E+02
7 34	2.0995485475E+00	1.0350004053E+02	-8.1775937921E+02
7 35	2.0995485475E+00	1.0400004053E+02	-8.1775936606E+02
7 36	2.0995485475E+00	1.0450004053E+02	-8.1775931327E+02
7 37	2.0995485475E+00	1.0500004053E+02	-8.1775928506E+02
7 38	2.0995485475E+00	1.0550004053E+02	-8.1775923856E+02
7 39	2.0995485475E+00	1.0600004053E+02	-8.1775921581E+02
7 40	2.0995485475E+00	1.0650004053E+02	-8.1775915975E+02
7 41	2.0995485475E+00	1.0700004053E+02	-8.1775915004E+02
7 42	2.0995485475E+00	1.0750004053E+02	-8.1775907575E+02
7 43	2.0995485475E+00	1.0800004053E+02	-8.1775908694E+02
7 44	2.0995485475E+00	1.0850004053E+02	-8.1775905555E+02
7 45	2.0995485475E+00	1.0900004053E+02	-8.1775902308E+02
7 46	2.0995485475E+00	1.0950004053E+02	-8.1775898672E+02
7 47	2.0995485475E+00	1.1000004053E+02	-8.1775895685E+02
7 48	2.0995485475E+00	1.1050004053E+02	-8.1775895241E+02
7 49	2.0995485475E+00	1.1100004053E+02	-8.1775892102E+02
7 50	2.0995485475E+00	1.1150004053E+02	-8.1775888937E+02
7 51	2.0995485475E+00	1.1200004053E+02	-8.1775885803E+02
7 52	2.0995485475E+00	1.1250004053E+02	-8.1775882726E+02
7 53	2.0995485475E+00	1.1300004053E+02	-8.1775879636E+02
7 54	2.0995485475E+00	1.1350004053E+02	-8.1775875726E+02
7 55	2.0995485475E+00	1.1400004053E+02	-8.1775873399E+02
7 56	2.0995485475E+00	1.1450004053E+02	-8.1775869950E+02

7 57	2.0995485475E+00	1.1500004053E+02	-8.1775867049E+02
7 58	2.0995485475E+00	1.1550004053E+02	-8.1775864147E+02
7 59	2.0995485475E+00	1.1600004053E+02	-8.1775861201E+02
7 60	2.0995485475E+00	1.1650004053E+02	-8.1775858225E+02
7 61	2.0995485475E+00	1.1700004053E+02	-8.1775855213E+02
8 1	2.1095485475E+00	8.7000040532E+01	-8.1776034520E+02
8 2	2.1095485475E+00	8.7500040532E+01	-8.1776036875E+02
8 3	2.1095485475E+00	8.8000040532E+01	-8.1776038885E+02
8 4	2.1095485475E+00	8.8500040532E+01	-8.1776040558E+02
8 5	2.1095485475E+00	8.9000040532E+01	-8.1776041890E+02
8 6	2.1095485475E+00	8.9500040532E+01	-8.1776041648E+02
8 7	2.1095485475E+00	9.0000040532E+01	-8.1776043521E+02
8 8	2.1095485475E+00	9.0500040532E+01	-8.1776041111E+02
8 9	2.1095485475E+00	9.1000040532E+01	-8.1776043979E+02
8 10	2.1095485475E+00	9.1500040532E+01	-8.1776041160E+02
8 11	2.1095485475E+00	9.2000040532E+01	-8.1776043177E+02
8 12	2.1095485475E+00	9.2500040532E+01	-8.1776039808E+02
8 13	2.1095485475E+00	9.3000040532E+01	-8.1776041276E+02
8 14	2.1095485475E+00	9.3500040532E+01	-8.1776037768E+02
8 15	2.1095485475E+00	9.4000040532E+01	-8.1776038443E+02
8 16	2.1095485475E+00	9.4500040532E+01	-8.1776034473E+02
8 17	2.1095485475E+00	9.5000040532E+01	-8.1776034818E+02
8 18	2.1095485475E+00	9.5500040532E+01	-8.1776030399E+02
8 19	2.1095485475E+00	9.6000040532E+01	-8.1776030498E+02
8 20	2.1095485475E+00	9.6500040532E+01	-8.1776025736E+02
8 21	2.1095485475E+00	9.7000040532E+01	-8.1776025598E+02
8 22	2.1095485475E+00	9.7500040532E+01	-8.1776020368E+02
8 23	2.1095485475E+00	9.8000040532E+01	-8.1775891337E+02
8 24	2.1095485475E+00	9.8500040532E+01	-8.1776015197E+02
8 25	2.1095485475E+00	9.9000040532E+01	-8.1776012061E+02
8 26	2.1095485475E+00	9.9500040532E+01	-8.1776009519E+02
8 27	2.1095485475E+00	1.0000004053E+02	-8.1776007060E+02
8 28	2.1095485475E+00	1.0050004053E+02	-8.1776004051E+02
8 29	2.1095485475E+00	1.0100004053E+02	-8.1776001142E+02
8 30	2.1095485475E+00	1.0150004053E+02	-8.1775997841E+02
8 31	2.1095485475E+00	1.0200004053E+02	-8.1775992627E+02
8 32	2.1095485475E+00	1.0250004053E+02	-8.1775965205E+02
8 33	2.1095485475E+00	1.0300004053E+02	-8.1775987642E+02
8 34	2.1095485475E+00	1.0350004053E+02	-8.1775983828E+02
8 35	2.1095485475E+00	1.0400004053E+02	-8.1775977706E+02
8 36	2.1095485475E+00	1.0450004053E+02	-8.1775975959E+02
8 37	2.1095485475E+00	1.0500004053E+02	-8.1775971388E+02
8 38	2.1095485475E+00	1.0550004053E+02	-8.1775967255E+02
8 39	2.1095485475E+00	1.0600004053E+02	-8.1775964487E+02
8 40	2.1095485475E+00	1.0650004053E+02	-8.1775958869E+02
8 41	2.1095485475E+00	1.0700004053E+02	-8.1775957941E+02
8 42	2.1095485475E+00	1.0750004053E+02	-8.1775951927E+02
8 43	2.1095485475E+00	1.0800004053E+02	-8.1775951639E+02
8 44	2.1095485475E+00	1.0850004053E+02	-8.1775945854E+02
8 45	2.1095485475E+00	1.0900004053E+02	-8.1775945190E+02
8 46	2.1095485475E+00	1.0950004053E+02	-8.1775938149E+02
8 47	2.1095485475E+00	1.1000004053E+02	-8.1775938524E+02

8 48	2.1095485475E+00	1.1050004053E+02	-8.1775938656E+02
8 49	2.1095485475E+00	1.1100004053E+02	-8.1775935473E+02
8 50	2.1095485475E+00	1.1150004053E+02	-8.1775932282E+02
8 51	2.1095485475E+00	1.1200004053E+02	-8.1775929125E+02
8 52	2.1095485475E+00	1.1250004053E+02	-8.1775926041E+02
8 53	2.1095485475E+00	1.1300004053E+02	-8.1775922931E+02
8 54	2.1095485475E+00	1.1350004053E+02	-8.1775919235E+02
8 55	2.1095485475E+00	1.1400004053E+02	-8.1775916517E+02
8 56	2.1095485475E+00	1.1450004053E+02	-8.1775913435E+02
8 57	2.1095485475E+00	1.1500004053E+02	-8.1775910531E+02
8 58	2.1095485475E+00	1.1550004053E+02	-8.1775907601E+02
8 59	2.1095485475E+00	1.1600004053E+02	-8.1775904648E+02
8 60	2.1095485475E+00	1.1650004053E+02	-8.1775901644E+02
8 61	2.1095485475E+00	1.1700004053E+02	-8.1775898609E+02
9 1	2.1195485475E+00	8.7000040532E+01	-8.1776073123E+02
9 2	2.1195485475E+00	8.7500040532E+01	-8.1776075486E+02
9 3	2.1195485475E+00	8.8000040532E+01	-8.1776077442E+02
9 4	2.1195485475E+00	8.8500040532E+01	-8.1776079080E+02
9 5	2.1195485475E+00	8.9000040532E+01	-8.1776080349E+02
9 6	2.1195485475E+00	8.9500040532E+01	-8.1776076697E+02
9 7	2.1195485475E+00	9.0000040532E+01	-8.1776081922E+02
9 8	2.1195485475E+00	9.0500040532E+01	-8.1776079347E+02
9 9	2.1195485475E+00	9.1000040532E+01	-8.1776082207E+02
9 10	2.1195485475E+00	9.1500040532E+01	-8.1776079597E+02
9 11	2.1195485475E+00	9.2000040532E+01	-8.1776081279E+02
9 12	2.1195485475E+00	9.2500040532E+01	-8.1776078366E+02
9 13	2.1195485475E+00	9.3000040532E+01	-8.1776079396E+02
9 14	2.1195485475E+00	9.3500040532E+01	-8.1776076008E+02
9 15	2.1195485475E+00	9.4000040532E+01	-8.1776076488E+02
9 16	2.1195485475E+00	9.4500040532E+01	-8.1776072974E+02
9 17	2.1195485475E+00	9.5000040532E+01	-8.1776072702E+02
9 18	2.1195485475E+00	9.5500040532E+01	-8.1776068676E+02
9 19	2.1195485475E+00	9.6000040532E+01	-8.1776068382E+02
9 20	2.1195485475E+00	9.6500040532E+01	-8.1776063744E+02
9 21	2.1195485475E+00	9.7000040532E+01	-8.1776063435E+02
9 22	2.1195485475E+00	9.7500040532E+01	-8.1776058625E+02
9 23	2.1195485475E+00	9.8000040532E+01	-8.1776056067E+02
9 24	2.1195485475E+00	9.8500040532E+01	-8.1776053422E+02
9 25	2.1195485475E+00	9.9000040532E+01	-8.1776050752E+02
9 26	2.1195485475E+00	9.9500040532E+01	-8.1776047989E+02
9 27	2.1195485475E+00	1.0000004053E+02	-8.1776045164E+02
9 28	2.1195485475E+00	1.0050004053E+02	-8.1776042198E+02
9 29	2.1195485475E+00	1.0100004053E+02	-8.1776038715E+02
9 30	2.1195485475E+00	1.0150004053E+02	-8.1776035928E+02
9 31	2.1195485475E+00	1.0200004053E+02	-8.1776031940E+02
9 32	2.1195485475E+00	1.0250004053E+02	-8.1776029177E+02
9 33	2.1195485475E+00	1.0300004053E+02	-8.1776025590E+02
9 34	2.1195485475E+00	1.0350004053E+02	-8.1776021936E+02
9 35	2.1195485475E+00	1.0400004053E+02	-8.1776018138E+02
9 36	2.1195485475E+00	1.0450004053E+02	-8.1776013992E+02
9 37	2.1195485475E+00	1.0500004053E+02	-8.1776008967E+02
9 38	2.1195485475E+00	1.0550004053E+02	-8.1776005378E+02

9	39	2.1195485475E+00	1.0600004053E+02	-8.1776002068E+02
9	40	2.1195485475E+00	1.0650004053E+02	-8.1775996741E+02
9	41	2.1195485475E+00	1.0700004053E+02	-8.1775995561E+02
9	42	2.1195485475E+00	1.0750004053E+02	-8.1775989513E+02
9	43	2.1195485475E+00	1.0800004053E+02	-8.1775989243E+02
9	44	2.1195485475E+00	1.0850004053E+02	-8.1775982390E+02
9	45	2.1195485475E+00	1.0900004053E+02	-8.1775982812E+02
9	46	2.1195485475E+00	1.0950004053E+02	-8.1775972474E+02
9	47	2.1195485475E+00	1.1000004053E+02	-8.1775976032E+02
9	48	2.1195485475E+00	1.1050004053E+02	-8.1775976783E+02
9	49	2.1195485475E+00	1.1100004053E+02	-8.1775973542E+02
9	50	2.1195485475E+00	1.1150004053E+02	-8.1775970360E+02
9	51	2.1195485475E+00	1.1200004053E+02	-8.1775967192E+02
9	52	2.1195485475E+00	1.1250004053E+02	-8.1775963439E+02
9	53	2.1195485475E+00	1.1300004053E+02	-8.1775960919E+02
9	54	2.1195485475E+00	1.1350004053E+02	-8.1775957443E+02
9	55	2.1195485475E+00	1.1400004053E+02	-8.1775954225E+02
9	56	2.1195485475E+00	1.1450004053E+02	-8.1775951635E+02
9	57	2.1195485475E+00	1.1500004053E+02	-8.1775948724E+02
9	58	2.1195485475E+00	1.1550004053E+02	-8.1775945788E+02
9	59	2.1195485475E+00	1.1600004053E+02	-8.1775942815E+02
9	60	2.1195485475E+00	1.1650004053E+02	-8.1775939808E+02
9	61	2.1195485475E+00	1.1700004053E+02	-8.1775936752E+02
10	1	2.1295485475E+00	8.7000040532E+01	-8.1776106634E+02
10	2	2.1295485475E+00	8.7500040532E+01	-8.1776109105E+02
10	3	2.1295485475E+00	8.8000040532E+01	-8.1776110936E+02
10	4	2.1295485475E+00	8.8500040532E+01	-8.1776112504E+02
10	5	2.1295485475E+00	8.9000040532E+01	-8.1776113718E+02
10	6	2.1295485475E+00	8.9500040532E+01	-8.1776112747E+02
10	7	2.1295485475E+00	9.0000040532E+01	-8.1776115171E+02
10	8	2.1295485475E+00	9.0500040532E+01	-8.1776113296E+02
10	9	2.1295485475E+00	9.1000040532E+01	-8.1776115337E+02
10	10	2.1295485475E+00	9.1500040532E+01	-8.1776113276E+02
10	11	2.1295485475E+00	9.2000040532E+01	-8.1776114323E+02
10	12	2.1295485475E+00	9.2500040532E+01	-8.1776111962E+02
10	13	2.1295485475E+00	9.3000040532E+01	-8.1776112365E+02
10	14	2.1295485475E+00	9.3500040532E+01	-8.1776081289E+02
10	15	2.1295485475E+00	9.4000040532E+01	-8.1776109386E+02
10	16	2.1295485475E+00	9.4500040532E+01	-8.1776106091E+02
10	17	2.1295485475E+00	9.5000040532E+01	-8.1776105556E+02
10	18	2.1295485475E+00	9.5500040532E+01	-8.1776101632E+02
10	19	2.1295485475E+00	9.6000040532E+01	-8.1776101205E+02
10	20	2.1295485475E+00	9.6500040532E+01	-8.1776096809E+02
10	21	2.1295485475E+00	9.7000040532E+01	-8.1776096187E+02
10	22	2.1295485475E+00	9.7500040532E+01	-8.1776091760E+02
10	23	2.1295485475E+00	9.8000040532E+01	-8.1776089113E+02
10	24	2.1295485475E+00	9.8500040532E+01	-8.1776086511E+02
10	25	2.1295485475E+00	9.9000040532E+01	-8.1776083829E+02
10	26	2.1295485475E+00	9.9500040532E+01	-8.1776081051E+02
10	27	2.1295485475E+00	1.0000004053E+02	-8.1776078168E+02
10	28	2.1295485475E+00	1.0050004053E+02	-8.1776075172E+02
10	29	2.1295485475E+00	1.0100004053E+02	-8.1776071395E+02

10	30	2.1295485475E+00	1.0150004053E+02	-8.1776068793E+02
10	31	2.1295485475E+00	1.0200004053E+02	-8.1776064612E+02
10	32	2.1295485475E+00	1.0250004053E+02	-8.1776061981E+02
10	33	2.1295485475E+00	1.0300004053E+02	-8.1776058411E+02
10	34	2.1295485475E+00	1.0350004053E+02	-8.1776054762E+02
10	35	2.1295485475E+00	1.0400004053E+02	-8.1776050964E+02
10	36	2.1295485475E+00	1.0450004053E+02	-8.1776046955E+02
10	37	2.1295485475E+00	1.0500004053E+02	-8.1776041478E+02
10	38	2.1295485475E+00	1.0550004053E+02	-8.1776038497E+02
10	39	2.1295485475E+00	1.0600004053E+02	-8.1776034571E+02
10	40	2.1295485475E+00	1.0650004053E+02	-8.1775970280E+02
10	41	2.1295485475E+00	1.0700004053E+02	-8.1776028092E+02
10	42	2.1295485475E+00	1.0750004053E+02	-8.1776021216E+02
10	43	2.1295485475E+00	1.0800004053E+02	-8.1776021777E+02
10	44	2.1295485475E+00	1.0850004053E+02	-8.1776015406E+02
10	45	2.1295485475E+00	1.0900004053E+02	-8.1776015311E+02
10	46	2.1295485475E+00	1.0950004053E+02	-8.1776006881E+02
10	47	2.1295485475E+00	1.1000004053E+02	-8.1776008430E+02
10	48	2.1295485475E+00	1.1050004053E+02	-8.1776009865E+02
10	49	2.1295485475E+00	1.1100004053E+02	-8.1776006611E+02
10	50	2.1295485475E+00	1.1150004053E+02	-8.1776003371E+02
10	51	2.1295485475E+00	1.1200004053E+02	-8.1776000180E+02
10	52	2.1295485475E+00	1.1250004053E+02	-8.1775996556E+02
10	53	2.1295485475E+00	1.1300004053E+02	-8.1775993872E+02
10	54	2.1295485475E+00	1.1350004053E+02	-8.1775990617E+02
10	55	2.1295485475E+00	1.1400004053E+02	-8.1775986990E+02
10	56	2.1295485475E+00	1.1450004053E+02	-8.1775984820E+02
10	57	2.1295485475E+00	1.1500004053E+02	-8.1775981902E+02
10	58	2.1295485475E+00	1.1550004053E+02	-8.1775978951E+02
10	59	2.1295485475E+00	1.1600004053E+02	-8.1775975961E+02
10	60	2.1295485475E+00	1.1650004053E+02	-8.1775972928E+02
10	61	2.1295485475E+00	1.1700004053E+02	-8.1775969865E+02
11	1	2.1395485475E+00	8.7000040532E+01	-8.1776135468E+02
11	2	2.1395485475E+00	8.7500040532E+01	-8.1776137705E+02
11	3	2.1395485475E+00	8.8000040532E+01	-8.1776139521E+02
11	4	2.1395485475E+00	8.8500040532E+01	-8.1776139112E+02
11	5	2.1395485475E+00	8.9000040532E+01	-8.1776142188E+02
11	6	2.1395485475E+00	8.9500040532E+01	-8.1776141242E+02
11	7	2.1395485475E+00	9.0000040532E+01	-8.1776143527E+02
11	8	2.1395485475E+00	9.0500040532E+01	-8.1776142278E+02
11	9	2.1395485475E+00	9.1000040532E+01	-8.1776143244E+02
11	10	2.1395485475E+00	9.1500040532E+01	-8.1776141921E+02
11	11	2.1395485475E+00	9.2000040532E+01	-8.1776142532E+02
11	12	2.1395485475E+00	9.2500040532E+01	-8.1776140151E+02
11	13	2.1395485475E+00	9.3000040532E+01	-8.1776140455E+02
11	14	2.1395485475E+00	9.3500040532E+01	-8.1776137964E+02
11	15	2.1395485475E+00	9.4000040532E+01	-8.1776137435E+02
11	16	2.1395485475E+00	9.4500040532E+01	-8.1776134372E+02
11	17	2.1395485475E+00	9.5000040532E+01	-8.1776133589E+02
11	18	2.1395485475E+00	9.5500040532E+01	-8.1776130043E+02
11	19	2.1395485475E+00	9.6000040532E+01	-8.1776129117E+02
11	20	2.1395485475E+00	9.6500040532E+01	-8.1776125140E+02

11	21	2.1395485475E+00	9.7000040532E+01	-8.1776124036E+02
11	22	2.1395485475E+00	9.7500040532E+01	-8.1776119610E+02
11	23	2.1395485475E+00	9.8000040532E+01	-8.1776117285E+02
11	24	2.1395485475E+00	9.8500040532E+01	-8.1776114622E+02
11	25	2.1395485475E+00	9.9000040532E+01	-8.1776111065E+02
11	26	2.1395485475E+00	9.9500040532E+01	-8.1776109009E+02
11	27	2.1395485475E+00	1.0000004053E+02	-8.1776106227E+02
11	28	2.1395485475E+00	1.0050004053E+02	-8.1776103199E+02
11	29	2.1395485475E+00	1.0100004053E+02	-8.1776099490E+02
11	30	2.1395485475E+00	1.0150004053E+02	-8.1776096775E+02
11	31	2.1395485475E+00	1.0200004053E+02	-8.1776092352E+02
11	32	2.1395485475E+00	1.0250004053E+02	-8.1776089921E+02
11	33	2.1395485475E+00	1.0300004053E+02	-8.1776086341E+02
11	34	2.1395485475E+00	1.0350004053E+02	-8.1776082647E+02
11	35	2.1395485475E+00	1.0400004053E+02	-8.1776078874E+02
11	36	2.1395485475E+00	1.0450004053E+02	-8.1776074707E+02
11	37	2.1395485475E+00	1.0500004053E+02	-8.1776069275E+02
11	38	2.1395485475E+00	1.0550004053E+02	-8.1776066531E+02
11	39	2.1395485475E+00	1.0600004053E+02	-8.1776062201E+02
11	40	2.1395485475E+00	1.0650004053E+02	-8.1776052380E+02
11	41	2.1395485475E+00	1.0700004053E+02	-8.1776055808E+02
11	42	2.1395485475E+00	1.0750004053E+02	-8.1776048311E+02
11	43	2.1395485475E+00	1.0800004053E+02	-8.1776049504E+02
11	44	2.1395485475E+00	1.0850004053E+02	-8.1776042756E+02
11	45	2.1395485475E+00	1.0900004053E+02	-8.1776042972E+02
11	46	2.1395485475E+00	1.0950004053E+02	-8.1776034413E+02
11	47	2.1395485475E+00	1.1000004053E+02	-8.1776036112E+02
11	48	2.1395485475E+00	1.1050004053E+02	-8.1776038120E+02
11	49	2.1395485475E+00	1.1100004053E+02	-8.1776034849E+02
11	50	2.1395485475E+00	1.1150004053E+02	-8.1776031589E+02
11	51	2.1395485475E+00	1.1200004053E+02	-8.1776028367E+02
11	52	2.1395485475E+00	1.1250004053E+02	-8.1776024909E+02
11	53	2.1395485475E+00	1.1300004053E+02	-8.1776022005E+02
11	54	2.1395485475E+00	1.1350004053E+02	-8.1776019046E+02
11	55	2.1395485475E+00	1.1400004053E+02	-8.1776014910E+02
11	56	2.1395485475E+00	1.1450004053E+02	-8.1776013232E+02
11	57	2.1395485475E+00	1.1500004053E+02	-8.1776010301E+02
11	58	2.1395485475E+00	1.1550004053E+02	-8.1776007337E+02
11	59	2.1395485475E+00	1.1600004053E+02	-8.1776004330E+02
11	60	2.1395485475E+00	1.1650004053E+02	-8.1776001282E+02
11	61	2.1395485475E+00	1.1700004053E+02	-8.1775998193E+02
12	1	2.1495485475E+00	8.7000040532E+01	-8.1776159414E+02
12	2	2.1495485475E+00	8.7500040532E+01	-8.1776159029E+02
12	3	2.1495485475E+00	8.8000040532E+01	-8.1776163398E+02
12	4	2.1495485475E+00	8.8500040532E+01	-8.1776163483E+02
12	5	2.1495485475E+00	8.9000040532E+01	-8.1776165915E+02
12	6	2.1495485475E+00	8.9500040532E+01	-8.1776165598E+02
12	7	2.1495485475E+00	9.0000040532E+01	-8.1776167172E+02
12	8	2.1495485475E+00	9.0500040532E+01	-8.1776165188E+02
12	9	2.1495485475E+00	9.1000040532E+01	-8.1776167201E+02
12	10	2.1495485475E+00	9.1500040532E+01	-8.1776165882E+02
12	11	2.1495485475E+00	9.2000040532E+01	-8.1776166063E+02

12	12	2.1495485475E+00	9.2500040532E+01	-8.1776164306E+02
12	13	2.1495485475E+00	9.3000040532E+01	-8.1776163910E+02
12	14	2.1495485475E+00	9.3500040532E+01	-8.1776161659E+02
12	15	2.1495485475E+00	9.4000040532E+01	-8.1776160828E+02
12	16	2.1495485475E+00	9.4500040532E+01	-8.1776158054E+02
12	17	2.1495485475E+00	9.5000040532E+01	-8.1776156956E+02
12	18	2.1495485475E+00	9.5500040532E+01	-8.1776153687E+02
12	19	2.1495485475E+00	9.6000040532E+01	-8.1776152437E+02
12	20	2.1495485475E+00	9.6500040532E+01	-8.1776148744E+02
12	21	2.1495485475E+00	9.7000040532E+01	-8.1776147336E+02
12	22	2.1495485475E+00	9.7500040532E+01	-8.1776143519E+02
12	23	2.1495485475E+00	9.8000040532E+01	-8.1776140823E+02
12	24	2.1495485475E+00	9.8500040532E+01	-8.1776138182E+02
12	25	2.1495485475E+00	9.9000040532E+01	-8.1776135374E+02
12	26	2.1495485475E+00	9.9500040532E+01	-8.1776132497E+02
12	27	2.1495485475E+00	1.0000004053E+02	-8.1776129573E+02
12	28	2.1495485475E+00	1.0050004053E+02	-8.1776126160E+02
12	29	2.1495485475E+00	1.0100004053E+02	-8.1776122649E+02
12	30	2.1495485475E+00	1.0150004053E+02	-8.1776120104E+02
12	31	2.1495485475E+00	1.0200004053E+02	-8.1776115511E+02
12	32	2.1495485475E+00	1.0250004053E+02	-8.1776113114E+02
12	33	2.1495485475E+00	1.0300004053E+02	-8.1776109547E+02
12	34	2.1495485475E+00	1.0350004053E+02	-8.1776105872E+02
12	35	2.1495485475E+00	1.0400004053E+02	-8.1776102100E+02
12	36	2.1495485475E+00	1.0450004053E+02	-8.1776098239E+02
12	37	2.1495485475E+00	1.0500004053E+02	-8.1776092364E+02
12	38	2.1495485475E+00	1.0550004053E+02	-8.1776085541E+02
12	39	2.1495485475E+00	1.0600004053E+02	-8.1776085280E+02
12	40	2.1495485475E+00	1.0650004053E+02	-8.1776078815E+02
12	41	2.1495485475E+00	1.0700004053E+02	-8.1776078878E+02
12	42	2.1495485475E+00	1.0750004053E+02	-8.1776071919E+02
12	43	2.1495485475E+00	1.0800004053E+02	-8.1776072605E+02
12	44	2.1495485475E+00	1.0850004053E+02	-8.1776064785E+02
12	45	2.1495485475E+00	1.0900004053E+02	-8.1776066061E+02
12	46	2.1495485475E+00	1.0950004053E+02	-8.1776057345E+02
12	47	2.1495485475E+00	1.1000004053E+02	-8.1776059129E+02
12	48	2.1495485475E+00	1.1050004053E+02	-8.1776061787E+02
12	49	2.1495485475E+00	1.1100004053E+02	-8.1776058522E+02
12	50	2.1495485475E+00	1.1150004053E+02	-8.1776055239E+02
12	51	2.1495485475E+00	1.1200004053E+02	-8.1776051991E+02
12	52	2.1495485475E+00	1.1250004053E+02	-8.1776048750E+02
12	53	2.1495485475E+00	1.1300004053E+02	-8.1776045578E+02
12	54	2.1495485475E+00	1.1350004053E+02	-8.1776042924E+02
12	55	2.1495485475E+00	1.1400004053E+02	-8.1776038208E+02
12	56	2.1495485475E+00	1.1450004053E+02	-8.1776037103E+02
12	57	2.1495485475E+00	1.1500004053E+02	-8.1776034164E+02
12	58	2.1495485475E+00	1.1550004053E+02	-8.1776031182E+02
12	59	2.1495485475E+00	1.1600004053E+02	-8.1776028159E+02
12	60	2.1495485475E+00	1.1650004053E+02	-8.1776025088E+02
12	61	2.1495485475E+00	1.1700004053E+02	-8.1776021964E+02
13	1	2.1595485475E+00	8.7000040532E+01	-8.1776179003E+02
13	2	2.1595485475E+00	8.7500040532E+01	-8.1776179916E+02

