

Iridium(III)-bis(oxazolinyl)phenyl Catalysts for Enantioselective C-H Functionalization

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Supporting Information (SI 2) – Computational Data

Table S1. Cartesian coordinates of all calculated structures:

18-eq:

1	6	0	1.173735	2.669542	-0.284417
2	6	0	-0.006776	1.969174	0.005250
3	6	0	-1.193987	2.659047	0.285865
4	6	0	-1.196924	4.057686	0.279845
5	6	0	-0.021652	4.766271	-0.010626
6	6	0	1.163461	4.065402	-0.294597
7	1	0	-2.110982	4.606224	0.498161
8	1	0	2.071752	4.620149	-0.521877
9	6	0	2.244554	1.732765	-0.539066
10	8	0	3.495978	2.072007	-0.838705
11	7	0	1.989057	0.449906	-0.471082
12	77	0	-0.001673	0.042155	0.012916
13	6	0	-2.257360	1.715139	0.543786
14	8	0	-3.515558	2.043277	0.828787
15	7	0	-1.989006	0.433697	0.491043
16	6	0	-0.020095	6.265781	-0.018308
17	1	0	0.659750	6.670937	0.738288
18	1	0	0.312397	6.662471	-0.982823
19	1	0	-1.015500	6.668349	0.181739
20	6	0	-3.628987	-1.041219	-0.602833
21	1	0	-2.787171	-1.675098	-0.903184
22	1	0	-3.752844	-0.289968	-1.392266
23	6	0	4.200623	0.822129	-1.114275
24	1	0	4.432726	0.812057	-2.180970
25	1	0	5.130975	0.835512	-0.541570
26	6	0	-4.202930	0.787421	1.123231
27	1	0	-4.416273	0.781546	2.194152
28	1	0	-5.142617	0.787756	0.566089
29	6	0	-3.226916	-0.318136	0.688281
30	1	0	-3.080853	-1.054451	1.488091
31	6	0	3.229690	-0.291933	-0.687744
32	1	0	3.080077	-1.017679	-1.497072
33	6	0	3.644221	-1.033400	0.588496
34	1	0	2.805167	-1.671931	0.888849
35	1	0	3.772603	-0.295109	1.389135
36	6	0	4.896021	-1.839439	0.400121
37	6	0	6.127076	-1.371268	0.869753
38	6	0	4.862292	-3.058829	-0.287164
39	6	0	7.295670	-2.100666	0.661754

40	1	0	6.164004	-0.430427	1.416385
41	6	0	6.026938	-3.790973	-0.495188
42	1	0	3.909723	-3.437717	-0.654354
43	6	0	7.248220	-3.313048	-0.021385
44	1	0	8.242176	-1.723117	1.038208
45	1	0	5.982168	-4.738420	-1.025406
46	1	0	8.157165	-3.885885	-0.182069
47	6	0	-4.883743	-1.847172	-0.434293
48	6	0	-4.857850	-3.071629	0.244522
49	6	0	-6.110225	-1.374975	-0.912169
50	6	0	-6.025076	-3.804130	0.436266
51	1	0	-3.909052	-3.453649	0.617871
52	6	0	-7.281412	-2.105006	-0.721027
53	1	0	-6.141262	-0.429833	-1.451850
54	6	0	-7.241541	-3.322041	-0.045755
55	1	0	-5.986164	-4.755228	0.960492
56	1	0	-8.224062	-1.723897	-1.103678
57	1	0	-8.152558	-3.895096	0.102331
58	17	0	0.540290	-0.118267	2.365167
59	17	0	-0.522314	-0.092894	-2.341769
60	8	0	-0.072813	-2.303812	0.085099
61	1	0	0.368842	-2.569552	0.902680
62	1	0	0.449689	-2.690111	-0.628756

18-ax:

1	6	0	1.267425	2.757647	-0.261405
2	6	0	0.041286	2.098624	-0.096011
3	6	0	-1.124420	2.817057	0.197771
4	6	0	-1.063918	4.209877	0.313974
5	6	0	0.156016	4.880007	0.137007
6	6	0	1.322077	4.147849	-0.147656
7	1	0	-1.958342	4.782710	0.549573
8	1	0	2.267361	4.673123	-0.269825
9	6	0	2.315158	1.789464	-0.508948
10	8	0	3.602279	2.084717	-0.656720
11	7	0	1.998008	0.519436	-0.576899
12	77	0	-0.019098	0.163445	-0.204485
13	6	0	-2.228864	1.898209	0.373498
14	8	0	-3.457727	2.246395	0.735774
15	7	0	-2.016177	0.616133	0.193580
16	6	0	0.220528	6.374571	0.240882
17	1	0	1.077883	6.699972	0.836853
18	1	0	0.327176	6.839647	-0.745176
19	1	0	-0.683128	6.783898	0.698223
20	6	0	-3.684852	-0.974506	-0.702978
21	1	0	-2.822276	-1.580693	-1.008413
22	1	0	-3.935926	-0.308373	-1.538342
23	6	0	4.281087	0.819146	-0.938483
24	1	0	4.630283	0.867664	-1.971603
25	1	0	5.140356	0.752222	-0.267176
26	6	0	-4.221831	1.004787	0.863727
27	1	0	-4.585893	0.956307	1.890444
28	1	0	-5.073614	1.076932	0.181377
29	6	0	-3.240871	-0.122731	0.488588

