Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Halogenation Effects in Intramolecular Furan Diels-Alder Reactions: Broad Scope Synthetic and Computational Studies

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Cartesian coordinates and absolute energy values for all starting materials, products and transition states for reactions **a-z**

REACTION a

1a

E=-745.245226 au

1	6	0	-1.916498	2.373880	1.398222
2	6	0	-0.621319	1.897673	1.209336
3	6	0	-0.299088	1.188829	0.055263
4	6	0	-1.279170	0.962361	-0.909391
5	6	0	-2.576331	1.427701	-0.718929
6	6	0	-2.902744	2.130052	0.441383
7	1	0	-2.160047	2.948630	2.284771
8	1	0	0.136480	2.092809	1.959710
9	1	0	0.709531	0.821386	-0.095386
10	1	0	-1.034688	0.418937	-1.815083
11	1	0	-3.332597	1.263619	-1.474695
12	7	0	-4.246815	2.596801	0.675530
13	6	0	-4.765157	3.517758	-0.218756
14	8	0	-4.115460	3.923601	-1.171886
15	8	0	-7.011580	3.716599	0.934841
16	6	0	-6.136842	4.064627	-0.064114
17	6	0	-5.806569	0.843856	1.599882
18	1	0	-6.266000	0.441604	2.501357
19	6	0	-6.039637	0.260361	0.431192
20	1	0	-5.605646	0.630220	-0.490127
21	1	0	-6.679227	-0.611080	0.357281
22	6	0	-6.732443	4.977941	-0.888580
23	1	0	-6.266638	5.417677	-1.754202
24	6	0	-8.041343	5.205741	-0.374790
25	1	0	-8.797015	5.864779	-0.771177
26	6	0	-8.156027	4.416181	0.727307
27	1	0	-8.945930	4.242317	1.438670
28	6	0	-4.940904	2.053624	1.851497
29	1	0	-5.538058	2.833341	2.323717
30	1	0	-4.171431	1.780709	2.578267

2a

E=-745.255138 au

1	6	0	0.996813	-0.045943	-0.484048
2	6	0	0.631559	1.872901	0.371984
3	6	0	0.963865	0.847429	-1.775818
4	1	0	1.931195	0.805486	-2.280687
5	1	0	0.191456	0.545145	-2.484141
6	6	0	0.700141	2.235887	-1.141676
7	1	0	-0.226099	2.696133	-1.488561
8	1	0	1.546970	-0.980405	-0.564405

9	8	0	1.648966	0.849986	0.435324
10	6	0	1.054256	3.131892	1.107262
11	8	0	0.809010	3.394476	2.264888
12	6	0	1.834216	3.271463	-1.144567
13	1	0	2.809002	2.792762	-1.279464
14	1	0	1.707739	4.031575	-1.917890
15	6	0	2.454936	5.099786	0.477411
16	6	0	2.196983	5.843747	1.640895
17	6	0	3.423576	5.567350	-0.424298
18	6	0	2.896373	7.021741	1.878626
19	1	0	1.465706	5.487276	2.348495
20	6	0	4.111700	6.750556	-0.171532
21	1	0	3.656799	5.007617	-1.319954
22	6	0	3.853820	7.487162	0.979870
23	1	0	2.683946	7.582102	2.782361
24	1	0	4.857009	7.090336	-0.882038
25	1	0	4.391472	8.407534	1.175502
26	7	0	1.753887	3.903005	0.189785
27	6	0	-0.630933	1.088374	0.650745
28	6	0	-0.414929	-0.104913	0.094093
29	1	0	-1.526928	1.480628	1.109435
30	1	0	-1.104103	-0.930934	-0.015258

TS a

E = -745.208573 au

1	6	0	-3.526613	-0.349515	0.872757
2	6	0	-1.787411	0.644430	0.089394
3	6	0	-2.751076	-1.796492	-0.559162
4	1	0	-2.645407	-2.569019	0.194686
5	1	0	-3.570509	-1.946603	-1.250483
6	6	0	-1.618501	-1.076321	-0.972426
7	1	0	-1.597150	-0.701834	-1.991088
8	1	0	-4.079558	-0.884273	1.631064
9	8	0	-2.233991	-0.031691	1.206137
10	6	0	-0.335574	1.036059	0.071575
11	8	0	0.039386	2.186726	0.192136
12	6	0	-0.250506	-1.349834	-0.382839
13	1	0	-0.353482	-1.916150	0.548337
14	1	0	0.361509	-1.939852	-1.070066
15	6	0	1.879976	-0.062467	-0.042947
16	6	0	2.632083	1.090423	-0.316362
17	6	0	2.551707	-1.241317	0.313354
18	6	0	4.019922	1.048490	-0.232487
19	1	0	2.127018	2.006967	-0.575399
20	6	0	3.941177	-1.268414	0.387608
21	1	0	1.994716	-2.137942	0.550687

22	6	0	4.685339	-0.124843	0.115182
23	1	0	4.584843	1.948707	-0.447651
24	1	0	4.438611	-2.190396	0.667190
25	1	0	5.767250	-0.146577	0.174691
26	7	0	0.460964	-0.072411	-0.136713
27	6	0	-2.900666	1.297876	-0.499978
28	6	0	-4.009345	0.642909	-0.018440
29	1	0	-2.844736	2.039938	-1.281139
30	1	0	-5.036077	0.757729	-0.331402

REACTION b

1b

E= -3317.529463 au

1	6	0	3.617365	-1.093453	0.201004
2	6	0	5.002406	-1.074959	0.049346
3	6	0	5.630878	0.016711	-0.540949
4	6	0	4.860715	1.090629	-0.985084
5	6	0	3.477513	1.075706	-0.847549
6	6	0	2.845322	-0.019654	-0.250528
7	1	0	3.138803	-1.938350	0.680557
8	1	0	5.587664	-1.915469	0.405052
9	1	0	6.708847	0.033335	-0.652888
10	1	0	5.338204	1.946848	-1.448099
11	1	0	2.888100	1.914816	-1.188436
12	7	0	1.411777	-0.074457	-0.150263
13	6	0	0.740652	1.025415	0.357518
14	8	0	1.326040	2.005982	0.794359
15	8	0	-1.586716	0.150454	-0.172746
16	6	0	-2.861079	1.730409	0.781405
17	6	0	-2.846063	0.568125	0.072683
18	6	0	-1.491219	2.059752	0.989622
19	1	0	-1.085059	2.913672	1.505407
20	6	0	-0.742964	1.079687	0.401119
21	6	0	0.325357	-2.220116	0.630721
22	1	0	-0.206055	-3.116809	0.317397
23	6	0	0.524858	-1.994595	1.924320
24	1	0	1.043579	-1.111760	2.281800
25	1	0	0.167842	-2.690317	2.674294
26	6	0	0.761058	-1.343041	-0.516505
27	1	0	1.475984	-1.890541	-1.135894
28	1	0	-0.095968	-1.143576	-1.160063
29	1	0	-3.733782	2.271219	1.106385
30	35	0	-4.231257	-0.497344	-0.597409

2b

E= -3317.545914 au

1	6	0	2.442250	0.095766	0.201601
2	6	0	0.539666	1.016512	0.307255
3	6	0	1.840083	-0.666432	1.428758
4	1	0	1.766021	-1.728864	1.195147
5	1	0	2.439216	-0.544221	2.330517
6	6	0	0.453528	0.020705	1.502347
7	1	0	0.286213	0.540310	2.446865
8	8	0	1.294840	0.214025	-0.638682
9	6	0	-0.893211	1.224180	-0.151365
10	8	0	-1.295910	2.163099	-0.802816
11	6	0	-0.790628	-0.794846	1.119147
12	1	0	-0.525220	-1.663345	0.508802
13	1	0	-1.350163	-1.137925	1.991178
14	6	0	-2.973851	-0.140080	0.041128
15	6	0	-3.840918	0.839420	-0.469796
16	6	0	-3.469657	-1.431843	0.273245
17	6	0	-5.167974	0.518008	-0.733200
18	1	0	-3.466760	1.831252	-0.666682
19	6	0	-4.801730	-1.734698	0.006830
20	1	0	-2.820232	-2.211404	0.647862
21	6	0	-5.660726	-0.763449	-0.496843
22	1	0	-5.823190	1.286429	-1.128052
23	1	0	-5.162294	-2.740377	0.191518
24	1	0	-6.697294	-1.001325	-0.704882
25	7	0	-1.617554	0.148955	0.338196
26	6	0	1.515350	2.126449	0.626624
27	6	0	2.714898	1.545590	0.585717
28	1	0	1.249752	3.130183	0.925056
29	1	0	3.685041	1.943164	0.843693
30	35	0	3.894511	-0.825579	-0.710431

TS b

E=-3317.495354 au

1	6	0	2.532740	0.253219	0.028759
2	6	0	0.575899	1.127350	0.087845
3	6	0	1.657334	-0.627721	1.843171
4	1	0	1.813323	-1.629291	1.459898
5	1	0	2.346453	-0.321159	2.619436
6	6	0	0.392237	-0.036018	1.758211
7	1	0	0.122106	0.706871	2.502418
8	8	0	1.307590	0.157687	-0.573375
9	6	0	-0.888599	1.213873	-0.242465

10	8	0	-1.358920	2.139743	-0.874993
11	6	0	-0.785850	-0.771116	1.153577
12	1	0	-0.431941	-1.627738	0.571639
13	1	0	-1.451021	-1.145902	1.935692
14	6	0	-2.938755	-0.146984	0.017676
15	6	0	-3.856915	0.856416	-0.327017
16	6	0	-3.383074	-1.474554	0.101931
17	6	0	-5.184066	0.523557	-0.578323
18	1	0	-3.524580	1.878608	-0.409530
19	6	0	-4.715429	-1.790336	-0.146784
20	1	0	-2.690665	-2.269795	0.343992
21	6	0	-5.625009	-0.794550	-0.488724
22	1	0	-5.880111	1.311459	-0.843610
23	1	0	-5.036341	-2.823702	-0.078748
24	1	0	-6.661781	-1.041909	-0.684597
25	7	0	-1.574945	0.147795	0.299294
26	6	0	1.469737	2.154849	0.482474
27	6	0	2.723423	1.592972	0.458761
28	1	0	1.176067	3.117201	0.872443
29	1	0	3.655822	2.006495	0.808466
30	35	0	3.890168	-0.858882	-0.700005

REACTION c

1c

E= -3317.528415 au

1	6	0	-4.008733	0.622760	0.354532
2	6	0	-5.325887	0.186479	0.482810
3	6	0	-5.675747	-1.110358	0.120689
4	6	0	-4.696445	-1.968572	-0.377398
5	6	0	-3.382211	-1.538160	-0.518775
6	6	0	-3.029225	-0.235792	-0.151401
7	1	0	-3.741456	1.627124	0.659018
8	1	0	-6.074626	0.864042	0.877495
9	1	0	-6.699167	-1.451187	0.226604
10	1	0	-4.956312	-2.981239	-0.664480
11	1	0	-2.627405	-2.211331	-0.899495
12	7	0	-1.686135	0.242375	-0.343445
13	6	0	-0.634695	-0.536242	0.109832
14	8	0	-0.808072	-1.571835	0.735020
15	8	0	1.185338	0.877241	-0.953571
16	6	0	3.007311	-0.101638	-0.146523
17	6	0	2.542165	0.896397	-0.945997
18	1	0	3.022194	1.654021	-1.540331
19	6	0	1.875297	-0.786834	0.374415
20	1	0	1.855020	-1.635435	1.035911

21	6	0	0.780836	-0.152551	-0.142528
22	6	0	-1.203646	2.698801	0.014254
23	1	0	-1.035508	3.656212	-0.475694
24	6	0	-1.110370	2.613588	1.336365
25	1	0	-1.266090	1.679554	1.865148
26	1	0	-0.869582	3.482409	1.937277
27	6	0	-1.528729	1.578052	-0.941765
28	1	0	-2.469382	1.802542	-1.451122
29	1	0	-0.769503	1.541955	-1.723099
30	35	0	4.821632	-0.490403	0.196978

2c

E= -3317.544072 au

1	6	0	2.048327	0.929539	0.905392
2	6	0	0.488715	-0.255909	0.059311
3	6	0	1.444827	1.940231	-0.129865
4	1	0	1.058931	2.816060	0.395144
5	1	0	2.171870	2.272848	-0.871368
6	6	0	0.309863	1.072589	-0.730225
7	1	0	0.416035	0.918254	-1.804786
8	1	0	2.606915	1.352503	1.735761
9	8	0	0.860803	0.263837	1.359030
10	6	0	-0.886248	-0.900958	0.085702
11	8	0	-1.113541	-2.074736	0.282682
12	6	0	-1.146728	1.424276	-0.391580
13	1	0	-1.209422	2.037136	0.512879
14	1	0	-1.650465	1.949548	-1.205071
15	6	0	-3.206600	-0.000482	-0.097648
16	6	0	-3.847807	-1.249795	-0.133294
17	6	0	-3.988684	1.160662	-0.001642
18	6	0	-5.235429	-1.316667	-0.074572
19	1	0	-3.257302	-2.149827	-0.193787
20	6	0	-5.376734	1.074720	0.052515
21	1	0	-3.522587	2.135515	0.044862
22	6	0	-6.010807	-0.162788	0.016080
23	1	0	-5.713058	-2.289704	-0.102769
24	1	0	-5.960016	1.985522	0.128702
25	1	0	-7.091640	-0.227950	0.059507
26	7	0	-1.795385	0.114379	-0.169272
27	6	0	1.753301	-0.958601	-0.386407
28	6	0	2.722408	-0.199411	0.123905
29	1	0	1.815160	-1.804165	-1.053730
30	35	0	4.586136	-0.304390	-0.153719

TS c

E= -3317.495300 au

1	6	0	2.140742	0.749531	1.084735
2	6	0	0.528590	-0.421882	0.264859
3	6	0	1.333145	2.070345	-0.447976
4	1	0	1.133595	2.857818	0.270495
5	1	0	2.182395	2.247655	-1.095960
6	6	0	0.280490	1.257595	-0.889514
7	1	0	0.345683	0.833115	-1.886228
8	1	0	2.627734	1.344929	1.841912
9	8	0	0.865284	0.334582	1.368477
10	6	0	-0.888507	-0.919860	0.189975
11	8	0	-1.179268	-2.090682	0.342179
12	6	0	-1.132478	1.435458	-0.376311
13	1	0	-1.125138	2.047822	0.531054
14	1	0	-1.755201	1.941579	-1.118576
15	6	0	-3.170695	-0.002733	-0.076515
16	6	0	-3.817116	-1.222163	-0.329211
17	6	0	-3.947268	1.133775	0.193222
18	6	0	-5.206485	-1.286936	-0.308838
19	1	0	-3.231945	-2.106397	-0.523033
20	6	0	-5.336644	1.053801	0.203854
21	1	0	-3.474081	2.081555	0.412666
22	6	0	-5.976148	-0.156095	-0.046629
23	1	0	-5.689138	-2.237657	-0.505901
24	1	0	-5.916625	1.944816	0.416540
25	1	0	-7.058069	-0.217653	-0.036010
26	7	0	-1.752166	0.115054	-0.104767
27	6	0	1.709581	-1.009558	-0.250868
28	6	0	2.729324	-0.245099	0.262480
29	1	0	1.759217	-1.779059	-1.003973
30	35	0	4.557126	-0.295205	-0.202698

REACTION d

1d

E= -3317.527662 au

1	6	0	-3.426617	0.349837	0.707145
2	6	0	-4.688432	-0.241558	0.728783
3	6	0	-5.014795	-1.238277	-0.184751
4	6	0	-4.067878	-1.637596	-1.127355
5	6	0	-2.811755	-1.044628	-1.163679
6	6	0	-2.481191	-0.043951	-0.243610
7	1	0	-3.173997	1.106006	1.439882
8	1	0	-5.411009	0.074763	1.472660
9	1	0	-5.994197	-1.701988	-0.162904

10	1	0	-4.309429	-2.413057	-1.845507
11	1	0	-2.082052	-1.361857	-1.895662
12	7	0	-1.203275	0.607358	-0.311494
13	6	0	-0.061686	-0.180509	-0.386713
14	8	0	-0.085946	-1.391010	-0.244934
15	8	0	1.350228	1.594710	-1.425922
16	6	0	2.668525	1.887823	-1.567033
17	1	0	2.895973	2.753838	-2.165426
18	6	0	2.518357	0.055244	-0.326168
19	6	0	1.251101	0.463508	-0.653737
20	6	0	-0.736483	2.509034	1.287301
21	1	0	-0.675941	3.590745	1.395704
22	6	0	-0.436377	1.729683	2.320404
23	1	0	-0.481045	0.647796	2.260246
24	1	0	-0.131800	2.154066	3.269691
25	6	0	-1.164888	2.061714	-0.088503
26	1	0	-2.170940	2.436461	-0.293733
27	1	0	-0.520791	2.527897	-0.833457
28	35	0	3.031317	-1.421273	0.718609
29	6	0	3.434042	0.982649	-0.907293
30	1	0	4.508632	0.958241	-0.837026