13	3	2.1595485475E+00	8.8000040532E+01	-8.1776182838E+02
13	4	2.1595485475E+00	8.8500040532E+01	-8.1776183365E+02
13	5	2.1595485475E+00	8.9000040532E+01	-8.1776184907E+02
13	6	2.1595485475E+00	8.9500040532E+01	-8.1776185361E+02
13	7	2.1595485475E+00	9.0000040532E+01	-8.1776186415E+02
13	8	2.1595485475E+00	9.0500040532E+01	-8.1776185799E+02
13	9	2.1595485475E+00	9.1000040532E+01	-8.1776186354E+02
13	10	2.1595485475E+00	9.1500040532E+01	-8.1776185471E+02
13	11	2.1595485475E+00	9.2000040532E+01	-8.1776184815E+02
13	12	2.1595485475E+00	9.2500040532E+01	-8.1776183789E+02
13	13	2.1595485475E+00	9.3000040532E+01	-8.1776182925E+02
13	14	2.1595485475E+00	9.3500040532E+01	-8.1776180991E+02
13	15	2.1595485475E+00	9.4000040532E+01	-8.1776179795E+02
13	16	2.1595485475E+00	9.4500040532E+01	-8.1776176005E+02
13	17	2.1595485475E+00	9.5000040532E+01	-8.1776175583E+02
13	18	2.1595485475E+00	9.5500040532E+01	-8.1776172944E+02
13	19	2.1595485475E+00	9.6000040532E+01	-8.1776171335E+02
13	20	2.1595485475E+00	9.6500040532E+01	-8.1776167973E+02
13	21	2.1595485475E+00	9.7000040532E+01	-8.1776165899E+02
13	22	2.1595485475E+00	9.7500040532E+01	-8.1776161319E+02
13	23	2.1595485475E+00	9.8000040532E+01	-8.1776160000E+02
13	24	2.1595485475E+00	9.8500040532E+01	-8.1776156865E+02
13	25	2.1595485475E+00	9.9000040532E+01	-8.1776154463E+02
13	26	2.1595485475E+00	9.9500040532E+01	-8.1776151585E+02
13	27	2.1595485475E+00	1.0000004053E+02	-8.1776148492E+02
13	28	2.1595485475E+00	1.0050004053E+02	-8.1776145439E+02
13	29	2.1595485475E+00	1.0100004053E+02	-8.1776141407E+02
13	30	2.1595485475E+00	1.0150004053E+02	-8.1776138889E+02
13	31	2.1595485475E+00	1.0200004053E+02	-8.1776134208E+02
13	32	2.1595485475E+00	1.0250004053E+02	-8.1776131947E+02
13	33	2.1595485475E+00	1.0300004053E+02	-8.1776128387E+02
13	34	2.1595485475E+00	1.0350004053E+02	-8.1776124671E+02
13	35	2.1595485475E+00	1.0400004053E+02	-8.1776120893E+02
13	36	2.1595485475E+00	1.0450004053E+02	-8.1776111778E+02
13	37	2.1595485475E+00	1.0500004053E+02	-8.1776111000E+02
13	38	2.1595485475E+00	1.0550004053E+02	-8.1776105016E+02
13	39	2.1595485475E+00	1.0600004053E+02	-8.1776103977E+02
13	40	2.1595485475E+00	1.0650004053E+02	-8.1776098088E+02
13	41	2.1595485475E+00	1.0700004053E+02	-8.1776097572E+02
13	42	2.1595485475E+00	1.0750004053E+02	-8.1776090930E+02
13	43	2.1595485475E+00	1.0800004053E+02	-8.1776091304E+02
13	44	2.1595485475E+00	1.0850004053E+02	-8.1776083954E+02
13	45	2.1595485475E+00	1.0900004053E+02	-8.1776084764E+02
13	46	2.1595485475E+00	1.0950004053E+02	-8.1776077074E+02
13	47	2.1595485475E+00	1.1000004053E+02	-8.1776077747E+02
13	48	2.1595485475E+00	1.1050004053E+02	-8.1776081178E+02
13	49	2.1595485475E+00	1.1100004053E+02	-8.1776077875E+02
13	50	2.1595485475E+00	1.1150004053E+02	-8.1776074552E+02
13	51	2.1595485475E+00	1.1200004053E+02	-8.1776071284E+02
13	52	2.1595485475E+00	1.1250004053E+02	-8.1776068290E+02
13	53	2.1595485475E+00	1.1300004053E+02	-8.1776064809E+02
13	54	2.1595485475E+00	1.1350004053E+02	-8.1776062500E+02

13	55	2.1595485475E+00	1.1400004053E+02	-8.1776057143E+02
13	56	2.1595485475E+00	1.1450004053E+02	-8.1776056680E+02
13	57	2.1595485475E+00	1.1500004053E+02	-8.1776053726E+02
13	58	2.1595485475E+00	1.1550004053E+02	-8.1776050722E+02
13	59	2.1595485475E+00	1.1600004053E+02	-8.1776047681E+02
13	60	2.1595485475E+00	1.1650004053E+02	-8.1776044589E+02
13	61	2.1595485475E+00	1.1700004053E+02	-8.1776041451E+02
14	1	2.1695485475E+00	8.7000040532E+01	-8.1776193955E+02
14	2	2.1695485475E+00	8.7500040532E+01	-8.1776195835E+02
14	3	2.1695485475E+00	8.8000040532E+01	-8.1776198046E+02
14	4	2.1695485475E+00	8.8500040532E+01	-8.1776199065E+02
14	5	2.1695485475E+00	8.9000040532E+01	-8.1776200386E+02
14	6	2.1695485475E+00	8.9500040532E+01	-8.1776200929E+02
14	7	2.1695485475E+00	9.0000040532E+01	-8.1776201444E+02
14	8	2.1695485475E+00	9.0500040532E+01	-8.1776201493E+02
14	9	2.1695485475E+00	9.1000040532E+01	-8.1776201294E+02
14	10	2.1695485475E+00	9.1500040532E+01	-8.1776200822E+02
14	11	2.1695485475E+00	9.2000040532E+01	-8.1776200023E+02
14	12	2.1695485475E+00	9.2500040532E+01	-8.1776199001E+02
14	13	2.1695485475E+00	9.3000040532E+01	-8.1776197756E+02
14	14	2.1695485475E+00	9.3500040532E+01	-8.1776196131E+02
14	15	2.1695485475E+00	9.4000040532E+01	-8.1776194587E+02
14	16	2.1695485475E+00	9.4500040532E+01	-8.1776192090E+02
14	17	2.1695485475E+00	9.5000040532E+01	-8.1776190631E+02
14	18	2.1695485475E+00	9.5500040532E+01	-8.1776188002E+02
14	19	2.1695485475E+00	9.6000040532E+01	-8.1776186018E+02
14	20	2.1695485475E+00	9.6500040532E+01	-8.1776182989E+02
14	21	2.1695485475E+00	9.7000040532E+01	-8.1776180847E+02
14	22	2.1695485475E+00	9.7500040532E+01	-8.1776177267E+02
14	23	2.1695485475E+00	9.8000040532E+01	-8.1776174855E+02
14	24	2.1695485475E+00	9.8500040532E+01	-8.1776172062E+02
14	25	2.1695485475E+00	9.9000040532E+01	-8.1776169221E+02
14	26	2.1695485475E+00	9.9500040532E+01	-8.1776164924E+02
14	27	2.1695485475E+00	1.0000004053E+02	-8.1776163289E+02
14	28	2.1695485475E+00	1.0050004053E+02	-8.1776158786E+02
14	29	2.1695485475E+00	1.0100004053E+02	-8.1776155901E+02
14	30	2.1695485475E+00	1.0150004053E+02	-8.1776153595E+02
14	31	2.1695485475E+00	1.0200004053E+02	-8.1776148690E+02
14	32	2.1695485475E+00	1.0250004053E+02	-8.1776146596E+02
14	33	2.1695485475E+00	1.0300004053E+02	-8.1776142974E+02
14	34	2.1695485475E+00	1.0350004053E+02	-8.1776087875E+02
14	35	2.1695485475E+00	1.0400004053E+02	-8.1776135498E+02
14	36	2.1695485475E+00	1.0450004053E+02	-8.1776126937E+02
14	37	2.1695485475E+00	1.0500004053E+02	-8.1776125704E+02
14	38	2.1695485475E+00	1.0550004053E+02	-8.1776120451E+02
14	39	2.1695485475E+00	1.0600004053E+02	-8.1776118469E+02
14	40	2.1695485475E+00	1.0650004053E+02	-8.1776113478E+02
14	41	2.1695485475E+00	1.0700004053E+02	-8.1776112095E+02
14	42	2.1695485475E+00	1.0750004053E+02	-8.1776106280E+02
14	43	2.1695485475E+00	1.0800004053E+02	-8.1776105832E+02
14	44	2.1695485475E+00	1.0850004053E+02	-8.1776099140E+02
14	45	2.1695485475E+00	1.0900004053E+02	-8.1776099326E+02

14	46	2.1695485475E+00	1.0950004053E+02	-8.1776092039E+02
14	47	2.1695485475E+00	1.1000004053E+02	-8.1776092269E+02
14	48	2.1695485475E+00	1.1050004053E+02	-8.1776096433E+02
14	49	2.1695485475E+00	1.1100004053E+02	-8.1776093114E+02
14	50	2.1695485475E+00	1.1150004053E+02	-8.1776089734E+02
14	51	2.1695485475E+00	1.1200004053E+02	-8.1776086486E+02
14	52	2.1695485475E+00	1.1250004053E+02	-8.1776083789E+02
14	53	2.1695485475E+00	1.1300004053E+02	-8.1776079952E+02
14	54	2.1695485475E+00	1.1350004053E+02	-8.1776078007E+02
14	55	2.1695485475E+00	1.1400004053E+02	-8.1776073530E+02
14	56	2.1695485475E+00	1.1450004053E+02	-8.1776072171E+02
14	57	2.1695485475E+00	1.1500004053E+02	-8.1776069204E+02
14	58	2.1695485475E+00	1.1550004053E+02	-8.1776066187E+02
14	59	2.1695485475E+00	1.1600004053E+02	-8.1776063128E+02
14	60	2.1695485475E+00	1.1650004053E+02	-8.1776060009E+02
14	61	2.1695485475E+00	1.1700004053E+02	-8.1776056848E+02
15	1	2.1795485475E+00	8.7000040532E+01	-8.1776205642E+02
15	2	2.1795485475E+00	8.7500040532E+01	-8.1776207542E+02
15	3	2.1795485475E+00	8.8000040532E+01	-8.1776209241E+02
15	4	2.1795485475E+00	8.8500040532E+01	-8.1776210714E+02
15	5	2.1795485475E+00	8.9000040532E+01	-8.1776211113E+02
15	6	2.1795485475E+00	8.9500040532E+01	-8.1776212466E+02
15	7	2.1795485475E+00	9.0000040532E+01	-8.1776212440E+02
15	8	2.1795485475E+00	9.0500040532E+01	-8.1776211809E+02
15	9	2.1795485475E+00	9.1000040532E+01	-8.1776212205E+02
15	10	2.1795485475E+00	9.1500040532E+01	-8.1776212154E+02
15	11	2.1795485475E+00	9.2000040532E+01	-8.1776210531E+02
15	12	2.1795485475E+00	9.2500040532E+01	-8.1776208972E+02
15	13	2.1795485475E+00	9.3000040532E+01	-8.1776208555E+02
15	14	2.1795485475E+00	9.3500040532E+01	-8.1776207266E+02
15	15	2.1795485475E+00	9.4000040532E+01	-8.1776205345E+02
15	16	2.1795485475E+00	9.4500040532E+01	-8.1776203513E+02
15	17	2.1795485475E+00	9.5000040532E+01	-8.1776201356E+02
15	18	2.1795485475E+00	9.5500040532E+01	-8.1776199063E+02
15	19	2.1795485475E+00	9.6000040532E+01	-8.1776196705E+02
15	20	2.1795485475E+00	9.6500040532E+01	-8.1776194008E+02
15	21	2.1795485475E+00	9.7000040532E+01	-8.1776191503E+02
15	22	2.1795485475E+00	9.7500040532E+01	-8.1776188579E+02
15	23	2.1795485475E+00	9.8000040532E+01	-8.1776185804E+02
15	24	2.1795485475E+00	9.8500040532E+01	-8.1776181562E+02
15	25	2.1795485475E+00	9.9000040532E+01	-8.1776180068E+02
15	26	2.1795485475E+00	9.9500040532E+01	-8.1776176721E+02
15	27	2.1795485475E+00	1.0000004053E+02	-8.1776174055E+02
15	28	2.1795485475E+00	1.0050004053E+02	-8.1776170532E+02
15	29	2.1795485475E+00	1.0100004053E+02	-8.1776166456E+02
15	30	2.1795485475E+00	1.0150004053E+02	-8.1776162976E+02
15	31	2.1795485475E+00	1.0200004053E+02	-8.1776159161E+02
15	32	2.1795485475E+00	1.0250004053E+02	-8.1776157292E+02
15	33	2.1795485475E+00	1.0300004053E+02	-8.1776153597E+02
15	34	2.1795485475E+00	1.0350004053E+02	-8.1776144924E+02
15	35	2.1795485475E+00	1.0400004053E+02	-8.1776145782E+02
15	36	2.1795485475E+00	1.0450004053E+02	-8.1776138446E+02

15	37	2.1795485475E+00	1.0500004053E+02	-8.1776136424E+02
15	38	2.1795485475E+00	1.0550004053E+02	-8.1776131847E+02
15	39	2.1795485475E+00	1.0600004053E+02	-8.1776128955E+02
15	40	2.1795485475E+00	1.0650004053E+02	-8.1776124859E+02
15	41	2.1795485475E+00	1.0700004053E+02	-8.1776122635E+02
15	42	2.1795485475E+00	1.0750004053E+02	-8.1776117756E+02
15	43	2.1795485475E+00	1.0800004053E+02	-8.1776116400E+02
15	44	2.1795485475E+00	1.0850004053E+02	-8.1776110490E+02
15	45	2.1795485475E+00	1.0900004053E+02	-8.1776109936E+02
15	46	2.1795485475E+00	1.0950004053E+02	-8.1776103329E+02
15	47	2.1795485475E+00	1.1000004053E+02	-8.1776102840E+02
15	48	2.1795485475E+00	1.1050004053E+02	-8.1776107806E+02
15	49	2.1795485475E+00	1.1100004053E+02	-8.1776104489E+02
15	50	2.1795485475E+00	1.1150004053E+02	-8.1776101275E+02
15	51	2.1795485475E+00	1.1200004053E+02	-8.1776098321E+02
15	52	2.1795485475E+00	1.1250004053E+02	-8.1776095419E+02
15	53	2.1795485475E+00	1.1300004053E+02	-8.1776091830E+02
15	54	2.1795485475E+00	1.1350004053E+02	-8.1776089669E+02
15	55	2.1795485475E+00	1.1400004053E+02	-8.1776084756E+02
15	56	2.1795485475E+00	1.1450004053E+02	-8.1776083823E+02
15	57	2.1795485475E+00	1.1500004053E+02	-8.1776080839E+02
15	58	2.1795485475E+00	1.1550004053E+02	-8.1776077800E+02
15	59	2.1795485475E+00	1.1600004053E+02	-8.1776074719E+02
15	60	2.1795485475E+00	1.1650004053E+02	-8.1776071573E+02
15	61	2.1795485475E+00	1.1700004053E+02	-8.1776068384E+02
16	1	2.1895485475E+00	8.7000040532E+01	-8.1776213104E+02
16	2	2.1895485475E+00	8.7500040532E+01	-8.1776215449E+02
16	3	2.1895485475E+00	8.8000040532E+01	-8.1776216601E+02
16	4	2.1895485475E+00	8.8500040532E+01	-8.1776218544E+02
16	5	2.1895485475E+00	8.9000040532E+01	-8.1776218741E+02
16	6	2.1895485475E+00	8.9500040532E+01	-8.1776218986E+02
16	7	2.1895485475E+00	9.0000040532E+01	-8.1776219614E+02
16	8	2.1895485475E+00	9.0500040532E+01	-8.1776220299E+02
16	9	2.1895485475E+00	9.1000040532E+01	-8.1776218956E+02
16	10	2.1895485475E+00	9.1500040532E+01	-8.1776219665E+02
16	11	2.1895485475E+00	9.2000040532E+01	-8.1776217911E+02
16	12	2.1895485475E+00	9.2500040532E+01	-8.1776217290E+02
16	13	2.1895485475E+00	9.3000040532E+01	-8.1776215211E+02
16	14	2.1895485475E+00	9.3500040532E+01	-8.1776213257E+02
16	15	2.1895485475E+00	9.4000040532E+01	-8.1776211968E+02
16	16	2.1895485475E+00	9.4500040532E+01	-8.1776209460E+02
16	17	2.1895485475E+00	9.5000040532E+01	-8.1776207941E+02
16	18	2.1895485475E+00	9.5500040532E+01	-8.1776206328E+02
16	19	2.1895485475E+00	9.6000040532E+01	-8.1776203583E+02
16	20	2.1895485475E+00	9.6500040532E+01	-8.1776199887E+02
16	21	2.1895485475E+00	9.7000040532E+01	-8.1776198001E+02
16	22	2.1895485475E+00	9.7500040532E+01	-8.1776195750E+02
16	23	2.1895485475E+00	9.8000040532E+01	-8.1776192927E+02
16	24	2.1895485475E+00	9.8500040532E+01	-8.1776189660E+02
16	25	2.1895485475E+00	9.9000040532E+01	-8.1776187123E+02
16	26	2.1895485475E+00	9.9500040532E+01	-8.1776184113E+02
16	27	2.1895485475E+00	1.0000004053E+02	-8.1776181038E+02

16	28	2.1895485475E+00	1.0050004053E+02	-8.1776177862E+02
16	29	2.1895485475E+00	1.0100004053E+02	-8.1776173108E+02
16	30	2.1895485475E+00	1.0150004053E+02	-8.1776170878E+02
16	31	2.1895485475E+00	1.0200004053E+02	-8.1776165836E+02
16	32	2.1895485475E+00	1.0250004053E+02	-8.1776158838E+02
16	33	2.1895485475E+00	1.0300004053E+02	-8.1776160512E+02
16	34	2.1895485475E+00	1.0350004053E+02	-8.1776152613E+02
16	35	2.1895485475E+00	1.0400004053E+02	-8.1776152975E+02
16	36	2.1895485475E+00	1.0450004053E+02	-8.1776144504E+02
16	37	2.1895485475E+00	1.0500004053E+02	-8.1776143356E+02
16	38	2.1895485475E+00	1.0550004053E+02	-8.1776139403E+02
16	39	2.1895485475E+00	1.0600004053E+02	-8.1776135378E+02
16	40	2.1895485475E+00	1.0650004053E+02	-8.1776132541E+02
16	41	2.1895485475E+00	1.0700004053E+02	-8.1776129417E+02
16	42	2.1895485475E+00	1.0750004053E+02	-8.1776125504E+02
16	43	2.1895485475E+00	1.0800004053E+02	-8.1776123211E+02
16	44	2.1895485475E+00	1.0850004053E+02	-8.1776118240E+02
16	45	2.1895485475E+00	1.0900004053E+02	-8.1776116777E+02
16	46	2.1895485475E+00	1.0950004053E+02	-8.1776110971E+02
16	47	2.1895485475E+00	1.1000004053E+02	-8.1776109706E+02
16	48	2.1895485475E+00	1.1050004053E+02	-8.1776115508E+02
16	49	2.1895485475E+00	1.1100004053E+02	-8.1776112251E+02
16	50	2.1895485475E+00	1.1150004053E+02	-8.1776109219E+02
16	51	2.1895485475E+00	1.1200004053E+02	-8.1776106322E+02
16	52	2.1895485475E+00	1.1250004053E+02	-8.1776103434E+02
16	53	2.1895485475E+00	1.1300004053E+02	-8.1776100583E+02
16	54	2.1895485475E+00	1.1350004053E+02	-8.1776097697E+02
16	55	2.1895485475E+00	1.1400004053E+02	-8.1776094790E+02
16	56	2.1895485475E+00	1.1450004053E+02	-8.1776091829E+02
16	57	2.1895485475E+00	1.1500004053E+02	-8.1776088844E+02
16	58	2.1895485475E+00	1.1550004053E+02	-8.1776085782E+02
16	59	2.1895485475E+00	1.1600004053E+02	-8.1776082679E+02
16	60	2.1895485475E+00	1.1650004053E+02	-8.1776079507E+02
16	61	2.1895485475E+00	1.1700004053E+02	-8.1776076288E+02
17	1	2.1995485475E+00	8.7000040532E+01	-8.1776216907E+02
17	2	2.1995485475E+00	8.7500040532E+01	-8.1776219698E+02
17	3	2.1995485475E+00	8.8000040532E+01	-8.1776220303E+02
17	4	2.1995485475E+00	8.8500040532E+01	-8.1776222740E+02
17	5	2.1995485475E+00	8.9000040532E+01	-8.1776222365E+02
17	6	2.1995485475E+00	8.9500040532E+01	-8.1776224069E+02
17	7	2.1995485475E+00	9.0000040532E+01	-8.1776223146E+02
17	8	2.1995485475E+00	9.0500040532E+01	-8.1776224586E+02
17	9	2.1995485475E+00	9.1000040532E+01	-8.1776222774E+02
17	10	2.1995485475E+00	9.1500040532E+01	-8.1776223558E+02
17	11	2.1995485475E+00	9.2000040532E+01	-8.1776220986E+02
17	12	2.1995485475E+00	9.2500040532E+01	-8.1776221412E+02
17	13	2.1995485475E+00	9.3000040532E+01	-8.1776218912E+02
17	14	2.1995485475E+00	9.3500040532E+01	-8.1776217997E+02
17	15	2.1995485475E+00	9.4000040532E+01	-8.1776215635E+02
17	16	2.1995485475E+00	9.4500040532E+01	-8.1776214157E+02
17	17	2.1995485475E+00	9.5000040532E+01	-8.1776211580E+02
17	18	2.1995485475E+00	9.5500040532E+01	-8.1776209995E+02

17	19	2.1995485475E+00	9.6000040532E+01	-8.1776206520E+02
17	20	2.1995485475E+00	9.6500040532E+01	-8.1776204522E+02
17	21	2.1995485475E+00	9.7000040532E+01	-8.1776201555E+02
17	22	2.1995485475E+00	9.7500040532E+01	-8.1776199324E+02
17	23	2.1995485475E+00	9.8000040532E+01	-8.1776196466E+02
17	24	2.1995485475E+00	9.8500040532E+01	-8.1776193549E+02
17	25	2.1995485475E+00	9.9000040532E+01	-8.1776190548E+02
17	26	2.1995485475E+00	9.9500040532E+01	-8.1776186108E+02
17	27	2.1995485475E+00	1.0000004053E+02	-8.1776184175E+02
17	28	2.1995485475E+00	1.0050004053E+02	-8.1776140170E+02
17	29	2.1995485475E+00	1.0100004053E+02	-8.1776176237E+02
17	30	2.1995485475E+00	1.0150004053E+02	-8.1776174535E+02
17	31	2.1995485475E+00	1.0200004053E+02	-8.1776168924E+02
17	32	2.1995485475E+00	1.0250004053E+02	-8.1776161508E+02
17	33	2.1995485475E+00	1.0300004053E+02	-8.1776163503E+02
17	34	2.1995485475E+00	1.0350004053E+02	-8.1776155112E+02
17	35	2.1995485475E+00	1.0400004053E+02	-8.1776156295E+02
17	36	2.1995485475E+00	1.0450004053E+02	-8.1776149752E+02
17	37	2.1995485475E+00	1.0500004053E+02	-8.1776146797E+02
17	38	2.1995485475E+00	1.0550004053E+02	-8.1776143414E+02
17	39	2.1995485475E+00	1.0600004053E+02	-8.1776137595E+02
17	40	2.1995485475E+00	1.0650004053E+02	-8.1776136638E+02
17	41	2.1995485475E+00	1.0700004053E+02	-8.1776132641E+02
17	42	2.1995485475E+00	1.0750004053E+02	-8.1776129674E+02
17	43	2.1995485475E+00	1.0800004053E+02	-8.1776126450E+02
17	44	2.1995485475E+00	1.0850004053E+02	-8.1776122441E+02
17	45	2.1995485475E+00	1.0900004053E+02	-8.1776120074E+02
17	46	2.1995485475E+00	1.0950004053E+02	-8.1776114765E+02
17	47	2.1995485475E+00	1.1000004053E+02	-8.1776113072E+02
17	48	2.1995485475E+00	1.1050004053E+02	-8.1776119767E+02
17	49	2.1995485475E+00	1.1100004053E+02	-8.1776116723E+02
17	50	2.1995485475E+00	1.1150004053E+02	-8.1776113781E+02
17	51	2.1995485475E+00	1.1200004053E+02	-8.1776110922E+02
17	52	2.1995485475E+00	1.1250004053E+02	-8.1776108061E+02
17	53	2.1995485475E+00	1.1300004053E+02	-8.1776105205E+02
17	54	2.1995485475E+00	1.1350004053E+02	-8.1776102329E+02
17	55	2.1995485475E+00	1.1400004053E+02	-8.1776099413E+02
17	56	2.1995485475E+00	1.1450004053E+02	-8.1776096447E+02
17	57	2.1995485475E+00	1.1500004053E+02	-8.1776093433E+02
17	58	2.1995485475E+00	1.1550004053E+02	-8.1776090355E+02
17	59	2.1995485475E+00	1.1600004053E+02	-8.1776087225E+02
17	60	2.1995485475E+00	1.1650004053E+02	-8.1776084022E+02
17	61	2.1995485475E+00	1.1700004053E+02	-8.1776080780E+02
18	1	2.2095485475E+00	8.7000040532E+01	-8.1776217256E+02
18	2	2.2095485475E+00	8.7500040532E+01	-8.1776220524E+02
18	3	2.2095485475E+00	8.8000040532E+01	-8.1776220557E+02
18	4	2.2095485475E+00	8.8500040532E+01	-8.1776223490E+02
18	5	2.2095485475E+00	8.9000040532E+01	-8.1776222540E+02
18	6	2.2095485475E+00	8.9500040532E+01	-8.1776225000E+02
18	7	2.2095485475E+00	9.0000040532E+01	-8.1776223240E+02
18	8	2.2095485475E+00	9.0500040532E+01	-8.1776223854E+02
18	9	2.2095485475E+00	9.1000040532E+01	-8.1776222453E+02