2d

E= -3317.542566 au

1	6	0	2.247204	2.196900	0.789720
2	6	0	0.991454	0.526969	0.349928
3	6	0	1.574374	2.679082	-0.544146
4	1	0	0.981907	3.576850	-0.355839
5	1	0	2.297774	2.900524	-1.329639
6	6	0	0.684149	1.451337	-0.862550
7	1	0	0.941970	0.970135	-1.806849
8	1	0	2.617332	2.977697	1.449684
9	8	0	1.144774	1.497626	1.401035
10	6	0	-2.651097	-0.019824	-0.067586
11	6	0	-3.065342	-1.305120	0.318993
12	6	0	-3.622561	0.923039	-0.437041
13	6	0	-4.419096	-1.621915	0.328608
14	1	0	-2.329680	-2.034107	0.618543
15	6	0	-4.973227	0.587120	-0.424595
16	1	0	-3.335780	1.925648	-0.724075
17	6	0	-5.382255	-0.686213	-0.042613
18	1	0	-4.719878	-2.618992	0.630421
19	1	0	-5.705795	1.332941	-0.712262
20	1	0	-6.434434	-0.945385	-0.032309
21	7	0	-1.280084	0.338678	-0.107534
22	6	0	2.412740	0.006907	0.216672
23	35	0	2.878433	-1.693969	-0.444302

24	6	0	3.202977	1.052471	0.463432
25	1	0	4.275168	1.125793	0.358141
26	6	0	-0.254028	-0.320783	0.554223
27	6	0	-0.840076	1.595524	-0.746849
28	1	0	-1.113705	2.452962	-0.123851
29	1	0	-1.323496	1.702737	-1.719555
30	8	0	-0.315681	-1.352827	1.183182

TS d

E= -3317.495465 au

1	6	0	2.392028	2.082167	0.990946
2	6	0	1.051199	0.448099	0.559592
3	6	0	1.511459	2.616746	-0.983365
4	1	0	1.109936	3.553869	-0.613832
5	1	0	2.379572	2.708980	-1.622804
6	6	0	0.671636	1.499632	-1.103637
7	1	0	0.911300	0.765652	-1.868110
8	1	0	2.681841	2.990848	1.497234
9	8	0	1.168077	1.575767	1.345826
10	6	0	-2.609230	0.001539	-0.035602
11	6	0	-3.016766	-1.326390	0.160807
12	6	0	-3.583551	0.988102	-0.243947
13	6	0	-4.370669	-1.644368	0.144257
14	1	0	-2.278101	-2.091693	0.337465
15	6	0	-4.934381	0.653166	-0.262540
16	1	0	-3.295951	2.022584	-0.377030
17	6	0	-5.337383	-0.664242	-0.068941
18	1	0	-4.668531	-2.675715	0.296561
19	1	0	-5.671194	1.432117	-0.423398
20	1	0	-6.389505	-0.923794	-0.082074
21	7	0	-1.233550	0.365371	-0.051292
22	6	0	2.370960	-0.041941	0.348728
23	35	0	2.795471	-1.685677	-0.464589
24	6	0	3.221459	1.012840	0.583328
25	1	0	4.279745	1.065221	0.382805
26	6	0	-0.256028	-0.296218	0.662275
27	6	0	-0.803941	1.586083	-0.771071
28	1	0	-0.997203	2.475882	-0.162916
29	1	0	-1.403259	1.662680	-1.681614
30	8	0	-0.381330	-1.330370	1.285723

REACTION e

1e

E=-745.244017 au

1	6	0	1.780326	-0.495510	1.010028
2	6	0	3.035696	-1.091712	1.082757
3	6	0	3.928758	-0.991105	0.017432
4	6	0	3.564801	-0.279701	-1.122987
5	6	0	2.314283	0.329343	-1.194789
6	6	0	1.415780	0.216045	-0.133109
7	1	0	1.088179	-0.567432	1.837371
8	1	0	3.315552	-1.639658	1.975419
9	1	0	4.904202	-1.460156	0.078259
10	1	0	4.256178	-0.187376	-1.952959
11	1	0	2.034067	0.903876	-2.070854
12	7	0	0.116974	0.827465	-0.257703
13	8	0	-1.151391	-2.005665	-0.175431
14	6	0	-3.329173	-2.125626	0.309218
15	1	0	-4.279161	-2.497151	0.658700
16	6	0	-2.138929	-2.775712	0.361620
17	1	0	-1.833344	-3.741356	0.727018
18	6	0	-3.060611	-0.856822	-0.300982
19	1	0	-3.765393	-0.066549	-0.505112
20	6	0	-1.726810	-0.831193	-0.575952
21	6	0	-1.576892	2.487404	0.494897
22	1	0	-2.215475	2.476548	1.372514
23	6	0	-1.863263	3.269827	-0.542129
24	1	0	-1.210147	3.341436	-1.406022
25	1	0	-2.749758	3.894030	-0.549569
26	6	0	-0.279296	1.754663	0.691029
27	8	0	0.396129	2.038980	1.663613
28	6	0	-0.835296	0.191258	-1.199783
29	1	0	-0.236725	-0.270768	-1.986155
30	1	0	-1.461149	0.948836	-1.663643

2e

E=-745.262361 au

1	6	0	1.068474	0.041085	-0.464541
2	6	0	0.554207	1.966623	0.310005
3	6	0	1.000832	0.874797	-1.791988
4	1	0	1.980857	0.914302	-2.268915
5	1	0	0.278357	0.485215	-2.509913
6	6	0	0.607443	2.253592	-1.217869
7	1	0	1.684863	-0.853807	-0.496058
8	8	0	1.630994	1.016628	0.428372
9	6	0	2.439505	5.142017	0.293381
10	6	0	2.233054	5.749793	1.542499
11	6	0	3.375193	5.711409	-0.587327
12	6	0	2.943295	6.891798	1.901105
13	1	0	1.514892	5.343299	2.241623
14	6	0	4.073646	6.853763	-0.212508

15	1	0	3.539566	5.257766	-1.551105
16	6	0	3.868859	7.453360	1.028159
17	1	0	2.764726	7.341163	2.871688
18	1	0	4.792183	7.276302	-0.906217
19	1	0	4.421480	8.342220	1.309162
20	7	0	1.703426	3.979478	-0.041568
21	6	0	1.634264	3.377828	-1.296344
22	6	0	0.906458	3.274555	0.977786
23	1	0	0.007613	3.842688	1.243814
24	1	0	1.497138	3.103381	1.879939
25	8	0	2.246171	3.702134	-2.291976
26	1	0	-0.336338	2.633698	-1.617729
27	6	0	-0.660360	1.100437	0.595169
28	1	0	-1.606009	1.440519	0.994607
29	6	0	-0.348278	-0.095909	0.092169
30	1	0	-0.980748	-0.967541	-0.005191

TS e

E=-745.211434 au

1	6	0	3.396962	-0.035382	1.103463
2	6	0	1.769355	-0.914847	-0.001409
3	6	0	2.764928	1.605664	-0.256661
4	1	0	2.532037	2.283395	0.555600
5	1	0	3.672201	1.826893	-0.803171
6	6	0	1.721746	0.918512	-0.883463
7	1	0	1.835122	0.640045	-1.927561
8	1	0	3.843379	0.420005	1.974265
9	8	0	2.080529	-0.389810	1.233769
10	6	0	-1.849151	-0.077584	-0.087199
11	6	0	-2.514303	-1.288881	-0.337600
12	6	0	-2.601974	1.022716	0.354956
13	6	0	-3.888858	-1.398619	-0.148195
14	1	0	-1.969898	-2.152099	-0.696618
15	6	0	-3.975788	0.897766	0.533492
16	1	0	-2.108964	1.962061	0.541657
17	6	0	-4.631147	-0.306450	0.288032
18	1	0	-4.376401	-2.345833	-0.350542
19	1	0	-4.537245	1.759874	0.876377
20	1	0	-5.701601	-0.391628	0.434296
21	7	0	-0.440981	-0.011754	-0.276224
22	6	0	2.955198	-1.476754	-0.542134
23	6	0	3.993476	-0.894672	0.151865
24	1	0	3.011990	-2.082181	-1.434164
25	1	0	5.050100	-0.960883	-0.058269
26	6	0	0.280501	1.163185	-0.491930
27	6	0	0.335047	-1.260703	-0.221410
28	1	0	0.248639	-1.837101	-1.149739

29	1	0	-0.048529	-1.878231	0.596020
30	8	0	-0.193017	2.279092	-0.408198

REACTION f

1f

E= -3317.527322 au

1	6	0	3.643559	-0.742150	0.074549
2	6	0	4.239134	-1.997815	0.074011
3	6	0	3.481446	-3.140891	-0.177712
4	6	0	2.117035	-3.016012	-0.418156
5	6	0	1.508920	-1.761816	-0.404966
6	6	0	2.271666	-0.616090	-0.166769
7	1	0	4.235265	0.140862	0.274151
8	1	0	5.302962	-2.081782	0.265525
9	1	0	3.950864	-4.117842	-0.181844
10	1	0	1.512954	-3.896702	-0.604942
11	1	0	0.441255	-1.679777	-0.560067
12	7	0	1.673359	0.689658	-0.204618
13	8	0	-1.333488	-0.079411	-0.464067
14	6	0	-2.619762	0.239401	-0.180416
15	6	0	-0.719661	1.079960	-0.883118
16	6	0	1.437965	2.991883	0.714948
17	1	0	0.815416	3.335153	1.534801
18	6	0	1.916119	3.849946	-0.182325
19	1	0	2.585932	3.537976	-0.977561
20	1	0	1.679337	4.906838	-0.134067
21	6	0	-2.865828	1.555104	-0.405453
22	1	0	-3.802267	2.066670	-0.260376
23	6	0	-1.621070	2.098901	-0.862555
24	1	0	-1.422347	3.123250	-1.134014
25	6	0	0.714894	0.994047	-1.289781
26	1	0	0.844496	0.214766	-2.042028
27	1	0	0.974210	1.940028	-1.762444
28	35	0	-3.715513	-1.147592	0.434102
29	6	0	1.883658	1.563653	0.853360
30	8	0	2.443852	1.236907	1.882560

2f

E= -3317.552551 au

1	6	0	2.404368	0.189043	0.113476
2	6	0	0.558330	1.217231	0.317264
3	6	0	1.807327	-0.575528	1.338873
4	1	0	1.625154	-1.617436	1.077745
5	1	0	2.451208	-0.534884	2.216509

6	6	0	0.483767	0.206982	1.497767
7	1	0	0.389008	0.692163	2.472692
8	8	0	1.235496	0.403912	-0.672036
9	6	0	-2.921652	0.027107	-0.039179
10	6	0	-3.632251	1.039245	-0.703789
11	6	0	-3.559442	-1.201870	0.199535
12	6	0	-4.943662	0.827797	-1.119157
13	1	0	-3.174142	1.999441	-0.898325
14	6	0	-4.870857	-1.393867	-0.220783
15	1	0	-3.026376	-1.986025	0.712020
16	6	0	-5.573862	-0.388839	-0.881271
17	1	0	-5.470418	1.625567	-1.630755
18	1	0	-5.344910	-2.349918	-0.028281
19	1	0	-6.594813	-0.552156	-1.205691
20	7	0	-1.586945	0.272939	0.370956
21	6	0	2.777105	1.609787	0.526450
22	1	0	3.776141	1.940974	0.767216
23	6	0	-0.820183	-0.531011	1.209895
24	6	0	-0.873381	1.478102	-0.084381
25	1	0	-1.262850	2.380293	0.401461
26	1	0	-0.958682	1.594367	-1.166553
27	8	0	-1.129794	-1.607863	1.671640
28	6	0	1.616757	2.258940	0.633185
29	1	0	1.435756	3.260925	0.997285
30	35	0	3.762964	-0.780314	-0.886747

TS f

E= -3317.497305 au

1	6	0	2.494413	0.336223	-0.128591
2	6	0	0.598637	1.343070	-0.037790
3	6	0	1.647869	-0.341202	1.832830
4	1	0	1.673096	-1.380198	1.529759
5	1	0	2.423658	-0.032888	2.520885
6	6	0	0.448158	0.362963	1.762957
7	1	0	0.297272	1.206118	2.431652
8	8	0	1.233592	0.282810	-0.652164
9	6	0	-2.875794	0.020544	-0.034632
10	6	0	-3.665164	1.011436	-0.638965
11	6	0	-3.414378	-1.265964	0.125047
12	6	0	-4.955492	0.724082	-1.074565
13	1	0	-3.286911	2.017754	-0.762417
14	6	0	-4.707761	-1.535291	-0.310232
15	1	0	-2.824808	-2.034563	0.596560
16	6	0	-5.487249	-0.550841	-0.912949
17	1	0	-5.544737	1.507938	-1.537210
18	1	0	-5.104914	-2.535610	-0.178188

19	1	0	-6.492370	-0.774157	-1.251018
20	7	0	-1.553187	0.348238	0.378344
21	6	0	2.793908	1.681279	0.195076
22	1	0	3.766707	2.052870	0.474182
23	6	0	-0.844492	-0.323319	1.373267
24	6	0	-0.866213	1.462687	-0.289781
25	1	0	-1.204650	2.436878	0.082310
26	1	0	-1.082465	1.418035	-1.361182
27	8	0	-1.225668	-1.342097	1.913132
28	6	0	1.578539	2.327410	0.245474
29	1	0	1.377178	3.323785	0.609528
30	35	0	3.724056	-0.933937	-0.815254

REACTION g

1g

E= -3317.527389 au

1	6	0	4.104274	0.308581	0.002801
2	6	0	5.192919	-0.548219	0.112309
3	6	0	5.010465	-1.930470	0.099367
4	6	0	3.724196	-2.447964	-0.013212
5	6	0	2.625375	-1.595644	-0.108629
6	6	0	2.810668	-0.211134	-0.110301
7	1	0	4.251230	1.379945	0.016818
8	1	0	6.190015	-0.132098	0.201977
9	1	0	5.862789	-2.595148	0.180123
10	1	0	3.566202	-3.520614	-0.014496
11	1	0	1.626241	-2.007347	-0.162522
12	7	0	1.696260	0.682342	-0.264771
13	8	0	-0.658205	-1.325037	-0.058381
14	6	0	-2.734671	-0.545210	-0.071922
15	6	0	-1.940686	-1.567819	0.333828
16	1	0	-2.120439	-2.477654	0.878388
17	6	0	-1.900109	0.397016	-0.751818
18	1	0	-2.200372	1.332674	-1.192832
19	6	0	-0.643232	-0.124235	-0.715601
20	6	0	0.502033	2.780515	0.345822
21	1	0	-0.178906	2.960084	1.171411
22	6	0	0.520304	3.590038	-0.709807
23	1	0	1.230700	3.463509	-1.520850
24	1	0	-0.157411	4.432814	-0.785707
25	35	0	-4.594058	-0.393973	0.217720
26	6	0	0.661779	0.352497	-1.268052
27	1	0	1.092463	-0.411838	-1.916398
28	1	0	0.454994	1.220410	-1.891609
29	6	0	1.536300	1.729745	0.633922
30	8	0	2.218584	1.855252	1.632964

2g

E= -3317.551343 au

1	6	0	1.978139	0.641688	1.012767
2	6	0	0.505980	-0.466936	-0.075738
3	6	0	1.395113	1.766876	0.093577
4	1	0	0.918060	2.538663	0.698427
5	1	0	2.146833	2.234131	-0.542840
6	6	0	0.346187	0.949469	-0.693431
7	1	0	0.510438	0.967913	-1.773858
8	1	0	2.472800	0.962690	1.924986
9	8	0	0.796872	-0.117955	1.296276
10	6	0	-3.172786	-0.165236	-0.087138
11	6	0	-3.692024	-1.469389	-0.117981
12	6	0	-4.058416	0.910237	0.095513
13	6	0	-5.057694	-1.692027	0.032345
14	1	0	-3.040052	-2.319568	-0.265785
15	6	0	-5.420008	0.668556	0.241219
16	1	0	-3.673110	1.916608	0.116521
17	6	0	-5.932773	-0.626414	0.213102
18	1	0	-5.432733	-2.709016	0.004624
19	1	0	-6.086672	1.512069	0.382510
20	1	0	-6.995785	-0.801213	0.330363
21	7	0	-1.777264	0.028630	-0.240004
22	6	0	1.826585	-1.061710	-0.538729
23	6	0	2.737075	-0.351307	0.128133
24	1	0	1.972462	-1.782876	-1.329144
25	35	0	4.613580	-0.356383	-0.065595
26	6	0	-0.852045	-1.116708	-0.194279
27	1	0	-0.925267	-1.726584	-1.102020
28	1	0	-1.057856	-1.746887	0.673157
29	6	0	-1.128187	1.245181	-0.437372
30	8	0	-1.633679	2.347131	-0.442901

TS g

E= -3317.498532 au

1	6	0	2.047936	0.431060	1.180036
2	6	0	0.541407	-0.658253	0.081169
3	6	0	1.298853	1.945999	-0.260666
4	1	0	0.989531	2.626913	0.523097
5	1	0	2.202716	2.219268	-0.789704
6	6	0	0.336128	1.151585	-0.882870
7	1	0	0.501090	0.835481	-1.908846
8	1	0	2.444748	0.950008	2.038255
9	8	0	0.773170	-0.054250	1.297568

10	6	0	-3.134358	-0.158241	-0.094630
11	6	0	-3.689361	-1.416932	-0.373310
12	6	0	-3.979721	0.865180	0.361807
13	6	0	-5.050684	-1.647898	-0.198113
14	1	0	-3.068187	-2.221992	-0.743776
15	6	0	-5.339186	0.620071	0.526004
16	1	0	-3.570722	1.840160	0.568887
17	6	0	-5.886362	-0.631074	0.251702
18	1	0	-5.454405	-2.628893	-0.422459
19	1	0	-5.975317	1.423691	0.880114
20	1	0	-6.946679	-0.810102	0.386347
21	7	0	-1.734229	0.032046	-0.268856
22	6	0	1.780773	-1.123018	-0.422700
23	6	0	2.732419	-0.413319	0.275689
24	1	0	1.925822	-1.747001	-1.290205
25	35	0	4.586993	-0.341257	-0.060833
26	6	0	-0.849851	-1.138371	-0.162256
27	1	0	-0.855438	-1.744436	-1.075704
28	1	0	-1.198119	-1.768268	0.661614
29	6	0	-1.127303	1.263759	-0.516682
30	8	0	-1.708716	2.329443	-0.473510

REACTION h

1h

E= -3317.529255 au

1	6	0	3.550799	0.917326	-0.468858
2	6	0	4.817693	0.398641	-0.710139
3	6	0	5.023638	-0.979902	-0.741699
4	6	0	3.950718	-1.836685	-0.516277
5	6	0	2.680809	-1.323842	-0.258553
6	6	0	2.472126	0.057037	-0.244545
7	1	0	3.394522	1.987358	-0.442341
8	1	0	5.646699	1.076284	-0.880276
9	1	0	6.011986	-1.380403	-0.935573
10	1	0	4.099185	-2.910662	-0.526080
11	1	0	1.858817	-1.995707	-0.047152
12	7	0	1.159435	0.601090	-0.033658
13	8	0	-0.394345	-1.690714	0.974272
14	6	0	-0.917621	-0.791858	0.087359
15	6	0	-0.361196	2.217702	1.086485
16	1	0	-0.784095	2.185394	2.085367
17	6	0	-0.906800	2.978903	0.142145
18	1	0	-0.471317	3.071631	-0.847609
19	1	0	-1.801778	3.559071	0.333823
20	6	0	-2.618482	-1.844687	1.138630
21	1	0	-3.607235	-2.142731	1.445102

22	6	0	-2.277479	-0.859631	0.157294
23	6	0	0.029146	-0.006137	-0.760669
24	1	0	0.467615	-0.648130	-1.527514
25	1	0	-0.550850	0.754053	-1.282548
26	6	0	0.971909	1.538586	0.975641
27	8	0	1.850267	1.847177	1.758523
28	35	0	-3.507243	0.145678	-0.865299
29	6	0	-1.433597	-2.311139	1.602576
30	1	0	-1.163448	-3.040104	2.347180

2h

E= -3317.551656 au

1	6	0	2.096767	2.044268	1.072807
2	6	0	0.993824	0.331953	0.415355
3	6	0	1.458284	2.602194	-0.245537
4	1	0	0.767865	3.416153	-0.021221
5	1	0	2.197686	2.957912	-0.963404
6	6	0	0.699961	1.344639	-0.724261
7	1	0	1.025888	0.990949	-1.705784
8	1	0	2.371810	2.782445	1.821701
9	8	0	1.024789	1.209193	1.551947
10	6	0	-2.629608	-0.204372	-0.011978
11	6	0	-2.907358	-1.506842	0.432432
12	6	0	-3.702513	0.640583	-0.342475
13	6	0	-4.221578	-1.950906	0.545387
14	1	0	-2.104777	-2.186135	0.685572
15	6	0	-5.008771	0.178478	-0.225630
16	1	0	-3.502242	1.641015	-0.689954
17	6	0	-5.282482	-1.113370	0.217956
18	1	0	-4.409260	-2.961440	0.890722
19	1	0	-5.822991	0.846326	-0.484384
20	1	0	-6.305154	-1.460597	0.306904
21	7	0	-1.281032	0.219655	-0.113727
22	6	0	2.461831	-0.067218	0.324780
23	35	0	3.091637	-1.677810	-0.435304
24	6	0	3.156890	1.004685	0.705294
25	1	0	4.224439	1.162886	0.671390
26	6	0	-0.825338	1.384941	-0.723416
27	6	0	-0.194705	-0.595764	0.458917
28	1	0	-0.015576	-1.499932	-0.131776
29	1	0	-0.425313	-0.880889	1.487286
30	8	0	-1.501496	2.267989	-1.206083

TS h

E= -3317.499870 au

1	6	0	2.181822	1.901882	1.354245
2	6	0	1.034509	0.215089	0.640973
3	6	0	1.414041	2.577317	-0.659854
4	1	0	0.878584	3.425377	-0.250761
5	1	0	2.331430	2.808666	-1.184411
6	6	0	0.710977	1.409223	-0.958285
7	1	0	1.084954	0.765374	-1.750953
8	1	0	2.335554	2.781590	1.959988
9	8	0	0.989033	1.255213	1.542517
10	6	0	-2.594181	-0.193962	-0.018787
11	6	0	-2.882266	-1.539597	0.259789
12	6	0	-3.661467	0.707345	-0.162094
13	6	0	-4.198551	-1.971458	0.394416
14	1	0	-2.085238	-2.264557	0.358424
15	6	0	-4.971300	0.257983	-0.030234
16	1	0	-3.457160	1.740989	-0.386210
17	6	0	-5.253519	-1.076783	0.249990
18	1	0	-4.392799	-3.016642	0.607792
19	1	0	-5.780789	0.970450	-0.144568
20	1	0	-6.278423	-1.413437	0.353441
21	7	0	-1.234837	0.211181	-0.131914
22	6	0	2.407291	-0.126097	0.490417
23	35	0	3.048567	-1.623598	-0.463158
24	6	0	3.136847	0.964879	0.908072
25	1	0	4.196835	1.131445	0.802420
26	6	0	-0.795380	1.348620	-0.806608
27	6	0	-0.200984	-0.609412	0.518342
28	1	0	0.031535	-1.511371	-0.056927
29	1	0	-0.560332	-0.917123	1.504542
30	8	0	-1.529931	2.201875	-1.262658

REACTION i

1i

E= -1204.414173 au

1	6	0	-2.583435	0.780065	0.396174
2	6	0	-3.976475	0.762810	0.425965
3	6	0	-4.676370	-0.333898	-0.066196
4	6	0	-3.970974	-1.413426	-0.595863
5	6	0	-2.581606	-1.399728	-0.639911
6	6	0	-1.877350	-0.299531	-0.140653
7	1	0	-2.048373	1.631053	0.799115
8	1	0	-4.509955	1.608524	0.844820
9	1	0	-5.759720	-0.349778	-0.037240
10	1	0	-4.504934	-2.273209	-0.984497
11	1	0	-2.041929	-2.243039	-1.045890

12	7	0	-0.441173	-0.244090	-0.229885
13	6	0	0.298759	-1.348205	0.182190
14	8	0	-0.232205	-2.327034	0.684106
15	8	0	2.532169	-0.418100	-0.566017
16	6	0	3.921056	-2.031210	0.112052
17	1	0	4.826859	-2.586078	0.296328
18	6	0	3.825907	-0.823288	-0.507338
19	1	0	4.545821	-0.150617	-0.942460
20	6	0	2.591240	-2.401276	0.461961
21	1	0	2.254966	-3.292485	0.964355
22	6	0	1.773776	-1.392300	0.033327
23	6	0	0.709018	1.914983	0.334703
24	6	0	0.706510	1.742426	1.647758
25	1	0	0.258090	0.854547	2.075770
26	1	0	1.146268	2.468171	2.317613
27	6	0	0.145186	1.001518	-0.730682
28	1	0	-0.638134	1.536690	-1.270776
29	1	0	0.930049	0.789256	-1.454678
30	17	0	1.435179	3.360178	-0.375230

2i

E=-1204.422521 au

1	6	0	3.142822	0.152421	-1.367949
2	6	0	1.522305	0.709922	-0.088474
3	6	0	2.703788	-1.260521	-0.843638
4	1	0	2.383074	-1.890796	-1.674919
5	1	0	3.479895	-1.780808	-0.285582
6	6	0	1.510828	-0.847288	0.049740
7	1	0	3.665942	0.160892	-2.320859
8	8	0	1.850630	0.787192	-1.490142
9	6	0	0.087886	1.141964	0.164724
10	8	0	-0.264784	2.251782	0.496048
11	6	0	0.086966	-1.167777	-0.424892
12	1	0	0.079601	-1.317932	-1.508651
13	1	0	-0.320122	-2.052895	0.062672
14	6	0	-2.117602	-0.002138	-0.084379
15	6	0	-2.881406	1.025906	0.491250
16	6	0	-2.777575	-1.083603	-0.686955
17	6	0	-4.269657	0.957003	0.456615
18	1	0	-2.384323	1.867187	0.946795
19	6	0	-4.168149	-1.137645	-0.708842
20	1	0	-2.215707	-1.882636	-1.151899
21	6	0	-4.924415	-0.119333	-0.138122
22	1	0	-4.843780	1.759452	0.906187
23	1	0	-4.656853	-1.982657	-1.180672
24	1	0	-6.007037	-0.162552	-0.156956
25	7	0	-0.700484	0.025078	-0.062113

26	17	0	1.701327	-1.395335	1.778831
27	6	0	2.746283	1.300927	0.570382
28	1	0	2.762538	1.810304	1.521387
29	6	0	3.759841	0.935247	-0.215678
30	1	0	4.819338	1.075273	-0.052778

TS h

E= -1204.375827 au

1	6	0	3.265025	0.457646	-1.346988
2	6	0	1.550356	0.931096	-0.138664
3	6	0	2.613102	-1.501976	-0.739298
4	1	0	2.451751	-1.811077	-1.765244
5	1	0	3.460846	-1.957489	-0.246919
6	6	0	1.498671	-1.126074	0.024663
7	1	0	3.790486	0.344506	-2.284033
8	8	0	1.949082	0.834454	-1.454450
9	6	0	0.092586	1.189162	0.117431
10	8	0	-0.322736	2.253106	0.532533
11	6	0	0.091222	-1.155391	-0.531360
12	1	0	0.157341	-1.237305	-1.620856
13	1	0	-0.456018	-2.021801	-0.154771
14	6	0	-2.079238	0.029593	-0.129518
15	6	0	-2.823718	0.867742	0.712816
16	6	0	-2.755691	-0.872172	-0.962972
17	6	0	-4.212677	0.793590	0.710516
18	1	0	-2.315111	1.574609	1.348442
19	6	0	-4.145813	-0.939546	-0.949091
20	1	0	-2.204787	-1.514517	-1.637661
21	6	0	-4.883642	-0.107147	-0.113366
22	1	0	-4.773371	1.448016	1.368488
23	1	0	-4.648941	-1.643419	-1.602458
24	1	0	-5.966121	-0.158367	-0.104876
25	7	0	-0.655948	0.059967	-0.146088
26	6	0	2.676859	1.287489	0.642117
27	6	0	3.772177	0.960513	-0.121610
28	1	0	2.647807	1.592656	1.675376
29	1	0	4.810209	0.959753	0.174070
30	17	0	1.568910	-1.504880	1.776489

REACTION j

1j

E= -3317.537556 au

1	6	0	2.556434	-1.120804	0.425651

2	6	0	3.897077	-1.500365	0.445571
3	6	0	4.872454	-0.663565	-0.086379
4	6	0	4.495018	0.555975	-0.646574
5	6	0	3.158716	0.937429	-0.681200
6	6	0	2.178077	0.098940	-0.141544
7	1	0	1.808397	-1.772375	0.859990
8	1	0	4.174136	-2.450374	0.888290
9	1	0	5.915882	-0.956003	-0.064790
10	1	0	5.245373	1.216196	-1.066664
11	1	0	2.875464	1.887116	-1.111350
12	7	0	0.784740	0.453566	-0.218582
13	6	0	0.398142	1.736038	0.159870
14	8	0	1.194889	2.537114	0.624104
15	8	0	-2.014943	1.468643	-0.557774
16	6	0	-2.880862	3.420103	0.099633
17	1	0	-3.589585	4.212437	0.279119
18	6	0	-3.139349	2.225871	-0.499317
19	1	0	-4.025048	1.779115	-0.918859
20	6	0	-1.497148	3.402041	0.435516
21	1	0	-0.916271	4.168838	0.919639
22	6	0	-1.004966	2.195496	0.020491
23	6	0	-0.918919	-1.257607	0.464457
24	6	0	-0.837153	-1.031696	1.766442
25	1	0	-0.143695	-0.288053	2.142442
26	1	0	-1.445483	-1.566309	2.482486
27	6	0	-0.144723	-0.593809	-0.652854
28	1	0	0.442048	-1.352756	-1.173339
29	1	0	-0.851531	-0.196897	-1.379157
30	35	0	-2.149121	-2.580750	-0.214770

2j

E= -3317.546294 au

1	6	0	2.809407	-1.422394	1.213348
2	6	0	1.250014	-1.023495	-0.196652
3	6	0	2.486051	0.071528	1.570897
4	1	0	2.147264	0.148789	2.605809
5	1	0	3.326878	0.746653	1.425710
6	6	0	1.328455	0.330053	0.578447
7	1	0	3.265424	-2.009499	2.006603
8	8	0	1.479012	-1.905765	0.922682
9	6	0	-0.185705	-1.119688	-0.685028
10	8	0	-0.572965	-1.813424	-1.598569
11	6	0	-0.103581	0.434042	1.119827
12	1	0	-0.167393	-0.067264	2.090948
13	1	0	-0.437807	1.464833	1.227835
14	6	0	-2.339365	-0.139504	0.113724
15	6	0	-3.113763	-0.588078	-0.968355

16	6	0	-2.982025	0.460894	1.206627
17	6	0	-4.494781	-0.428767	-0.942303
18	1	0	-2.631273	-1.062354	-1.807796
19	6	0	-4.365214	0.615681	1.213655
20	1	0	-2.413821	0.800487	2.062168
21	6	0	-5.131748	0.173233	0.140649
22	1	0	-5.077046	-0.780271	-1.786753
23	1	0	-4.840372	1.082539	2.069100
24	1	0	-6.208638	0.293957	0.148068
25	7	0	-0.927879	-0.270474	0.120119
26	6	0	2.481800	-1.242882	-1.043261
27	1	0	2.533565	-1.128894	-2.114865
28	6	0	3.458527	-1.470549	-0.164096
29	1	0	4.517107	-1.583579	-0.351950
30	35	0	1.675556	1.881171	-0.627242

TS j

E= -3317.499305 au

1	6	0	2.924710	-1.716314	0.966530
2	6	0	1.274044	-1.241900	-0.328282
3	6	0	2.430204	0.273731	1.617803
4	1	0	2.217616	-0.069249	2.624278
5	1	0	3.336471	0.853016	1.511659
6	6	0	1.348082	0.514221	0.758841
7	1	0	3.388532	-2.220684	1.801685
8	8	0	1.584603	-1.967327	0.801281
9	6	0	-0.175237	-1.173006	-0.718330
10	8	0	-0.620111	-1.747904	-1.692109
11	6	0	-0.088345	0.324176	1.196027
12	1	0	-0.085184	-0.266439	2.118405
13	1	0	-0.565619	1.282923	1.406139
14	6	0	-2.290553	-0.202959	0.122714
15	6	0	-3.022684	-0.319077	-1.067620
16	6	0	-2.969665	0.090443	1.313631
17	6	0	-4.402285	-0.142411	-1.051023
18	1	0	-2.513047	-0.557641	-1.987202
19	6	0	-4.349657	0.271690	1.312984
20	1	0	-2.429983	0.163418	2.248870
21	6	0	-5.075240	0.155905	0.131587
22	1	0	-4.953564	-0.234804	-1.980073
23	1	0	-4.855146	0.497119	2.245242
24	1	0	-6.150058	0.294612	0.132123
25	7	0	-0.875470	-0.358070	0.147946
26	6	0	2.430158	-1.175026	-1.144217
27	1	0	2.455769	-0.817703	-2.160561
28	6	0	3.486114	-1.452375	-0.309244
29	1	0	4.540573	-1.371516	-0.524967