18 10	2.2095485475E+00	9.1500040532E+01	-8.1776224014E+02
18 11	2.2095485475E+00	9.2000040532E+01	-8.1776221303E+02
18 12	2.2095485475E+00	9.2500040532E+01	-8.1776220433E+02
18 13	2.2095485475E+00	9.3000040532E+01	-8.1776218851E+02
18 14	2.2095485475E+00	9.3500040532E+01	-8.1776218645E+02
18 15	2.2095485475E+00	9.4000040532E+01	-8.1776215539E+02
18 16	2.2095485475E+00	9.4500040532E+01	-8.1776214781E+02
18 17	2.2095485475E+00	9.5000040532E+01	-8.1776211454E+02
18 18	2.2095485475E+00	9.5500040532E+01	-8.1776208870E+02
18 19	2.2095485475E+00	9.6000040532E+01	-8.1776206708E+02
18 20	2.2095485475E+00	9.6500040532E+01	-8.1776205095E+02
18 21	2.2095485475E+00	9.7000040532E+01	-8.1776201043E+02
18 22	2.2095485475E+00	9.7500040532E+01	-8.1776199483E+02
18 23	2.2095485475E+00	9.8000040532E+01	-8.1776196595E+02
18 24	2.2095485475E+00	9.8500040532E+01	-8.1776192188E+02
18 25	2.2095485475E+00	9.9000040532E+01	-8.1776190619E+02
18 26	2.2095485475E+00	9.9500040532E+01	-8.1776187164E+02
18 27	2.2095485475E+00	1.0000004053E+02	-8.1776183253E+02
18 28	2.2095485475E+00	1.0050004053E+02	-8.1776172171E+02
18 29	2.2095485475E+00	1.0100004053E+02	-8.1776175971E+02
18 30	2.2095485475E+00	1.0150004053E+02	-8.1776169827E+02
18 31	2.2095485475E+00	1.0200004053E+02	-8.1776168621E+02
18 32	2.2095485475E+00	1.0250004053E+02	-8.1776163401E+02
18 33	2.2095485475E+00	1.0300004053E+02	-8.1776163796E+02
18 34	2.2095485475E+00	1.0350004053E+02	-8.1776157093E+02
18 35	2.2095485475E+00	1.0400004053E+02	-8.1776156268E+02
18 36	2.2095485475E+00	1.0450004053E+02	-8.1776150995E+02
18 37	2.2095485475E+00	1.0500004053E+02	-8.1776146260E+02
18 38	2.2095485475E+00	1.0550004053E+02	-8.1776144226E+02
18 39	2.2095485475E+00	1.0600004053E+02	-8.1776139427E+02
18 40	2.2095485475E+00	1.0650004053E+02	-8.1776137273E+02
18 41	2.2095485475E+00	1.0700004053E+02	-8.1776132414E+02
18 42	2.2095485475E+00	1.0750004053E+02	-8.1776129872E+02
18 43	2.2095485475E+00	1.0800004053E+02	-8.1776126315E+02
18 44	2.2095485475E+00	1.0850004053E+02	-8.1776123383E+02
18 45	2.2095485475E+00	1.0900004053E+02	-8.1776119969E+02
18 46	2.2095485475E+00	1.0950004053E+02	-8.1776116055E+02
18 47	2.2095485475E+00	1.1000004053E+02	-8.1776113166E+02
18 48	2.2095485475E+00	1.1050004053E+02	-8.1776120986E+02
18 49	2.2095485475E+00	1.1100004053E+02	-8.1776118044E+02
18 50	2.2095485475E+00	1.1150004053E+02	-8.1776115173E+02
18 51	2.2095485475E+00	1.1200004053E+02	-8.1776112348E+02
18 52	2.2095485475E+00	1.1250004053E+02	-8.1776109504E+02
18 53	2.2095485475E+00	1.1300004053E+02	-8.1776106656E+02
18 54	2.2095485475E+00	1.1350004053E+02	-8.1776103768E+02
18 55	2.2095485475E+00	1.1400004053E+02	-8.1776100846E+02
18 56	2.2095485475E+00	1.1450004053E+02	-8.1776097866E+02
18 57	2.2095485475E+00	1.1500004053E+02	-8.1776094831E+02
18 58	2.2095485475E+00	1.1550004053E+02	-8.1776091730E+02
18 59	2.2095485475E+00	1.1600004053E+02	-8.1776088581E+02
18 60	2.2095485475E+00	1.1650004053E+02	-8.1776085348E+02
18 61	2.2095485475E+00	1.1700004053E+02	-8.1776082074E+02

19	1	2.2195485475E+00	8.7000040532E+01	-8.1776214319E+02
19	2	2.2195485475E+00	8.7500040532E+01	-8.1776216817E+02
19	3	2.2195485475E+00	8.8000040532E+01	-8.1776217542E+02
19	4	2.2195485475E+00	8.8500040532E+01	-8.1776220963E+02
19	5	2.2195485475E+00	8.9000040532E+01	-8.1776219431E+02
19	6	2.2195485475E+00	8.9500040532E+01	-8.1776221214E+02
19	7	2.2195485475E+00	9.0000040532E+01	-8.1776220061E+02
19	8	2.2195485475E+00	9.0500040532E+01	-8.1776222140E+02
19	9	2.2195485475E+00	9.1000040532E+01	-8.1776219550E+02
19	10	2.2195485475E+00	9.1500040532E+01	-8.1776221224E+02
19	11	2.2195485475E+00	9.2000040532E+01	-8.1776218016E+02
19	12	2.2195485475E+00	9.2500040532E+01	-8.1776218571E+02
19	13	2.2195485475E+00	9.3000040532E+01	-8.1776215530E+02
19	14	2.2195485475E+00	9.3500040532E+01	-8.1776214356E+02
19	15	2.2195485475E+00	9.4000040532E+01	-8.1776212189E+02
19	16	2.2195485475E+00	9.4500040532E+01	-8.1776211456E+02
19	17	2.2195485475E+00	9.5000040532E+01	-8.1776208081E+02
19	18	2.2195485475E+00	9.5500040532E+01	-8.1776206885E+02
19	19	2.2195485475E+00	9.6000040532E+01	-8.1776203302E+02
19	20	2.2195485475E+00	9.6500040532E+01	-8.1776201704E+02
19	21	2.2195485475E+00	9.7000040532E+01	-8.1776197947E+02
19	22	2.2195485475E+00	9.7500040532E+01	-8.1776196413E+02
19	23	2.2195485475E+00	9.8000040532E+01	-8.1776193510E+02
19	24	2.2195485475E+00	9.8500040532E+01	-8.1776190107E+02
19	25	2.2195485475E+00	9.9000040532E+01	-8.1776187490E+02
19	26	2.2195485475E+00	9.9500040532E+01	-8.1776184376E+02
19	27	2.2195485475E+00	1.0000004053E+02	-8.1776181255E+02
19	28	2.2195485475E+00	1.0050004053E+02	-8.1776173252E+02
19	29	2.2195485475E+00	1.0100004053E+02	-8.1776172476E+02
19	30	2.2195485475E+00	1.0150004053E+02	-8.1776165914E+02
19	31	2.2195485475E+00	1.0200004053E+02	-8.1776164745E+02
19	32	2.2195485475E+00	1.0250004053E+02	-8.1776161458E+02
19	33	2.2195485475E+00	1.0300004053E+02	-8.1776160637E+02
19	34	2.2195485475E+00	1.0350004053E+02	-8.1776155153E+02
19	35	2.2195485475E+00	1.0400004053E+02	-8.1776153080E+02
19	36	2.2195485475E+00	1.0450004053E+02	-8.1776146871E+02
19	37	2.2195485475E+00	1.0500004053E+02	-8.1776143703E+02
19	38	2.2195485475E+00	1.0550004053E+02	-8.1776141364E+02
19	39	2.2195485475E+00	1.0600004053E+02	-8.1776135745E+02
19	40	2.2195485475E+00	1.0650004053E+02	-8.1776134888E+02
19	41	2.2195485475E+00	1.0700004053E+02	-8.1776129166E+02
19	42	2.2195485475E+00	1.0750004053E+02	-8.1776128020E+02
19	43	2.2195485475E+00	1.0800004053E+02	-8.1776122680E+02
19	44	2.2195485475E+00	1.0850004053E+02	-8.1776121145E+02
19	45	2.2195485475E+00	1.0900004053E+02	-8.1776116708E+02
19	46	2.2195485475E+00	1.0950004053E+02	-8.1776113545E+02
19	47	2.2195485475E+00	1.1000004053E+02	-8.1776110039E+02
19	48	2.2195485475E+00	1.1050004053E+02	-8.1776119309E+02
19	49	2.2195485475E+00	1.1100004053E+02	-8.1776116434E+02
19	50	2.2195485475E+00	1.1150004053E+02	-8.1776113624E+02
19	51	2.2195485475E+00	1.1200004053E+02	-8.1776110806E+02
19	52	2.2195485475E+00	1.1250004053E+02	-8.1776107992E+02

19	53	2.2195485475E+00	1.1300004053E+02	-8.1776105138E+02
19	54	2.2195485475E+00	1.1350004053E+02	-8.1776102233E+02
19	55	2.2195485475E+00	1.1400004053E+02	-8.1776099303E+02
19	56	2.2195485475E+00	1.1450004053E+02	-8.1776096308E+02
19	57	2.2195485475E+00	1.1500004053E+02	-8.1776093258E+02
19	58	2.2195485475E+00	1.1550004053E+02	-8.1776090134E+02
19	59	2.2195485475E+00	1.1600004053E+02	-8.1776086959E+02
19	60	2.2195485475E+00	1.1650004053E+02	-8.1776083703E+02
19	61	2.2195485475E+00	1.1700004053E+02	-8.1776080397E+02
20	1	2.2295485475E+00	8.7000040532E+01	-8.1776208170E+02
20	2	2.2295485475E+00	8.7500040532E+01	-8.1776212231E+02
20	3	2.2295485475E+00	8.8000040532E+01	-8.1776211397E+02
20	4	2.2295485475E+00	8.8500040532E+01	-8.1776215359E+02
20	5	2.2295485475E+00	8.9000040532E+01	-8.1776213211E+02
20	6	2.2295485475E+00	8.9500040532E+01	-8.1776216418E+02
20	7	2.2295485475E+00	9.0000040532E+01	-8.1776213781E+02
20	8	2.2295485475E+00	9.0500040532E+01	-8.1776216655E+02
20	9	2.2295485475E+00	9.1000040532E+01	-8.1776212894E+02
20	10	2.2295485475E+00	9.1500040532E+01	-8.1776215346E+02
20	11	2.2295485475E+00	9.2000040532E+01	-8.1776211646E+02
20	12	2.2295485475E+00	9.2500040532E+01	-8.1776212973E+02
20	13	2.2295485475E+00	9.3000040532E+01	-8.1776209137E+02
20	14	2.2295485475E+00	9.3500040532E+01	-8.1776209393E+02
20	15	2.2295485475E+00	9.4000040532E+01	-8.1776205773E+02
20	16	2.2295485475E+00	9.4500040532E+01	-8.1776205785E+02
20	17	2.2295485475E+00	9.5000040532E+01	-8.1776201648E+02
20	18	2.2295485475E+00	9.5500040532E+01	-8.1776201193E+02
20	19	2.2295485475E+00	9.6000040532E+01	-8.1776196849E+02
20	20	2.2295485475E+00	9.6500040532E+01	-8.1776196004E+02
20	21	2.2295485475E+00	9.7000040532E+01	-8.1776191129E+02
20	22	2.2295485475E+00	9.7500040532E+01	-8.1776190310E+02
20	23	2.2295485475E+00	9.8000040532E+01	-8.1776187375E+02
20	24	2.2295485475E+00	9.8500040532E+01	-8.1776184348E+02
20	25	2.2295485475E+00	9.9000040532E+01	-8.1776181299E+02
20	26	2.2295485475E+00	9.9500040532E+01	-8.1776173741E+02
20	27	2.2295485475E+00	1.0000004053E+02	-8.1776174761E+02
20	28	2.2295485475E+00	1.0050004053E+02	-8.1776166450E+02
20	29	2.2295485475E+00	1.0100004053E+02	-8.1776165942E+02
20	30	2.2295485475E+00	1.0150004053E+02	-8.1776161772E+02
20	31	2.2295485475E+00	1.0200004053E+02	-8.1776157242E+02
20	32	2.2295485475E+00	1.0250004053E+02	-8.1776154513E+02
20	33	2.2295485475E+00	1.0300004053E+02	-8.1776154485E+02
20	34	2.2295485475E+00	1.0350004053E+02	-8.1776148243E+02
20	35	2.2295485475E+00	1.0400004053E+02	-8.1776146938E+02
20	36	2.2295485475E+00	1.0450004053E+02	-8.1776143013E+02
20	37	2.2295485475E+00	1.0500004053E+02	-8.1776136681E+02
20	38	2.2295485475E+00	1.0550004053E+02	-8.1776136661E+02
20	39	2.2295485475E+00	1.0600004053E+02	-8.1776130175E+02
20	40	2.2295485475E+00	1.0650004053E+02	-8.1776129598E+02
20	41	2.2295485475E+00	1.0700004053E+02	-8.1776122972E+02
20	42	2.2295485475E+00	1.0750004053E+02	-8.1776122120E+02
20	43	2.2295485475E+00	1.0800004053E+02	-8.1776115470E+02

20	44	2.2295485475E+00	1.0850004053E+02	-8.1776115371E+02
20	45	2.2295485475E+00	1.0900004053E+02	-8.1776110136E+02
20	46	2.2295485475E+00	1.0950004053E+02	-8.1776108991E+02
20	47	2.2295485475E+00	1.1000004053E+02	-8.1776103870E+02
20	48	2.2295485475E+00	1.1050004053E+02	-8.1776114896E+02
20	49	2.2295485475E+00	1.1100004053E+02	-8.1776112095E+02
20	50	2.2295485475E+00	1.1150004053E+02	-8.1776109316E+02
20	51	2.2295485475E+00	1.1200004053E+02	-8.1776106537E+02
20	52	2.2295485475E+00	1.1250004053E+02	-8.1776103705E+02
20	53	2.2295485475E+00	1.1300004053E+02	-8.1776100859E+02
20	54	2.2295485475E+00	1.1350004053E+02	-8.1776097950E+02
20	55	2.2295485475E+00	1.1400004053E+02	-8.1776095014E+02
20	56	2.2295485475E+00	1.1450004053E+02	-8.1776091996E+02
20	57	2.2295485475E+00	1.1500004053E+02	-8.1776088935E+02
20	58	2.2295485475E+00	1.1550004053E+02	-8.1776085788E+02
20	59	2.2295485475E+00	1.1600004053E+02	-8.1776082589E+02
20	60	2.2295485475E+00	1.1650004053E+02	-8.1776079305E+02
20	61	2.2295485475E+00	1.1700004053E+02	-8.1776075980E+02
21	1	2.2395485475E+00	8.7000040532E+01	-8.1776199212E+02
21	2	2.2395485475E+00	8.7500040532E+01	-8.1776204003E+02
21	3	2.2395485475E+00	8.8000040532E+01	-8.1776202361E+02
21	4	2.2395485475E+00	8.8500040532E+01	-8.1776206812E+02
21	5	2.2395485475E+00	8.9000040532E+01	-8.1776204016E+02
21	6	2.2395485475E+00	8.9500040532E+01	-8.1776208094E+02
21	7	2.2395485475E+00	9.0000040532E+01	-8.1776204568E+02
21	8	2.2395485475E+00	9.0500040532E+01	-8.1776206705E+02
21	9	2.2395485475E+00	9.1000040532E+01	-8.1776203963E+02
21	10	2.2395485475E+00	9.1500040532E+01	-8.1776206581E+02
21	11	2.2395485475E+00	9.2000040532E+01	-8.1776202360E+02
21	12	2.2395485475E+00	9.2500040532E+01	-8.1776204146E+02
21	13	2.2395485475E+00	9.3000040532E+01	-8.1776199825E+02
21	14	2.2395485475E+00	9.3500040532E+01	-8.1776200849E+02
21	15	2.2395485475E+00	9.4000040532E+01	-8.1776196449E+02
21	16	2.2395485475E+00	9.4500040532E+01	-8.1776196887E+02
21	17	2.2395485475E+00	9.5000040532E+01	-8.1776192312E+02
21	18	2.2395485475E+00	9.5500040532E+01	-8.1776192258E+02
21	19	2.2395485475E+00	9.6000040532E+01	-8.1776187498E+02
21	20	2.2395485475E+00	9.6500040532E+01	-8.1776187054E+02
21	21	2.2395485475E+00	9.7000040532E+01	-8.1776182093E+02
21	22	2.2395485475E+00	9.7500040532E+01	-8.1776181336E+02
21	23	2.2395485475E+00	9.8000040532E+01	-8.1776178385E+02
21	24	2.2395485475E+00	9.8500040532E+01	-8.1776175353E+02
21	25	2.2395485475E+00	9.9000040532E+01	-8.1776172271E+02
21	26	2.2395485475E+00	9.9500040532E+01	-8.1776163982E+02
21	27	2.2395485475E+00	1.0000004053E+02	-8.1776166000E+02
21	28	2.2395485475E+00	1.0050004053E+02	-8.1776159448E+02
21	29	2.2395485475E+00	1.0100004053E+02	-8.1776156208E+02
21	30	2.2395485475E+00	1.0150004053E+02	-8.1776154128E+02
21	31	2.2395485475E+00	1.0200004053E+02	-8.1776149138E+02
21	32	2.2395485475E+00	1.0250004053E+02	-8.1776147864E+02
21	33	2.2395485475E+00	1.0300004053E+02	-8.1776145564E+02
21	34	2.2395485475E+00	1.0350004053E+02	-8.1776141677E+02

21	35	2.2395485475E+00	1.0400004053E+02	-8.1776137688E+02
21	36	2.2395485475E+00	1.0450004053E+02	-8.1776135634E+02
21	37	2.2395485475E+00	1.0500004053E+02	-8.1776127093E+02
21	38	2.2395485475E+00	1.0550004053E+02	-8.1776128313E+02
21	39	2.2395485475E+00	1.0600004053E+02	-8.1776120943E+02
21	40	2.2395485475E+00	1.0650004053E+02	-8.1776121798E+02
21	41	2.2395485475E+00	1.0700004053E+02	-8.1776113508E+02
21	42	2.2395485475E+00	1.0750004053E+02	-8.1776114771E+02
21	43	2.2395485475E+00	1.0800004053E+02	-8.1776107539E+02
21	44	2.2395485475E+00	1.0850004053E+02	-8.1776108068E+02
21	45	2.2395485475E+00	1.0900004053E+02	-8.1776100147E+02
21	46	2.2395485475E+00	1.0950004053E+02	-8.1776100874E+02
21	47	2.2395485475E+00	1.1000004053E+02	-8.1776094929E+02
21	48	2.2395485475E+00	1.1050004053E+02	-8.1776107980E+02
21	49	2.2395485475E+00	1.1100004053E+02	-8.1776105257E+02
21	50	2.2395485475E+00	1.1150004053E+02	-8.1776102480E+02
21	51	2.2395485475E+00	1.1200004053E+02	-8.1776099722E+02
21	52	2.2395485475E+00	1.1250004053E+02	-8.1776096906E+02
21	53	2.2395485475E+00	1.1300004053E+02	-8.1776094054E+02
21	54	2.2395485475E+00	1.1350004053E+02	-8.1776091146E+02
21	55	2.2395485475E+00	1.1400004053E+02	-8.1776088200E+02
21	56	2.2395485475E+00	1.1450004053E+02	-8.1776085156E+02
21	57	2.2395485475E+00	1.1500004053E+02	-8.1776082075E+02
21	58	2.2395485475E+00	1.1550004053E+02	-8.1776078915E+02
21	59	2.2395485475E+00	1.1600004053E+02	-8.1776075691E+02
21	60	2.2395485475E+00	1.1650004053E+02	-8.1776072391E+02
21	61	2.2395485475E+00	1.1700004053E+02	-8.1776069036E+02
22	1	2.2495485475E+00	8.7000040532E+01	-8.1776190727E+02
22	2	2.2495485475E+00	8.7500040532E+01	-8.1776191447E+02
22	3	2.2495485475E+00	8.8000040532E+01	-8.1776194308E+02
22	4	2.2495485475E+00	8.8500040532E+01	-8.1776195481E+02
22	5	2.2495485475E+00	8.9000040532E+01	-8.1776196277E+02
22	6	2.2495485475E+00	8.9500040532E+01	-8.1776195405E+02
22	7	2.2495485475E+00	9.0000040532E+01	-8.1776192622E+02
22	8	2.2495485475E+00	9.0500040532E+01	-8.1776196199E+02
22	9	2.2495485475E+00	9.1000040532E+01	-8.1776191919E+02
22	10	2.2495485475E+00	9.1500040532E+01	-8.1776195082E+02
22	11	2.2495485475E+00	9.2000040532E+01	-8.1776190299E+02
22	12	2.2495485475E+00	9.2500040532E+01	-8.1776192604E+02
22	13	2.2495485475E+00	9.3000040532E+01	-8.1776187765E+02
22	14	2.2495485475E+00	9.3500040532E+01	-8.1776187913E+02
22	15	2.2495485475E+00	9.4000040532E+01	-8.1776184377E+02
22	16	2.2495485475E+00	9.4500040532E+01	-8.1776184901E+02
22	17	2.2495485475E+00	9.5000040532E+01	-8.1776180262E+02
22	18	2.2495485475E+00	9.5500040532E+01	-8.1776180253E+02
22	19	2.2495485475E+00	9.6000040532E+01	-8.1776175439E+02
22	20	2.2495485475E+00	9.6500040532E+01	-8.1776175021E+02
22	21	2.2495485475E+00	9.7000040532E+01	-8.1776170003E+02
22	22	2.2495485475E+00	9.7500040532E+01	-8.1776168173E+02
22	23	2.2495485475E+00	9.8000040532E+01	-8.1776166718E+02
22	24	2.2495485475E+00	9.8500040532E+01	-8.1776158775E+02
22	25	2.2495485475E+00	9.9000040532E+01	-8.1776160332E+02

22	26	2.2495485475E+00	9.9500040532E+01	-8.1776154309E+02
22	27	2.2495485475E+00	1.0000004053E+02	-8.1776154049E+02
22	28	2.2495485475E+00	1.0050004053E+02	-8.1776149159E+02
22	29	2.2495485475E+00	1.0100004053E+02	-8.1776147909E+02
22	30	2.2495485475E+00	1.0150004053E+02	-8.1776141887E+02
22	31	2.2495485475E+00	1.0200004053E+02	-8.1776141173E+02
22	32	2.2495485475E+00	1.0250004053E+02	-8.1776137872E+02
22	33	2.2495485475E+00	1.0300004053E+02	-8.1776134059E+02
22	34	2.2495485475E+00	1.0350004053E+02	-8.1776131802E+02
22	35	2.2495485475E+00	1.0400004053E+02	-8.1776125183E+02
22	36	2.2495485475E+00	1.0450004053E+02	-8.1776124893E+02
22	37	2.2495485475E+00	1.0500004053E+02	-8.1776114887E+02
22	38	2.2495485475E+00	1.0550004053E+02	-8.1776118556E+02
22	39	2.2495485475E+00	1.0600004053E+02	-8.1776107532E+02
22	40	2.2495485475E+00	1.0650004053E+02	-8.1776110986E+02
22	41	2.2495485475E+00	1.0700004053E+02	-8.1776102242E+02
22	42	2.2495485475E+00	1.0750004053E+02	-8.1776103926E+02
22	43	2.2495485475E+00	1.0800004053E+02	-8.1776095806E+02
22	44	2.2495485475E+00	1.0850004053E+02	-8.1776097224E+02
22	45	2.2495485475E+00	1.0900004053E+02	-8.1776089747E+02
22	46	2.2495485475E+00	1.0950004053E+02	-8.1776091419E+02
22	47	2.2495485475E+00	1.1000004053E+02	-8.1776083039E+02
22	48	2.2495485475E+00	1.1050004053E+02	-8.1776098781E+02
22	49	2.2495485475E+00	1.1100004053E+02	-8.1776096098E+02
22	50	2.2495485475E+00	1.1150004053E+02	-8.1776093403E+02
22	51	2.2495485475E+00	1.1200004053E+02	-8.1776090626E+02
22	52	2.2495485475E+00	1.1250004053E+02	-8.1776087816E+02
22	53	2.2495485475E+00	1.1300004053E+02	-8.1776084962E+02
22	54	2.2495485475E+00	1.1350004053E+02	-8.1776082037E+02
22	55	2.2495485475E+00	1.1400004053E+02	-8.1776079077E+02
22	56	2.2495485475E+00	1.1450004053E+02	-8.1776076034E+02
22	57	2.2495485475E+00	1.1500004053E+02	-8.1776072932E+02
22	58	2.2495485475E+00	1.1550004053E+02	-8.1776069747E+02
22	59	2.2495485475E+00	1.1600004053E+02	-8.1776066500E+02
22	60	2.2495485475E+00	1.1650004053E+02	-8.1776063179E+02
22	61	2.2495485475E+00	1.1700004053E+02	-8.1776059802E+02
23	1	2.2595485475E+00	8.7000040532E+01	-8.1776176403E+02
23	2	2.2595485475E+00	8.7500040532E+01	-8.1776178537E+02
23	3	2.2595485475E+00	8.8000040532E+01	-8.1776179983E+02
23	4	2.2595485475E+00	8.8500040532E+01	-8.1776181572E+02
23	5	2.2595485475E+00	8.9000040532E+01	-8.1776181939E+02
23	6	2.2595485475E+00	8.9500040532E+01	-8.1776182425E+02
23	7	2.2595485475E+00	9.0000040532E+01	-8.1776178081E+02
23	8	2.2595485475E+00	9.0500040532E+01	-8.1776182487E+02
23	9	2.2595485475E+00	9.1000040532E+01	-8.1776177307E+02
23	10	2.2595485475E+00	9.1500040532E+01	-8.1776181017E+02
23	11	2.2595485475E+00	9.2000040532E+01	-8.1776175609E+02
23	12	2.2595485475E+00	9.2500040532E+01	-8.1776178510E+02
23	13	2.2595485475E+00	9.3000040532E+01	-8.1776173061E+02
23	14	2.2595485475E+00	9.3500040532E+01	-8.1776174821E+02
23	15	2.2595485475E+00	9.4000040532E+01	-8.1776169630E+02
23	16	2.2595485475E+00	9.4500040532E+01	-8.1776171139E+02

23	17	2.2595485475E+00	9.5000040532E+01	-8.1776165620E+02
23	18	2.2595485475E+00	9.5500040532E+01	-8.1776166489E+02
23	19	2.2595485475E+00	9.6000040532E+01	-8.1776160773E+02
23	20	2.2595485475E+00	9.6500040532E+01	-8.1776161270E+02
23	21	2.2595485475E+00	9.7000040532E+01	-8.1776155375E+02
23	22	2.2595485475E+00	9.7500040532E+01	-8.1776155078E+02
23	23	2.2595485475E+00	9.8000040532E+01	-8.1776152554E+02
23	24	2.2595485475E+00	9.8500040532E+01	-8.1776146573E+02
23	25	2.2595485475E+00	9.9000040532E+01	-8.1776145195E+02
23	26	2.2595485475E+00	9.9500040532E+01	-8.1776141504E+02
23	27	2.2595485475E+00	1.0000004053E+02	-8.1776138974E+02
23	28	2.2595485475E+00	1.0050004053E+02	-8.1776134460E+02
23	29	2.2595485475E+00	1.0100004053E+02	-8.1776133849E+02
23	30	2.2595485475E+00	1.0150004053E+02	-8.1776130337E+02
23	31	2.2595485475E+00	1.0200004053E+02	-8.1776126855E+02
23	32	2.2595485475E+00	1.0250004053E+02	-8.1776123269E+02
23	33	2.2595485475E+00	1.0300004053E+02	-8.1776119802E+02
23	34	2.2595485475E+00	1.0350004053E+02	-8.1776119248E+02
23	35	2.2595485475E+00	1.0400004053E+02	-8.1776112748E+02
23	36	2.2595485475E+00	1.0450004053E+02	-8.1776112924E+02
23	37	2.2595485475E+00	1.0500004053E+02	-8.1776100187E+02
23	38	2.2595485475E+00	1.0550004053E+02	-8.1776105669E+02
23	39	2.2595485475E+00	1.0600004053E+02	-8.1776093101E+02
23	40	2.2595485475E+00	1.0650004053E+02	-8.1776099110E+02
23	41	2.2595485475E+00	1.0700004053E+02	-8.1776088083E+02
23	42	2.2595485475E+00	1.0750004053E+02	-8.1776092087E+02
23	43	2.2595485475E+00	1.0800004053E+02	-8.1776081640E+02
23	44	2.2595485475E+00	1.0850004053E+02	-8.1776085462E+02
23	45	2.2595485475E+00	1.0900004053E+02	-8.1776075698E+02
23	46	2.2595485475E+00	1.0950004053E+02	-8.1776078561E+02
23	47	2.2595485475E+00	1.1000004053E+02	-8.1776068079E+02
23	48	2.2595485475E+00	1.1050004053E+02	-8.1776087515E+02
23	49	2.2595485475E+00	1.1100004053E+02	-8.1776084885E+02
23	50	2.2595485475E+00	1.1150004053E+02	-8.1776082183E+02
23	51	2.2595485475E+00	1.1200004053E+02	-8.1776079456E+02
23	52	2.2595485475E+00	1.1250004053E+02	-8.1776076646E+02
23	53	2.2595485475E+00	1.1300004053E+02	-8.1776073801E+02
23	54	2.2595485475E+00	1.1350004053E+02	-8.1776070869E+02
23	55	2.2595485475E+00	1.1400004053E+02	-8.1776067892E+02
23	56	2.2595485475E+00	1.1450004053E+02	-8.1776064827E+02
23	57	2.2595485475E+00	1.1500004053E+02	-8.1776061719E+02
23	58	2.2595485475E+00	1.1550004053E+02	-8.1776058517E+02
23	59	2.2595485475E+00	1.1600004053E+02	-8.1776055255E+02
23	60	2.2595485475E+00	1.1650004053E+02	-8.1776051917E+02
23	61	2.2595485475E+00	1.1700004053E+02	-8.1776048518E+02
24	1	2.2695485475E+00	8.7000040532E+01	-8.1776158947E+02
24	2	2.2695485475E+00	8.7500040532E+01	-8.1776162459E+02
24	3	2.2695485475E+00	8.8000040532E+01	-8.1776162505E+02
24	4	2.2695485475E+00	8.8500040532E+01	-8.1776165170E+02
24	5	2.2695485475E+00	8.9000040532E+01	-8.1776165928E+02
24	6	2.2695485475E+00	8.9500040532E+01	-8.1776166309E+02
24	7	2.2695485475E+00	9.0000040532E+01	-8.1776166339E+02