30	35	0	1.568803	1.983791	-0.518657

REACTION k

1k

E= -1204.407416 au

1	6	0	-2.543781	0.737420	-0.213443
2	6	0	-3.923552	0.625900	-0.056012
3	6	0	-4.521195	-0.626810	0.036768
4	6	0	-3.726239	-1.769565	-0.035542
5	6	0	-2.349653	-1.667998	-0.202846
6	6	0	-1.747105	-0.408395	-0.291383
7	1	0	-2.088054	1.718108	-0.262922
8	1	0	-4.526287	1.525020	0.005238
9	1	0	-5.593857	-0.713671	0.166379
10	1	0	-4.179846	-2.751911	0.034101
11	1	0	-1.740501	-2.558449	-0.248853
12	7	0	-0.334083	-0.276132	-0.521019
13	6	0	0.545799	-1.037285	0.235967
14	8	0	0.157947	-1.806288	1.101740
15	8	0	2.640986	-0.149320	-0.885231
16	6	0	4.225451	-1.280437	0.212017
17	1	0	5.194805	-1.634401	0.524273
18	6	0	3.976404	-0.358419	-0.756747
19	1	0	4.605255	0.216402	-1.415795
20	6	0	2.954351	-1.670567	0.721813
21	1	0	2.735154	-2.379530	1.502098
22	6	0	2.013911	-0.960143	0.029312
23	6	0	0.673489	2.688652	-0.030291
24	6	0	0.072605	0.666596	-1.568621
25	1	0	-0.780932	0.763548	-2.245286
26	1	0	0.870289	0.220472	-2.163865
27	6	0	0.513439	2.056815	-1.187115
28	1	0	0.759948	2.660684	-2.059305
29	1	0	1.015314	3.713452	0.009682
30	17	0	0.393663	2.048440	1.570945

2k

E= -1204.418801 au

1	6	0	-3.139756	-0.299076	-0.638601
2	6	0	-1.289940	-1.091481	0.062342
3	6	0	-2.761139	0.754562	0.459990
4	6	0	-1.384630	0.203047	0.921587

5	1	0	-1.384613	-0.008453	1.991390
6	1	0	-3.817660	0.056770	-1.408781
7	8	0	-1.849109	-0.609215	-1.178119
8	6	0	0.195685	-1.382881	-0.060924
9	8	0	0.682056	-2.457779	-0.338588
10	6	0	-0.081523	0.914399	0.528565
11	1	0	-0.219308	1.554766	-0.343730
12	1	0	0.321494	1.515038	1.345052
13	6	0	2.239933	0.039960	0.086420
14	6	0	3.162725	-1.017713	0.042037
15	6	0	2.713260	1.358664	0.012953
16	6	0	4.521597	-0.744658	-0.070135
17	1	0	2.809013	-2.035553	0.081990
18	6	0	4.077253	1.613018	-0.095845
19	1	0	2.023911	2.192013	0.025406
20	6	0	4.991276	0.565256	-0.137194
21	1	0	5.220178	-1.573273	-0.103361
22	1	0	4.420050	2.640001	-0.153365
23	1	0	6.052835	0.765453	-0.222951
24	7	0	0.847518	-0.193915	0.217742
25	1	0	-3.483515	0.802014	1.269718
26	17	0	-2.731947	2.444899	-0.212965
27	6	0	-3.492143	-1.591694	0.098913
28	1	0	-4.493699	-1.951253	0.288609
29	6	0	-2.330205	-2.097166	0.513914
30	1	0	-2.136160	-2.972871	1.115764

TS k

E= -1204.370863 au

1	6	0	-3.220460	-0.564641	-0.759852
2	6	0	-1.294394	-1.227140	-0.075144
3	6	0	-2.635293	0.957578	0.753440
4	6	0	-1.377219	0.406958	1.065773
5	1	0	-1.300008	-0.025002	2.058243
6	1	0	-3.890025	-0.065598	-1.443965
7	8	0	-1.907859	-0.600213	-1.139562
8	6	0	0.204380	-1.374463	-0.140767
9	8	0	0.746546	-2.431014	-0.400772
10	6	0	-0.071208	0.945896	0.523518
11	1	0	-0.252509	1.577580	-0.347905
12	1	0	0.435339	1.550797	1.279806
13	6	0	2.223378	0.043860	0.060975
14	6	0	3.151004	-1.001140	0.189592
15	6	0	2.694043	1.346489	-0.160424
16	6	0	4.512783	-0.733267	0.097966
17	1	0	2.801994	-2.009387	0.343081

18	6	0	4.060244	1.598303	-0.244876
19	1	0	2.000911	2.167548	-0.284884
20	6	0	4.979018	0.561676	-0.116154
21	1	0	5.215409	-1.552782	0.199751
22	1	0	4.401242	2.612602	-0.419004
23	1	0	6.042455	0.759078	-0.183788
24	7	0	0.821814	-0.181676	0.169472
25	6	0	-2.241980	-2.113404	0.511039
26	6	0	-3.472059	-1.664144	0.095214
27	1	0	-2.014922	-2.863495	1.252564
28	1	0	-4.446017	-1.989857	0.427669
29	1	0	-3.435816	0.929716	1.476987
30	17	0	-2.770215	2.431470	-0.236705

REACTION l

1l

E= -1204.409264 au

1	6	0	2.484962	0.139674	-1.077503
2	6	0	3.849064	0.341138	-1.267105
3	6	0	4.739648	0.174729	-0.208019
4	6	0	4.261200	-0.204624	1.043663
5	6	0	2.897720	-0.414959	1.235473
6	6	0	2.005539	-0.234819	0.178282
7	1	0	1.792145	0.252701	-1.901272
8	1	0	4.216327	0.628180	-2.245839
9	1	0	5.801094	0.334061	-0.359509
10	1	0	4.948321	-0.347944	1.869814
11	1	0	2.521554	-0.730593	2.202201
12	7	0	0.593882	-0.406858	0.415908
13	6	0	-0.052605	-1.406191	-0.291106
14	8	0	0.550222	-2.130480	-1.069359
15	8	0	-2.322126	-1.039774	0.784448
16	6	0	-3.560986	-2.546478	-0.307340
17	1	0	-4.405880	-3.139248	-0.619030
18	6	0	-3.560993	-1.585394	0.654288
19	1	0	-4.319052	-1.187754	1.308137
20	6	0	-2.228512	-2.605045	-0.807964
21	1	0	-1.829040	-3.248379	-1.573580
22	6	0	-1.503814	-1.672704	-0.120912
23	6	0	-1.743823	2.261387	0.363112
24	1	0	-2.557560	1.804838	0.908998
25	6	0	-0.057008	0.647820	1.220940
26	1	0	0.684174	0.979436	1.951605
27	1	0	-0.892995	0.232635	1.774141
28	6	0	-0.491814	1.828017	0.388251

29	1	0	0.271827	2.329218	-0.197957
30	17	0	-2.261431	3.645152	-0.574950

2l

E= -1204.420059 au

1	6	0	-2.915830	0.408461	1.077130
2	6	0	-1.152617	0.952504	-0.001827
3	6	0	-2.542209	-0.949206	0.383856
4	1	0	-2.309938	-1.696072	1.138967
5	6	0	-1.301695	-0.532379	-0.439691
6	1	0	-1.464840	-0.638129	-1.511175
7	1	0	-3.514668	0.311904	1.978900
8	8	0	-1.583729	0.852152	1.380103
9	6	0	0.330684	1.259713	-0.105811
10	8	0	0.817727	2.366936	-0.175754
11	6	0	0.061897	-1.113691	-0.035627
12	1	0	0.042508	-1.516189	0.982074
13	1	0	0.396002	-1.900106	-0.714439
14	6	0	2.389895	-0.152275	-0.062446
15	6	0	3.284865	0.886907	-0.365347
16	6	0	2.903923	-1.410335	0.287184
17	6	0	4.655041	0.655743	-0.315511
18	1	0	2.901705	1.861143	-0.622625
19	6	0	4.278577	-1.624128	0.328984
20	1	0	2.240190	-2.226082	0.539846
21	6	0	5.164152	-0.594655	0.028131
22	1	0	5.330975	1.469873	-0.552054
23	1	0	4.652690	-2.603960	0.603689
24	1	0	6.234109	-0.762933	0.062085
25	7	0	0.985066	0.037109	-0.113100
26	17	0	-3.883118	-1.669933	-0.601515
27	6	0	-2.252564	1.783249	-0.619194
28	1	0	-2.139698	2.437748	-1.470995
29	6	0	-3.360881	1.419227	0.027161
30	1	0	-4.382886	1.704393	-0.173555

TS l

E= -1204.373175 au

1	6	0	-2.897802	0.685500	1.291852
2	6	0	-1.149979	1.116012	0.111692
3	6	0	-2.478908	-1.214058	0.199371
4	1	0	-2.437874	-1.797235	1.108209
5	6	0	-1.312468	-0.781736	-0.452603
6	1	0	-1.350500	-0.719706	-1.534885
7	1	0	-3.420923	0.436462	2.202943

8	8	0	-1.542319	0.836003	1.408749
9	6	0	0.331911	1.275241	-0.106025
10	8	0	0.856722	2.349015	-0.324218
11	6	0	0.055632	-1.122116	0.106924
12	1	0	-0.025086	-1.410105	1.159585
13	1	0	0.495444	-1.959259	-0.440714
14	6	0	2.363896	-0.142131	-0.036427
15	6	0	3.235366	0.781954	-0.632738
16	6	0	2.899678	-1.286759	0.571661
17	6	0	4.606974	0.551524	-0.613406
18	1	0	2.836964	1.673451	-1.089511
19	6	0	4.274129	-1.505272	0.577455
20	1	0	2.252352	-2.004228	1.058121
21	6	0	5.137271	-0.588685	-0.014501
22	1	0	5.265910	1.276078	-1.078615
23	1	0	4.666516	-2.395956	1.055087
24	1	0	6.207471	-0.758965	-0.007579
25	7	0	0.953292	0.044619	-0.046201
26	6	0	-2.229740	1.775308	-0.536031
27	6	0	-3.347463	1.467305	0.202696
28	1	0	-2.173122	2.267669	-1.494194
29	1	0	-4.378585	1.664700	-0.044766
30	17	0	-3.885753	-1.655171	-0.780356

REACTION m

1m

E= -785.934987 au

1	8	0	3.427910	0.338276	-0.425905
2	6	0	3.893641	-1.146199	1.177223
3	1	0	4.388354	-1.643250	1.996577
4	6	0	4.285685	0.008655	0.579641
5	1	0	5.111340	0.682672	0.732524
6	6	0	2.705530	-1.564215	0.494145
7	1	0	2.100687	-2.435097	0.690226
8	6	0	2.461311	-0.630887	-0.466595
9	6	0	1.379584	-0.467245	-1.482769
10	1	0	1.787080	0.050562	-2.355174
11	1	0	1.040228	-1.454254	-1.792532
12	6	0	0.165228	1.729548	-1.108204
13	1	0	-0.826130	2.045097	-1.444079
14	1	0	0.867174	2.025513	-1.896158
15	6	0	0.509075	2.482801	0.154213
16	1	0	0.463044	3.564991	0.041402
17	6	0	0.839459	1.960963	1.328727
18	1	0	0.904681	0.889840	1.482662
19	1	0	1.067308	2.595218	2.177464

20	7	0	0.192824	0.271786	-1.029141
21	6	0	-0.861489	-0.470234	-0.557102
22	8	0	-0.839445	-1.683621	-0.453341
23	8	0	-1.909271	0.323424	-0.245142
24	6	0	-3.151723	-0.235456	0.320877
25	6	0	-4.007964	1.014222	0.529076
26	1	0	-4.973808	0.739539	0.959893
27	1	0	-3.508757	1.710944	1.205657
28	1	0	-4.184523	1.522230	-0.421733
29	6	0	-2.858687	-0.920586	1.658221
30	1	0	-3.799148	-1.227900	2.123710
31	1	0	-2.231967	-1.799445	1.517780
32	1	0	-2.354137	-0.227095	2.335675
33	6	0	-3.808609	-1.183236	-0.686311
34	1	0	-4.789675	-1.489994	-0.313211
35	1	0	-3.953469	-0.675400	-1.643510
36	1	0	-3.197843	-2.070097	-0.844931

2m

E= -785.941139 au

1	6	0	3.844672	0.673277	0.722585
2	6	0	2.301823	-0.586320	-0.064470
3	6	0	1.943075	0.795720	-0.731789
4	1	0	1.954566	0.727728	-1.821038
5	1	0	4.424263	1.095196	1.540195
6	8	0	2.762573	-0.126764	1.223296
7	6	0	0.511124	1.021969	-0.227832
8	1	0	0.513731	1.523257	0.746237
9	1	0	-0.100243	1.608622	-0.912792
10	7	0	-0.025547	-0.341635	-0.109093
11	6	0	4.547584	-0.306286	-0.211901
12	1	0	5.592459	-0.272548	-0.488559
13	6	0	3.586119	-1.096547	-0.691811
14	1	0	3.654597	-1.858577	-1.456122
15	6	0	3.061612	1.703861	-0.168743
16	1	0	3.685480	2.155465	-0.941378
17	1	0	2.656639	2.501817	0.457246
18	6	0	1.013105	-1.370958	0.028507
19	1	0	0.929435	-2.113538	-0.770571
20	1	0	0.939094	-1.894696	0.984409
21	6	0	-1.336288	-0.684647	0.006485
22	8	0	-1.720209	-1.831500	0.147303
23	8	0	-2.128409	0.416342	-0.065311
24	6	0	-3.595069	0.300425	0.013017
25	6	0	-4.048212	1.756078	-0.106706
26	1	0	-5.138123	1.816887	-0.057050
27	1	0	-3.629009	2.355097	0.704668

28	1	0	-3.719631	2.183372	-1.056768
29	6	0	-4.121200	-0.530316	-1.160828
30	1	0	-3.772164	-0.109646	-2.107703
31	1	0	-3.786688	-1.563645	-1.087910
32	1	0	-5.214561	-0.511275	-1.163084
33	6	0	-4.005528	-0.284944	1.367267
34	1	0	-3.575154	0.306010	2.180079
35	1	0	-5.094371	-0.254782	1.464503
36	1	0	-3.670024	-1.315813	1.464299

TS m

E= -785.897566 au

1	6	0	4.017398	0.384266	0.771857
2	6	0	2.360008	-0.760279	-0.001821
3	6	0	1.845517	1.146369	-0.701245
4	1	0	1.805910	0.975159	-1.772518
5	1	0	4.585613	0.846708	1.566099
6	8	0	2.857774	-0.235473	1.173083
7	6	0	0.506372	1.080434	-0.006969
8	1	0	0.609003	1.424715	1.029915
9	1	0	-0.229589	1.718893	-0.495348
10	7	0	0.000049	-0.299704	-0.047571
11	6	0	4.525196	-0.330199	-0.347826
12	1	0	5.500023	-0.192114	-0.790437
13	6	0	3.468158	-1.056712	-0.840552
14	1	0	3.417588	-1.614268	-1.763894
15	6	0	2.914314	1.904729	-0.191815
16	1	0	3.631594	2.340050	-0.876691
17	1	0	2.757083	2.480123	0.715252
18	6	0	1.001080	-1.371879	0.072090
19	1	0	0.864542	-2.099029	-0.731222
20	1	0	0.876880	-1.906363	1.019387
21	6	0	-1.313305	-0.661987	0.001419
22	8	0	-1.682435	-1.822378	0.043524
23	8	0	-2.126306	0.424126	-0.011820
24	6	0	-3.592442	0.273854	0.003903
25	6	0	-4.072427	1.725652	-0.024438
26	1	0	-5.164412	1.761430	-0.007709
27	1	0	-3.693246	2.271273	0.842423
28	1	0	-3.722268	2.228770	-0.928538
29	6	0	-4.060203	-0.476849	-1.246029
30	1	0	-3.688072	0.019435	-2.146228
31	1	0	-3.707357	-1.506542	-1.237799
32	1	0	-5.153014	-0.477287	-1.285377
33	6	0	-4.036793	-0.417620	1.296031
34	1	0	-3.650964	0.122087	2.164886
35	1	0	-5.128789	-0.418620	1.353707

36	1	0	-3.680368	-1.445352	1.331170

REACTION n

1n

E= -1245.104643 au

1	8	0	3.344071	-0.310854	-0.433071
2	6	0	3.787984	-1.815115	1.157709
3	1	0	4.279546	-2.330755	1.967328
4	6	0	4.205744	-0.669922	0.559000
5	1	0	5.053015	-0.021198	0.702519
6	6	0	2.578246	-2.194781	0.490078
7	1	0	1.953097	-3.050247	0.691000
8	6	0	2.348753	-1.250728	-0.463846
9	6	0	1.259288	-1.049080	-1.463485
10	1	0	1.676524	-0.578955	-2.358207
11	1	0	0.852948	-2.020271	-1.739414
12	6	0	0.199375	1.220341	-1.088629
13	1	0	-0.766506	1.618252	-1.404749
14	1	0	0.923357	1.480674	-1.866476
15	6	0	0.603518	1.924259	0.189078
16	6	0	0.894887	1.392164	1.364706
17	1	0	0.874961	0.316927	1.488746
18	1	0	1.169131	2.003362	2.213266
19	7	0	0.126795	-0.229426	-1.004218
20	6	0	-0.987550	-0.893995	-0.541607
21	8	0	-1.056942	-2.105061	-0.452572
22	8	0	-1.965413	-0.023129	-0.219928
23	6	0	-3.262064	-0.486239	0.319244
24	6	0	-4.014180	0.826826	0.536234
25	1	0	-5.006441	0.625800	0.946825
26	1	0	-3.471850	1.469327	1.232794
27	1	0	-4.132180	1.363682	-0.407614
28	6	0	-3.044117	-1.215740	1.646727
29	1	0	-4.012962	-1.454470	2.093668
30	1	0	-2.488076	-2.139693	1.498190
31	1	0	-2.496309	-0.577197	2.344358
32	6	0	-3.976014	-1.359581	-0.715281
33	1	0	-4.986059	-1.587709	-0.364249
34	1	0	-4.059940	-0.827026	-1.666194
35	1	0	-3.440199	-2.292988	-0.877946
36	17	0	0.650201	3.679434	-0.032902

2n

E= -1245.110462 au

1	6	0	3.562448	-0.508754	1.247323
2	6	0	2.063773	-0.749066	-0.271578
3	6	0	1.760813	0.706116	0.266611
4	1	0	4.079925	-0.827250	2.148640
5	8	0	2.421682	-1.350108	0.988378
6	6	0	0.316844	0.553495	0.757346
7	1	0	0.322909	0.190966	1.790782
8	1	0	-0.248423	1.481397	0.713473
9	7	0	-0.250728	-0.450019	-0.146587
10	6	0	4.316029	-0.597057	-0.072077
11	1	0	5.379951	-0.450888	-0.196746
12	6	0	3.385803	-0.752828	-1.014261
13	1	0	3.504574	-0.760195	-2.087532
14	6	0	2.871931	0.899685	1.321115
15	1	0	3.540411	1.723984	1.079823
16	1	0	2.450648	1.064990	2.314224
17	6	0	0.757434	-1.281415	-0.812883
18	1	0	0.695831	-1.167893	-1.898522
19	1	0	0.635295	-2.339402	-0.570986
20	6	0	-1.574578	-0.664825	-0.381646
21	8	0	-1.986685	-1.515324	-1.147431
22	8	0	-2.333191	0.188512	0.349360
23	6	0	-3.804396	0.175402	0.244341
24	6	0	-4.214486	1.291222	1.206003
25	1	0	-5.302584	1.388308	1.225912
26	1	0	-3.866506	1.073054	2.218112
27	1	0	-3.786784	2.245784	0.891506
28	6	0	-4.234347	0.508081	-1.187201
29	1	0	-3.784897	1.451573	-1.507724
30	1	0	-3.936491	-0.278225	-1.878577
31	1	0	-5.321503	0.619181	-1.224756
32	6	0	-4.349884	-1.175511	0.715084
33	1	0	-3.986846	-1.398988	1.721650
34	1	0	-5.442251	-1.138221	0.747580
35	1	0	-4.043930	-1.975009	0.042841
36	17	0	1.818060	1.955004	-1.066772

TS n

E= -1245.066150 au

1	6	0	3.826500	-0.577220	1.013399
2	6	0	2.138180	-1.012447	-0.258195
3	6	0	1.677807	0.969463	0.395887
4	1	0	4.420382	-0.704557	1.907306
5	8	0	2.658328	-1.304417	0.984915
6	6	0	0.332318	0.503290	0.894241

7	1	0	0.469507	0.114816	1.911450
8	1	0	-0.385253	1.320283	0.938154
9	7	0	-0.205785	-0.533485	0.012952
10	6	0	4.301218	-0.465869	-0.323320
11	1	0	5.269608	-0.089543	-0.615661
12	6	0	3.223199	-0.739100	-1.129220
13	1	0	3.148508	-0.616117	-2.198101
14	6	0	2.774400	1.197408	1.243865
15	1	0	3.474046	1.983119	0.992940
16	1	0	2.621152	1.048639	2.307289
17	6	0	0.756897	-1.501828	-0.535446
18	1	0	0.595255	-1.607473	-1.609030
19	1	0	0.609660	-2.487959	-0.081996
20	6	0	-1.528778	-0.740740	-0.253506
21	8	0	-1.925340	-1.646927	-0.963174
22	8	0	-2.308019	0.176610	0.368212
23	6	0	-3.772048	0.181304	0.179926
24	6	0	-4.210063	1.372504	1.032756
25	1	0	-5.295571	1.487665	0.986718
26	1	0	-3.920627	1.225093	2.075608
27	1	0	-3.747738	2.294126	0.672407
28	6	0	-4.111996	0.414703	-1.294268
29	1	0	-3.623581	1.323261	-1.655687
30	1	0	-3.792142	-0.426409	-1.906610
31	1	0	-5.192484	0.541980	-1.404128
32	6	0	-4.373090	-1.120785	0.716097
33	1	0	-4.072155	-1.276323	1.755531
34	1	0	-5.464434	-1.060443	0.683724
35	1	0	-4.048207	-1.973207	0.122501
36	17	0	1.574562	1.997131	-1.069765

REACTION o

1o

E= -3358.228043 au

1	8	0	3.059661	-1.436785	-0.400033
2	6	0	3.083795	-3.035380	1.160107
3	1	0	3.413676	-3.669329	1.967750
4	6	0	3.780331	-2.011095	0.603097
5	1	0	4.753032	-1.586583	0.784693
6	6	0	1.839755	-3.102431	0.452326
7	1	0	1.022065	-3.786454	0.614038
8	6	0	1.871036	-2.111823	-0.481339
9	6	0	0.890812	-1.634888	-1.501261
10	1	0	1.435170	-1.212462	-2.349439

11	1	0	0.307571	-2.484604	-1.851770
12	6	0	0.277163	0.789581	-1.086622
13	1	0	-0.599864	1.367845	-1.381928
14	1	0	1.027752	0.924824	-1.870714
15	6	0	0.819410	1.373217	0.200832
16	6	0	0.998610	0.774121	1.366196
17	1	0	0.759489	-0.277549	1.472180
18	1	0	1.391054	1.296838	2.227257
19	7	0	-0.067642	-0.622553	-1.029491
20	6	0	-1.282260	-1.076769	-0.565950
21	8	0	-1.572455	-2.256174	-0.496855
22	8	0	-2.080797	-0.047423	-0.219055
23	6	0	-3.437483	-0.275602	0.322892
24	6	0	-3.932711	1.148100	0.576896
25	1	0	-4.942040	1.123262	0.994518
26	1	0	-3.276081	1.662585	1.281371
27	1	0	-3.956644	1.719629	-0.353497
28	6	0	-3.352251	-1.062304	1.633152
29	1	0	-4.345623	-1.121488	2.085792
30	1	0	-2.983973	-2.072235	1.462216
31	1	0	-2.688238	-0.554318	2.337002
32	6	0	-4.306426	-0.977873	-0.723052
33	1	0	-5.336028	-1.038243	-0.360105
34	1	0	-4.309123	-0.409620	-1.656878
35	1	0	-3.943942	-1.984838	-0.921834
36	35	0	1.257008	3.245787	-0.002580

2o

E= -3358.234877

1	6	0	3.209734	-1.480671	1.078623
2	6	0	1.785881	-1.011466	-0.460213
3	6	0	1.570556	0.170585	0.564378
4	1	0	3.645679	-2.149963	1.815970
5	8	0	2.019540	-2.056686	0.506110
6	6	0	0.094963	-0.013142	0.934783
7	1	0	0.021198	-0.726112	1.763870
8	1	0	-0.398341	0.910960	1.225594
9	7	0	-0.500609	-0.565522	-0.284214
10	6	0	4.028143	-1.166475	-0.165780
11	1	0	5.105985	-1.091760	-0.204343
12	6	0	3.144036	-0.881965	-1.122133
13	1	0	3.323117	-0.518635	-2.123006
14	6	0	2.636008	-0.130889	1.640724
15	1	0	3.385208	0.652806	1.733222
16	1	0	2.172756	-0.292214	2.615895
17	6	0	0.473265	-1.188420	-1.187152
18	1	0	0.480566	-0.684658	-2.157357

19	1	0	0.255087	-2.245957	-1.350445
20	6	0	-1.828304	-0.599356	-0.584981
21	8	0	-2.268664	-1.090939	-1.606668
22	8	0	-2.555076	-0.019832	0.402107
23	6	0	-4.022348	0.090046	0.299719
24	6	0	-4.392015	0.805776	1.599377
25	1	0	-5.473911	0.947819	1.655009
26	1	0	-4.073894	0.219403	2.464250
27	1	0	-3.910411	1.784836	1.648963
28	6	0	-4.403840	0.939748	-0.915434
29	1	0	-3.898731	1.908258	-0.873052
30	1	0	-4.132181	0.439803	-1.843397
31	1	0	-5.482659	1.118143	-0.912094
32	6	0	-4.649008	-1.306181	0.251670
33	1	0	-4.319552	-1.898074	1.109688
34	1	0	-5.738160	-1.220044	0.295914
35	1	0	-4.372817	-1.826389	-0.663724
36	35	0	1.813329	1.960130	-0.292153

TS o

E= -3358.189660 au

1	6	0	3.536880	-1.394650	0.923469
2	6	0	1.887938	-1.292537	-0.465753
3	6	0	1.529536	0.430579	0.750082
4	1	0	4.073936	-1.830808	1.753701
5	8	0	2.322434	-1.980850	0.646782
6	6	0	0.138673	-0.065383	1.057414
7	1	0	0.214656	-0.754429	1.909104
8	1	0	-0.530004	0.745345	1.338863
9	7	0	-0.429274	-0.746169	-0.106348
10	6	0	4.084915	-0.932848	-0.305539
11	1	0	5.091000	-0.568202	-0.445790
12	6	0	3.032768	-0.865793	-1.185612
13	1	0	3.021131	-0.426804	-2.170479
14	6	0	2.601847	0.312442	1.649508
15	1	0	3.367227	1.076113	1.664727
16	1	0	2.391926	-0.136621	2.615109
17	6	0	0.491388	-1.561851	-0.913975
18	1	0	0.374261	-1.309910	-1.968927
19	1	0	0.258358	-2.626111	-0.802093
20	6	0	-1.754128	-0.780472	-0.435651
21	8	0	-2.180943	-1.400973	-1.391923
22	8	0	-2.497139	-0.049790	0.429708
23	6	0	-3.953948	0.095955	0.244552
24	6	0	-4.346202	0.997580	1.415671

25	1	0	-5.423220	1.180989	1.403184
26	1	0	-4.085256	0.526914	2.366204
27	1	0	-3.829762	1.957872	1.351977
28	6	0	-4.249336	0.781750	-1.091884
29	1	0	-3.706812	1.728212	-1.158682
30	1	0	-3.960357	0.148066	-1.928405
31	1	0	-5.319137	0.996557	-1.163202
32	6	0	-4.635733	-1.270252	0.360199
33	1	0	-4.364751	-1.749134	1.304843
34	1	0	-5.721263	-1.139437	0.344778
35	1	0	-4.347159	-1.921748	-0.462590
36	35	0	1.547364	2.001489	-0.419980

REACTION p

1p

E= -1245.101772

1	8	0	2.929861	-1.070830	-0.319102
2	6	0	2.813597	-2.702585	1.201230
3	1	0	3.081294	-3.373521	2.002051
4	6	0	3.585670	-1.709143	0.689096
5	1	0	4.576160	-1.347760	0.907320
6	6	0	1.589923	-2.679951	0.456716
7	1	0	0.731004	-3.320791	0.576794
8	6	0	1.706903	-1.672003	-0.451603
9	6	0	0.790247	-1.117545	-1.493170
10	1	0	1.387307	-0.666954	-2.289746
11	1	0	0.200246	-1.927668	-1.917444
12	6	0	0.300476	1.265879	-0.792518
13	1	0	-0.532688	1.941690	-0.994229
14	1	0	1.080625	1.475548	-1.525201
15	7	0	-0.162034	-0.107306	-1.010410
16	6	0	-1.397096	-0.549427	-0.608118
17	8	0	-1.772585	-1.702019	-0.714086
18	8	0	-2.128484	0.467015	-0.090558
19	6	0	-3.525636	0.258041	0.343326
20	6	0	-3.935640	1.652543	0.817437
21	1	0	-4.967426	1.637386	1.176425
22	1	0	-3.290320	1.987454	1.632533
23	1	0	-3.863486	2.374117	0.000747
24	6	0	-3.572426	-0.744130	1.499665
25	1	0	-4.591410	-0.799678	1.892235
26	1	0	-3.266171	-1.735226	1.170845
27	1	0	-2.914774	-0.419252	2.310219
28	6	0	-4.382067	-0.185588	-0.845299

29	1	0	-5.432905	-0.218624	-0.545191
30	1	0	-4.286415	0.527753	-1.668109
31	1	0	-4.084883	-1.172477	-1.195528
32	6	0	0.812586	1.514272	0.601819
33	1	0	0.185917	1.152233	1.411352
34	6	0	1.928252	2.139468	0.951787
35	1	0	2.233087	2.293739	1.976833
36	17	0	3.080588	2.821816	-0.181251

2p

E= -1245.104331 au

1	6	0	3.586092	-0.046925	0.569893
2	6	0	1.875844	-1.186900	-0.026428
3	1	0	4.228737	0.432314	1.302321
4	8	0	2.423301	-0.612426	1.178413
5	6	0	0.290853	0.594365	-0.378878
6	1	0	0.380090	1.197817	0.526645
7	1	0	-0.254135	1.170105	-1.124855
8	7	0	-0.402986	-0.672536	-0.102679
9	6	0	4.139470	-1.231505	-0.220701
10	1	0	5.175437	-1.375346	-0.493820
11	6	0	3.072792	-1.943789	-0.582687
12	1	0	3.024187	-2.813864	-1.222721
13	6	0	2.945803	0.917226	-0.490965
14	1	0	3.596654	1.098835	-1.341180
15	6	0	0.504926	-1.787466	0.186893
16	1	0	0.317237	-2.626224	-0.489753
17	1	0	0.393096	-2.150495	1.211555
18	6	0	-1.743464	-0.832186	0.075986
19	8	0	-2.253007	-1.893131	0.386652
20	8	0	-2.399167	0.332307	-0.149949
21	6	0	-3.866383	0.413095	-0.026017
22	6	0	-4.146550	1.877864	-0.363354
23	1	0	-5.219119	2.078106	-0.304994
24	1	0	-3.630852	2.538204	0.337168
25	1	0	-3.803943	2.111618	-1.373799
26	6	0	-4.533376	-0.516500	-1.043622
27	1	0	-4.177619	-0.290808	-2.052459
28	1	0	-4.319930	-1.559738	-0.817725
29	1	0	-5.615973	-0.363917	-1.023506
30	6	0	-4.288795	0.097811	1.411702
31	1	0	-3.757888	0.747922	2.111976
32	1	0	-5.361120	0.278645	1.525844
33	1	0	-4.077909	-0.940043	1.663327
34	6	0	1.667468	0.124914	-0.871243
35	1	0	1.634041	-0.077659	-1.942669
36	17	0	2.652518	2.574015	0.203706

TS p

E= -1245.059953 au

1	6	0	-3.794457	-0.368544	-0.431095
2	6	0	-1.890032	-1.324555	-0.109228
3	1	0	-4.518419	0.175414	-1.019604
4	8	0	-2.624988	-0.671449	-1.076868
5	6	0	-0.275940	0.703661	0.178193
6	1	0	-0.494733	1.224857	-0.758323
7	1	0	0.399651	1.329910	0.759561
8	7	0	0.393913	-0.576541	-0.080474
9	6	0	-4.027902	-1.370584	0.549479
10	1	0	-4.942629	-1.502015	1.107314
11	6	0	-2.817101	-1.982760	0.753036
12	1	0	-2.552805	-2.699609	1.516171
13	6	0	-2.771439	1.103662	0.731480
14	1	0	-3.435139	1.276214	1.565556
15	6	0	-0.484366	-1.687894	-0.472628
16	1	0	-0.169286	-2.598062	0.039395
17	1	0	-0.420802	-1.877822	-1.549625
18	6	0	1.741696	-0.764833	-0.185309
19	8	0	2.239262	-1.830613	-0.501030
20	8	0	2.421966	0.366918	0.117741
21	6	0	3.897172	0.396021	0.096235
22	6	0	4.203904	1.838445	0.500346
23	1	0	5.284142	2.001363	0.519074
24	1	0	3.759108	2.538866	-0.209812
25	1	0	3.803557	2.052426	1.493839
26	6	0	4.459557	-0.587590	1.126002
27	1	0	4.037098	-0.383820	2.113522
28	1	0	4.233480	-1.615584	0.848862
29	1	0	5.544631	-0.468459	1.190172
30	6	0	4.405594	0.109101	-1.319170
31	1	0	3.948665	0.800638	-2.031891
32	1	0	5.489151	0.251528	-1.354466
33	1	0	4.174289	-0.911547	-1.618541
34	6	0	-1.553494	0.422555	0.931671
35	1	0	-1.401885	0.039570	1.935574
36	17	0	-2.843796	2.503704	-0.376252