24	8	2.2695485475E+00	9.0500040532E+01	-8.1776165710E+02
24	9	2.2695485475E+00	9.1000040532E+01	-8.1776160094E+02
24	10	2.2695485475E+00	9.1500040532E+01	-8.1776164542E+02
24	11	2.2695485475E+00	9.2000040532E+01	-8.1776158735E+02
24	12	2.2695485475E+00	9.2500040532E+01	-8.1776160635E+02
24	13	2.2695485475E+00	9.3000040532E+01	-8.1776156092E+02
24	14	2.2695485475E+00	9.3500040532E+01	-8.1776158713E+02
24	15	2.2695485475E+00	9.4000040532E+01	-8.1776156757E+02
24	16	2.2695485475E+00	9.4500040532E+01	-8.1776153165E+02
24	17	2.2695485475E+00	9.5000040532E+01	-8.1776009516E+02
24	18	2.2695485475E+00	9.5500040532E+01	-8.1776148419E+02
24	19	2.2695485475E+00	9.6000040532E+01	-8.1776143650E+02
24	20	2.2695485475E+00	9.6500040532E+01	-8.1776143235E+02
24	21	2.2695485475E+00	9.7000040532E+01	-8.1776138432E+02
24	22	2.2695485475E+00	9.7500040532E+01	-8.1776139002E+02
24	23	2.2695485475E+00	9.8000040532E+01	-8.1776136047E+02
24	24	2.2695485475E+00	9.8500040532E+01	-8.1776131391E+02
24	25	2.2695485475E+00	9.9000040532E+01	-8.1776129996E+02
24	26	2.2695485475E+00	9.9500040532E+01	-8.1776126172E+02
24	27	2.2695485475E+00	1.0000004053E+02	-8.1776123865E+02
24	28	2.2695485475E+00	1.0050004053E+02	-8.1776120600E+02
24	29	2.2695485475E+00	1.0100004053E+02	-8.1776117240E+02
24	30	2.2695485475E+00	1.0150004053E+02	-8.1776115825E+02
24	31	2.2695485475E+00	1.0200004053E+02	-8.1776109613E+02
24	32	2.2695485475E+00	1.0250004053E+02	-8.1776109956E+02
24	33	2.2695485475E+00	1.0300004053E+02	-8.1776102630E+02
24	34	2.2695485475E+00	1.0350004053E+02	-8.1776104710E+02
24	35	2.2695485475E+00	1.0400004053E+02	-8.1776096694E+02
24	36	2.2695485475E+00	1.0450004053E+02	-8.1776098486E+02
24	37	2.2695485475E+00	1.0500004053E+02	-8.1776083262E+02
24	38	2.2695485475E+00	1.0550004053E+02	-8.1776091859E+02
24	39	2.2695485475E+00	1.0600004053E+02	-8.1776076267E+02
24	40	2.2695485475E+00	1.0650004053E+02	-8.1776084342E+02
24	41	2.2695485475E+00	1.0700004053E+02	-8.1776071129E+02
24	42	2.2695485475E+00	1.0750004053E+02	-8.1776077842E+02
24	43	2.2695485475E+00	1.0800004053E+02	-8.1776064899E+02
24	44	2.2695485475E+00	1.0850004053E+02	-8.1776071246E+02
24	45	2.2695485475E+00	1.0900004053E+02	-8.1776059111E+02
24	46	2.2695485475E+00	1.0950004053E+02	-8.1776065306E+02
24	47	2.2695485475E+00	1.1000004053E+02	-8.1776053333E+02
24	48	2.2695485475E+00	1.1050004053E+02	-8.1776074416E+02
24	49	2.2695485475E+00	1.1100004053E+02	-8.1776071848E+02
24	50	2.2695485475E+00	1.1150004053E+02	-8.1776069170E+02
24	51	2.2695485475E+00	1.1200004053E+02	-8.1776066477E+02
24	52	2.2695485475E+00	1.1250004053E+02	-8.1776063646E+02
24	53	2.2695485475E+00	1.1300004053E+02	-8.1776060801E+02
24	54	2.2695485475E+00	1.1350004053E+02	-8.1776057865E+02
24	55	2.2695485475E+00	1.1400004053E+02	-8.1776054883E+02
24	56	2.2695485475E+00	1.1450004053E+02	-8.1776051805E+02
24	57	2.2695485475E+00	1.1500004053E+02	-8.1776048688E+02
24	58	2.2695485475E+00	1.1550004053E+02	-8.1776045471E+02
24	59	2.2695485475E+00	1.1600004053E+02	-8.1776042205E+02

24	60	2.2695485475E+00	1.1650004053E+02	-8.1776038855E+02
24	61	2.2695485475E+00	1.1700004053E+02	-8.1776035447E+02
25	1	2.2795485475E+00	8.7000040532E+01	-8.1776141746E+02
25	2	2.2795485475E+00	8.7500040532E+01	-8.1776143752E+02
25	3	2.2795485475E+00	8.8000040532E+01	-8.1776145302E+02
25	4	2.2795485475E+00	8.8500040532E+01	-8.1776146460E+02
25	5	2.2795485475E+00	8.9000040532E+01	-8.1776147221E+02
25	6	2.2795485475E+00	8.9500040532E+01	-8.1776147276E+02
25	7	2.2795485475E+00	9.0000040532E+01	-8.1776147630E+02
25	8	2.2795485475E+00	9.0500040532E+01	-8.1776147320E+02
25	9	2.2795485475E+00	9.1000040532E+01	-8.1776146719E+02
25	10	2.2795485475E+00	9.1500040532E+01	-8.1776144449E+02
25	11	2.2795485475E+00	9.2000040532E+01	-8.1776144701E+02
25	12	2.2795485475E+00	9.2500040532E+01	-8.1776142970E+02
25	13	2.2795485475E+00	9.3000040532E+01	-8.1776141784E+02
25	14	2.2795485475E+00	9.3500040532E+01	-8.1776138520E+02
25	15	2.2795485475E+00	9.4000040532E+01	-8.1776137783E+02
25	16	2.2795485475E+00	9.4500040532E+01	-8.1776135572E+02
25	17	2.2795485475E+00	9.5000040532E+01	-8.1776129535E+02
25	18	2.2795485475E+00	9.5500040532E+01	-8.1776130842E+02
25	19	2.2795485475E+00	9.6000040532E+01	-8.1776128738E+02
25	20	2.2795485475E+00	9.6500040532E+01	-8.1776125572E+02
25	21	2.2795485475E+00	9.7000040532E+01	-8.1776123206E+02
25	22	2.2795485475E+00	9.7500040532E+01	-8.1776117290E+02
25	23	2.2795485475E+00	9.8000040532E+01	-8.1776117405E+02
25	24	2.2795485475E+00	9.8500040532E+01	-8.1776112182E+02
25	25	2.2795485475E+00	9.9000040532E+01	-8.1776111132E+02
25	26	2.2795485475E+00	9.9500040532E+01	-8.1776107114E+02
25	27	2.2795485475E+00	1.0000004053E+02	-8.1776105093E+02
25	28	2.2795485475E+00	1.0050004053E+02	-8.1776103961E+02
25	29	2.2795485475E+00	1.0100004053E+02	-8.1776097860E+02
25	30	2.2795485475E+00	1.0150004053E+02	-8.1776099058E+02
25	31	2.2795485475E+00	1.0200004053E+02	-8.1776092867E+02
25	32	2.2795485475E+00	1.0250004053E+02	-8.1776093874E+02
25	33	2.2795485475E+00	1.0300004053E+02	-8.1776085987E+02
25	34	2.2795485475E+00	1.0350004053E+02	-8.1776088395E+02
25	35	2.2795485475E+00	1.0400004053E+02	-8.1776078778E+02
25	36	2.2795485475E+00	1.0450004053E+02	-8.1776082408E+02
25	37	2.2795485475E+00	1.0500004053E+02	-8.1776063895E+02
25	38	2.2795485475E+00	1.0550004053E+02	-8.1776075893E+02
25	39	2.2795485475E+00	1.0600004053E+02	-8.1776057398E+02
25	40	2.2795485475E+00	1.0650004053E+02	-8.1776069024E+02
25	41	2.2795485475E+00	1.0700004053E+02	-8.1776052425E+02
25	42	2.2795485475E+00	1.0750004053E+02	-8.1776062041E+02
25	43	2.2795485475E+00	1.0800004053E+02	-8.1776045406E+02
25	44	2.2795485475E+00	1.0850004053E+02	-8.1776054511E+02
25	45	2.2795485475E+00	1.0900004053E+02	-8.1776039698E+02
25	46	2.2795485475E+00	1.0950004053E+02	-8.1776048482E+02
25	47	2.2795485475E+00	1.1000004053E+02	-8.1776034927E+02
25	48	2.2795485475E+00	1.1050004053E+02	-8.1776059237E+02
25	49	2.2795485475E+00	1.1100004053E+02	-8.1776057232E+02
25	50	2.2795485475E+00	1.1150004053E+02	-8.1776054545E+02

25	51	2.2795485475E+00	1.1200004053E+02	-8.1776051861E+02
25	52	2.2795485475E+00	1.1250004053E+02	-8.1776049055E+02
25	53	2.2795485475E+00	1.1300004053E+02	-8.1776046218E+02
25	54	2.2795485475E+00	1.1350004053E+02	-8.1776043273E+02
25	55	2.2795485475E+00	1.1400004053E+02	-8.1776040287E+02
25	56	2.2795485475E+00	1.1450004053E+02	-8.1776037206E+02
25	57	2.2795485475E+00	1.1500004053E+02	-8.1776034072E+02
25	58	2.2795485475E+00	1.1550004053E+02	-8.1776030859E+02
25	59	2.2795485475E+00	1.1600004053E+02	-8.1776027587E+02
25	60	2.2795485475E+00	1.1650004053E+02	-8.1776024233E+02
25	61	2.2795485475E+00	1.1700004053E+02	-8.1776020817E+02
26	1	2.2895485475E+00	8.7000040532E+01	-8.1776120460E+02
26	2	2.2895485475E+00	8.7500040532E+01	-8.1776122859E+02
26	3	2.2895485475E+00	8.8000040532E+01	-8.1776124432E+02
26	4	2.2895485475E+00	8.8500040532E+01	-8.1776125588E+02
26	5	2.2895485475E+00	8.9000040532E+01	-8.1776126358E+02
26	6	2.2895485475E+00	8.9500040532E+01	-8.1776126740E+02
26	7	2.2895485475E+00	9.0000040532E+01	-8.1776126425E+02
26	8	2.2895485475E+00	9.0500040532E+01	-8.1776125156E+02
26	9	2.2895485475E+00	9.1000040532E+01	-8.1776125563E+02
26	10	2.2895485475E+00	9.1500040532E+01	-8.1776124674E+02
26	11	2.2895485475E+00	9.2000040532E+01	-8.1776123579E+02
26	12	2.2895485475E+00	9.2500040532E+01	-8.1776122566E+02
26	13	2.2895485475E+00	9.3000040532E+01	-8.1776120714E+02
26	14	2.2895485475E+00	9.3500040532E+01	-8.1776118888E+02
26	15	2.2895485475E+00	9.4000040532E+01	-8.1776116084E+02
26	16	2.2895485475E+00	9.4500040532E+01	-8.1776115291E+02
26	17	2.2895485475E+00	9.5000040532E+01	-8.1776113012E+02
26	18	2.2895485475E+00	9.5500040532E+01	-8.1776110586E+02
26	19	2.2895485475E+00	9.6000040532E+01	-8.1776107763E+02
26	20	2.2895485475E+00	9.6500040532E+01	-8.1776105335E+02
26	21	2.2895485475E+00	9.7000040532E+01	-8.1776102579E+02
26	22	2.2895485475E+00	9.7500040532E+01	-8.1776098902E+02
26	23	2.2895485475E+00	9.8000040532E+01	-8.1776096853E+02
26	24	2.2895485475E+00	9.8500040532E+01	-8.1776094135E+02
26	25	2.2895485475E+00	9.9000040532E+01	-8.1776089677E+02
26	26	2.2895485475E+00	9.9500040532E+01	-8.1776089445E+02
26	27	2.2895485475E+00	1.0000004053E+02	-8.1776083791E+02
26	28	2.2895485475E+00	1.0050004053E+02	-8.1776085198E+02
26	29	2.2895485475E+00	1.0100004053E+02	-8.1776079168E+02
26	30	2.2895485475E+00	1.0150004053E+02	-8.1776078213E+02
26	31	2.2895485475E+00	1.0200004053E+02	-8.1776072533E+02
26	32	2.2895485475E+00	1.0250004053E+02	-8.1776075768E+02
26	33	2.2895485475E+00	1.0300004053E+02	-8.1776073295E+02
26	34	2.2895485475E+00	1.0350004053E+02	-8.1776070558E+02
26	35	2.2895485475E+00	1.0400004053E+02	-8.1776067795E+02
26	36	2.2895485475E+00	1.0450004053E+02	-8.1776064820E+02
26	37	2.2895485475E+00	1.0500004053E+02	-8.1776043364E+02
26	38	2.2895485475E+00	1.0550004053E+02	-8.1776058555E+02
26	39	2.2895485475E+00	1.0600004053E+02	-8.1776036702E+02
26	40	2.2895485475E+00	1.0650004053E+02	-8.1776051392E+02
26	41	2.2895485475E+00	1.0700004053E+02	-8.1776031503E+02

26	42	2.2895485475E+00	1.0750004053E+02	-8.1776045772E+02
26	43	2.2895485475E+00	1.0800004053E+02	-8.1776026675E+02
26	44	2.2895485475E+00	1.0850004053E+02	-8.1776039424E+02
26	45	2.2895485475E+00	1.0900004053E+02	-8.1776021391E+02
26	46	2.2895485475E+00	1.0950004053E+02	-8.1776033165E+02
26	47	2.2895485475E+00	1.1000004053E+02	-8.1776013986E+02
26	48	2.2895485475E+00	1.1050004053E+02	-8.1776044045E+02
26	49	2.2895485475E+00	1.1100004053E+02	-8.1776041023E+02
26	50	2.2895485475E+00	1.1150004053E+02	-8.1776037851E+02
26	51	2.2895485475E+00	1.1200004053E+02	-8.1776035909E+02
26	52	2.2895485475E+00	1.1250004053E+02	-8.1776033117E+02
26	53	2.2895485475E+00	1.1300004053E+02	-8.1776030285E+02
26	54	2.2895485475E+00	1.1350004053E+02	-8.1776027339E+02
26	55	2.2895485475E+00	1.1400004053E+02	-8.1776024345E+02
26	56	2.2895485475E+00	1.1450004053E+02	-8.1776021269E+02
26	57	2.2895485475E+00	1.1500004053E+02	-8.1776018138E+02
26	58	2.2895485475E+00	1.1550004053E+02	-8.1776014919E+02
26	59	2.2895485475E+00	1.1600004053E+02	-8.1776011653E+02
26	60	2.2895485475E+00	1.1650004053E+02	-8.1776008299E+02
26	61	2.2895485475E+00	1.1700004053E+02	-8.1776004895E+02
27	1	2.2995485475E+00	8.7000040532E+01	-8.1776097894E+02
27	2	2.2995485475E+00	8.7500040532E+01	-8.1776099923E+02
27	3	2.2995485475E+00	8.8000040532E+01	-8.1776101519E+02
27	4	2.2995485475E+00	8.8500040532E+01	-8.1776102697E+02
27	5	2.2995485475E+00	8.9000040532E+01	-8.1776103487E+02
27	6	2.2995485475E+00	8.9500040532E+01	-8.1776102506E+02
27	7	2.2995485475E+00	9.0000040532E+01	-8.1776102632E+02
27	8	2.2995485475E+00	9.0500040532E+01	-8.1776103330E+02
27	9	2.2995485475E+00	9.1000040532E+01	-8.1776101799E+02
27	10	2.2995485475E+00	9.1500040532E+01	-8.1776102289E+02
27	11	2.2995485475E+00	9.2000040532E+01	-8.1776099875E+02
27	12	2.2995485475E+00	9.2500040532E+01	-8.1776098401E+02
27	13	2.2995485475E+00	9.3000040532E+01	-8.1776097040E+02
27	14	2.2995485475E+00	9.3500040532E+01	-8.1776096681E+02
27	15	2.2995485475E+00	9.4000040532E+01	-8.1776094819E+02
27	16	2.2995485475E+00	9.4500040532E+01	-8.1776091049E+02
27	17	2.2995485475E+00	9.5000040532E+01	-8.1776090506E+02
27	18	2.2995485475E+00	9.5500040532E+01	-8.1776085068E+02
27	19	2.2995485475E+00	9.6000040532E+01	-8.1776084260E+02
27	20	2.2995485475E+00	9.6500040532E+01	-8.1776080727E+02
27	21	2.2995485475E+00	9.7000040532E+01	-8.1776079836E+02
27	22	2.2995485475E+00	9.7500040532E+01	-8.1776078046E+02
27	23	2.2995485475E+00	9.8000040532E+01	-8.1776074207E+02
27	24	2.2995485475E+00	9.8500040532E+01	-8.1776073613E+02
27	25	2.2995485475E+00	9.9000040532E+01	-8.1776068889E+02
27	26	2.2995485475E+00	9.9500040532E+01	-8.1776069346E+02
27	27	2.2995485475E+00	1.0000004053E+02	-8.1776063264E+02
27	28	2.2995485475E+00	1.0050004053E+02	-8.1776062830E+02
27	29	2.2995485475E+00	1.0100004053E+02	-8.1776057093E+02
27	30	2.2995485475E+00	1.0150004053E+02	-8.1776060346E+02
27	31	2.2995485475E+00	1.0200004053E+02	-8.1776049744E+02
27	32	2.2995485475E+00	1.0250004053E+02	-8.1776056479E+02

27	33	2.2995485475E+00	1.0300004053E+02	-8.1776053465E+02
27	34	2.2995485475E+00	1.0350004053E+02	-8.1776051621E+02
27	35	2.2995485475E+00	1.0400004053E+02	-8.1776048958E+02
27	36	2.2995485475E+00	1.0450004053E+02	-8.1776045483E+02
27	37	2.2995485475E+00	1.0500004053E+02	-8.1776020516E+02
27	38	2.2995485475E+00	1.0550004053E+02	-8.1776040476E+02
27	39	2.2995485475E+00	1.0600004053E+02	-8.1776014434E+02
27	40	2.2995485475E+00	1.0650004053E+02	-8.1776035661E+02
27	41	2.2995485475E+00	1.0700004053E+02	-8.1776008794E+02
27	42	2.2995485475E+00	1.0750004053E+02	-8.1776029686E+02
27	43	2.2995485475E+00	1.0800004053E+02	-8.1776012003E+02
27	44	2.2995485475E+00	1.0850004053E+02	-8.1776023404E+02
27	45	2.2995485475E+00	1.0900004053E+02	-8.1776000042E+02
27	46	2.2995485475E+00	1.0950004053E+02	-8.1776017042E+02
27	47	2.2995485475E+00	1.1000004053E+02	-8.1775994393E+02
27	48	2.2995485475E+00	1.1050004053E+02	-8.1776027861E+02
27	49	2.2995485475E+00	1.1100004053E+02	-8.1776024755E+02
27	50	2.2995485475E+00	1.1150004053E+02	-8.1776021601E+02
27	51	2.2995485475E+00	1.1200004053E+02	-8.1776018913E+02
27	52	2.2995485475E+00	1.1250004053E+02	-8.1776016051E+02
27	53	2.2995485475E+00	1.1300004053E+02	-8.1776013226E+02
27	54	2.2995485475E+00	1.1350004053E+02	-8.1776010299E+02
27	55	2.2995485475E+00	1.1400004053E+02	-8.1776007302E+02
27	56	2.2995485475E+00	1.1450004053E+02	-8.1776004229E+02
27	57	2.2995485475E+00	1.1500004053E+02	-8.1776001095E+02
27	58	2.2995485475E+00	1.1550004053E+02	-8.1775995765E+02
27	59	2.2995485475E+00	1.1600004053E+02	-8.1775994637E+02
27	60	2.2995485475E+00	1.1650004053E+02	-8.1775989522E+02
27	61	2.2995485475E+00	1.1700004053E+02	-8.1775987918E+02
28	1	2.3095485475E+00	8.7000040532E+01	-8.1776073027E+02
28	2	2.3095485475E+00	8.7500040532E+01	-8.1776075085E+02
28	3	2.3095485475E+00	8.8000040532E+01	-8.1776076715E+02
28	4	2.3095485475E+00	8.8500040532E+01	-8.1776076525E+02
28	5	2.3095485475E+00	8.9000040532E+01	-8.1776078755E+02
28	6	2.3095485475E+00	8.9500040532E+01	-8.1776078852E+02
28	7	2.3095485475E+00	9.0000040532E+01	-8.1776079308E+02
28	8	2.3095485475E+00	9.0500040532E+01	-8.1776079058E+02
28	9	2.3095485475E+00	9.1000040532E+01	-8.1776078569E+02
28	10	2.3095485475E+00	9.1500040532E+01	-8.1776076302E+02
28	11	2.3095485475E+00	9.2000040532E+01	-8.1776076741E+02
28	12	2.3095485475E+00	9.2500040532E+01	-8.1776075094E+02
28	13	2.3095485475E+00	9.3000040532E+01	-8.1776074047E+02
28	14	2.3095485475E+00	9.3500040532E+01	-8.1776070692E+02
28	15	2.3095485475E+00	9.4000040532E+01	-8.1776070205E+02
28	16	2.3095485475E+00	9.4500040532E+01	-8.1776068025E+02
28	17	2.3095485475E+00	9.5000040532E+01	-8.1776065999E+02
28	18	2.3095485475E+00	9.5500040532E+01	-8.1776062927E+02
28	19	2.3095485475E+00	9.6000040532E+01	-8.1776061489E+02
28	20	2.3095485475E+00	9.6500040532E+01	-8.1776059068E+02
28	21	2.3095485475E+00	9.7000040532E+01	-8.1776054685E+02
28	22	2.3095485475E+00	9.7500040532E+01	-8.1776053679E+02
28	23	2.3095485475E+00	9.8000040532E+01	-8.1776049253E+02

28 24	2.3095485475E+00	9.8500040532E+01	-8.1776049677E+02
28 25	2.3095485475E+00	9.9000040532E+01	-8.1776049598E+02
28 26	2.3095485475E+00	9.9500040532E+01	-8.1776045570E+02
28 27	2.3095485475E+00	1.0000004053E+02	-8.1776045762E+02
28 28	2.3095485475E+00	1.0050004053E+02	-8.1776043461E+02
28 29	2.3095485475E+00	1.0100004053E+02	-8.1776032688E+02
28 30	2.3095485475E+00	1.0150004053E+02	-8.1776040240E+02
28 31	2.3095485475E+00	1.0200004053E+02	-8.1776038209E+02
28 32	2.3095485475E+00	1.0250004053E+02	-8.1776036157E+02
28 33	2.3095485475E+00	1.0300004053E+02	-8.1776031409E+02
28 34	2.3095485475E+00	1.0350004053E+02	-8.1776031289E+02
28 35	2.3095485475E+00	1.0400004053E+02	-8.1776028597E+02
28 36	2.3095485475E+00	1.0450004053E+02	-8.1776027830E+02
28 37	2.3095485475E+00	1.0500004053E+02	-8.1775996888E+02
28 38	2.3095485475E+00	1.0550004053E+02	-8.1776024153E+02
28 39	2.3095485475E+00	1.0600004053E+02	-8.1775990777E+02
28 40	2.3095485475E+00	1.0650004053E+02	-8.1776018912E+02
28 41	2.3095485475E+00	1.0700004053E+02	-8.1775986150E+02
28 42	2.3095485475E+00	1.0750004053E+02	-8.1776013034E+02
28 43	2.3095485475E+00	1.0800004053E+02	-8.1776009984E+02
28 44	2.3095485475E+00	1.0850004053E+02	-8.1776006849E+02
28 45	2.3095485475E+00	1.0900004053E+02	-8.1776003672E+02
28 46	2.3095485475E+00	1.0950004053E+02	-8.1776000424E+02
28 47	2.3095485475E+00	1.1000004053E+02	-8.1775972027E+02
28 48	2.3095485475E+00	1.1050004053E+02	-8.1776010890E+02
28 49	2.3095485475E+00	1.1100004053E+02	-8.1776007817E+02
28 50	2.3095485475E+00	1.1150004053E+02	-8.1776004624E+02
28 51	2.3095485475E+00	1.1200004053E+02	-8.1776001377E+02
28 52	2.3095485475E+00	1.1250004053E+02	-8.1775998090E+02
28 53	2.3095485475E+00	1.1300004053E+02	-8.1775995302E+02
28 54	2.3095485475E+00	1.1350004053E+02	-8.1775992362E+02
28 55	2.3095485475E+00	1.1400004053E+02	-8.1775989399E+02
28 56	2.3095485475E+00	1.1450004053E+02	-8.1775986334E+02
28 57	2.3095485475E+00	1.1500004053E+02	-8.1775983210E+02
28 58	2.3095485475E+00	1.1550004053E+02	-8.1775979097E+02
28 59	2.3095485475E+00	1.1600004053E+02	-8.1775976779E+02
28 60	2.3095485475E+00	1.1650004053E+02	-8.1775972843E+02
28 61	2.3095485475E+00	1.1700004053E+02	-8.1775970117E+02
29 1	2.3195485475E+00	8.7000040532E+01	-8.1776046025E+02
29 2	2.3195485475E+00	8.7500040532E+01	-8.1776047037E+02
29 3	2.3195485475E+00	8.8000040532E+01	-8.1776050160E+02
29 4	2.3195485475E+00	8.8500040532E+01	-8.1776051070E+02
29 5	2.3195485475E+00	8.9000040532E+01	-8.1776051949E+02
29 6	2.3195485475E+00	8.9500040532E+01	-8.1776052795E+02
29 7	2.3195485475E+00	9.0000040532E+01	-8.1776052618E+02
29 8	2.3195485475E+00	9.0500040532E+01	-8.1776051372E+02
29 9	2.3195485475E+00	9.1000040532E+01	-8.1776052017E+02
29 10	2.3195485475E+00	9.1500040532E+01	-8.1776051264E+02
29 11	2.3195485475E+00	9.2000040532E+01	-8.1776050331E+02
29 12	2.3195485475E+00	9.2500040532E+01	-8.1776049509E+02
29 13	2.3195485475E+00	9.3000040532E+01	-8.1776047784E+02
29 14	2.3195485475E+00	9.3500040532E+01	-8.1776046058E+02