REACTION q

1q

E= -1245.100919 au

1	8	0	-3.175880	-0.822701	0.658861
2	6	0	-3.586594	-1.271713	-1.490654

3	1	0	-4.078977	-1.313977	-2.449106
4	6	0	-4.060883	-0.675513	-0.366498
5	1	0	-4.963058	-0.135747	-0.134334
6	6	0	-2.314305	-1.829670	-1.139338
7	1	0	-1.632982	-2.374454	-1.773198
8	6	0	-2.107875	-1.529514	0.172749
9	6	0	-0.977240	-1.781041	1.114684
10	1	0	-1.369318	-1.855609	2.132188
11	1	0	-0.506881	-2.727516	0.853769
12	6	0	-0.035263	0.419560	1.959940
13	1	0	0.950357	0.660387	2.365542
14	1	0	-0.665780	0.147746	2.814149
15	6	0	-1.011386	1.767221	0.068325
16	1	0	-1.006626	0.960129	-0.649918
17	7	0	0.081615	-0.759454	1.109332
18	6	0	1.162328	-0.982914	0.288655
19	8	0	1.261508	-1.951750	-0.441196
20	8	0	2.076214	0.002105	0.415884
21	6	0	3.318621	0.005075	-0.385065
22	6	0	4.002089	1.292236	0.076383
23	1	0	4.948254	1.424673	-0.453665
24	1	0	3.366168	2.156805	-0.124515
25	1	0	4.208596	1.255649	1.148419
26	6	0	2.979741	0.074345	-1.876081
27	1	0	3.900015	0.199418	-2.452915
28	1	0	2.479026	-0.833822	-2.206755
29	1	0	2.333342	0.932080	-2.078207
30	6	0	4.168349	-1.219418	-0.037196
31	1	0	5.135914	-1.146675	-0.541234
32	1	0	4.349518	-1.261336	1.040034
33	1	0	3.676413	-2.138650	-0.349885
34	6	0	-0.602213	1.666267	1.322755
35	1	0	-0.655873	2.533361	1.975065
36	17	0	-1.643903	3.258997	-0.600065

2q

E= -1245.107186 au

1	6	0	3.363441	-0.361071	1.032857
2	6	0	1.712491	-1.121179	-0.109377
3	1	0	3.943282	-0.243295	1.944426
4	8	0	2.147016	-1.078221	1.273401
5	6	0	0.151630	0.722962	0.073797
6	1	0	0.128846	0.985547	1.137415
7	1	0	-0.317762	1.531415	-0.485521
8	7	0	-0.555010	-0.542189	-0.166453
9	6	0	3.982627	-1.147462	-0.114629
10	1	0	5.036593	-1.198631	-0.343858

11	6	0	2.954586	-1.635761	-0.808646
12	1	0	2.968174	-2.177710	-1.744075
13	6	0	0.329402	-1.709890	-0.260903
14	1	0	0.205073	-2.213289	-1.224242
15	1	0	0.125346	-2.437497	0.528108
16	6	0	-1.905739	-0.718713	-0.158127
17	8	0	-2.438058	-1.803629	-0.300005
18	8	0	-2.540810	0.465802	0.019306
19	6	0	-4.013828	0.539116	0.054749
20	6	0	-4.265418	2.032851	0.263355
21	1	0	-5.339084	2.229115	0.314000
22	1	0	-3.805647	2.373347	1.193691
23	1	0	-3.845418	2.612329	-0.561815
24	6	0	-4.598253	0.071747	-1.281097
25	1	0	-4.156543	0.637111	-2.105933
26	1	0	-4.413057	-0.989082	-1.439761
27	1	0	-5.677474	0.247289	-1.289119
28	6	0	-4.548942	-0.272085	1.237846
29	1	0	-4.077697	0.059196	2.166921
30	1	0	-5.627447	-0.117503	1.329812
31	1	0	-4.355249	-1.334609	1.102254
32	6	0	1.583486	0.421610	-0.393514
33	1	0	1.710219	0.660332	-1.448699
34	6	0	2.740579	0.965994	0.471693
35	1	0	2.385864	1.582199	1.293845
36	17	0	3.925617	2.011101	-0.423054

TS q

E= -1245.063197 au

1	6	0	3.444853	-0.703520	1.071267
2	6	0	1.736053	-1.325093	-0.090559
3	1	0	3.976567	-0.518676	1.993040
4	8	0	2.168758	-1.186668	1.214579
5	6	0	0.155229	0.705155	0.287613
6	1	0	0.219339	0.782204	1.379782
7	1	0	-0.435160	1.549176	-0.069050
8	7	0	-0.528207	-0.531707	-0.110273
9	6	0	3.967141	-1.188261	-0.154824
10	1	0	4.992430	-1.103763	-0.478151
11	6	0	2.879999	-1.585597	-0.894545
12	1	0	2.855932	-1.882500	-1.932275
13	6	0	0.310460	-1.728340	-0.269182
14	1	0	0.161111	-2.165478	-1.259288
15	1	0	0.034278	-2.488297	0.468018
16	6	0	-1.881450	-0.698905	-0.172418
17	8	0	-2.405142	-1.763449	-0.445841
18	8	0	-2.531312	0.458239	0.099745

19	6	0	-4.005034	0.529744	0.054777
20	6	0	-4.275579	1.990262	0.417446
21	1	0	-5.351419	2.180379	0.430730
22	1	0	-3.869769	2.221230	1.404761
23	1	0	-3.814288	2.660274	-0.311490
24	6	0	-4.502655	0.219472	-1.359400
25	1	0	-4.015568	0.877247	-2.084131
26	1	0	-4.299267	-0.815731	-1.627721
27	1	0	-5.580754	0.393489	-1.414285
28	6	0	-4.608868	-0.409540	1.102448
29	1	0	-4.194863	-0.190330	2.090139
30	1	0	-5.691006	-0.259117	1.146813
31	1	0	-4.407205	-1.450549	0.857187
32	6	0	1.541476	0.719958	-0.316272
33	1	0	1.573189	0.852656	-1.392044
34	6	0	2.646099	1.178421	0.419955
35	1	0	2.517568	1.567942	1.420736
36	17	0	3.924798	2.072017	-0.433915

REACTION r

1r

E= -3776.698521 au

1	6	0	-3.642008	0.820492	0.209516
2	6	0	-5.027731	0.831943	0.062712
3	6	0	-5.681151	-0.246436	-0.524599
4	6	0	-4.936276	-1.336839	-0.971638
5	6	0	-3.552567	-1.351608	-0.839463
6	6	0	-2.896242	-0.270019	-0.244469
7	1	0	-3.145162	1.657139	0.684819
8	1	0	-5.593110	1.685577	0.418867
9	1	0	-6.759527	-0.239716	-0.632942
10	1	0	-5.433826	-2.182281	-1.433111
11	1	0	-2.982360	-2.202682	-1.183409
12	7	0	-1.458976	-0.247638	-0.150606
13	6	0	-0.808442	-1.363930	0.359240
14	8	0	-1.419673	-2.323139	0.804725
15	8	0	1.532891	-0.529665	-0.161898
16	6	0	2.784532	-0.979802	0.067909
17	6	0	0.671513	-1.454427	0.393009
18	6	0	-0.349590	1.875754	0.600347
19	6	0	-0.509968	1.670220	1.899148
20	1	0	-1.012675	0.777605	2.249942
21	1	0	-0.149150	2.376148	2.634248
22	6	0	-0.785432	0.991976	-0.547259
23	1	0	-1.480418	1.552136	-1.175323

24	1	0	0.082643	0.774924	-1.167669
25	6	0	2.775643	-2.158894	0.749690
26	1	0	3.637615	-2.726018	1.057962
27	6	0	1.400675	-2.463545	0.956624
28	1	0	0.978520	-3.319910	1.455371
29	35	0	4.189741	0.068450	-0.581329
30	17	0	0.462699	3.330466	0.019104

2r

E= -3776.712819 au

1	6	0	-2.425732	-0.069265	0.078411
2	6	0	-0.531022	0.640026	0.724219
3	6	0	-1.846226	0.411650	-1.293003
4	1	0	-1.771121	-0.430976	-1.980104
5	1	0	-2.436460	1.200485	-1.753376
6	6	0	-0.456492	0.896355	-0.815943
7	8	0	-1.250782	-0.618120	0.685679
8	6	0	2.973819	-0.323738	-0.014594
9	6	0	3.852403	-0.069127	1.050172
10	6	0	3.453285	-0.996747	-1.147925
11	6	0	5.176964	-0.483534	0.965320
12	1	0	3.491094	0.436585	1.931128
13	6	0	4.783244	-1.400837	-1.216862
14	1	0	2.794966	-1.221606	-1.976329
15	6	0	5.654297	-1.147565	-0.162450
16	1	0	5.842613	-0.278969	1.796280
17	1	0	5.132561	-1.920844	-2.101638
18	1	0	6.689175	-1.464089	-0.217348
19	7	0	1.617376	0.090820	0.027316
20	6	0	-1.527897	1.561341	1.386065
21	1	0	-1.282019	2.432062	1.974099
22	6	0	-2.717930	1.130304	0.967533
23	1	0	-3.697528	1.557871	1.119407
24	35	0	-3.839318	-1.397933	-0.050946
25	17	0	-0.148469	2.646676	-1.212204
26	6	0	0.780189	0.065115	-1.185916
27	1	0	0.483018	-0.959735	-1.427483
28	1	0	1.322086	0.490609	-2.029637
29	6	0	0.909342	0.436151	1.165225
30	8	0	1.318359	0.562652	2.297177

TS r

E= -3776.662768 au

1	6	0	-2.540820	-0.084960	0.287755
2	6	0	-0.576921	0.474597	0.940278

3	6	0	-1.669213	0.664635	-1.546368
4	1	0	-1.816868	-0.297373	-2.021298
5	1	0	-2.335163	1.452171	-1.869877
6	6	0	-0.397685	0.990548	-1.065222
7	8	0	-1.329956	-0.636799	0.613277
8	6	0	2.940028	-0.383641	-0.007624
9	6	0	3.860888	0.065342	0.949081
10	6	0	3.383869	-1.213751	-1.045993
11	6	0	5.195064	-0.317171	0.856276
12	1	0	3.527274	0.693853	1.759101
13	6	0	4.723409	-1.582010	-1.129734
14	1	0	2.686712	-1.589936	-1.783485
15	6	0	5.637033	-1.137292	-0.179238
16	1	0	5.895654	0.038065	1.603531
17	1	0	5.046872	-2.225997	-1.939635
18	1	0	6.679320	-1.427004	-0.243409
19	7	0	1.567688	-0.003225	0.040878
20	6	0	-1.448223	1.465305	1.453588
21	1	0	-1.136759	2.379192	1.933276
22	6	0	-2.706576	1.116573	1.027495
23	1	0	-3.624662	1.676731	1.104431
24	35	0	-3.926236	-1.325926	-0.095287
25	17	0	0.057917	2.722399	-1.102228
26	6	0	0.786591	0.058807	-1.210904
27	1	0	0.408403	-0.932134	-1.480843
28	1	0	1.450343	0.401875	-2.006892
29	6	0	0.885781	0.259140	1.209399
30	8	0	1.359876	0.352177	2.324116

REACTION s

1s

E= -3776.691528 au

1	6	0	-3.492400	0.884225	-0.432251
2	6	0	-4.880695	0.863297	-0.546222
3	6	0	-5.556852	-0.345237	-0.678215
4	6	0	-4.831035	-1.535040	-0.701383
5	6	0	-3.444454	-1.523131	-0.598511
6	6	0	-2.764472	-0.308444	-0.461604
7	1	0	-2.979438	1.829504	-0.308513
8	1	0	-5.430631	1.797220	-0.519328
9	1	0	-6.637553	-0.361849	-0.759789
10	1	0	-5.345968	-2.483462	-0.805411
11	1	0	-2.890601	-2.450212	-0.609225
12	7	0	-1.327739	-0.264582	-0.411703

13	6	0	-0.657216	-1.142079	0.424733
14	8	0	-1.242507	-1.938731	1.141707
15	8	0	1.669524	-0.364146	-0.245335
16	6	0	2.928484	-0.690382	0.114569
17	6	0	0.825521	-1.168016	0.496302
18	6	0	-0.672402	0.729832	-1.269350
19	1	0	-1.384071	0.966176	-2.064821
20	1	0	0.181038	0.269838	-1.769373
21	6	0	2.943253	-1.672219	1.057636
22	1	0	3.815630	-2.110192	1.512490
23	6	0	1.574359	-1.978603	1.301671
24	1	0	1.168431	-2.704087	1.986471
25	35	0	4.313208	0.239616	-0.735322
26	6	0	-0.202917	2.030799	-0.670276
27	1	0	0.272081	2.673286	-1.409955
28	6	0	-0.234960	2.546723	0.552812
29	1	0	0.178346	3.523011	0.763832
30	17	0	-0.896281	1.811115	1.993609

2s

E= -3776.706240

1	6	0	-2.255275	-0.401225	0.121643
2	6	0	-0.303725	-1.146416	0.490807
3	6	0	-1.729733	0.666116	1.165448
4	8	0	-1.080597	-0.662898	-0.635639
5	6	0	3.161159	0.062553	-0.029664
6	6	0	4.083779	-0.977670	-0.223784
7	6	0	3.593554	1.390373	-0.160728
8	6	0	5.404756	-0.678967	-0.538746
9	1	0	3.758146	-2.002254	-0.141067
10	6	0	4.920545	1.670564	-0.473267
11	1	0	2.899646	2.210714	-0.036290
12	6	0	5.835387	0.640047	-0.663412
13	1	0	6.104243	-1.494124	-0.686373
14	1	0	5.232998	2.703918	-0.572597
15	1	0	6.867748	0.860651	-0.908009
16	7	0	1.808387	-0.200519	0.308729
17	6	0	-1.225934	-2.188160	1.088883
18	1	0	-0.910935	-3.066904	1.632347
19	6	0	-2.451916	-1.707502	0.890964
20	1	0	-3.407093	-2.076462	1.232834
21	35	0	-3.743255	0.102742	-1.009152
22	6	0	0.918923	0.880840	0.785432
23	1	0	0.623938	1.528349	-0.041313
24	1	0	1.436156	1.481186	1.534681
25	6	0	1.146315	-1.398133	0.113190
26	8	0	1.597966	-2.457931	-0.262191

27	6	0	-0.285146	0.129812	1.375431
28	1	0	-0.102414	-0.100420	2.425562
29	17	0	-1.814392	2.378082	0.598281
30	1	0	-2.317636	0.648866	2.078109

TS s

E= -3776.656565 au

1	6	0	-2.366283	-0.633487	0.017720
2	6	0	-0.340094	-1.215627	0.431542
3	6	0	-1.508063	0.968338	1.479065
4	8	0	-1.128446	-0.635617	-0.552148
5	6	0	3.149437	0.047730	-0.061990
6	6	0	4.088117	-0.994635	-0.074230
7	6	0	3.568466	1.346148	-0.385278
8	6	0	5.412856	-0.727944	-0.404045
9	1	0	3.774491	-1.999830	0.157172
10	6	0	4.898584	1.596818	-0.708990
11	1	0	2.860055	2.163608	-0.403287
12	6	0	5.829447	0.562895	-0.720591
13	1	0	6.125944	-1.544628	-0.408885
14	1	0	5.200932	2.607390	-0.959167
15	1	0	6.864400	0.759423	-0.974778
16	7	0	1.787600	-0.176541	0.288097
17	6	0	-1.168910	-2.114897	1.167489
18	1	0	-0.813921	-2.836966	1.886591
19	6	0	-2.458255	-1.710670	0.934775
20	1	0	-3.368889	-2.051237	1.401285
21	35	0	-3.773412	0.016335	-1.055599
22	6	0	0.962092	0.948761	0.777087
23	1	0	0.626532	1.570074	-0.055096
24	1	0	1.579175	1.565670	1.434800
25	6	0	1.127714	-1.371095	0.107858
26	8	0	1.611606	-2.434255	-0.225576
27	6	0	-0.225617	0.389571	1.533054
28	1	0	0.034323	-0.048173	2.491817
29	17	0	-1.813268	2.446897	0.570751
30	1	0	-2.183468	0.889028	2.317050

REACTION t

1t

E= -3776.693343 au

1	6	0	-3.615959	0.650502	-0.490367
2	6	0	-5.001477	0.564551	-0.610878
3	6	0	-5.636321	-0.671825	-0.553571

4	6	0	-4.872465	-1.825148	-0.380537
5	6	0	-3.488830	-1.749523	-0.270179
6	6	0	-2.850271	-0.506481	-0.323188
7	1	0	-3.134378	1.620178	-0.519040
8	1	0	-5.581285	1.471403	-0.739776
9	1	0	-6.714608	-0.738002	-0.640551
10	1	0	-5.355318	-2.794780	-0.335833
11	1	0	-2.905013	-2.647717	-0.129191
12	7	0	-1.415085	-0.414540	-0.264740
13	6	0	-0.742988	-1.110640	0.729522
14	8	0	-1.331872	-1.727316	1.604781
15	8	0	1.582515	-0.619112	-0.170076
16	6	0	2.842712	-0.866593	0.245267
17	6	0	0.739617	-1.143916	0.789371
18	6	0	-0.530875	2.281593	0.485623
19	1	0	-1.061401	1.750144	1.263099
20	6	0	-0.760079	0.465837	-1.243917
21	1	0	-1.475911	0.616278	-2.055840
22	1	0	0.093008	-0.046015	-1.689007
23	6	0	2.858331	-1.530390	1.433992
24	1	0	3.731458	-1.844223	1.980610
25	6	0	1.489421	-1.709969	1.781706
26	1	0	1.084974	-2.197737	2.652789
27	35	0	4.225600	-0.270534	-0.864382
28	6	0	-0.308448	1.811974	-0.733201
29	1	0	0.241020	2.416554	-1.448806
30	17	0	0.020453	3.857410	1.007800

2t

E= -3776.709950 au

1	6	0	-2.175245	-0.328262	-0.027040
2	6	0	-0.255447	-0.728619	0.788310
3	6	0	-1.654799	1.130983	0.239021
4	1	0	-1.572856	1.657863	-0.707735
5	8	0	-0.956323	-0.913365	-0.475491
6	6	0	3.252401	0.117413	-0.080586
7	6	0	4.164128	-0.886425	0.283667
8	6	0	3.715873	1.228699	-0.800631
9	6	0	5.503312	-0.764103	-0.070147
10	1	0	3.816724	-1.751615	0.824911
11	6	0	5.060564	1.335757	-1.143089
12	1	0	3.034387	2.009452	-1.109724
13	6	0	5.963737	0.342030	-0.780755
14	1	0	6.193562	-1.548775	0.218447
15	1	0	5.396283	2.202422	-1.701182
16	1	0	7.010030	0.426560	-1.049632
17	7	0	1.879220	0.038675	0.271172

18	6	0	-1.226853	-1.331578	1.775256
19	1	0	-0.959953	-1.784888	2.718685
20	6	0	-2.434969	-1.052784	1.285755
21	1	0	-3.409698	-1.209949	1.720055
22	35	0	-3.563583	-0.460962	-1.374764
23	6	0	0.985095	1.201684	0.098430
24	1	0	0.769334	1.360966	-0.962530
25	1	0	1.463803	2.097980	0.495690
26	6	0	1.211719	-1.105661	0.675203
27	8	0	1.673584	-2.199826	0.912611
28	17	0	-2.744426	2.131666	1.271217
29	6	0	-0.281291	0.822813	0.882286
30	1	0	-0.222969	1.178474	1.909825

TS t

E= -3776.687910 au

1	6	0	-2.549683	-2.091162	1.137682
2	6	0	-3.763431	-2.769394	1.211896
3	6	0	-4.724645	-2.591546	0.218889
4	6	0	-4.469191	-1.734445	-0.849199
5	6	0	-3.258178	-1.051136	-0.924237
6	6	0	-2.299439	-1.228616	0.071059
7	1	0	-1.788358	-2.238419	1.895386
8	1	0	-3.953375	-3.443060	2.039581
9	1	0	-5.667861	-3.122723	0.275118
10	1	0	-5.212325	-1.596561	-1.626109
11	1	0	-3.050214	-0.385546	-1.752921
12	7	0	-1.051513	-0.509523	0.015064
13	6	0	-0.035207	-1.019191	-0.761998
14	8	0	-0.124940	-2.059997	-1.380996
15	8	0	2.258090	-0.614592	-0.019957
16	6	0	3.329303	0.153040	-0.342590
17	6	0	1.228965	-0.205042	-0.830516
18	6	0	-2.654116	2.492515	0.802206
19	1	0	-3.109807	2.169050	1.728853
20	6	0	-0.930583	0.702125	0.844911
21	1	0	0.131046	0.911726	0.983652
22	1	0	-1.350765	0.484995	1.829955
23	6	0	3.028487	1.036627	-1.328197
24	1	0	3.695858	1.756156	-1.771706
25	6	0	1.650992	0.797334	-1.646380
26	1	0	1.064092	1.296899	-2.400681
27	35	0	4.905931	-0.161608	0.614307
28	6	0	-1.610394	1.901224	0.238199
29	1	0	-1.211317	2.275297	-0.699231
30	17	0	-3.448027	3.891638	0.120542

REACTION u

1u

E= -3776.697852 au

1	6	0	-3.917944	-0.024918	0.480941
2	6	0	-5.211689	-0.537523	0.554262
3	6	0	-5.499978	-1.794500	0.032903
4	6	0	-4.484232	-2.534667	-0.570218
5	6	0	-3.193328	-2.026201	-0.657943
6	6	0	-2.902490	-0.765190	-0.129182
7	1	0	-3.700648	0.947320	0.905628
8	1	0	-5.989810	0.048710	1.029658
9	1	0	-6.504900	-2.195516	0.095909
10	1	0	-4.697064	-3.514820	-0.981579
11	1	0	-2.409862	-2.608659	-1.121103
12	7	0	-1.582613	-0.201671	-0.260644
13	6	0	-0.487918	-0.980612	0.090262
14	8	0	-0.612304	-2.095412	0.572001
15	8	0	1.246722	0.694508	-0.692398
16	6	0	0.903779	-0.495945	-0.103148
17	6	0	-1.241109	2.210595	0.346443
18	6	0	-1.125353	2.016514	1.651509
19	1	0	-1.215185	1.018020	2.060697
20	1	0	-0.939991	2.834498	2.333690
21	6	0	-1.494633	1.182495	-0.733541
22	1	0	-2.439944	1.418330	-1.225702
23	1	0	-0.720125	1.278012	-1.492889
24	6	0	3.125028	-0.337460	-0.112532
25	6	0	2.034910	-1.166806	0.269246
26	1	0	2.065284	-2.128715	0.750999
27	17	0	-1.100845	3.834129	-0.332648
28	6	0	2.600600	0.777685	-0.690789
29	1	0	3.033688	1.663656	-1.121171
30	35	0	4.960057	-0.698940	0.132551

2u

E= -3776.711443 au

1	6	0	-1.992364	0.320095	-1.384458
2	6	0	-0.447764	-0.431603	-0.109583
3	6	0	-1.412782	1.664777	-0.829528
4	8	0	-0.784865	-0.453105	-1.515778
5	6	0	3.247517	-0.114573	-0.086642
6	6	0	3.893227	-1.221351	0.486810
7	6	0	4.021949	0.895247	-0.676360
8	6	0	5.281303	-1.298698	0.463892

9	1	0	3.307049	-2.009076	0.932163
10	6	0	5.410633	0.802834	-0.686779
11	1	0	3.551702	1.751845	-1.140389
12	6	0	6.050446	-0.293044	-0.117313
13	1	0	5.763937	-2.160017	0.911882
14	1	0	5.989601	1.594579	-1.148614
15	1	0	7.131702	-0.363692	-0.127023
16	7	0	1.834429	0.008769	-0.072534
17	6	0	-1.721322	-0.910726	0.548670
18	1	0	-1.797259	-1.429050	1.490636
19	6	0	-2.677960	-0.420805	-0.239027
20	6	0	1.180857	1.285592	-0.415482
21	1	0	1.206176	1.452679	-1.496481
22	1	0	1.679950	2.113243	0.087179
23	6	0	0.932316	-1.020865	0.135570
24	8	0	1.160545	-2.167454	0.448616
25	6	0	-0.270028	1.111685	0.054761
26	1	0	-2.135246	2.248151	-0.261979
27	1	0	-2.531589	0.375249	-2.325864
28	35	0	-4.545078	-0.430628	0.012664
29	1	0	-1.029631	2.274535	-1.649291
30	17	0	-0.404781	1.642074	1.791906

TS u

E=-3776.662188 au

1	6	0	-2.112747	0.046832	-1.503960
2	6	0	-0.490002	-0.694131	-0.296905
3	6	0	-1.312359	1.877708	-0.721535
4	8	0	-0.838436	-0.450295	-1.607860
5	6	0	3.201832	-0.117888	-0.105977
6	6	0	3.833517	-1.064790	0.712144
7	6	0	3.987061	0.762321	-0.862916
8	6	0	5.222602	-1.118030	0.761699
9	1	0	3.239244	-1.755686	1.288312
10	6	0	5.376011	0.701838	-0.797447
11	1	0	3.521273	1.487231	-1.518021
12	6	0	6.002560	-0.238828	0.013964
13	1	0	5.696669	-1.855253	1.399819
14	1	0	5.965747	1.390881	-1.391373
15	1	0	7.084092	-0.287349	0.062480
16	7	0	1.781810	-0.017032	-0.172519
17	6	0	-1.659547	-1.001871	0.434552
18	1	0	-1.697330	-1.386417	1.439877
19	6	0	-2.688895	-0.513445	-0.334272
20	6	0	1.162865	1.289821	-0.481887
21	1	0	1.138700	1.457915	-1.563193
22	1	0	1.780096	2.068047	-0.028384

23	6	0	0.932303	-1.092873	-0.021760
24	8	0	1.239245	-2.217590	0.320431
25	6	0	-0.256044	1.360516	0.037582
26	1	0	-2.141432	2.355845	-0.217906
27	1	0	-2.613603	0.271433	-2.433584
28	35	0	-4.509102	-0.365660	0.126412
29	1	0	-1.097078	2.245853	-1.717719
30	17	0	-0.348936	1.593224	1.809568

REACTION v

1v

E= -3776.691210 au

1	6	0	-3.892223	0.338067	-0.014176
2	6	0	-5.205443	-0.068098	0.212661
3	6	0	-5.533550	-1.420032	0.207279
4	6	0	-4.537284	-2.364833	-0.032958
5	6	0	-3.225915	-1.968036	-0.270510
6	6	0	-2.895329	-0.609224	-0.260753
7	1	0	-3.643797	1.391337	0.011471
8	1	0	-5.967765	0.678418	0.404776
9	1	0	-6.553950	-1.736154	0.390900
10	1	0	-4.780687	-3.421301	-0.040170
11	1	0	-2.457420	-2.706234	-0.446694
12	7	0	-1.557860	-0.169755	-0.560710
13	6	0	-0.492795	-0.785879	0.074544
14	8	0	-0.646216	-1.686778	0.883782
15	8	0	1.287416	0.652301	-1.020621
16	6	0	0.912103	-0.383108	-0.201101
17	6	0	-1.430784	0.886598	-1.571466
18	1	0	-2.322256	0.818221	-2.200914
19	1	0	-0.590010	0.657494	-2.228341
20	6	0	3.134479	-0.245665	-0.176562
21	6	0	2.022883	-0.964933	0.341726
22	1	0	2.025386	-1.795595	1.025856
23	6	0	2.642285	0.724561	-0.994108
24	1	0	3.100901	1.495196	-1.588625
25	35	0	4.957635	-0.561582	0.192588
26	6	0	-1.291541	2.322301	-1.133286
27	1	0	-1.293814	3.009671	-1.977941
28	6	0	-1.153016	2.915302	0.046556
29	1	0	-1.060047	3.989019	0.130994
30	17	0	-1.089503	2.145722	1.613571

2v

E= -3776.706859 au

1	6	0	1.976730	0.609975	0.777034
2	6	0	0.369986	-0.586698	0.048306
3	6	0	1.433896	1.513940	-0.382762
4	8	0	0.768821	0.045738	1.288676
5	6	0	-3.315216	-0.232690	-0.110583
6	6	0	-3.992938	-1.460908	-0.049342
7	6	0	-4.058896	0.956596	-0.097450
8	6	0	-5.381548	-1.480455	0.020939
9	1	0	-3.430867	-2.381043	-0.043358
10	6	0	-5.448495	0.917577	-0.030134
11	1	0	-3.562367	1.917064	-0.124573
12	6	0	-6.119991	-0.299217	0.028583
13	1	0	-5.889018	-2.437424	0.068647
14	1	0	-6.003156	1.849014	-0.018758
15	1	0	-7.201938	-0.327310	0.082052
16	7	0	-1.900467	-0.169345	-0.198499
17	6	0	1.608012	-1.377570	-0.328566
18	1	0	1.631415	-2.292526	-0.899767
19	6	0	2.609254	-0.614771	0.107280
20	6	0	-1.216263	1.099455	-0.530818
21	1	0	-1.246110	1.785488	0.316889
22	1	0	-1.707980	1.570987	-1.382539
23	6	0	-1.024373	-1.183931	0.142412
24	8	0	-1.279033	-2.328286	0.448283
25	6	0	0.221195	0.667277	-0.858171
26	1	0	2.550995	1.116179	1.546461
27	35	0	4.465805	-0.820628	-0.141392
28	1	0	0.304443	0.423191	-1.917597
29	1	0	2.166029	1.674570	-1.169019
30	17	0	1.029544	3.182242	0.209631

TS v

E= -3776.657065 au

1	6	0	2.098876	0.421930	0.999399
2	6	0	0.407387	-0.703155	0.288636
3	6	0	1.294254	1.672576	-0.651241
4	8	0	0.808759	0.113399	1.325646
5	6	0	-3.286254	-0.233671	-0.098449
6	6	0	-3.957011	-1.460931	-0.207788
7	6	0	-4.037501	0.944063	0.023455
8	6	0	-5.347484	-1.492919	-0.193555
9	1	0	-3.391105	-2.375007	-0.286710
10	6	0	-5.428400	0.895322	0.030801
11	1	0	-3.545347	1.901459	0.130281
12	6	0	-6.092891	-0.322125	-0.077306
13	1	0	-5.850073	-2.449834	-0.278688
14	1	0	-5.989600	1.817650	0.128886

15	1	0	-7.175919	-0.358774	-0.069121
16	7	0	-1.863879	-0.153233	-0.128441
17	6	0	1.548341	-1.399321	-0.194518
18	1	0	1.540685	-2.223871	-0.888778
19	6	0	2.617565	-0.657675	0.244450
20	6	0	-1.216388	1.119472	-0.525392
21	1	0	-1.221793	1.826511	0.306020
22	1	0	-1.801864	1.551547	-1.340776
23	6	0	-1.028361	-1.163322	0.294859
24	8	0	-1.346165	-2.294550	0.605421
25	6	0	0.201660	0.851344	-0.978128
26	1	0	2.620385	1.086864	1.670100
27	35	0	4.430195	-0.844779	-0.237949
28	1	0	0.277921	0.340625	-1.932208
29	1	0	2.134321	1.758780	-1.324415
30	17	0	1.061719	3.199038	0.231343

REACTION w

1w

E= -3776.692887 au

1	6	0	3.950261	0.121791	-0.029147
2	6	0	5.252839	-0.304208	-0.281149
3	6	0	5.546265	-1.662004	-0.353906
4	6	0	4.526025	-2.593359	-0.166241
5	6	0	3.225838	-2.177183	0.096111
6	6	0	2.929632	-0.812457	0.164721
7	1	0	3.729682	1.181492	0.008366
8	1	0	6.034004	0.432561	-0.429960
9	1	0	6.558227	-1.992957	-0.556429
10	1	0	4.742400	-3.654328	-0.219022
11	1	0	2.439123	-2.905162	0.233086
12	7	0	1.599877	-0.364819	0.488446
13	6	0	0.527114	-0.918316	-0.194225
14	8	0	0.677607	-1.706864	-1.114679
15	8	0	-1.257954	0.187729	1.230819
16	6	0	-0.877273	-0.578046	0.157354
17	6	0	1.152426	2.429771	-0.292997
18	1	0	1.274168	1.745671	-1.120983
19	6	0	1.479531	0.693560	1.502452
20	1	0	2.415526	0.693426	2.066561
21	1	0	0.698430	0.432579	2.216561
22	6	0	-3.100944	-0.450307	0.168499
23	6	0	-1.985528	-0.995004	-0.525047
24	1	0	-1.984849	-1.614144	-1.405327
25	6	0	-2.613341	0.256701	1.224133

26	1	0	-3.075904	0.828425	2.009547
27	35	0	-4.921476	-0.658839	-0.277999
28	6	0	1.219850	2.087183	0.985164
29	1	0	1.078844	2.844455	1.751069
30	17	0	0.846441	4.069732	-0.818004

2w

E= -3776.707520 au

1	6	0	1.844365	0.352452	1.153733
2	6	0	0.217815	-0.516592	0.069888
3	6	0	1.260352	1.603255	0.405617
4	8	0	0.606882	-0.303063	1.457185
5	6	0	-3.460148	-0.041281	-0.071441
6	6	0	-4.155505	-1.224957	-0.366970
7	6	0	-4.189732	1.116679	0.236850
8	6	0	-5.545881	-1.231287	-0.352355
9	1	0	-3.605494	-2.124641	-0.591412
10	6	0	-5.581311	1.092349	0.243641
11	1	0	-3.682410	2.039150	0.484671
12	6	0	-6.269644	-0.079746	-0.051199
13	1	0	-6.066365	-2.154078	-0.582747
14	1	0	-6.124321	1.998900	0.485875
15	1	0	-7.353088	-0.096777	-0.044762
16	7	0	-2.042082	0.012822	-0.091109
17	6	0	1.442477	-1.187191	-0.508909
18	1	0	1.456867	-1.892077	-1.325490
19	6	0	2.455402	-0.622676	0.148168
20	6	0	-1.330509	1.306487	-0.036327
21	1	0	-1.395134	1.732809	0.969656
22	1	0	-1.782437	2.006389	-0.740875
23	6	0	-1.189776	-1.078282	-0.039877
24	8	0	-1.475488	-2.254555	-0.082333
25	6	0	0.117679	0.955559	-0.410421
26	1	0	2.420214	0.567694	2.049114
27	35	0	4.305847	-0.871572	-0.089491
28	1	0	0.895228	2.316906	1.140190
29	1	0	0.274066	1.055235	-1.483477
30	17	0	2.459303	2.515181	-0.594824