29	15	2.3195485475E+00	9.4000040532E+01	-8.1776043400E+02
29	16	2.3195485475E+00	9.4500040532E+01	-8.1776042785E+02
29	17	2.3195485475E+00	9.5000040532E+01	-8.1776039297E+02
29	18	2.3195485475E+00	9.5500040532E+01	-8.1776038562E+02
29	19	2.3195485475E+00	9.6000040532E+01	-8.1776036254E+02
29	20	2.3195485475E+00	9.6500040532E+01	-8.1776035247E+02
29	21	2.3195485475E+00	9.7000040532E+01	-8.1776033511E+02
29	22	2.3195485475E+00	9.7500040532E+01	-8.1776031523E+02
29	23	2.3195485475E+00	9.8000040532E+01	-8.1776030083E+02
29	24	2.3195485475E+00	9.8500040532E+01	-8.1776028160E+02
29	25	2.3195485475E+00	9.9000040532E+01	-8.1776025869E+02
29	26	2.3195485475E+00	9.9500040532E+01	-8.1776024791E+02
29	27	2.3195485475E+00	1.0000004053E+02	-8.1776022560E+02
29	28	2.3195485475E+00	1.0050004053E+02	-8.1776022032E+02
29	29	2.3195485475E+00	1.0100004053E+02	-8.1776020492E+02
29	30	2.3195485475E+00	1.0150004053E+02	-8.1776017258E+02
29	31	2.3195485475E+00	1.0200004053E+02	-8.1776016408E+02
29	32	2.3195485475E+00	1.0250004053E+02	-8.1776015550E+02
29	33	2.3195485475E+00	1.0300004053E+02	-8.1776015197E+02
29	34	2.3195485475E+00	1.0350004053E+02	-8.1776014067E+02
29	35	2.3195485475E+00	1.0400004053E+02	-8.1776012685E+02
29	36	2.3195485475E+00	1.0450004053E+02	-8.1776011020E+02
29	37	2.3195485475E+00	1.0500004053E+02	-8.1776009104E+02
29	38	2.3195485475E+00	1.0550004053E+02	-8.1776006154E+02
29	39	2.3195485475E+00	1.0600004053E+02	-8.1775966026E+02
29	40	2.3195485475E+00	1.0650004053E+02	-8.1776001836E+02
29	41	2.3195485475E+00	1.0700004053E+02	-8.1775960912E+02
29	42	2.3195485475E+00	1.0750004053E+02	-8.1775996071E+02
29	43	2.3195485475E+00	1.0800004053E+02	-8.1775993070E+02
29	44	2.3195485475E+00	1.0850004053E+02	-8.1775989977E+02
29	45	2.3195485475E+00	1.0900004053E+02	-8.1775986861E+02
29	46	2.3195485475E+00	1.0950004053E+02	-8.1775983578E+02
29	47	2.3195485475E+00	1.1000004053E+02	-8.1775948304E+02
29	48	2.3195485475E+00	1.1050004053E+02	-8.1775993365E+02
29	49	2.3195485475E+00	1.1100004053E+02	-8.1775990307E+02
29	50	2.3195485475E+00	1.1150004053E+02	-8.1775987141E+02
29	51	2.3195485475E+00	1.1200004053E+02	-8.1775983869E+02
29	52	2.3195485475E+00	1.1250004053E+02	-8.1775980507E+02
29	53	2.3195485475E+00	1.1300004053E+02	-8.1775977147E+02
29	54	2.3195485475E+00	1.1350004053E+02	-8.1775973823E+02
29	55	2.3195485475E+00	1.1400004053E+02	-8.1775970887E+02
29	56	2.3195485475E+00	1.1450004053E+02	-8.1775967734E+02
29	57	2.3195485475E+00	1.1500004053E+02	-8.1775964713E+02
29	58	2.3195485475E+00	1.1550004053E+02	-8.1775961891E+02
29	59	2.3195485475E+00	1.1600004053E+02	-8.1775958334E+02
29	60	2.3195485475E+00	1.1650004053E+02	-8.1775955624E+02
29	61	2.3195485475E+00	1.1700004053E+02	-8.1775951719E+02
30	1	2.3295485475E+00	8.7000040532E+01	-8.1776016697E+02
30	2	2.3295485475E+00	8.7500040532E+01	-8.1776019889E+02
30	3	2.3295485475E+00	8.8000040532E+01	-8.1776021991E+02
30	4	2.3295485475E+00	8.8500040532E+01	-8.1776023317E+02
30	5	2.3295485475E+00	8.9000040532E+01	-8.1776022918E+02

30	6	2.3295485475E+00	8.9500040532E+01	-8.1776023408E+02
30	7	2.3295485475E+00	9.0000040532E+01	-8.1776023704E+02
30	8	2.3295485475E+00	9.0500040532E+01	-8.1776024665E+02
30	9	2.3295485475E+00	9.1000040532E+01	-8.1776023351E+02
30	10	2.3295485475E+00	9.1500040532E+01	-8.1776024056E+02
30	11	2.3295485475E+00	9.2000040532E+01	-8.1776021778E+02
30	12	2.3295485475E+00	9.2500040532E+01	-8.1776020302E+02
30	13	2.3295485475E+00	9.3000040532E+01	-8.1776019400E+02
30	14	2.3295485475E+00	9.3500040532E+01	-8.1776019299E+02
30	15	2.3295485475E+00	9.4000040532E+01	-8.1776014454E+02
30	16	2.3295485475E+00	9.4500040532E+01	-8.1776013554E+02
30	17	2.3295485475E+00	9.5000040532E+01	-8.1776010480E+02
30	18	2.3295485475E+00	9.5500040532E+01	-8.1776011030E+02
30	19	2.3295485475E+00	9.6000040532E+01	-8.1776011543E+02
30	20	2.3295485475E+00	9.6500040532E+01	-8.1776008410E+02
30	21	2.3295485475E+00	9.7000040532E+01	-8.1776007897E+02
30	22	2.3295485475E+00	9.7500040532E+01	-8.1776007316E+02
30	23	2.3295485475E+00	9.8000040532E+01	-8.1776006025E+02
30	24	2.3295485475E+00	9.8500040532E+01	-8.1776004652E+02
30	25	2.3295485475E+00	9.9000040532E+01	-8.1776000200E+02
30	26	2.3295485475E+00	9.9500040532E+01	-8.1776002084E+02
30	27	2.3295485475E+00	1.0000004053E+02	-8.1775997439E+02
30	28	2.3295485475E+00	1.0050004053E+02	-8.1775998544E+02
30	29	2.3295485475E+00	1.0100004053E+02	-8.1775998872E+02
30	30	2.3295485475E+00	1.0150004053E+02	-8.1775998479E+02
30	31	2.3295485475E+00	1.0200004053E+02	-8.1775998178E+02
30	32	2.3295485475E+00	1.0250004053E+02	-8.1775997758E+02
30	33	2.3295485475E+00	1.0300004053E+02	-8.1775997103E+02
30	34	2.3295485475E+00	1.0350004053E+02	-8.1775995388E+02
30	35	2.3295485475E+00	1.0400004053E+02	-8.1775994991E+02
30	36	2.3295485475E+00	1.0450004053E+02	-8.1775992653E+02
30	37	2.3295485475E+00	1.0500004053E+02	-8.1775990574E+02
30	38	2.3295485475E+00	1.0550004053E+02	-8.1775989585E+02
30	39	2.3295485475E+00	1.0600004053E+02	-8.1775987230E+02
30	40	2.3295485475E+00	1.0650004053E+02	-8.1775984686E+02
30	41	2.3295485475E+00	1.0700004053E+02	-8.1775936432E+02
30	42	2.3295485475E+00	1.0750004053E+02	-8.1775979002E+02
30	43	2.3295485475E+00	1.0800004053E+02	-8.1775976036E+02
30	44	2.3295485475E+00	1.0850004053E+02	-8.1775973011E+02
30	45	2.3295485475E+00	1.0900004053E+02	-8.1775969971E+02
30	46	2.3295485475E+00	1.0950004053E+02	-8.1775966716E+02
30	47	2.3295485475E+00	1.1000004053E+02	-8.1775963305E+02
30	48	2.3295485475E+00	1.1050004053E+02	-8.1775975501E+02
30	49	2.3295485475E+00	1.1100004053E+02	-8.1775972479E+02
30	50	2.3295485475E+00	1.1150004053E+02	-8.1775969309E+02
30	51	2.3295485475E+00	1.1200004053E+02	-8.1775966042E+02
30	52	2.3295485475E+00	1.1250004053E+02	-8.1775962667E+02
30	53	2.3295485475E+00	1.1300004053E+02	-8.1775959272E+02
30	54	2.3295485475E+00	1.1350004053E+02	-8.1775955916E+02
30	55	2.3295485475E+00	1.1400004053E+02	-8.1775952984E+02
30	56	2.3295485475E+00	1.1450004053E+02	-8.1775950169E+02
30	57	2.3295485475E+00	1.1500004053E+02	-8.1775947356E+02

30	58	2.3295485475E+00	1.1550004053E+02	-8.1775944377E+02
30	59	2.3295485475E+00	1.1600004053E+02	-8.1775941271E+02
30	60	2.3295485475E+00	1.1650004053E+02	-8.1775938033E+02
30	61	2.3295485475E+00	1.1700004053E+02	-8.1775934639E+02
31	1	2.3395485475E+00	8.7000040532E+01	-8.1775988311E+02
31	2	2.3395485475E+00	8.7500040532E+01	-8.1775990541E+02
31	3	2.3395485475E+00	8.8000040532E+01	-8.1775992376E+02
31	4	2.3395485475E+00	8.8500040532E+01	-8.1775992273E+02
31	5	2.3395485475E+00	8.9000040532E+01	-8.1775994842E+02
31	6	2.3395485475E+00	8.9500040532E+01	-8.1775995146E+02
31	7	2.3395485475E+00	9.0000040532E+01	-8.1775995888E+02
31	8	2.3395485475E+00	9.0500040532E+01	-8.1775995907E+02
31	9	2.3395485475E+00	9.1000040532E+01	-8.1775995681E+02
31	10	2.3395485475E+00	9.1500040532E+01	-8.1775993518E+02
31	11	2.3395485475E+00	9.2000040532E+01	-8.1775994418E+02
31	12	2.3395485475E+00	9.2500040532E+01	-8.1775992960E+02
31	13	2.3395485475E+00	9.3000040532E+01	-8.1775989011E+02
31	14	2.3395485475E+00	9.3500040532E+01	-8.1775990901E+02
31	15	2.3395485475E+00	9.4000040532E+01	-8.1775989377E+02
31	16	2.3395485475E+00	9.4500040532E+01	-8.1775988083E+02
31	17	2.3395485475E+00	9.5000040532E+01	-8.1775987543E+02
31	18	2.3395485475E+00	9.5500040532E+01	-8.1775986194E+02
31	19	2.3395485475E+00	9.6000040532E+01	-8.1775984624E+02
31	20	2.3395485475E+00	9.6500040532E+01	-8.1775984319E+02
31	21	2.3395485475E+00	9.7000040532E+01	-8.1775980404E+02
31	22	2.3395485475E+00	9.7500040532E+01	-8.1775982531E+02
31	23	2.3395485475E+00	9.8000040532E+01	-8.1775980318E+02
31	24	2.3395485475E+00	9.8500040532E+01	-8.1775980696E+02
31	25	2.3395485475E+00	9.9000040532E+01	-8.1775979838E+02
31	26	2.3395485475E+00	9.9500040532E+01	-8.1775977889E+02
31	27	2.3395485475E+00	1.0000004053E+02	-8.1775978843E+02
31	28	2.3395485475E+00	1.0050004053E+02	-8.1775978976E+02
31	29	2.3395485475E+00	1.0100004053E+02	-8.1775979286E+02
31	30	2.3395485475E+00	1.0150004053E+02	-8.1775978825E+02
31	31	2.3395485475E+00	1.0200004053E+02	-8.1775978225E+02
31	32	2.3395485475E+00	1.0250004053E+02	-8.1775978666E+02
31	33	2.3395485475E+00	1.0300004053E+02	-8.1775977904E+02
31	34	2.3395485475E+00	1.0350004053E+02	-8.1775978352E+02
31	35	2.3395485475E+00	1.0400004053E+02	-8.1775976255E+02
31	36	2.3395485475E+00	1.0450004053E+02	-8.1775975991E+02
31	37	2.3395485475E+00	1.0500004053E+02	-8.1775974344E+02
31	38	2.3395485475E+00	1.0550004053E+02	-8.1775972359E+02
31	39	2.3395485475E+00	1.0600004053E+02	-8.1775970136E+02
31	40	2.3395485475E+00	1.0650004053E+02	-8.1775967608E+02
31	41	2.3395485475E+00	1.0700004053E+02	-8.1775910716E+02
31	42	2.3395485475E+00	1.0750004053E+02	-8.1775962030E+02
31	43	2.3395485475E+00	1.0800004053E+02	-8.1775959099E+02
31	44	2.3395485475E+00	1.0850004053E+02	-8.1775956150E+02
31	45	2.3395485475E+00	1.0900004053E+02	-8.1775953197E+02
31	46	2.3395485475E+00	1.0950004053E+02	-8.1775950043E+02
31	47	2.3395485475E+00	1.1000004053E+02	-8.1775946657E+02
31	48	2.3395485475E+00	1.1050004053E+02	-8.1775957618E+02

31	49	2.3395485475E+00	1.1100004053E+02	-8.1775954511E+02
31	50	2.3395485475E+00	1.1150004053E+02	-8.1775951355E+02
31	51	2.3395485475E+00	1.1200004053E+02	-8.1775948118E+02
31	52	2.3395485475E+00	1.1250004053E+02	-8.1775944703E+02
31	53	2.3395485475E+00	1.1300004053E+02	-8.1775941319E+02
31	54	2.3395485475E+00	1.1350004053E+02	-8.1775937997E+02
31	55	2.3395485475E+00	1.1400004053E+02	-8.1775935215E+02
31	56	2.3395485475E+00	1.1450004053E+02	-8.1775932511E+02
31	57	2.3395485475E+00	1.1500004053E+02	-8.1775929617E+02
31	58	2.3395485475E+00	1.1550004053E+02	-8.1775926609E+02
31	59	2.3395485475E+00	1.1600004053E+02	-8.1775923497E+02
31	60	2.3395485475E+00	1.1650004053E+02	-8.1775920202E+02
31	61	2.3395485475E+00	1.1700004053E+02	-8.1775916780E+02
32	1	2.3495485475E+00	8.7000040532E+01	-8.1775956830E+02
32	2	2.3495485475E+00	8.7500040532E+01	-8.1775957912E+02
32	3	2.3495485475E+00	8.8000040532E+01	-8.1775961078E+02
32	4	2.3495485475E+00	8.8500040532E+01	-8.1775962566E+02
32	5	2.3495485475E+00	8.9000040532E+01	-8.1775963765E+02
32	6	2.3495485475E+00	8.9500040532E+01	-8.1775964940E+02
32	7	2.3495485475E+00	9.0000040532E+01	-8.1775965056E+02
32	8	2.3495485475E+00	9.0500040532E+01	-8.1775963920E+02
32	9	2.3495485475E+00	9.1000040532E+01	-8.1775965134E+02
32	10	2.3495485475E+00	9.1500040532E+01	-8.1775964683E+02
32	11	2.3495485475E+00	9.2000040532E+01	-8.1775964176E+02
32	12	2.3495485475E+00	9.2500040532E+01	-8.1775963714E+02
32	13	2.3495485475E+00	9.3000040532E+01	-8.1775962705E+02
32	14	2.3495485475E+00	9.3500040532E+01	-8.1775959495E+02
32	15	2.3495485475E+00	9.4000040532E+01	-8.1775959916E+02
32	16	2.3495485475E+00	9.4500040532E+01	-8.1775960832E+02
32	17	2.3495485475E+00	9.5000040532E+01	-8.1775960261E+02
32	18	2.3495485475E+00	9.5500040532E+01	-8.1775959635E+02
32	19	2.3495485475E+00	9.6000040532E+01	-8.1775955920E+02
32	20	2.3495485475E+00	9.6500040532E+01	-8.1775958571E+02
32	21	2.3495485475E+00	9.7000040532E+01	-8.1775958096E+02
32	22	2.3495485475E+00	9.7500040532E+01	-8.1775957630E+02
32	23	2.3495485475E+00	9.8000040532E+01	-8.1775952919E+02
32	24	2.3495485475E+00	9.8500040532E+01	-8.1775955607E+02
32	25	2.3495485475E+00	9.9000040532E+01	-8.1775954946E+02
32	26	2.3495485475E+00	9.9500040532E+01	-8.1775957455E+02
32	27	2.3495485475E+00	1.0000004053E+02	-8.1775958450E+02
32	28	2.3495485475E+00	1.0050004053E+02	-8.1775958638E+02
32	29	2.3495485475E+00	1.0100004053E+02	-8.1775960273E+02
32	30	2.3495485475E+00	1.0150004053E+02	-8.1775960868E+02
32	31	2.3495485475E+00	1.0200004053E+02	-8.1775961339E+02
32	32	2.3495485475E+00	1.0250004053E+02	-8.1775961442E+02
32	33	2.3495485475E+00	1.0300004053E+02	-8.1775961302E+02
32	34	2.3495485475E+00	1.0350004053E+02	-8.1775959847E+02
32	35	2.3495485475E+00	1.0400004053E+02	-8.1775959983E+02
32	36	2.3495485475E+00	1.0450004053E+02	-8.1775958776E+02
32	37	2.3495485475E+00	1.0500004053E+02	-8.1775957270E+02
32	38	2.3495485475E+00	1.0550004053E+02	-8.1775955411E+02
32	39	2.3495485475E+00	1.0600004053E+02	-8.1775953269E+02

32	40	2.3495485475E+00	1.0650004053E+02	-8.1775950840E+02
32	41	2.3495485475E+00	1.0700004053E+02	-8.1775948173E+02
32	42	2.3495485475E+00	1.0750004053E+02	-8.1775945319E+02
32	43	2.3495485475E+00	1.0800004053E+02	-8.1775942413E+02
32	44	2.3495485475E+00	1.0850004053E+02	-8.1775939561E+02
32	45	2.3495485475E+00	1.0900004053E+02	-8.1775936749E+02
32	46	2.3495485475E+00	1.0950004053E+02	-8.1775933935E+02
32	47	2.3495485475E+00	1.1000004053E+02	-8.1775930831E+02
32	48	2.3495485475E+00	1.1050004053E+02	-8.1775927868E+02
32	49	2.3495485475E+00	1.1100004053E+02	-8.1775936644E+02
32	50	2.3495485475E+00	1.1150004053E+02	-8.1775933324E+02
32	51	2.3495485475E+00	1.1200004053E+02	-8.1775930178E+02
32	52	2.3495485475E+00	1.1250004053E+02	-8.1775926598E+02
32	53	2.3495485475E+00	1.1300004053E+02	-8.1775923430E+02
32	54	2.3495485475E+00	1.1350004053E+02	-8.1775920196E+02
32	55	2.3495485475E+00	1.1400004053E+02	-8.1775917439E+02
32	56	2.3495485475E+00	1.1450004053E+02	-8.1775914711E+02
32	57	2.3495485475E+00	1.1500004053E+02	-8.1775911840E+02
32	58	2.3495485475E+00	1.1550004053E+02	-8.1775908828E+02
32	59	2.3495485475E+00	1.1600004053E+02	-8.1775905634E+02
32	60	2.3495485475E+00	1.1650004053E+02	-8.1775902308E+02
32	61	2.3495485475E+00	1.1700004053E+02	-8.1775898834E+02
33	1	2.3595485475E+00	8.7000040532E+01	-8.1775924828E+02
33	2	2.3595485475E+00	8.7500040532E+01	-8.1775926849E+02
33	3	2.3595485475E+00	8.8000040532E+01	-8.1775927973E+02
33	4	2.3595485475E+00	8.8500040532E+01	-8.1775930976E+02
33	5	2.3595485475E+00	8.9000040532E+01	-8.1775930882E+02
33	6	2.3595485475E+00	8.9500040532E+01	-8.1775931558E+02
33	7	2.3595485475E+00	9.0000040532E+01	-8.1775932443E+02
33	8	2.3595485475E+00	9.0500040532E+01	-8.1775933830E+02
33	9	2.3595485475E+00	9.1000040532E+01	-8.1775932852E+02
33	10	2.3595485475E+00	9.1500040532E+01	-8.1775934138E+02
33	11	2.3595485475E+00	9.2000040532E+01	-8.1775932240E+02
33	12	2.3595485475E+00	9.2500040532E+01	-8.1775930056E+02
33	13	2.3595485475E+00	9.3000040532E+01	-8.1775931984E+02
33	14	2.3595485475E+00	9.3500040532E+01	-8.1775932394E+02
33	15	2.3595485475E+00	9.4000040532E+01	-8.1775928802E+02
33	16	2.3595485475E+00	9.4500040532E+01	-8.1775930655E+02
33	17	2.3595485475E+00	9.5000040532E+01	-8.1775932716E+02
33	18	2.3595485475E+00	9.5500040532E+01	-8.1775932674E+02
33	19	2.3595485475E+00	9.6000040532E+01	-8.1775932706E+02
33	20	2.3595485475E+00	9.6500040532E+01	-8.1775929670E+02
33	21	2.3595485475E+00	9.7000040532E+01	-8.1775931236E+02
33	22	2.3595485475E+00	9.7500040532E+01	-8.1775932071E+02
33	23	2.3595485475E+00	9.8000040532E+01	-8.1775933316E+02
33	24	2.3595485475E+00	9.8500040532E+01	-8.1775934052E+02
33	25	2.3595485475E+00	9.9000040532E+01	-8.1775928501E+02
33	26	2.3595485475E+00	9.9500040532E+01	-8.1775936356E+02
33	27	2.3595485475E+00	1.0000004053E+02	-8.1775938904E+02
33	28	2.3595485475E+00	1.0050004053E+02	-8.1775940352E+02
33	29	2.3595485475E+00	1.0100004053E+02	-8.1775940422E+02
33	30	2.3595485475E+00	1.0150004053E+02	-8.1775941621E+02

33	31	2.3595485475E+00	1.0200004053E+02	-8.1775942323E+02
33	32	2.3595485475E+00	1.0250004053E+02	-8.1775942746E+02
33	33	2.3595485475E+00	1.0300004053E+02	-8.1775942945E+02
33	34	2.3595485475E+00	1.0350004053E+02	-8.1775943676E+02
33	35	2.3595485475E+00	1.0400004053E+02	-8.1775942066E+02
33	36	2.3595485475E+00	1.0450004053E+02	-8.1775942002E+02
33	37	2.3595485475E+00	1.0500004053E+02	-8.1775940633E+02
33	38	2.3595485475E+00	1.0550004053E+02	-8.1775938883E+02
33	39	2.3595485475E+00	1.0600004053E+02	-8.1775936850E+02
33	40	2.3595485475E+00	1.0650004053E+02	-8.1775934500E+02
33	41	2.3595485475E+00	1.0700004053E+02	-8.1775931905E+02
33	42	2.3595485475E+00	1.0750004053E+02	-8.1775929086E+02
33	43	2.3595485475E+00	1.0800004053E+02	-8.1775926169E+02
33	44	2.3595485475E+00	1.0850004053E+02	-8.1775923393E+02
33	45	2.3595485475E+00	1.0900004053E+02	-8.1775920949E+02
33	46	2.3595485475E+00	1.0950004053E+02	-8.1775918271E+02
33	47	2.3595485475E+00	1.1000004053E+02	-8.1775915221E+02
33	48	2.3595485475E+00	1.1050004053E+02	-8.1775911992E+02
33	49	2.3595485475E+00	1.1100004053E+02	-8.1775919987E+02
33	50	2.3595485475E+00	1.1150004053E+02	-8.1775916536E+02
33	51	2.3595485475E+00	1.1200004053E+02	-8.1775912716E+02
33	52	2.3595485475E+00	1.1250004053E+02	-8.1775909533E+02
33	53	2.3595485475E+00	1.1300004053E+02	-8.1775906050E+02
33	54	2.3595485475E+00	1.1350004053E+02	-8.1775876396E+02
33	55	2.3595485475E+00	1.1400004053E+02	-8.1775899377E+02
33	56	2.3595485475E+00	1.1450004053E+02	-8.1775896946E+02
33	57	2.3595485475E+00	1.1500004053E+02	-8.1775894032E+02
33	58	2.3595485475E+00	1.1550004053E+02	-8.1775891011E+02
33	59	2.3595485475E+00	1.1600004053E+02	-8.1775887782E+02
33	60	2.3595485475E+00	1.1650004053E+02	-8.1775884398E+02
33	61	2.3595485475E+00	1.1700004053E+02	-8.1775880870E+02
34	1	2.3695485475E+00	8.7000040532E+01	-8.1775891401E+02
34	2	2.3695485475E+00	8.7500040532E+01	-8.1775893973E+02
34	3	2.3695485475E+00	8.8000040532E+01	-8.1775896201E+02
34	4	2.3695485475E+00	8.8500040532E+01	-8.1775896337E+02
34	5	2.3695485475E+00	8.9000040532E+01	-8.1775899524E+02
34	6	2.3695485475E+00	8.9500040532E+01	-8.1775900243E+02
34	7	2.3695485475E+00	9.0000040532E+01	-8.1775901528E+02
34	8	2.3695485475E+00	9.0500040532E+01	-8.1775902076E+02
34	9	2.3695485475E+00	9.1000040532E+01	-8.1775902348E+02
34	10	2.3695485475E+00	9.1500040532E+01	-8.1775898053E+02
34	11	2.3695485475E+00	9.2000040532E+01	-8.1775902188E+02
34	12	2.3695485475E+00	9.2500040532E+01	-8.1775901875E+02
34	13	2.3695485475E+00	9.3000040532E+01	-8.1775899687E+02
34	14	2.3695485475E+00	9.3500040532E+01	-8.1775903813E+02
34	15	2.3695485475E+00	9.4000040532E+01	-8.1775896130E+02
34	16	2.3695485475E+00	9.4500040532E+01	-8.1775904546E+02
34	17	2.3695485475E+00	9.5000040532E+01	-8.1775904051E+02
34	18	2.3695485475E+00	9.5500040532E+01	-8.1775902969E+02
34	19	2.3695485475E+00	9.6000040532E+01	-8.1775905026E+02
34	20	2.3695485475E+00	9.6500040532E+01	-8.1775906694E+02
34	21	2.3695485475E+00	9.7000040532E+01	-8.1775902906E+02

34	22	2.3695485475E+00	9.7500040532E+01	-8.1775909032E+02
34	23	2.3695485475E+00	9.8000040532E+01	-8.1775910655E+02
34	24	2.3695485475E+00	9.8500040532E+01	-8.1775912049E+02
34	25	2.3695485475E+00	9.9000040532E+01	-8.1775915467E+02
34	26	2.3695485475E+00	9.9500040532E+01	-8.1775917820E+02
34	27	2.3695485475E+00	1.0000004053E+02	-8.1775918783E+02
34	28	2.3695485475E+00	1.0050004053E+02	-8.1775920704E+02
34	29	2.3695485475E+00	1.0100004053E+02	-8.1775923559E+02
34	30	2.3695485475E+00	1.0150004053E+02	-8.1775924933E+02
34	31	2.3695485475E+00	1.0200004053E+02	-8.1775926014E+02
34	32	2.3695485475E+00	1.0250004053E+02	-8.1775926759E+02
34	33	2.3695485475E+00	1.0300004053E+02	-8.1775927104E+02
34	34	2.3695485475E+00	1.0350004053E+02	-8.1775927080E+02
34	35	2.3695485475E+00	1.0400004053E+02	-8.1775926663E+02
34	36	2.3695485475E+00	1.0450004053E+02	-8.1775925826E+02
34	37	2.3695485475E+00	1.0500004053E+02	-8.1775924627E+02
34	38	2.3695485475E+00	1.0550004053E+02	-8.1775923025E+02
34	39	2.3695485475E+00	1.0600004053E+02	-8.1775921128E+02
34	40	2.3695485475E+00	1.0650004053E+02	-8.1775918900E+02
34	41	2.3695485475E+00	1.0700004053E+02	-8.1775916379E+02
34	42	2.3695485475E+00	1.0750004053E+02	-8.1775913601E+02
34	43	2.3695485475E+00	1.0800004053E+02	-8.1775910666E+02
34	44	2.3695485475E+00	1.0850004053E+02	-8.1775907946E+02
34	45	2.3695485475E+00	1.0900004053E+02	-8.1775905668E+02
34	46	2.3695485475E+00	1.0950004053E+02	-8.1775903007E+02
34	47	2.3695485475E+00	1.1000004053E+02	-8.1775899960E+02
34	48	2.3695485475E+00	1.1050004053E+02	-8.1775896594E+02
34	49	2.3695485475E+00	1.1100004053E+02	-8.1775903705E+02
34	50	2.3695485475E+00	1.1150004053E+02	-8.1775900134E+02
34	51	2.3695485475E+00	1.1200004053E+02	-8.1775896478E+02
34	52	2.3695485475E+00	1.1250004053E+02	-8.1775892856E+02
34	53	2.3695485475E+00	1.1300004053E+02	-8.1775889209E+02
34	54	2.3695485475E+00	1.1350004053E+02	-8.1775885661E+02
34	55	2.3695485475E+00	1.1400004053E+02	-8.1775882312E+02
34	56	2.3695485475E+00	1.1450004053E+02	-8.1775879504E+02
34	57	2.3695485475E+00	1.1500004053E+02	-8.1775876492E+02
34	58	2.3695485475E+00	1.1550004053E+02	-8.1775873320E+02
34	59	2.3695485475E+00	1.1600004053E+02	-8.1775870083E+02
34	60	2.3695485475E+00	1.1650004053E+02	-8.1775866648E+02
34	61	2.3695485475E+00	1.1700004053E+02	-8.1775863052E+02
35	1	2.3795485475E+00	8.7000040532E+01	-8.1775857073E+02
35	2	2.3795485475E+00	8.7500040532E+01	-8.1775858050E+02
35	3	2.3795485475E+00	8.8000040532E+01	-8.1775861847E+02
35	4	2.3795485475E+00	8.8500040532E+01	-8.1775863791E+02
35	5	2.3795485475E+00	8.9000040532E+01	-8.1775865550E+02
35	6	2.3795485475E+00	8.9500040532E+01	-8.1775867335E+02
35	7	2.3795485475E+00	9.0000040532E+01	-8.1775868014E+02
35	8	2.3795485475E+00	9.0500040532E+01	-8.1775860039E+02
35	9	2.3795485475E+00	9.1000040532E+01	-8.1775869357E+02
35	10	2.3795485475E+00	9.1500040532E+01	-8.1775868823E+02
35	11	2.3795485475E+00	9.2000040532E+01	-8.1775869811E+02
35	12	2.3795485475E+00	9.2500040532E+01	-8.1775872339E+02

35	13	2.3795485475E+00	9.3000040532E+01	-8.1775865965E+02
35	14	2.3795485475E+00	9.3500040532E+01	-8.1775874793E+02
35	15	2.3795485475E+00	9.4000040532E+01	-8.1775875942E+02
35	16	2.3795485475E+00	9.4500040532E+01	-8.1775877162E+02
35	17	2.3795485475E+00	9.5000040532E+01	-8.1775874043E+02
35	18	2.3795485475E+00	9.5500040532E+01	-8.1775879166E+02
35	19	2.3795485475E+00	9.6000040532E+01	-8.1775876076E+02
35	20	2.3795485475E+00	9.6500040532E+01	-8.1775882517E+02
35	21	2.3795485475E+00	9.7000040532E+01	-8.1775884262E+02
35	22	2.3795485475E+00	9.7500040532E+01	-8.1775885969E+02
35	23	2.3795485475E+00	9.8000040532E+01	-8.1775888185E+02
35	24	2.3795485475E+00	9.8500040532E+01	-8.1775893292E+02
35	25	2.3795485475E+00	9.9000040532E+01	-8.1775895093E+02
35	26	2.3795485475E+00	9.9500040532E+01	-8.1775897809E+02
35	27	2.3795485475E+00	1.0000004053E+02	-8.1775901817E+02
35	28	2.3795485475E+00	1.0050004053E+02	-8.1775904144E+02
35	29	2.3795485475E+00	1.0100004053E+02	-8.1775906205E+02
35	30	2.3795485475E+00	1.0150004053E+02	-8.1775906123E+02
35	31	2.3795485475E+00	1.0200004053E+02	-8.1775908556E+02
35	32	2.3795485475E+00	1.0250004053E+02	-8.1775910371E+02
35	33	2.3795485475E+00	1.0300004053E+02	-8.1775911067E+02
35	34	2.3795485475E+00	1.0350004053E+02	-8.1775911356E+02
35	35	2.3795485475E+00	1.0400004053E+02	-8.1775911167E+02
35	36	2.3795485475E+00	1.0450004053E+02	-8.1775910569E+02
35	37	2.3795485475E+00	1.0500004053E+02	-8.1775909602E+02
35	38	2.3795485475E+00	1.0550004053E+02	-8.1775908238E+02
35	39	2.3795485475E+00	1.0600004053E+02	-8.1775906546E+02
35	40	2.3795485475E+00	1.0650004053E+02	-8.1775904488E+02
35	41	2.3795485475E+00	1.0700004053E+02	-8.1775902109E+02
35	42	2.3795485475E+00	1.0750004053E+02	-8.1775899413E+02
35	43	2.3795485475E+00	1.0800004053E+02	-8.1775896482E+02
35	44	2.3795485475E+00	1.0850004053E+02	-8.1775893535E+02
35	45	2.3795485475E+00	1.0900004053E+02	-8.1775891190E+02
35	46	2.3795485475E+00	1.0950004053E+02	-8.1775888580E+02
35	47	2.3795485475E+00	1.1000004053E+02	-8.1775885618E+02
35	48	2.3795485475E+00	1.1050004053E+02	-8.1775882273E+02
35	49	2.3795485475E+00	1.1100004053E+02	-8.1775888417E+02
35	50	2.3795485475E+00	1.1150004053E+02	-8.1775884583E+02
35	51	2.3795485475E+00	1.1200004053E+02	-8.1775880705E+02
35	52	2.3795485475E+00	1.1250004053E+02	-8.1775876877E+02
35	53	2.3795485475E+00	1.1300004053E+02	-8.1775873043E+02
35	54	2.3795485475E+00	1.1350004053E+02	-8.1775869296E+02
35	55	2.3795485475E+00	1.1400004053E+02	-8.1775857059E+02
35	56	2.3795485475E+00	1.1450004053E+02	-8.1775862513E+02
35	57	2.3795485475E+00	1.1500004053E+02	-8.1775859344E+02
35	58	2.3795485475E+00	1.1550004053E+02	-8.1775856133E+02
35	59	2.3795485475E+00	1.1600004053E+02	-8.1775852798E+02
35	60	2.3795485475E+00	1.1650004053E+02	-8.1775849277E+02
35	61	2.3795485475E+00	1.1700004053E+02	-8.1775845618E+02
36	1	2.3895485475E+00	8.7000040532E+01	-8.1775821991E+02
36	2	2.3895485475E+00	8.7500040532E+01	-8.1775824470E+02
36	3	2.3895485475E+00	8.8000040532E+01	-8.1775826006E+02

36	4	2.3895485475E+00	8.8500040532E+01	-8.1775829796E+02
36	5	2.3895485475E+00	8.9000040532E+01	-8.1775830180E+02
36	6	2.3895485475E+00	8.9500040532E+01	-8.1775823742E+02
36	7	2.3895485475E+00	9.0000040532E+01	-8.1775833059E+02
36	8	2.3895485475E+00	9.0500040532E+01	-8.1775831156E+02
36	9	2.3895485475E+00	9.1000040532E+01	-8.1775834921E+02
36	10	2.3895485475E+00	9.1500040532E+01	-8.1775838297E+02
36	11	2.3895485475E+00	9.2000040532E+01	-8.1775836028E+02
36	12	2.3895485475E+00	9.2500040532E+01	-8.1775839426E+02
36	13	2.3895485475E+00	9.3000040532E+01	-8.1775844334E+02
36	14	2.3895485475E+00	9.3500040532E+01	-8.1775842724E+02
36	15	2.3895485475E+00	9.4000040532E+01	-8.1775846774E+02
36	16	2.3895485475E+00	9.4500040532E+01	-8.1775845215E+02
36	17	2.3895485475E+00	9.5000040532E+01	-8.1775842846E+02
36	18	2.3895485475E+00	9.5500040532E+01	-8.1775854203E+02
36	19	2.3895485475E+00	9.6000040532E+01	-8.1775845975E+02
36	20	2.3895485475E+00	9.6500040532E+01	-8.1775858334E+02
36	21	2.3895485475E+00	9.7000040532E+01	-8.1775863049E+02
36	22	2.3895485475E+00	9.7500040532E+01	-8.1775867104E+02
36	23	2.3895485475E+00	9.8000040532E+01	-8.1775871047E+02
36	24	2.3895485475E+00	9.8500040532E+01	-8.1775874794E+02
36	25	2.3895485475E+00	9.9000040532E+01	-8.1775878334E+02
36	26	2.3895485475E+00	9.9500040532E+01	-8.1775881620E+02
36	27	2.3895485475E+00	1.0000004053E+02	-8.1775883794E+02
36	28	2.3895485475E+00	1.0050004053E+02	-8.1775884623E+02
36	29	2.3895485475E+00	1.0100004053E+02	-8.1775889092E+02
36	30	2.3895485475E+00	1.0150004053E+02	-8.1775891819E+02
36	31	2.3895485475E+00	1.0200004053E+02	-8.1775893586E+02
36	32	2.3895485475E+00	1.0250004053E+02	-8.1775895031E+02
36	33	2.3895485475E+00	1.0300004053E+02	-8.1775896084E+02
36	34	2.3895485475E+00	1.0350004053E+02	-8.1775896865E+02
36	35	2.3895485475E+00	1.0400004053E+02	-8.1775896958E+02
36	36	2.3895485475E+00	1.0450004053E+02	-8.1775896761E+02
36	37	2.3895485475E+00	1.0500004053E+02	-8.1775896172E+02
36	38	2.3895485475E+00	1.0550004053E+02	-8.1775895170E+02
36	39	2.3895485475E+00	1.0600004053E+02	-8.1775893775E+02
36	40	2.3895485475E+00	1.0650004053E+02	-8.1775892034E+02
36	41	2.3895485475E+00	1.0700004053E+02	-8.1775889920E+02
36	42	2.3895485475E+00	1.0750004053E+02	-8.1775887489E+02
36	43	2.3895485475E+00	1.0800004053E+02	-8.1775884749E+02
36	44	2.3895485475E+00	1.0850004053E+02	-8.1775881774E+02
36	45	2.3895485475E+00	1.0900004053E+02	-8.1775878758E+02
36	46	2.3895485475E+00	1.0950004053E+02	-8.1775876062E+02
36	47	2.3895485475E+00	1.1000004053E+02	-8.1775873385E+02
36	48	2.3895485475E+00	1.1050004053E+02	-8.1775870340E+02
36	49	2.3895485475E+00	1.1100004053E+02	-8.1775875804E+02
36	50	2.3895485475E+00	1.1150004053E+02	-8.1775871778E+02
36	51	2.3895485475E+00	1.1200004053E+02	-8.1775867751E+02
36	52	2.3895485475E+00	1.1250004053E+02	-8.1775863619E+02
36	53	2.3895485475E+00	1.1300004053E+02	-8.1775859431E+02
36	54	2.3895485475E+00	1.1350004053E+02	-8.1775855212E+02
36	55	2.3895485475E+00	1.1400004053E+02	-8.1775851020E+02

36	56	2.3895485475E+00	1.1450004053E+02	-8.1775846986E+02
36	57	2.3895485475E+00	1.1500004053E+02	-8.1775843415E+02
36	58	2.3895485475E+00	1.1550004053E+02	-8.1775839494E+02
36	59	2.3895485475E+00	1.1600004053E+02	-8.1775836111E+02
36	60	2.3895485475E+00	1.1650004053E+02	-8.1775800322E+02
36	61	2.3895485475E+00	1.1700004053E+02	-8.1775829241E+02
37	1	2.3995485475E+00	8.7000040532E+01	-8.1775786310E+02
37	2	2.3995485475E+00	8.7500040532E+01	-8.1775789489E+02
37	3	2.3995485475E+00	8.8000040532E+01	-8.1775792371E+02
37	4	2.3995485475E+00	8.8500040532E+01	-8.1775792807E+02
37	5	2.3995485475E+00	8.9000040532E+01	-8.1775797156E+02
37	6	2.3995485475E+00	8.9500040532E+01	-8.1775793447E+02
37	7	2.3995485475E+00	9.0000040532E+01	-8.1775800781E+02
37	8	2.3995485475E+00	9.0500040532E+01	-8.1775801116E+02
37	9	2.3995485475E+00	9.1000040532E+01	-8.1775804645E+02
37	10	2.3995485475E+00	9.1500040532E+01	-8.1775799503E+02
37	11	2.3995485475E+00	9.2000040532E+01	-8.1775801085E+02
37	12	2.3995485475E+00	9.2500040532E+01	-8.1775812259E+02
37	13	2.3995485475E+00	9.3000040532E+01	-8.1775814468E+02
37	14	2.3995485475E+00	9.3500040532E+01	-8.1775817430E+02
37	15	2.3995485475E+00	9.4000040532E+01	-8.1775816504E+02
37	16	2.3995485475E+00	9.4500040532E+01	-8.1775822573E+02
37	17	2.3995485475E+00	9.5000040532E+01	-8.1775826751E+02
37	18	2.3995485475E+00	9.5500040532E+01	-8.1775829047E+02
37	19	2.3995485475E+00	9.6000040532E+01	-8.1775834366E+02
37	20	2.3995485475E+00	9.6500040532E+01	-8.1775839348E+02
37	21	2.3995485475E+00	9.7000040532E+01	-8.1775844283E+02
37	22	2.3995485475E+00	9.7500040532E+01	-8.1775847690E+02
37	23	2.3995485475E+00	9.8000040532E+01	-8.1775852087E+02
37	24	2.3995485475E+00	9.8500040532E+01	-8.1775855757E+02
37	25	2.3995485475E+00	9.9000040532E+01	-8.1775860689E+02
37	26	2.3995485475E+00	9.9500040532E+01	-8.1775865318E+02
37	27	2.3995485475E+00	1.0000004053E+02	-8.1775868604E+02
37	28	2.3995485475E+00	1.0050004053E+02	-8.1775871651E+02
37	29	2.3995485475E+00	1.0100004053E+02	-8.1775874350E+02
37	30	2.3995485475E+00	1.0150004053E+02	-8.1775876808E+02
37	31	2.3995485475E+00	1.0200004053E+02	-8.1775879013E+02
37	32	2.3995485475E+00	1.0250004053E+02	-8.1775880944E+02
37	33	2.3995485475E+00	1.0300004053E+02	-8.1775882681E+02
37	34	2.3995485475E+00	1.0350004053E+02	-8.1775883913E+02
37	35	2.3995485475E+00	1.0400004053E+02	-8.1775884775E+02
37	36	2.3995485475E+00	1.0450004053E+02	-8.1775885148E+02
37	37	2.3995485475E+00	1.0500004053E+02	-8.1775885109E+02
37	38	2.3995485475E+00	1.0550004053E+02	-8.1775884613E+02
37	39	2.3995485475E+00	1.0600004053E+02	-8.1775883738E+02
37	40	2.3995485475E+00	1.0650004053E+02	-8.1775882446E+02
37	41	2.3995485475E+00	1.0700004053E+02	-8.1775880824E+02
37	42	2.3995485475E+00	1.0750004053E+02	-8.1775878843E+02
37	43	2.3995485475E+00	1.0800004053E+02	-8.1775876557E+02
37	44	2.3995485475E+00	1.0850004053E+02	-8.1775873983E+02
37	45	2.3995485475E+00	1.0900004053E+02	-8.1775871162E+02
37	46	2.3995485475E+00	1.0950004053E+02	-8.1775868195E+02

37	47	2.3995485475E+00	1.1000004053E+02	-8.1775865335E+02
37	48	2.3995485475E+00	1.1050004053E+02	-8.1775862629E+02
37	49	2.3995485475E+00	1.1100004053E+02	-8.1775868836E+02
37	50	2.3995485475E+00	1.1150004053E+02	-8.1775864970E+02
37	51	2.3995485475E+00	1.1200004053E+02	-8.1775861029E+02
37	52	2.3995485475E+00	1.1250004053E+02	-8.1775857123E+02
37	53	2.3995485475E+00	1.1300004053E+02	-8.1775853205E+02
37	54	2.3995485475E+00	1.1350004053E+02	-8.1775849188E+02
37	55	2.3995485475E+00	1.1400004053E+02	-8.1775845077E+02
37	56	2.3995485475E+00	1.1450004053E+02	-8.1775840875E+02
37	57	2.3995485475E+00	1.1500004053E+02	-8.1775836616E+02
37	58	2.3995485475E+00	1.1550004053E+02	-8.1775832349E+02
37	59	2.3995485475E+00	1.1600004053E+02	-8.1775828072E+02
37	60	2.3995485475E+00	1.1650004053E+02	-8.1775823799E+02
37	61	2.3995485475E+00	1.1700004053E+02	-8.1775819386E+02
38	1	2.4095485475E+00	8.7000040532E+01	-8.1775750221E+02
38	2	2.4095485475E+00	8.7500040532E+01	-8.1775751621E+02
38	3	2.4095485475E+00	8.8000040532E+01	-8.1775756434E+02
38	4	2.4095485475E+00	8.8500040532E+01	-8.1775759121E+02
38	5	2.4095485475E+00	8.9000040532E+01	-8.1775762296E+02
38	6	2.4095485475E+00	8.9500040532E+01	-8.1775762118E+02
38	7	2.4095485475E+00	9.0000040532E+01	-8.1775766656E+02
38	8	2.4095485475E+00	9.0500040532E+01	-8.1775769957E+02
38	9	2.4095485475E+00	9.1000040532E+01	-8.1775773664E+02
38	10	2.4095485475E+00	9.1500040532E+01	-8.1775773465E+02
38	11	2.4095485475E+00	9.2000040532E+01	-8.1775780700E+02
38	12	2.4095485475E+00	9.2500040532E+01	-8.1775784115E+02
38	13	2.4095485475E+00	9.3000040532E+01	-8.1775783627E+02
38	14	2.4095485475E+00	9.3500040532E+01	-8.1775791144E+02
38	15	2.4095485475E+00	9.4000040532E+01	-8.1775785323E+02
38	16	2.4095485475E+00	9.4500040532E+01	-8.1775798995E+02
38	17	2.4095485475E+00	9.5000040532E+01	-8.1775801419E+02
38	18	2.4095485475E+00	9.5500040532E+01	-8.1775809901E+02
38	19	2.4095485475E+00	9.6000040532E+01	-8.1775815897E+02
38	20	2.4095485475E+00	9.6500040532E+01	-8.1775820511E+02
38	21	2.4095485475E+00	9.7000040532E+01	-8.1775825606E+02
38	22	2.4095485475E+00	9.7500040532E+01	-8.1775832976E+02
38	23	2.4095485475E+00	9.8000040532E+01	-8.1775838154E+02
38	24	2.4095485475E+00	9.8500040532E+01	-8.1775842987E+02
38	25	2.4095485475E+00	9.9000040532E+01	-8.1775847547E+02
38	26	2.4095485475E+00	9.9500040532E+01	-8.1775851901E+02
38	27	2.4095485475E+00	1.0000004053E+02	-8.1775856012E+02
38	28	2.4095485475E+00	1.0050004053E+02	-8.1775859789E+02
38	29	2.4095485475E+00	1.0100004053E+02	-8.1775863125E+02
38	30	2.4095485475E+00	1.0150004053E+02	-8.1775865996E+02
38	31	2.4095485475E+00	1.0200004053E+02	-8.1775868375E+02
38	32	2.4095485475E+00	1.0250004053E+02	-8.1775870332E+02
38	33	2.4095485475E+00	1.0300004053E+02	-8.1775871916E+02
38	34	2.4095485475E+00	1.0350004053E+02	-8.1775873249E+02
38	35	2.4095485475E+00	1.0400004053E+02	-8.1775874903E+02
38	36	2.4095485475E+00	1.0450004053E+02	-8.1775876188E+02
38	37	2.4095485475E+00	1.0500004053E+02	-8.1775876954E+02

38	38	2.4095485475E+00	1.0550004053E+02	-8.1775877195E+02
38	39	2.4095485475E+00	1.0600004053E+02	-8.1775876879E+02
38	40	2.4095485475E+00	1.0650004053E+02	-8.1775876221E+02
38	41	2.4095485475E+00	1.0700004053E+02	-8.1775875033E+02
38	42	2.4095485475E+00	1.0750004053E+02	-8.1775873554E+02
38	43	2.4095485475E+00	1.0800004053E+02	-8.1775871756E+02
38	44	2.4095485475E+00	1.0850004053E+02	-8.1775869627E+02
38	45	2.4095485475E+00	1.0900004053E+02	-8.1775867245E+02
38	46	2.4095485475E+00	1.0950004053E+02	-8.1775864610E+02
38	47	2.4095485475E+00	1.1000004053E+02	-8.1775861834E+02
38	48	2.4095485475E+00	1.1050004053E+02	-8.1775859115E+02
38	49	2.4095485475E+00	1.1100004053E+02	-8.1775865687E+02
38	50	2.4095485475E+00	1.1150004053E+02	-8.1775862184E+02
38	51	2.4095485475E+00	1.1200004053E+02	-8.1775858611E+02
38	52	2.4095485475E+00	1.1250004053E+02	-8.1775854993E+02
38	53	2.4095485475E+00	1.1300004053E+02	-8.1775851407E+02
38	54	2.4095485475E+00	1.1350004053E+02	-8.1775847765E+02
38	55	2.4095485475E+00	1.1400004053E+02	-8.1775844023E+02
38	56	2.4095485475E+00	1.1450004053E+02	-8.1775840160E+02
38	57	2.4095485475E+00	1.1500004053E+02	-8.1775836191E+02
38	58	2.4095485475E+00	1.1550004053E+02	-8.1775832144E+02
38	59	2.4095485475E+00	1.1600004053E+02	-8.1775828078E+02
38	60	2.4095485475E+00	1.1650004053E+02	-8.1775824012E+02
38	61	2.4095485475E+00	1.1700004053E+02	-8.1775819986E+02
39	1	2.4195485475E+00	8.7000040532E+01	-8.1775713454E+02
39	2	2.4195485475E+00	8.7500040532E+01	-8.1775717110E+02
39	3	2.4195485475E+00	8.8000040532E+01	-8.1775719364E+02
39	4	2.4195485475E+00	8.8500040532E+01	-8.1775724427E+02
39	5	2.4195485475E+00	8.9000040532E+01	-8.1775726968E+02
39	6	2.4195485475E+00	8.9500040532E+01	-8.1775729736E+02
39	7	2.4195485475E+00	9.0000040532E+01	-8.1775734305E+02
39	8	2.4195485475E+00	9.0500040532E+01	-8.1775728487E+02
39	9	2.4195485475E+00	9.1000040532E+01	-8.1775743297E+02
39	10	2.4195485475E+00	9.1500040532E+01	-8.1775746659E+02
39	11	2.4195485475E+00	9.2000040532E+01	-8.1775750917E+02
39	12	2.4195485475E+00	9.2500040532E+01	-8.1775747025E+02
39	13	2.4195485475E+00	9.3000040532E+01	-8.1775751956E+02
39	14	2.4195485475E+00	9.3500040532E+01	-8.1775765668E+02
39	15	2.4195485475E+00	9.4000040532E+01	-8.1775771571E+02
39	16	2.4195485475E+00	9.4500040532E+01	-8.1775777445E+02
39	17	2.4195485475E+00	9.5000040532E+01	-8.1775775342E+02
39	18	2.4195485475E+00	9.5500040532E+01	-8.1775791219E+02
39	19	2.4195485475E+00	9.6000040532E+01	-8.1775797545E+02
39	20	2.4195485475E+00	9.6500040532E+01	-8.1775806734E+02
39	21	2.4195485475E+00	9.7000040532E+01	-8.1775813442E+02
39	22	2.4195485475E+00	9.7500040532E+01	-8.1775820033E+02
39	23	2.4195485475E+00	9.8000040532E+01	-8.1775824007E+02
39	24	2.4195485475E+00	9.8500040532E+01	-8.1775832742E+02
39	25	2.4195485475E+00	9.9000040532E+01	-8.1775835700E+02
39	26	2.4195485475E+00	9.9500040532E+01	-8.1775844179E+02
39	27	2.4195485475E+00	1.0000004053E+02	-8.1775849170E+02
39	28	2.4195485475E+00	1.0050004053E+02	-8.1775853653E+02

39	29	2.4195485475E+00	1.0100004053E+02	-8.1775857592E+02
39	30	2.4195485475E+00	1.0150004053E+02	-8.1775861006E+02
39	31	2.4195485475E+00	1.0200004053E+02	-8.1775863852E+02
39	32	2.4195485475E+00	1.0250004053E+02	-8.1775866250E+02
39	33	2.4195485475E+00	1.0300004053E+02	-8.1775868066E+02
39	34	2.4195485475E+00	1.0350004053E+02	-8.1775869396E+02
39	35	2.4195485475E+00	1.0400004053E+02	-8.1775870232E+02
39	36	2.4195485475E+00	1.0450004053E+02	-8.1775870729E+02
39	37	2.4195485475E+00	1.0500004053E+02	-8.1775871270E+02
39	38	2.4195485475E+00	1.0550004053E+02	-8.1775872471E+02
39	39	2.4195485475E+00	1.0600004053E+02	-8.1775873009E+02
39	40	2.4195485475E+00	1.0650004053E+02	-8.1775872837E+02
39	41	2.4195485475E+00	1.0700004053E+02	-8.1775872229E+02
39	42	2.4195485475E+00	1.0750004053E+02	-8.1775871190E+02
39	43	2.4195485475E+00	1.0800004053E+02	-8.1775869811E+02
39	44	2.4195485475E+00	1.0850004053E+02	-8.1775868093E+02
39	45	2.4195485475E+00	1.0900004053E+02	-8.1775866093E+02
39	46	2.4195485475E+00	1.0950004053E+02	-8.1775863826E+02
39	47	2.4195485475E+00	1.1000004053E+02	-8.1775861355E+02
39	48	2.4195485475E+00	1.1050004053E+02	-8.1775858777E+02
39	49	2.4195485475E+00	1.1100004053E+02	-8.1775865433E+02
39	50	2.4195485475E+00	1.1150004053E+02	-8.1775862176E+02
39	51	2.4195485475E+00	1.1200004053E+02	-8.1775858913E+02
39	52	2.4195485475E+00	1.1250004053E+02	-8.1775855633E+02
39	53	2.4195485475E+00	1.1300004053E+02	-8.1775852395E+02
39	54	2.4195485475E+00	1.1350004053E+02	-8.1775849127E+02
39	55	2.4195485475E+00	1.1400004053E+02	-8.1775845755E+02
39	56	2.4195485475E+00	1.1450004053E+02	-8.1775842254E+02
39	57	2.4195485475E+00	1.1500004053E+02	-8.1775838636E+02
39	58	2.4195485475E+00	1.1550004053E+02	-8.1775834905E+02
39	59	2.4195485475E+00	1.1600004053E+02	-8.1775831116E+02
39	60	2.4195485475E+00	1.1650004053E+02	-8.1775827298E+02
39	61	2.4195485475E+00	1.1700004053E+02	-8.1775823519E+02
40	1	2.4295485475E+00	8.7000040532E+01	-8.1775677522E+02
40	2	2.4295485475E+00	8.7500040532E+01	-8.1775681690E+02
40	3	2.4295485475E+00	8.8000040532E+01	-8.1775685588E+02
40	4	2.4295485475E+00	8.8500040532E+01	-8.1775677907E+02
40	5	2.4295485475E+00	8.9000040532E+01	-8.1775690738E+02
40	6	2.4295485475E+00	8.9500040532E+01	-8.1775686793E+02
40	7	2.4295485475E+00	9.0000040532E+01	-8.1775702213E+02
40	8	2.4295485475E+00	9.0500040532E+01	-8.1775703420E+02
40	9	2.4295485475E+00	9.1000040532E+01	-8.1775712873E+02
40	10	2.4295485475E+00	9.1500040532E+01	-8.1775719059E+02
40	11	2.4295485475E+00	9.2000040532E+01	-8.1775720317E+02
40	12	2.4295485475E+00	9.2500040532E+01	-8.1775728011E+02
40	13	2.4295485475E+00	9.3000040532E+01	-8.1775736636E+02
40	14	2.4295485475E+00	9.3500040532E+01	-8.1775743361E+02
40	15	2.4295485475E+00	9.4000040532E+01	-8.1775753100E+02
40	16	2.4295485475E+00	9.4500040532E+01	-8.1775761557E+02
40	17	2.4295485475E+00	9.5000040532E+01	-8.1775770089E+02
40	18	2.4295485475E+00	9.5500040532E+01	-8.1775778535E+02
40	19	2.4295485475E+00	9.6000040532E+01	-8.1775786937E+02