TS w

E= -3776.658641 au

1	6	0	1.880652	0.031619	1.355964
2	6	0	0.241659	-0.694225	0.156752
3	6	0	1.161387	1.829513	0.205047

4	8	0	0.566913	-0.331541	1.455035
5	6	0	-3.432714	-0.043717	-0.041152
6	6	0	-4.129753	-1.110875	-0.627350
7	6	0	-4.158811	1.008907	0.534744
8	6	0	-5.520739	-1.109665	-0.630010
9	1	0	-3.582805	-1.932609	-1.060524
10	6	0	-5.550333	0.997492	0.518660
11	1	0	-3.646249	1.833658	1.011812
12	6	0	-6.240862	-0.060791	-0.063305
13	1	0	-6.043851	-1.941891	-1.087427
14	1	0	-6.091774	1.820623	0.971001
15	1	0	-7.324431	-0.069235	-0.073790
16	7	0	-2.009968	0.006414	-0.030918
17	6	0	1.415013	-1.199381	-0.465190
18	1	0	1.459285	-1.725269	-1.404860
19	6	0	2.451071	-0.706932	0.291424
20	6	0	-1.321037	1.308288	0.112149
21	1	0	-1.296963	1.618942	1.161138
22	1	0	-1.889894	2.053368	-0.449191
23	6	0	-1.191737	-1.102603	-0.070973
24	8	0	-1.523009	-2.252168	-0.280781
25	6	0	0.087390	1.194653	-0.437389
26	1	0	2.359738	0.366489	2.262987
27	35	0	4.297205	-0.833459	-0.055826
28	1	0	1.025007	2.399649	1.112910
29	1	0	0.142225	1.118676	-1.518176
30	17	0	2.474057	2.482337	-0.775636

REACTION x

1x

E= -3776.696471 au

1	6	0	3.367061	-0.179516	-0.553058
2	6	0	4.581394	-0.849176	-0.693344
3	6	0	4.806459	-2.046578	-0.022885
4	6	0	3.807077	-2.568909	0.797517
5	6	0	2.598640	-1.901279	0.953022
6	6	0	2.369723	-0.699141	0.275639
7	1	0	3.196509	0.738979	-1.100510
8	1	0	5.346067	-0.432442	-1.338959
9	1	0	5.748739	-2.569582	-0.137506
10	1	0	3.970514	-3.500367	1.327540
11	1	0	1.828392	-2.313501	1.590218
12	7	0	1.140010	0.017762	0.478386
13	6	0	-0.062226	-0.677384	0.361304
14	8	0	-0.118959	-1.811763	-0.078244
15	8	0	-1.342159	0.910456	1.794101

16	6	0	-1.324401	-0.023274	0.786761
17	6	0	0.538696	1.730530	-1.861738
18	6	0	1.213880	1.476708	0.589390
19	1	0	2.231613	1.732183	0.890240
20	1	0	0.562711	1.830774	1.385911
21	6	0	-2.618586	-0.260672	0.398722
22	6	0	-2.635796	1.253274	2.020097
23	1	0	-2.800197	1.979719	2.797924
24	6	0	0.875124	2.226526	-0.680301
25	6	0	-3.464810	0.572694	1.188944
26	1	0	-4.538511	0.638731	1.133970
27	35	0	-3.237070	-1.427020	-0.938575
28	1	0	0.306055	2.371719	-2.700596
29	1	0	0.491882	0.658734	-2.009584
30	17	0	0.961714	3.974944	-0.436735

2x

E= -3776.708543 au

1	6	0	-2.093731	1.945992	-1.363688
2	6	0	-0.875054	0.350739	-0.616197
3	6	0	-1.471858	2.640236	-0.105640
4	8	0	-0.961788	1.157113	-1.803547
5	6	0	2.766357	-0.085021	-0.069196
6	6	0	3.181110	-1.423637	-0.148250
7	6	0	3.733085	0.920747	0.073882
8	6	0	4.535468	-1.731090	-0.082451
9	1	0	2.447111	-2.203818	-0.271439
10	6	0	5.084556	0.594362	0.141509
11	1	0	3.442764	1.961876	0.122208
12	6	0	5.495581	-0.732158	0.064118
13	1	0	4.839242	-2.770058	-0.144134
14	1	0	5.815367	1.387648	0.251190
15	1	0	6.548124	-0.984637	0.116156
16	7	0	1.393190	0.267409	-0.115947
17	6	0	-2.306921	-0.139383	-0.478234
18	6	0	-3.068407	0.865052	-0.915058
19	6	0	0.944020	1.618011	0.263868
20	1	0	1.181045	2.338265	-0.525222
21	1	0	1.423385	1.930540	1.190768
22	6	0	0.376952	-0.515101	-0.639716
23	8	0	0.444397	-1.647792	-1.056408
24	6	0	-0.578455	1.489818	0.415421
25	1	0	-2.426787	2.610240	-2.157151
26	1	0	-4.144680	0.948415	-0.895586
27	35	0	-2.843043	-1.764867	0.295554
28	1	0	-2.211401	2.955638	0.627711
29	1	0	-0.878072	3.505632	-0.405053

30	17	0	-0.969354	1.020750	2.129131

TS x

E= -3776.660130 au

1	6	0	-2.270093	1.857601	-1.474243
2	6	0	-0.942988	0.274325	-0.855827
3	6	0	-1.410707	2.706093	0.304826
4	8	0	-1.047196	1.300830	-1.767231
5	6	0	2.706016	-0.052892	-0.111939
6	6	0	3.098733	-1.395763	-0.024246
7	6	0	3.687949	0.947055	-0.104690
8	6	0	4.449106	-1.716217	0.066172
9	1	0	2.352713	-2.174159	-0.040926
10	6	0	5.035221	0.611247	-0.006205
11	1	0	3.410446	1.989580	-0.191498
12	6	0	5.424564	-0.721664	0.078300
13	1	0	4.737149	-2.759238	0.133713
14	1	0	5.779485	1.399540	-0.003271
15	1	0	6.473789	-0.982666	0.152083
16	7	0	1.332168	0.316469	-0.189516
17	6	0	-2.262052	-0.179270	-0.583128
18	6	0	-3.106226	0.845064	-0.946215
19	6	0	0.908542	1.640492	0.309129
20	1	0	1.080126	2.409157	-0.451159
21	1	0	1.515592	1.882332	1.183565
22	6	0	0.370458	-0.456572	-0.806556
23	8	0	0.513802	-1.578753	-1.246230
24	6	0	-0.562757	1.649865	0.665450
25	1	0	-2.564277	2.682694	-2.106371
26	1	0	-4.167979	0.917724	-0.772855
27	35	0	-2.733420	-1.776205	0.286922
28	1	0	-2.246135	2.951931	0.945415
29	1	0	-0.991751	3.535723	-0.252098
30	17	0	-0.913064	0.839204	2.219437

REACTION y

1y

E= -3776.687808 au

1	6	0	-3.363900	-0.207212	0.308408
2	6	0	-4.510749	-0.975422	0.503210
3	6	0	-4.528333	-2.316747	0.133758
4	6	0	-3.391945	-2.888904	-0.436499
5	6	0	-2.248455	-2.125291	-0.644401

6	6	0	-2.231505	-0.778598	-0.272157
7	1	0	-3.345535	0.829246	0.617246
8	1	0	-5.385714	-0.522781	0.955940
9	1	0	-5.418368	-2.914889	0.292677
10	1	0	-3.394491	-3.934669	-0.722415
11	1	0	-1.362956	-2.571475	-1.076186
12	7	0	-1.071965	0.037660	-0.538314
13	6	0	0.147011	-0.379545	-0.024665
14	8	0	0.257672	-1.400090	0.632466
15	8	0	1.303961	1.753149	-0.618141
16	6	0	1.368550	0.425547	-0.272319
17	6	0	-1.666914	3.100791	0.071971
18	6	0	-1.252830	1.093031	-1.541423
19	1	0	-2.014187	0.731102	-2.239029
20	1	0	-0.338130	1.193404	-2.130031
21	6	0	2.692011	0.083900	-0.135984
22	6	0	2.570846	2.227945	-0.692607
23	1	0	2.668015	3.270446	-0.944880
24	6	0	-1.672725	2.472269	-1.097571
25	1	0	-2.036684	3.080672	-1.924100
26	6	0	3.467766	1.248057	-0.414439
27	1	0	4.541926	1.325950	-0.397312
28	35	0	3.436270	-1.583908	0.307209
29	17	0	-1.143280	2.462411	1.611253
30	1	0	-2.009838	4.121756	0.166385

2y

E= -3776.705661 au

1	6	0	2.315396	1.570355	0.910387
2	6	0	0.922624	0.041122	0.388847
3	6	0	1.721694	2.147203	-0.422746
4	8	0	1.155730	0.947908	1.480483
5	6	0	-2.748175	-0.205714	-0.054271
6	6	0	-3.259206	-1.475207	0.260351
7	6	0	-3.641658	0.828447	-0.370427
8	6	0	-4.633376	-1.687215	0.253971
9	1	0	-2.582808	-2.274286	0.518360
10	6	0	-5.014026	0.596879	-0.375041
11	1	0	-3.277304	1.820354	-0.600706
12	6	0	-5.520153	-0.660733	-0.063569
13	1	0	-5.011135	-2.673221	0.500273
14	1	0	-5.686362	1.411340	-0.620007
15	1	0	-6.589107	-0.838542	-0.066171
16	7	0	-1.352244	0.047958	-0.075236
17	6	0	2.297697	-0.593281	0.229352
18	6	0	3.174263	0.366174	0.527889
19	6	0	-0.820290	1.299336	-0.654915

20	1	0	-1.033204	2.145594	-0.000022
21	1	0	-1.283444	1.482599	-1.625364
22	6	0	-0.386701	-0.714329	0.559247
23	8	0	-0.524680	-1.762499	1.147945
24	6	0	0.688460	1.040972	-0.777004
25	1	0	2.742637	2.305621	1.585811
26	1	0	0.910995	0.595603	-1.747215
27	1	0	4.249860	0.353559	0.435731
28	35	0	2.613722	-2.299902	-0.491488
29	1	0	2.471101	2.281472	-1.197310
30	17	0	1.026265	3.808438	-0.173793

TS y

E= -3776.657818 au

1	6	0	2.546573	1.307678	1.185511
2	6	0	0.979612	-0.063559	0.629980
3	6	0	1.694474	2.118041	-0.765584
4	8	0	1.262248	0.966324	1.503007
5	6	0	-2.705517	-0.117207	-0.016044
6	6	0	-3.247512	-1.394316	0.192637
7	6	0	-3.571053	0.956473	-0.269477
8	6	0	-4.625346	-1.577124	0.145979
9	1	0	-2.593892	-2.225182	0.403762
10	6	0	-4.947574	0.755690	-0.317060
11	1	0	-3.181783	1.955125	-0.414906
12	6	0	-5.484320	-0.510739	-0.109656
13	1	0	-5.027425	-2.570629	0.309568
14	1	0	-5.598808	1.600234	-0.511841
15	1	0	-6.556409	-0.664888	-0.144869
16	7	0	-1.299092	0.107869	0.001991
17	6	0	2.218865	-0.724688	0.367196
18	6	0	3.212412	0.174327	0.676221
19	6	0	-0.745212	1.305968	-0.666073
20	1	0	-0.905213	2.193017	-0.050449
21	1	0	-1.279596	1.447380	-1.608640
22	6	0	-0.407978	-0.655100	0.723447
23	8	0	-0.646320	-1.666911	1.349667
24	6	0	0.732642	1.103286	-0.928488
25	1	0	2.950923	2.155323	1.717462
26	1	0	0.943009	0.406686	-1.735571
27	1	0	4.267655	0.091415	0.469886
28	35	0	2.391586	-2.329234	-0.596994
29	1	0	2.561115	2.163292	-1.406727
30	17	0	1.234160	3.749922	-0.238809

REACTION z

1z

E= -3776.691662 au

1	6	0	3.436697	0.348938	-0.145899
2	6	0	4.699698	-0.051648	-0.578299
3	6	0	5.025256	-1.401981	-0.645480
4	6	0	4.076795	-2.352820	-0.270049
5	6	0	2.819640	-1.961694	0.173756
6	6	0	2.489440	-0.603912	0.238131
7	1	0	3.189143	1.402950	-0.121696
8	1	0	5.423380	0.699992	-0.872571
9	1	0	6.005448	-1.712557	-0.987997
10	1	0	4.317952	-3.408753	-0.316239
11	1	0	2.089354	-2.705719	0.460253
12	7	0	1.208391	-0.195687	0.744930
13	6	0	0.066680	-0.810612	0.239818
14	8	0	0.095106	-1.547799	-0.729846
15	8	0	-1.328719	-0.321805	2.247560
16	6	0	-1.241757	-0.568388	0.898809
17	6	0	0.454431	2.434965	-0.318231
18	1	0	0.485518	1.647373	-1.058006
19	6	0	1.165937	0.986192	1.618360
20	1	0	2.168989	1.105667	2.035500
21	1	0	0.512283	0.792264	2.467950
22	6	0	-2.514600	-0.647739	0.393778
23	6	0	-2.644930	-0.240199	2.570630
24	1	0	-2.863564	-0.058218	3.609337
25	6	0	0.746014	2.280910	0.965612
26	1	0	0.683181	3.135052	1.634157
27	17	0	-0.029195	3.972409	-0.997276
28	6	0	-3.420762	-0.424189	1.472926
29	1	0	-4.496503	-0.410980	1.419433
30	35	0	-3.044569	-0.960524	-1.381595

2z

E= -3776.707279 au

1	6	0	2.219929	1.300701	1.402176
2	6	0	0.734758	-0.002325	0.582292
3	6	0	1.663788	2.163926	0.214391
4	8	0	0.979692	0.704280	1.819187
5	6	0	-2.916103	0.138037	-0.063789
6	6	0	-3.544514	-1.111176	0.065830
7	6	0	-3.704971	1.274326	-0.297991
8	6	0	-4.927891	-1.202684	-0.039584
9	1	0	-2.950950	-1.990226	0.258522

10	6	0	-5.088326	1.163124	-0.403733
11	1	0	-3.251674	2.252040	-0.388925
12	6	0	-5.710071	-0.074358	-0.275731
13	1	0	-5.396145	-2.175097	0.063703
14	1	0	-5.677814	2.055073	-0.583445
15	1	0	-6.787325	-0.158838	-0.356988
16	7	0	-1.505821	0.273492	0.020806
17	6	0	2.058203	-0.718038	0.383569
18	6	0	2.992892	0.106343	0.858164
19	6	0	-0.843588	1.538391	-0.354648
20	1	0	-1.043320	2.308626	0.397293
21	1	0	-1.225687	1.885339	-1.316019
22	6	0	-0.639293	-0.653741	0.579170
23	8	0	-0.897038	-1.757653	1.001244
24	6	0	0.649268	1.182459	-0.417594
25	1	0	2.674889	1.868480	2.209412
26	1	0	1.189846	3.061810	0.603595
27	1	0	0.933845	0.890907	-1.427565
28	17	0	2.942128	2.751864	-0.925617
29	1	0	4.065973	0.015569	0.797667
30	35	0	2.276207	-2.311793	-0.589314

TS z

E= -3776.659370 au

1	6	0	2.219568	1.121367	1.749788
2	6	0	0.729834	-0.118852	0.800740
3	6	0	1.594178	2.249716	-0.123459
4	8	0	0.907114	0.748829	1.862439
5	6	0	-2.897938	0.137529	-0.046341
6	6	0	-3.499518	-1.122118	-0.184378
7	6	0	-3.705371	1.283669	-0.062114
8	6	0	-4.879086	-1.216266	-0.334218
9	1	0	-2.890812	-2.011617	-0.159440
10	6	0	-5.083984	1.172635	-0.218280
11	1	0	-3.268495	2.265655	0.062313
12	6	0	-5.680122	-0.076860	-0.354914
13	1	0	-5.328548	-2.197199	-0.440086
14	1	0	-5.690180	2.071406	-0.225929
15	1	0	-6.753801	-0.162270	-0.474334
16	7	0	-1.487931	0.279695	0.089910
17	6	0	1.992640	-0.736742	0.561118
18	6	0	2.941443	0.083764	1.126316
19	6	0	-0.838838	1.557275	-0.272959
20	1	0	-0.962801	2.292766	0.528205
21	1	0	-1.330430	1.945288	-1.168179
22	6	0	-0.665273	-0.675262	0.648716

23	8	0	-0.968584	-1.801843	0.980523
24	6	0	0.634453	1.316015	-0.543110
25	1	0	2.567829	1.839162	2.476934
26	1	0	1.322874	3.138574	0.428016
27	1	0	0.838782	0.787716	-1.469371
28	17	0	3.023214	2.521808	-1.125922
29	1	0	4.011959	0.024872	1.016670
30	35	0	2.280696	-2.178688	-0.608246