40	20	2.4295485475E+00	9.6500040532E+01	-8.1775795302E+02
40	21	2.4295485475E+00	9.7000040532E+01	-8.1775800842E+02
40	22	2.4295485475E+00	9.7500040532E+01	-8.1775811874E+02
40	23	2.4295485475E+00	9.8000040532E+01	-8.1775819615E+02
40	24	2.4295485475E+00	9.8500040532E+01	-8.1775826934E+02
40	25	2.4295485475E+00	9.9000040532E+01	-8.1775833685E+02
40	26	2.4295485475E+00	9.9500040532E+01	-8.1775839900E+02
40	27	2.4295485475E+00	1.0000004053E+02	-8.1775845504E+02
40	28	2.4295485475E+00	1.0050004053E+02	-8.1775850562E+02
40	29	2.4295485475E+00	1.0100004053E+02	-8.1775855033E+02
40	30	2.4295485475E+00	1.0150004053E+02	-8.1775858939E+02
40	31	2.4295485475E+00	1.0200004053E+02	-8.1775862231E+02
40	32	2.4295485475E+00	1.0250004053E+02	-8.1775864977E+02
40	33	2.4295485475E+00	1.0300004053E+02	-8.1775867156E+02
40	34	2.4295485475E+00	1.0350004053E+02	-8.1775868801E+02
40	35	2.4295485475E+00	1.0400004053E+02	-8.1775869932E+02
40	36	2.4295485475E+00	1.0450004053E+02	-8.1775870566E+02
40	37	2.4295485475E+00	1.0500004053E+02	-8.1775870793E+02
40	38	2.4295485475E+00	1.0550004053E+02	-8.1775870662E+02
40	39	2.4295485475E+00	1.0600004053E+02	-8.1775871743E+02
40	40	2.4295485475E+00	1.0650004053E+02	-8.1775872289E+02
40	41	2.4295485475E+00	1.0700004053E+02	-8.1775872071E+02
40	42	2.4295485475E+00	1.0750004053E+02	-8.1775871428E+02
40	43	2.4295485475E+00	1.0800004053E+02	-8.1775870372E+02
40	44	2.4295485475E+00	1.0850004053E+02	-8.1775869004E+02
40	45	2.4295485475E+00	1.0900004053E+02	-8.1775867318E+02
40	46	2.4295485475E+00	1.0950004053E+02	-8.1775865362E+02
40	47	2.4295485475E+00	1.1000004053E+02	-8.1775863185E+02
40	48	2.4295485475E+00	1.1050004053E+02	-8.1775860855E+02
40	49	2.4295485475E+00	1.1100004053E+02	-8.1775867497E+02
40	50	2.4295485475E+00	1.1150004053E+02	-8.1775864469E+02
40	51	2.4295485475E+00	1.1200004053E+02	-8.1775861483E+02
40	52	2.4295485475E+00	1.1250004053E+02	-8.1775858522E+02
40	53	2.4295485475E+00	1.1300004053E+02	-8.1775855632E+02
40	54	2.4295485475E+00	1.1350004053E+02	-8.1775852715E+02
40	55	2.4295485475E+00	1.1400004053E+02	-8.1775849705E+02
40	56	2.4295485475E+00	1.1450004053E+02	-8.1775846559E+02
40	57	2.4295485475E+00	1.1500004053E+02	-8.1775843280E+02
40	58	2.4295485475E+00	1.1550004053E+02	-8.1775839880E+02
40	59	2.4295485475E+00	1.1600004053E+02	-8.1775836398E+02
40	60	2.4295485475E+00	1.1650004053E+02	-8.1775832869E+02
40	61	2.4295485475E+00	1.1700004053E+02	-8.1775829367E+02
41	1	2.4395485475E+00	8.7000040532E+01	-8.1775640813E+02
41	2	2.4395485475E+00	8.7500040532E+01	-8.1775632022E+02
41	3	2.4395485475E+00	8.8000040532E+01	-8.1775650232E+02
41	4	2.4395485475E+00	8.8500040532E+01	-8.1775649776E+02
41	5	2.4395485475E+00	8.9000040532E+01	-8.1775660323E+02
41	6	2.4395485475E+00	8.9500040532E+01	-8.1775661250E+02
41	7	2.4395485475E+00	9.0000040532E+01	-8.1775669350E+02
41	8	2.4395485475E+00	9.0500040532E+01	-8.1775677803E+02
41	9	2.4395485475E+00	9.1000040532E+01	-8.1775681765E+02
41	10	2.4395485475E+00	9.1500040532E+01	-8.1775692045E+02

41	11	2.4395485475E+00	9.2000040532E+01	-8.1775689161E+02
41	12	2.4395485475E+00	9.2500040532E+01	-8.1775708521E+02
41	13	2.4395485475E+00	9.3000040532E+01	-8.1775718283E+02
41	14	2.4395485475E+00	9.3500040532E+01	-8.1775728172E+02
41	15	2.4395485475E+00	9.4000040532E+01	-8.1775735346E+02
41	16	2.4395485475E+00	9.4500040532E+01	-8.1775745519E+02
41	17	2.4395485475E+00	9.5000040532E+01	-8.1775755791E+02
41	18	2.4395485475E+00	9.5500040532E+01	-8.1775768852E+02
41	19	2.4395485475E+00	9.6000040532E+01	-8.1775776080E+02
41	20	2.4395485475E+00	9.6500040532E+01	-8.1775789268E+02
41	21	2.4395485475E+00	9.7000040532E+01	-8.1775798958E+02
41	22	2.4395485475E+00	9.7500040532E+01	-8.1775808054E+02
41	23	2.4395485475E+00	9.8000040532E+01	-8.1775816605E+02
41	24	2.4395485475E+00	9.8500040532E+01	-8.1775824585E+02
41	25	2.4395485475E+00	9.9000040532E+01	-8.1775831940E+02
41	26	2.4395485475E+00	9.9500040532E+01	-8.1775838677E+02
41	27	2.4395485475E+00	1.0000004053E+02	-8.1775844762E+02
41	28	2.4395485475E+00	1.0050004053E+02	-8.1775850286E+02
41	29	2.4395485475E+00	1.0100004053E+02	-8.1775855127E+02
41	30	2.4395485475E+00	1.0150004053E+02	-8.1775859399E+02
41	31	2.4395485475E+00	1.0200004053E+02	-8.1775863045E+02
41	32	2.4395485475E+00	1.0250004053E+02	-8.1775866105E+02
41	33	2.4395485475E+00	1.0300004053E+02	-8.1775868558E+02
41	34	2.4395485475E+00	1.0350004053E+02	-8.1775870471E+02
41	35	2.4395485475E+00	1.0400004053E+02	-8.1775871819E+02
41	36	2.4395485475E+00	1.0450004053E+02	-8.1775872664E+02
41	37	2.4395485475E+00	1.0500004053E+02	-8.1775873006E+02
41	38	2.4395485475E+00	1.0550004053E+02	-8.1775872947E+02
41	39	2.4395485475E+00	1.0600004053E+02	-8.1775872691E+02
41	40	2.4395485475E+00	1.0650004053E+02	-8.1775874169E+02
41	41	2.4395485475E+00	1.0700004053E+02	-8.1775874329E+02
41	42	2.4395485475E+00	1.0750004053E+02	-8.1775873998E+02
41	43	2.4395485475E+00	1.0800004053E+02	-8.1775873225E+02
41	44	2.4395485475E+00	1.0850004053E+02	-8.1775872115E+02
41	45	2.4395485475E+00	1.0900004053E+02	-8.1775870679E+02
41	46	2.4395485475E+00	1.0950004053E+02	-8.1775868980E+02
41	47	2.4395485475E+00	1.1000004053E+02	-8.1775867059E+02
41	48	2.4395485475E+00	1.1050004053E+02	-8.1775864972E+02
41	49	2.4395485475E+00	1.1100004053E+02	-8.1775871552E+02
41	50	2.4395485475E+00	1.1150004053E+02	-8.1775868771E+02
41	51	2.4395485475E+00	1.1200004053E+02	-8.1775866048E+02
41	52	2.4395485475E+00	1.1250004053E+02	-8.1775863426E+02
41	53	2.4395485475E+00	1.1300004053E+02	-8.1775860888E+02
41	54	2.4395485475E+00	1.1350004053E+02	-8.1775858312E+02
41	55	2.4395485475E+00	1.1400004053E+02	-8.1775855634E+02
41	56	2.4395485475E+00	1.1450004053E+02	-8.1775852812E+02
41	57	2.4395485475E+00	1.1500004053E+02	-8.1775849860E+02
41	58	2.4395485475E+00	1.1550004053E+02	-8.1775846775E+02
41	59	2.4395485475E+00	1.1600004053E+02	-8.1775843610E+02
41	60	2.4395485475E+00	1.1650004053E+02	-8.1775840388E+02
41	61	2.4395485475E+00	1.1700004053E+02	-8.1775837180E+02
42	1	2.4495485475E+00	8.7000040532E+01	-8.1775605417E+02

42	2	2.4495485475E+00	8.7500040532E+01	-8.1775603277E+02
42	3	2.4495485475E+00	8.8000040532E+01	-8.1775614946E+02
42	4	2.4495485475E+00	8.8500040532E+01	-8.1775621144E+02
42	5	2.4495485475E+00	8.9000040532E+01	-8.1775628573E+02
42	6	2.4495485475E+00	8.9500040532E+01	-8.1775635366E+02
42	7	2.4495485475E+00	9.0000040532E+01	-8.1775635943E+02
42	8	2.4495485475E+00	9.0500040532E+01	-8.1775651771E+02
42	9	2.4495485475E+00	9.1000040532E+01	-8.1775650157E+02
42	10	2.4495485475E+00	9.1500040532E+01	-8.1775669645E+02
42	11	2.4495485475E+00	9.2000040532E+01	-8.1775680935E+02
42	12	2.4495485475E+00	9.2500040532E+01	-8.1775689236E+02
42	13	2.4495485475E+00	9.3000040532E+01	-8.1775704519E+02
42	14	2.4495485475E+00	9.3500040532E+01	-8.1775716581E+02
42	15	2.4495485475E+00	9.4000040532E+01	-8.1775728793E+02
42	16	2.4495485475E+00	9.4500040532E+01	-8.1775741088E+02
42	17	2.4495485475E+00	9.5000040532E+01	-8.1775753315E+02
42	18	2.4495485475E+00	9.5500040532E+01	-8.1775765390E+02
42	19	2.4495485475E+00	9.6000040532E+01	-8.1775776991E+02
42	20	2.4495485475E+00	9.6500040532E+01	-8.1775787952E+02
42	21	2.4495485475E+00	9.7000040532E+01	-8.1775798332E+02
42	22	2.4495485475E+00	9.7500040532E+01	-8.1775808069E+02
42	23	2.4495485475E+00	9.8000040532E+01	-8.1775817102E+02
42	24	2.4495485475E+00	9.8500040532E+01	-8.1775825533E+02
42	25	2.4495485475E+00	9.9000040532E+01	-8.1775833258E+02
42	26	2.4495485475E+00	9.9500040532E+01	-8.1775840380E+02
42	27	2.4495485475E+00	1.0000004053E+02	-8.1775846769E+02
42	28	2.4495485475E+00	1.0050004053E+02	-8.1775852584E+02
42	29	2.4495485475E+00	1.0100004053E+02	-8.1775857705E+02
42	30	2.4495485475E+00	1.0150004053E+02	-8.1775862257E+02
42	31	2.4495485475E+00	1.0200004053E+02	-8.1775866139E+02
42	32	2.4495485475E+00	1.0250004053E+02	-8.1775869408E+02
42	33	2.4495485475E+00	1.0300004053E+02	-8.1775872067E+02
42	34	2.4495485475E+00	1.0350004053E+02	-8.1775874160E+02
42	35	2.4495485475E+00	1.0400004053E+02	-8.1775875676E+02
42	36	2.4495485475E+00	1.0450004053E+02	-8.1775876658E+02
42	37	2.4495485475E+00	1.0500004053E+02	-8.1775877153E+02
42	38	2.4495485475E+00	1.0550004053E+02	-8.1775877203E+02
42	39	2.4495485475E+00	1.0600004053E+02	-8.1775876948E+02
42	40	2.4495485475E+00	1.0650004053E+02	-8.1775878452E+02
42	41	2.4495485475E+00	1.0700004053E+02	-8.1775878865E+02
42	42	2.4495485475E+00	1.0750004053E+02	-8.1775878736E+02
42	43	2.4495485475E+00	1.0800004053E+02	-8.1775878155E+02
42	44	2.4495485475E+00	1.0850004053E+02	-8.1775877231E+02
42	45	2.4495485475E+00	1.0900004053E+02	-8.1775876009E+02
42	46	2.4495485475E+00	1.0950004053E+02	-8.1775874526E+02
42	47	2.4495485475E+00	1.1000004053E+02	-8.1775872820E+02
42	48	2.4495485475E+00	1.1050004053E+02	-8.1775870991E+02
42	49	2.4495485475E+00	1.1100004053E+02	-8.1775877417E+02
42	50	2.4495485475E+00	1.1150004053E+02	-8.1775874908E+02
42	51	2.4495485475E+00	1.1200004053E+02	-8.1775872483E+02
42	52	2.4495485475E+00	1.1250004053E+02	-8.1775870208E+02
42	53	2.4495485475E+00	1.1300004053E+02	-8.1775868014E+02

42	54	2.4495485475E+00	1.1350004053E+02	-8.1775865761E+02
42	55	2.4495485475E+00	1.1400004053E+02	-8.1775863391E+02
42	56	2.4495485475E+00	1.1450004053E+02	-8.1775860873E+02
42	57	2.4495485475E+00	1.1500004053E+02	-8.1775858223E+02
42	58	2.4495485475E+00	1.1550004053E+02	-8.1775855440E+02
42	59	2.4495485475E+00	1.1600004053E+02	-8.1775852580E+02
42	60	2.4495485475E+00	1.1650004053E+02	-8.1775849660E+02
42	61	2.4495485475E+00	1.1700004053E+02	-8.1775846765E+02
43	1	2.4595485475E+00	8.7000040532E+01	-8.1775569585E+02
43	2	2.4595485475E+00	8.7500040532E+01	-8.1775574120E+02
43	3	2.4595485475E+00	8.8000040532E+01	-8.1775579020E+02
43	4	2.4595485475E+00	8.8500040532E+01	-8.1775591982E+02
43	5	2.4595485475E+00	8.9000040532E+01	-8.1775596472E+02
43	6	2.4595485475E+00	8.9500040532E+01	-8.1775609051E+02
43	7	2.4595485475E+00	9.0000040532E+01	-8.1775617818E+02
43	8	2.4595485475E+00	9.0500040532E+01	-8.1775623467E+02
43	9	2.4595485475E+00	9.1000040532E+01	-8.1775641287E+02
43	10	2.4595485475E+00	9.1500040532E+01	-8.1775651161E+02
43	11	2.4595485475E+00	9.2000040532E+01	-8.1775669239E+02
43	12	2.4595485475E+00	9.2500040532E+01	-8.1775683607E+02
43	13	2.4595485475E+00	9.3000040532E+01	-8.1775697870E+02
43	14	2.4595485475E+00	9.3500040532E+01	-8.1775712373E+02
43	15	2.4595485475E+00	9.4000040532E+01	-8.1775726554E+02
43	16	2.4595485475E+00	9.4500040532E+01	-8.1775740633E+02
43	17	2.4595485475E+00	9.5000040532E+01	-8.1775754117E+02
43	18	2.4595485475E+00	9.5500040532E+01	-8.1775767024E+02
43	19	2.4595485475E+00	9.6000040532E+01	-8.1775779111E+02
43	20	2.4595485475E+00	9.6500040532E+01	-8.1775790600E+02
43	21	2.4595485475E+00	9.7000040532E+01	-8.1775801355E+02
43	22	2.4595485475E+00	9.7500040532E+01	-8.1775811430E+02
43	23	2.4595485475E+00	9.8000040532E+01	-8.1775820766E+02
43	24	2.4595485475E+00	9.8500040532E+01	-8.1775829434E+02
43	25	2.4595485475E+00	9.9000040532E+01	-8.1775837402E+02
43	26	2.4595485475E+00	9.9500040532E+01	-8.1775844745E+02
43	27	2.4595485475E+00	1.0000004053E+02	-8.1775851320E+02
43	28	2.4595485475E+00	1.0050004053E+02	-8.1775857348E+02
43	29	2.4595485475E+00	1.0100004053E+02	-8.1775862607E+02
43	30	2.4595485475E+00	1.0150004053E+02	-8.1775867307E+02
43	31	2.4595485475E+00	1.0200004053E+02	-8.1775871318E+02
43	32	2.4595485475E+00	1.0250004053E+02	-8.1775874745E+02
43	33	2.4595485475E+00	1.0300004053E+02	-8.1775877531E+02
43	34	2.4595485475E+00	1.0350004053E+02	-8.1775879745E+02
43	35	2.4595485475E+00	1.0400004053E+02	-8.1775881374E+02
43	36	2.4595485475E+00	1.0450004053E+02	-8.1775882469E+02
43	37	2.4595485475E+00	1.0500004053E+02	-8.1775883060E+02
43	38	2.4595485475E+00	1.0550004053E+02	-8.1775883205E+02
43	39	2.4595485475E+00	1.0600004053E+02	-8.1775883062E+02
43	40	2.4595485475E+00	1.0650004053E+02	-8.1775884984E+02
43	41	2.4595485475E+00	1.0700004053E+02	-8.1775885453E+02
43	42	2.4595485475E+00	1.0750004053E+02	-8.1775885431E+02
43	43	2.4595485475E+00	1.0800004053E+02	-8.1775885000E+02
43	44	2.4595485475E+00	1.0850004053E+02	-8.1775884240E+02

43	45	2.4595485475E+00	1.0900004053E+02	-8.1775883184E+02
43	46	2.4595485475E+00	1.0950004053E+02	-8.1775881874E+02
43	47	2.4595485475E+00	1.1000004053E+02	-8.1775880363E+02
43	48	2.4595485475E+00	1.1050004053E+02	-8.1775878780E+02
43	49	2.4595485475E+00	1.1100004053E+02	-8.1775885005E+02
43	50	2.4595485475E+00	1.1150004053E+02	-8.1775882772E+02
43	51	2.4595485475E+00	1.1200004053E+02	-8.1775880694E+02
43	52	2.4595485475E+00	1.1250004053E+02	-8.1775878792E+02
43	53	2.4595485475E+00	1.1300004053E+02	-8.1775876916E+02
43	54	2.4595485475E+00	1.1350004053E+02	-8.1775874956E+02
43	55	2.4595485475E+00	1.1400004053E+02	-8.1775872873E+02
43	56	2.4595485475E+00	1.1450004053E+02	-8.1775870637E+02
43	57	2.4595485475E+00	1.1500004053E+02	-8.1775868266E+02
43	58	2.4595485475E+00	1.1550004053E+02	-8.1775865772E+02
43	59	2.4595485475E+00	1.1600004053E+02	-8.1775863204E+02
43	60	2.4595485475E+00	1.1650004053E+02	-8.1775860591E+02
43	61	2.4595485475E+00	1.1700004053E+02	-8.1775858006E+02
44	1	2.4695485475E+00	8.7000040532E+01	-8.1775535475E+02
44	2	2.4695485475E+00	8.7500040532E+01	-8.1775544533E+02
44	3	2.4695485475E+00	8.8000040532E+01	-8.1775554160E+02
44	4	2.4695485475E+00	8.8500040532E+01	-8.1775563880E+02
44	5	2.4695485475E+00	8.9000040532E+01	-8.1775563974E+02
44	6	2.4695485475E+00	8.9500040532E+01	-8.1775585113E+02
44	7	2.4695485475E+00	9.0000040532E+01	-8.1775593846E+02
44	8	2.4695485475E+00	9.0500040532E+01	-8.1775616278E+02
44	9	2.4695485475E+00	9.1000040532E+01	-8.1775627238E+02
44	10	2.4695485475E+00	9.1500040532E+01	-8.1775649853E+02
44	11	2.4695485475E+00	9.2000040532E+01	-8.1775661921E+02
44	12	2.4695485475E+00	9.2500040532E+01	-8.1775683095E+02
44	13	2.4695485475E+00	9.3000040532E+01	-8.1775699285E+02
44	14	2.4695485475E+00	9.3500040532E+01	-8.1775715379E+02
44	15	2.4695485475E+00	9.4000040532E+01	-8.1775730732E+02
44	16	2.4695485475E+00	9.4500040532E+01	-8.1775745456E+02
44	17	2.4695485475E+00	9.5000040532E+01	-8.1775759363E+02
44	18	2.4695485475E+00	9.5500040532E+01	-8.1775772639E+02
44	19	2.4695485475E+00	9.6000040532E+01	-8.1775785012E+02
44	20	2.4695485475E+00	9.6500040532E+01	-8.1775796690E+02
44	21	2.4695485475E+00	9.7000040532E+01	-8.1775807610E+02
44	22	2.4695485475E+00	9.7500040532E+01	-8.1775817841E+02
44	23	2.4695485475E+00	9.8000040532E+01	-8.1775827314E+02
44	24	2.4695485475E+00	9.8500040532E+01	-8.1775836077E+02
44	25	2.4695485475E+00	9.9000040532E+01	-8.1775844149E+02
44	26	2.4695485475E+00	9.9500040532E+01	-8.1775851569E+02
44	27	2.4695485475E+00	1.0000004053E+02	-8.1775858210E+02
44	28	2.4695485475E+00	1.0050004053E+02	-8.1775864328E+02
44	29	2.4695485475E+00	1.0100004053E+02	-8.1775869682E+02
44	30	2.4695485475E+00	1.0150004053E+02	-8.1775874441E+02
44	31	2.4695485475E+00	1.0200004053E+02	-8.1775878532E+02
44	32	2.4695485475E+00	1.0250004053E+02	-8.1775881995E+02
44	33	2.4695485475E+00	1.0300004053E+02	-8.1775884840E+02
44	34	2.4695485475E+00	1.0350004053E+02	-8.1775887125E+02
44	35	2.4695485475E+00	1.0400004053E+02	-8.1775888814E+02

44	36	2.4695485475E+00	1.0450004053E+02	-8.1775889981E+02
44	37	2.4695485475E+00	1.0500004053E+02	-8.1775890652E+02
44	38	2.4695485475E+00	1.0550004053E+02	-8.1775890903E+02
44	39	2.4695485475E+00	1.0600004053E+02	-8.1775890954E+02
44	40	2.4695485475E+00	1.0650004053E+02	-8.1775893363E+02
44	41	2.4695485475E+00	1.0700004053E+02	-8.1775893908E+02
44	42	2.4695485475E+00	1.0750004053E+02	-8.1775893952E+02
44	43	2.4695485475E+00	1.0800004053E+02	-8.1775893646E+02
44	44	2.4695485475E+00	1.0850004053E+02	-8.1775893001E+02
44	45	2.4695485475E+00	1.0900004053E+02	-8.1775892078E+02
44	46	2.4695485475E+00	1.0950004053E+02	-8.1775890925E+02
44	47	2.4695485475E+00	1.1000004053E+02	-8.1775889602E+02
44	48	2.4695485475E+00	1.1050004053E+02	-8.1775888291E+02
44	49	2.4695485475E+00	1.1100004053E+02	-8.1775894236E+02
44	50	2.4695485475E+00	1.1150004053E+02	-8.1775892324E+02
44	51	2.4695485475E+00	1.1200004053E+02	-8.1775890643E+02
44	52	2.4695485475E+00	1.1250004053E+02	-8.1775889088E+02
44	53	2.4695485475E+00	1.1300004053E+02	-8.1775887503E+02
44	54	2.4695485475E+00	1.1350004053E+02	-8.1775885812E+02
44	55	2.4695485475E+00	1.1400004053E+02	-8.1775883984E+02
44	56	2.4695485475E+00	1.1450004053E+02	-8.1775882006E+02
44	57	2.4695485475E+00	1.1500004053E+02	-8.1775879898E+02
44	58	2.4695485475E+00	1.1550004053E+02	-8.1775877682E+02
44	59	2.4695485475E+00	1.1600004053E+02	-8.1775875395E+02
44	60	2.4695485475E+00	1.1650004053E+02	-8.1775873084E+02
44	61	2.4695485475E+00	1.1700004053E+02	-8.1775870808E+02
45	1	2.4795485475E+00	8.7000040532E+01	-8.1775505474E+02
45	2	2.4795485475E+00	8.7500040532E+01	-8.1775516433E+02
45	3	2.4795485475E+00	8.8000040532E+01	-8.1775525972E+02
45	4	2.4795485475E+00	8.8500040532E+01	-8.1775540843E+02
45	5	2.4795485475E+00	8.9000040532E+01	-8.1775558138E+02
45	6	2.4795485475E+00	8.9500040532E+01	-8.1775577148E+02
45	7	2.4795485475E+00	9.0000040532E+01	-8.1775570503E+02
45	8	2.4795485475E+00	9.0500040532E+01	-8.1775615954E+02
45	9	2.4795485475E+00	9.1000040532E+01	-8.1775634787E+02
45	10	2.4795485475E+00	9.1500040532E+01	-8.1775653509E+02
45	11	2.4795485475E+00	9.2000040532E+01	-8.1775671772E+02
45	12	2.4795485475E+00	9.2500040532E+01	-8.1775689709E+02
45	13	2.4795485475E+00	9.3000040532E+01	-8.1775704258E+02
45	14	2.4795485475E+00	9.3500040532E+01	-8.1775723546E+02
45	15	2.4795485475E+00	9.4000040532E+01	-8.1775739289E+02
45	16	2.4795485475E+00	9.4500040532E+01	-8.1775754251E+02
45	17	2.4795485475E+00	9.5000040532E+01	-8.1775768284E+02
45	18	2.4795485475E+00	9.5500040532E+01	-8.1775781605E+02
45	19	2.4795485475E+00	9.6000040532E+01	-8.1775794045E+02
45	20	2.4795485475E+00	9.6500040532E+01	-8.1775805808E+02
45	21	2.4795485475E+00	9.7000040532E+01	-8.1775816728E+02
45	22	2.4795485475E+00	9.7500040532E+01	-8.1775826979E+02
45	23	2.4795485475E+00	9.8000040532E+01	-8.1775836417E+02
45	24	2.4795485475E+00	9.8500040532E+01	-8.1775845217E+02
45	25	2.4795485475E+00	9.9000040532E+01	-8.1775853245E+02
45	26	2.4795485475E+00	9.9500040532E+01	-8.1775860638E+02

45	27	2.4795485475E+00	1.0000004053E+02	-8.1775867312E+02
45	28	2.4795485475E+00	1.0050004053E+02	-8.1775873352E+02
45	29	2.4795485475E+00	1.0100004053E+02	-8.1775878710E+02
45	30	2.4795485475E+00	1.0150004053E+02	-8.1775883457E+02
45	31	2.4795485475E+00	1.0200004053E+02	-8.1775887537E+02
45	32	2.4795485475E+00	1.0250004053E+02	-8.1775891045E+02
45	33	2.4795485475E+00	1.0300004053E+02	-8.1775893894E+02
45	34	2.4795485475E+00	1.0350004053E+02	-8.1775896204E+02
45	35	2.4795485475E+00	1.0400004053E+02	-8.1775897932E+02
45	36	2.4795485475E+00	1.0450004053E+02	-8.1775899144E+02
45	37	2.4795485475E+00	1.0500004053E+02	-8.1775899864E+02
45	38	2.4795485475E+00	1.0550004053E+02	-8.1775900901E+02
45	39	2.4795485475E+00	1.0600004053E+02	-8.1775902301E+02
45	40	2.4795485475E+00	1.0650004053E+02	-8.1775903517E+02
45	41	2.4795485475E+00	1.0700004053E+02	-8.1775904051E+02
45	42	2.4795485475E+00	1.0750004053E+02	-8.1775904184E+02
45	43	2.4795485475E+00	1.0800004053E+02	-8.1775903945E+02
45	44	2.4795485475E+00	1.0850004053E+02	-8.1775903404E+02
45	45	2.4795485475E+00	1.0900004053E+02	-8.1775902602E+02
45	46	2.4795485475E+00	1.0950004053E+02	-8.1775901551E+02
45	47	2.4795485475E+00	1.1000004053E+02	-8.1775900439E+02
45	48	2.4795485475E+00	1.1050004053E+02	-8.1775899497E+02
45	49	2.4795485475E+00	1.1100004053E+02	-8.1775905077E+02
45	50	2.4795485475E+00	1.1150004053E+02	-8.1775903560E+02
45	51	2.4795485475E+00	1.1200004053E+02	-8.1775902260E+02
45	52	2.4795485475E+00	1.1250004053E+02	-8.1775901019E+02
45	53	2.4795485475E+00	1.1300004053E+02	-8.1775899682E+02
45	54	2.4795485475E+00	1.1350004053E+02	-8.1775898227E+02
45	55	2.4795485475E+00	1.1400004053E+02	-8.1775896635E+02
45	56	2.4795485475E+00	1.1450004053E+02	-8.1775894897E+02
45	57	2.4795485475E+00	1.1500004053E+02	-8.1775893037E+02
45	58	2.4795485475E+00	1.1550004053E+02	-8.1775891084E+02
45	59	2.4795485475E+00	1.1600004053E+02	-8.1775889076E+02
45	60	2.4795485475E+00	1.1650004053E+02	-8.1775887064E+02
45	61	2.4795485475E+00	1.1700004053E+02	-8.1775885087E+02
46	1	2.4895485475E+00	8.7000040532E+01	-8.1775477275E+02
46	2	2.4895485475E+00	8.7500040532E+01	-8.1775496526E+02
46	3	2.4895485475E+00	8.8000040532E+01	-8.1775498009E+02
46	4	2.4895485475E+00	8.8500040532E+01	-8.1775538448E+02
46	5	2.4895485475E+00	8.9000040532E+01	-8.1775560410E+02
46	6	2.4895485475E+00	8.9500040532E+01	-8.1775582019E+02
46	7	2.4895485475E+00	9.0000040532E+01	-8.1775603145E+02
46	8	2.4895485475E+00	9.0500040532E+01	-8.1775623990E+02
46	9	2.4895485475E+00	9.1000040532E+01	-8.1775644161E+02
46	10	2.4895485475E+00	9.1500040532E+01	-8.1775663945E+02
46	11	2.4895485475E+00	9.2000040532E+01	-8.1775683052E+02
46	12	2.4895485475E+00	9.2500040532E+01	-8.1775701380E+02
46	13	2.4895485475E+00	9.3000040532E+01	-8.1775718864E+02
46	14	2.4895485475E+00	9.3500040532E+01	-8.1775735520E+02
46	15	2.4895485475E+00	9.4000040532E+01	-8.1775751261E+02
46	16	2.4895485475E+00	9.4500040532E+01	-8.1775766228E+02
46	17	2.4895485475E+00	9.5000040532E+01	-8.1775780241E+02

46	18	2.4895485475E+00	9.5500040532E+01	-8.1775793524E+02
46	19	2.4895485475E+00	9.6000040532E+01	-8.1775805879E+02
46	20	2.4895485475E+00	9.6500040532E+01	-8.1775817554E+02
46	21	2.4895485475E+00	9.7000040532E+01	-8.1775828378E+02
46	22	2.4895485475E+00	9.7500040532E+01	-8.1775838513E+02
46	23	2.4895485475E+00	9.8000040532E+01	-8.1775847869E+02
46	24	2.4895485475E+00	9.8500040532E+01	-8.1775856550E+02
46	25	2.4895485475E+00	9.9000040532E+01	-8.1775864489E+02
46	26	2.4895485475E+00	9.9500040532E+01	-8.1775871761E+02
46	27	2.4895485475E+00	1.0000004053E+02	-8.1775878324E+02
46	28	2.4895485475E+00	1.0050004053E+02	-8.1775884289E+02
46	29	2.4895485475E+00	1.0100004053E+02	-8.1775889570E+02
46	30	2.4895485475E+00	1.0150004053E+02	-8.1775894264E+02
46	31	2.4895485475E+00	1.0200004053E+02	-8.1775898295E+02
46	32	2.4895485475E+00	1.0250004053E+02	-8.1775901761E+02
46	33	2.4895485475E+00	1.0300004053E+02	-8.1775904623E+02
46	34	2.4895485475E+00	1.0350004053E+02	-8.1775906913E+02
46	35	2.4895485475E+00	1.0400004053E+02	-8.1775908651E+02
46	36	2.4895485475E+00	1.0450004053E+02	-8.1775909881E+02
46	37	2.4895485475E+00	1.0500004053E+02	-8.1775910684E+02
46	38	2.4895485475E+00	1.0550004053E+02	-8.1775912436E+02
46	39	2.4895485475E+00	1.0600004053E+02	-8.1775914273E+02
46	40	2.4895485475E+00	1.0650004053E+02	-8.1775915236E+02
46	41	2.4895485475E+00	1.0700004053E+02	-8.1775915808E+02
46	42	2.4895485475E+00	1.0750004053E+02	-8.1775915965E+02
46	43	2.4895485475E+00	1.0800004053E+02	-8.1775915810E+02
46	44	2.4895485475E+00	1.0850004053E+02	-8.1775915358E+02
46	45	2.4895485475E+00	1.0900004053E+02	-8.1775914657E+02
46	46	2.4895485475E+00	1.0950004053E+02	-8.1775913793E+02
46	47	2.4895485475E+00	1.1000004053E+02	-8.1775912833E+02
46	48	2.4895485475E+00	1.1050004053E+02	-8.1775912296E+02
46	49	2.4895485475E+00	1.1100004053E+02	-8.1775917525E+02
46	50	2.4895485475E+00	1.1150004053E+02	-8.1775916418E+02
46	51	2.4895485475E+00	1.1200004053E+02	-8.1775915453E+02
46	52	2.4895485475E+00	1.1250004053E+02	-8.1775914463E+02
46	53	2.4895485475E+00	1.1300004053E+02	-8.1775913357E+02
46	54	2.4895485475E+00	1.1350004053E+02	-8.1775912112E+02
46	55	2.4895485475E+00	1.1400004053E+02	-8.1775910735E+02
46	56	2.4895485475E+00	1.1450004053E+02	-8.1775909225E+02
46	57	2.4895485475E+00	1.1500004053E+02	-8.1775907603E+02
46	58	2.4895485475E+00	1.1550004053E+02	-8.1775905906E+02
46	59	2.4895485475E+00	1.1600004053E+02	-8.1775904173E+02
46	60	2.4895485475E+00	1.1650004053E+02	-8.1775902447E+02
46	61	2.4895485475E+00	1.1700004053E+02	-8.1775900770E+02
47	1	2.4995485475E+00	8.7000040532E+01	-8.1775449505E+02
47	2	2.4995485475E+00	8.7500040532E+01	-8.1775500493E+02
47	3	2.4995485475E+00	8.8000040532E+01	-8.1775524699E+02
47	4	2.4995485475E+00	8.8500040532E+01	-8.1775548471E+02
47	5	2.4995485475E+00	8.9000040532E+01	-8.1775571697E+02
47	6	2.4995485475E+00	8.9500040532E+01	-8.1775594503E+02
47	7	2.4995485475E+00	9.0000040532E+01	-8.1775614208E+02
47	8	2.4995485475E+00	9.0500040532E+01	-8.1775638255E+02

47 9	2.4995485475E+00	9.1000040532E+01	-8.1775659142E+02
47 10	2.4995485475E+00	9.1500040532E+01	-8.1775679173E+02
47 11	2.4995485475E+00	9.2000040532E+01	-8.1775698293E+02
47 12	2.4995485475E+00	9.2500040532E+01	-8.1775716694E+02
47 13	2.4995485475E+00	9.3000040532E+01	-8.1775734000E+02
47 14	2.4995485475E+00	9.3500040532E+01	-8.1775750590E+02
47 15	2.4995485475E+00	9.4000040532E+01	-8.1775766148E+02
47 16	2.4995485475E+00	9.4500040532E+01	-8.1775781000E+02
47 17	2.4995485475E+00	9.5000040532E+01	-8.1775794835E+02
47 18	2.4995485475E+00	9.5500040532E+01	-8.1775807935E+02
47 19	2.4995485475E+00	9.6000040532E+01	-8.1775820122E+02
47 20	2.4995485475E+00	9.6500040532E+01	-8.1775831630E+02
47 21	2.4995485475E+00	9.7000040532E+01	-8.1775842283E+02
47 22	2.4995485475E+00	9.7500040532E+01	-8.1775852246E+02
47 23	2.4995485475E+00	9.8000040532E+01	-8.1775861427E+02
47 24	2.4995485475E+00	9.8500040532E+01	-8.1775869927E+02
47 25	2.4995485475E+00	9.9000040532E+01	-8.1775877649E+02
47 26	2.4995485475E+00	9.9500040532E+01	-8.1775884767E+02
47 27	2.4995485475E+00	1.0000004053E+02	-8.1775891142E+02
47 28	2.4995485475E+00	1.0050004053E+02	-8.1775896960E+02
47 29	2.4995485475E+00	1.0100004053E+02	-8.1775902129E+02
47 30	2.4995485475E+00	1.0150004053E+02	-8.1775906709E+02
47 31	2.4995485475E+00	1.0200004053E+02	-8.1775910684E+02
47 32	2.4995485475E+00	1.0250004053E+02	-8.1775914090E+02
47 33	2.4995485475E+00	1.0300004053E+02	-8.1775916910E+02
47 34	2.4995485475E+00	1.0350004053E+02	-8.1775919198E+02
47 35	2.4995485475E+00	1.0400004053E+02	-8.1775920925E+02
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47 39	2.4995485475E+00	1.0600004053E+02	-8.1775927548E+02
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47 46	2.4995485475E+00	1.0950004053E+02	-8.1775927452E+02
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47 48	2.4995485475E+00	1.1050004053E+02	-8.1775926658E+02
47 49	2.4995485475E+00	1.1100004053E+02	-8.1775931556E+02
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47 57	2.4995485475E+00	1.1500004053E+02	-8.1775923516E+02
47 58	2.4995485475E+00	1.1550004053E+02	-8.1775922071E+02
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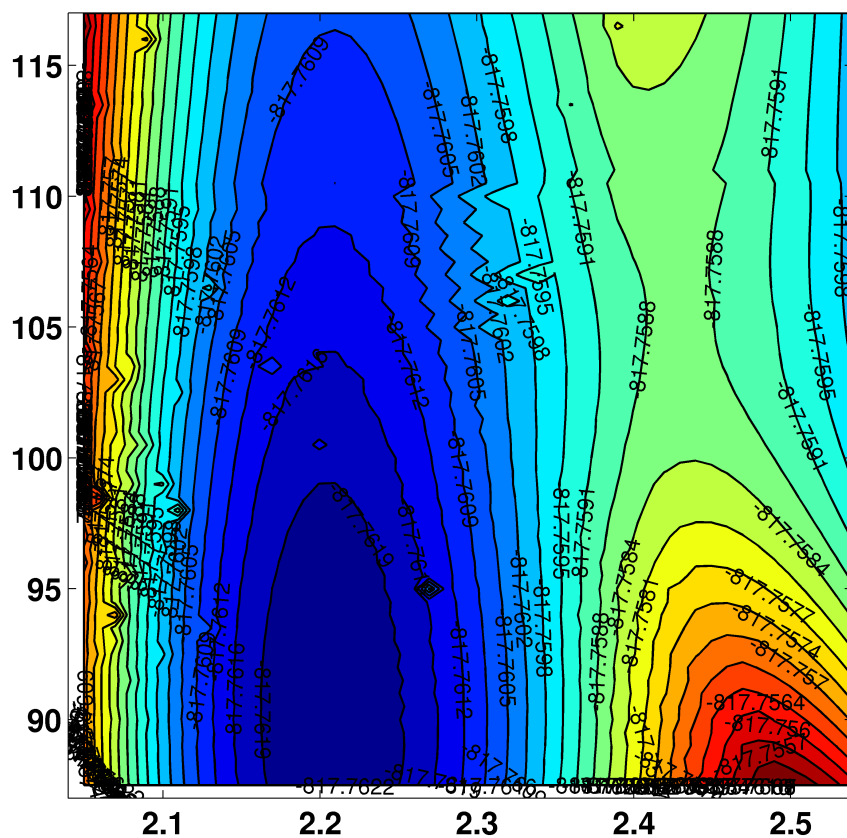
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50	44	2.5295485475E+00	1.0850004053E+02	-8.1775976765E+02
50	45	2.5295485475E+00	1.0900004053E+02	-8.1775976451E+02
50	46	2.5295485475E+00	1.0950004053E+02	-8.1775976399E+02
50	47	2.5295485475E+00	1.1000004053E+02	-8.1775976976E+02
50	48	2.5295485475E+00	1.1050004053E+02	-8.1775977444E+02
50	49	2.5295485475E+00	1.1100004053E+02	-8.1775981965E+02
50	50	2.5295485475E+00	1.1150004053E+02	-8.1775981895E+02
50	51	2.5295485475E+00	1.1200004053E+02	-8.1775981737E+02
50	52	2.5295485475E+00	1.1250004053E+02	-8.1775981472E+02
50	53	2.5295485475E+00	1.1300004053E+02	-8.1775981087E+02
50	54	2.5295485475E+00	1.1350004053E+02	-8.1775980583E+02
50	55	2.5295485475E+00	1.1400004053E+02	-8.1775979968E+02
50	56	2.5295485475E+00	1.1450004053E+02	-8.1775979289E+02
50	57	2.5295485475E+00	1.1500004053E+02	-8.1775978549E+02
50	58	2.5295485475E+00	1.1550004053E+02	-8.1775977816E+02
50	59	2.5295485475E+00	1.1600004053E+02	-8.1775977097E+02
50	60	2.5295485475E+00	1.1650004053E+02	-8.1775976437E+02
50	61	2.5295485475E+00	1.1700004053E+02	-8.1775975796E+02
51	1	2.5395485475E+00	8.7000040532E+01	-8.1775561585E+02
51	2	2.5395485475E+00	8.7500040532E+01	-8.1775589058E+02
51	3	2.5395485475E+00	8.8000040532E+01	-8.1775615550E+02
51	4	2.5395485475E+00	8.8500040532E+01	-8.1775640980E+02
51	5	2.5395485475E+00	8.9000040532E+01	-8.1775665227E+02
51	6	2.5395485475E+00	8.9500040532E+01	-8.1775688269E+02
51	7	2.5395485475E+00	9.0000040532E+01	-8.1775710134E+02
51	8	2.5395485475E+00	9.0500040532E+01	-8.1775730806E+02
51	9	2.5395485475E+00	9.1000040532E+01	-8.1775750292E+02
51	10	2.5395485475E+00	9.1500040532E+01	-8.1775768655E+02
51	11	2.5395485475E+00	9.2000040532E+01	-8.1775785982E+02
51	12	2.5395485475E+00	9.2500040532E+01	-8.1775802383E+02
51	13	2.5395485475E+00	9.3000040532E+01	-8.1775817874E+02
51	14	2.5395485475E+00	9.3500040532E+01	-8.1775832962E+02
51	15	2.5395485475E+00	9.4000040532E+01	-8.1775847172E+02
51	16	2.5395485475E+00	9.4500040532E+01	-8.1775860624E+02
51	17	2.5395485475E+00	9.5000040532E+01	-8.1775873224E+02
51	18	2.5395485475E+00	9.5500040532E+01	-8.1775885088E+02
51	19	2.5395485475E+00	9.6000040532E+01	-8.1775896028E+02
51	20	2.5395485475E+00	9.6500040532E+01	-8.1775906209E+02
51	21	2.5395485475E+00	9.7000040532E+01	-8.1775915718E+02
51	22	2.5395485475E+00	9.7500040532E+01	-8.1775924509E+02
51	23	2.5395485475E+00	9.8000040532E+01	-8.1775932475E+02
51	24	2.5395485475E+00	9.8500040532E+01	-8.1775939733E+02

51	25	2.5395485475E+00	9.9000040532E+01	-8.1775946277E+02
51	26	2.5395485475E+00	9.9500040532E+01	-8.1775952128E+02
51	27	2.5395485475E+00	1.0000004053E+02	-8.1775957312E+02
51	28	2.5395485475E+00	1.0050004053E+02	-8.1775962638E+02
51	29	2.5395485475E+00	1.0100004053E+02	-8.1775967445E+02
51	30	2.5395485475E+00	1.0150004053E+02	-8.1775971763E+02
51	31	2.5395485475E+00	1.0200004053E+02	-8.1775975284E+02
51	32	2.5395485475E+00	1.0250004053E+02	-8.1775978469E+02
51	33	2.5395485475E+00	1.0300004053E+02	-8.1775981111E+02
51	34	2.5395485475E+00	1.0350004053E+02	-8.1775983450E+02
51	35	2.5395485475E+00	1.0400004053E+02	-8.1775985985E+02
51	36	2.5395485475E+00	1.0450004053E+02	-8.1775988777E+02
51	37	2.5395485475E+00	1.0500004053E+02	-8.1775990586E+02
51	38	2.5395485475E+00	1.0550004053E+02	-8.1775992203E+02
51	39	2.5395485475E+00	1.0600004053E+02	-8.1775993407E+02
51	40	2.5395485475E+00	1.0650004053E+02	-8.1775994265E+02
51	41	2.5395485475E+00	1.0700004053E+02	-8.1775994827E+02
51	42	2.5395485475E+00	1.0750004053E+02	-8.1775995116E+02
51	43	2.5395485475E+00	1.0800004053E+02	-8.1775995158E+02
51	44	2.5395485475E+00	1.0850004053E+02	-8.1775995054E+02
51	45	2.5395485475E+00	1.0900004053E+02	-8.1775994899E+02
51	46	2.5395485475E+00	1.0950004053E+02	-8.1775995339E+02
51	47	2.5395485475E+00	1.1000004053E+02	-8.1775996114E+02
51	48	2.5395485475E+00	1.1050004053E+02	-8.1775996686E+02
51	49	2.5395485475E+00	1.1100004053E+02	-8.1776001121E+02
51	50	2.5395485475E+00	1.1150004053E+02	-8.1776001204E+02
51	51	2.5395485475E+00	1.1200004053E+02	-8.1776001200E+02
51	52	2.5395485475E+00	1.1250004053E+02	-8.1776001082E+02
51	53	2.5395485475E+00	1.1300004053E+02	-8.1776000846E+02
51	54	2.5395485475E+00	1.1350004053E+02	-8.1776000512E+02
51	55	2.5395485475E+00	1.1400004053E+02	-8.1776000081E+02
51	56	2.5395485475E+00	1.1450004053E+02	-8.1775999590E+02
51	57	2.5395485475E+00	1.1500004053E+02	-8.1775999054E+02
51	58	2.5395485475E+00	1.1550004053E+02	-8.1775998541E+02
51	59	2.5395485475E+00	1.1600004053E+02	-8.1775998032E+02
51	60	2.5395485475E+00	1.1650004053E+02	-8.1775997610E+02
51	61	2.5395485475E+00	1.1700004053E+02	-8.1775997234E+02

Total grid point: 3111

Labeled Contour Plot of Potential energy surface (B3PW91)



Born-Oppenhemer Molecular Dynamics (BOMD) plot data

<u>Simulation Time(pico sec)</u>	<u>C-I bond length (in Angstrom)</u>
2.499999944120646E-003	2.09878132727019
4.999999888241291E-003	3.05358535214344
7.499999832361937E-003	2.09224613946686
9.999999776482582E-003	3.07475039453303
1.249999972060323E-002	2.09182023000329

1.499999966472387E-002	3.07109069520163
1.749999960884452E-002	2.10501383421345
1.999999955296516E-002	3.09706156487016
2.249999949708581E-002	2.13611254845947
2.499999944120646E-002	3.11498125587137
2.749999938532710E-002	2.17157091510386
2.999999932944775E-002	3.14194427797232
3.249999927356839E-002	2.19797171992749
3.499999921768904E-002	3.12966488274384
3.749999916180968E-002	2.19711893243902
3.999999910593033E-002	3.13551927573552
4.249999905005097E-002	2.18494292543718
4.499999899417162E-002	3.13321661496217
4.749999893829226E-002	2.17860366663007
4.999999888241291E-002	3.13063732027170
5.249999882653356E-002	2.18460608692505
5.499999877065420E-002	3.09736536536037
5.749999871477485E-002	2.16588185877023
5.999999865889549E-002	3.06633901302873
6.249999860301614E-002	2.11834423005563
6.499999854713678E-002	3.05376021986812
6.749999849125743E-002	2.07413632053874
6.999999843537807E-002	3.04061276767644
7.249999837949872E-002	2.07150844302552
7.499999832361937E-002	3.02072476264985
7.749999826774001E-002	2.08822657710316
7.999999821186066E-002	2.99155716683168
8.249999815598130E-002	2.09726586518996
8.499999810010195E-002	2.99757660653218
8.749999804422259E-002	2.09862113207077
8.999999798834324E-002	3.00216625728040
9.249999793246388E-002	2.11626162690864
9.499999787658453E-002	3.01721061108203
9.749999782070518E-002	2.14220759749610
9.999999776482582E-002	3.02027064443255
0.102499997708946	2.16348437723964
0.104999997653067	3.05269009392994
0.107499997597188	2.16924917706957
0.109999997541308	3.07576748774188
0.112499997485429	2.17238884067033
0.114999997429550	3.09587362305198
0.117499997373670	2.17128214429747
0.119999997317791	3.09803014217970
0.122499997261912	2.16242199261037
0.124999997206032	3.12038326924690
0.127499997150153	2.14435101903723
0.129999997094274	3.14447060817302
0.132499997038394	2.13725381647150
0.134999996982515	3.14965216723149
0.137499996926636	2.14078569811063
0.139999996870756	3.13362063701703
0.142499996814877	2.14044491864776

0.144999996758997	3.12880589668295
0.147499996703118	2.13462801567744
0.149999996647239	3.14273525892351
0.152499996591359	2.14167426716459
0.154999996535480	3.13810535942517
0.157499996479601	2.16135703436707
0.159999996423721	3.10915678759965
0.162499996367842	2.16903289840933
0.164999996311963	3.09440307552943
0.167499996256083	2.16868366416151
0.169999996200204	3.09821144743560
0.172499996144325	2.17066740565523
0.174999996088445	3.08885393446744
0.177499996032566	2.17777482180344
0.179999995976686	3.05403151941004
0.182499995920807	2.16382372371180
0.184999995864928	3.03236964124593
0.187499995809048	2.14150508801567
0.189999995753169	3.03866788649023
0.192499995697290	2.12823038057302
0.194999995641410	3.03989230522300
0.197499995585531	2.13320876366051
0.199999995529652	3.02395103620512
0.202499995473772	2.12288576992122
0.204999995417893	3.01733548386420
0.207499995362014	2.09676831883377
0.209999995306134	3.04403395594152
0.212499995250255	2.08999182656201
0.214999995194376	3.06042234787472
0.217499995138496	2.12679813233932
0.219999995082617	3.05894910802942
0.222499995026737	2.16288840220895
0.224999994970858	3.06552470571304
0.227499994914979	2.16410079710743
0.229999994859099	3.11075862496996
0.232499994803220	2.15022524705878
0.234999994747341	3.14399745995365
0.237499994691461	2.16691354790195
0.239999994635582	3.15288574525132
0.242499994579703	2.20269605773720
0.244999994523823	3.13689129086489
0.247499994467944	2.22103944449980
0.249999994412065	3.15121118332840
0.252499994356185	2.20690949597259
0.254999994300306	3.15747707758837
0.257499994244426	2.18366670969290
0.259999994188547	3.14803999926145
0.262499994132668	2.16476202403728
0.264999994076788	3.11665894623104
0.267499994020909	2.15056681083546
0.269999993965030	3.11169071286913
0.272499993909150	2.14076606720562

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0.277499993797392	2.12872426095890
0.279999993741512	3.06763529504112
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0.284999993629754	3.02109544340261
0.287499993573874	2.08529750000090
0.289999993517995	3.01199447190827
0.292499993462116	2.08582499819544
0.294999993406236	3.01089529429686
0.297499993350357	2.10868922816450
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0.314999992959201	3.02952739410589
0.317499992903322	2.14464331228552
0.319999992847443	3.03384989370898
0.322499992791563	2.17718626575013
0.324999992735684	3.04158213334459
0.327499992679805	2.18414555804919
0.329999992623925	3.04374347553288
0.332499992568046	2.15547536852222
0.334999992512167	3.08795861681646
0.337499992456287	2.12246291569535
0.339999992400408	3.10305366414617
0.342499992344528	2.12160343891737
0.344999992288649	3.11841259649938
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0.362499991897494	2.12965556770174
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0.382499991450459	2.18252500848581
0.384999991394579	3.11620689264705
0.387499991338700	2.18807702346193
0.389999991282821	3.08488114807605
0.392499991226941	2.17853923143032
0.394999991171062	3.06542241735083
0.397499991115183	2.15627524171521
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0.402499991003424	2.13856446840281

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0.407499990891665	2.12273595958306
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0.417499990668148	2.07865670888678
0.419999990612268	3.01504679666834
0.422499990556389	2.08118260023334
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0.552499987650663	2.12167492594554
0.554999987594783	3.03033565503328
0.557499987538904	2.10252093845698
0.559999987483025	3.04822515387725
0.562499987427145	2.10442074550267
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0.567499987315387	2.13979956059277
0.569999987259507	3.09564491901268
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0.589999986812472	3.17543069617383
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0.609999986365438	3.12913725913582
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0.614999986253679	3.11172602414946
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0.629999985918403	3.05125766688639
0.632499985862523	2.09126130937886
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0.637499985750765	2.09810545206336
0.639999985694885	2.99902689048215
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0.654999985359609	3.01649007404848
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0.659999985247850	3.01936940604640
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0.669999985024333	3.06042998954036
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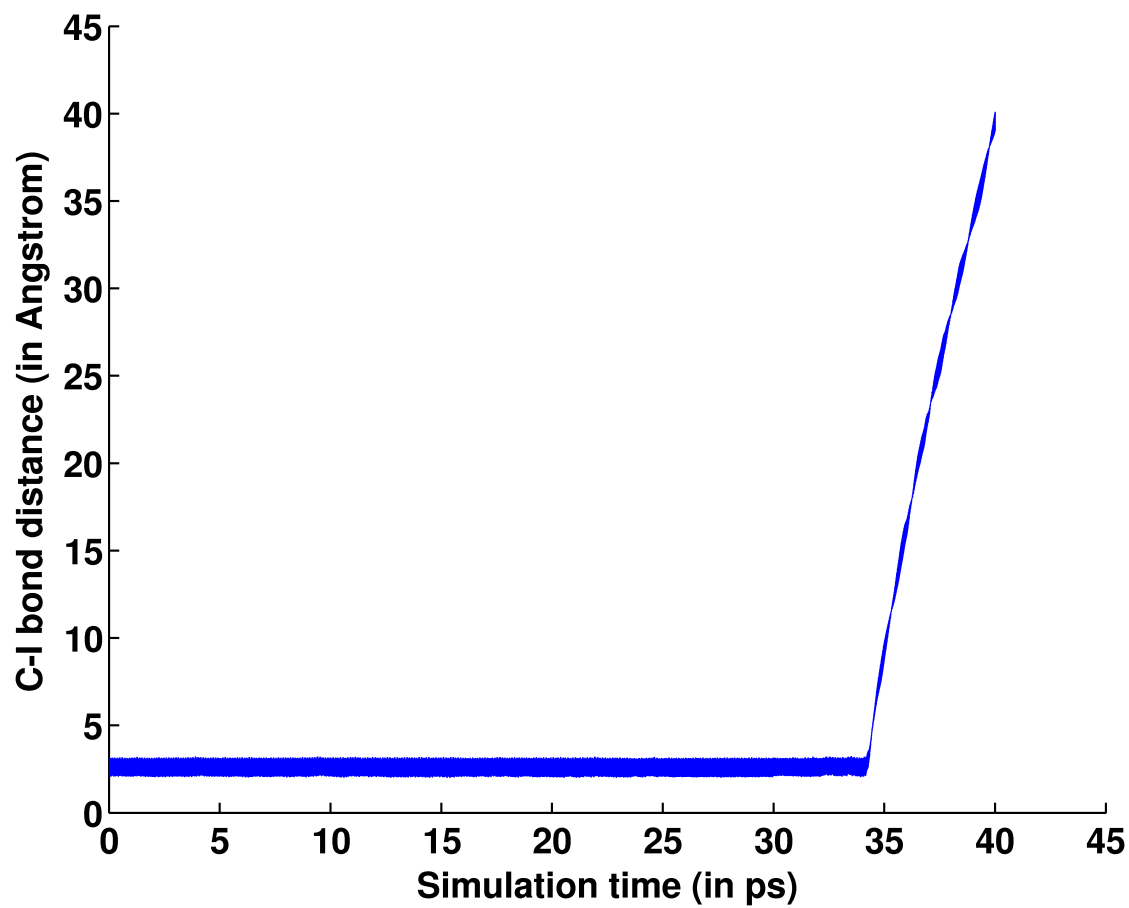
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Plot Of BOMD simulation