30	1	0	-3.045535	-0.784217	1.343458
31	6	0	3.222454	-0.270875	-0.698449
32	1	0	3.139313	-0.938754	-1.563912
33	6	0	3.441565	-1.106412	0.566511
34	1	0	2.540582	-1.715019	0.711696
35	1	0	3.502468	-0.424523	1.423406
36	6	0	4.670682	-1.963038	0.480296
37	6	0	5.831110	-1.625143	1.183534
38	6	0	4.689438	-3.103760	-0.331909
39	6	0	6.979587	-2.407858	1.086797
40	1	0	5.826416	-0.744388	1.823291
41	6	0	5.834654	-3.887597	-0.431398
42	1	0	3.791272	-3.381541	-0.881774
43	6	0	6.983981	-3.542054	0.279015
44	1	0	7.869354	-2.132980	1.646453
45	1	0	5.829653	-4.773572	-1.060234
46	1	0	7.876575	-4.156760	0.205049
47	6	0	-4.850856	-1.853981	-0.352500
48	6	0	-4.648716	-3.004665	0.419056
49	6	0	-6.154087	-1.525361	-0.736231
50	6	0	-5.721660	-3.805865	0.796318
51	1	0	-3.636543	-3.272990	0.718445
52	6	0	-7.231250	-2.325938	-0.359556
53	1	0	-6.324164	-0.638237	-1.344159
54	6	0	-7.017547	-3.467012	0.408867
55	1	0	-5.546415	-4.698400	1.390685
56	1	0	-8.237576	-2.057595	-0.669218
57	1	0	-7.855907	-4.092588	0.701648
58	17	0	0.379951	0.033384	2.136315
59	17	0	-0.111614	-2.396808	-0.649756
60	8	0	-0.370199	0.101508	-2.355367
61	1	0	-0.435718	-0.865962	-2.483251
62	1	0	-1.245523	0.454419	-2.571811

19-eq:

1	6	0	-0.870572	3.421721	0.324567
2	6	0	0.262136	2.641326	0.105606
3	6	0	1.501186	3.241545	-0.114048
4	6	0	1.615939	4.632490	-0.110588
5	6	0	0.476611	5.426831	0.114943
6	6	0	-0.768491	4.817831	0.329760
7	1	0	2.576678	5.113459	-0.284382
8	1	0	-1.645379	5.440144	0.496716
9	6	0	-2.020428	2.558648	0.495532
10	8	0	-3.269675	2.983150	0.645902
11	7	0	-1.853017	1.257358	0.475056
12	77	0	0.104912	0.624537	0.077642
13	6	0	2.495298	2.212073	-0.343738
14	8	0	3.777309	2.447236	-0.594832
15	7	0	2.130804	0.955298	-0.320425
16	6	0	0.602329	6.920987	0.125356
17	1	0	-0.371403	7.404160	0.231276
18	1	0	1.233894	7.263372	0.951674
19	1	0	1.062165	7.291777	-0.795882
20	6	0	3.548336	-0.862729	0.578186

21	1	0	2.630886	-1.446011	0.726658
22	1	0	3.713625	-0.282725	1.493919
23	6	0	-4.089608	1.788227	0.841678
24	1	0	-4.421203	1.795462	1.881655
25	1	0	-4.955601	1.872476	0.181604
26	6	0	4.410176	1.143342	-0.787430
27	1	0	4.835709	1.137375	-1.791588
28	1	0	5.216020	1.062226	-0.052492
29	6	0	3.292083	0.104382	-0.577733
30	1	0	3.100119	-0.477578	-1.486535
31	6	0	-3.165098	0.608031	0.504172
32	1	0	-3.188796	-0.141598	1.303756
33	6	0	-3.460074	-0.083303	-0.830615
34	1	0	-2.577898	-0.678204	-1.098522
35	1	0	-3.562563	0.683352	-1.608203
36	6	0	-4.682013	-0.950638	-0.754951
37	6	0	-5.915272	-0.512074	-1.245513
38	6	0	-4.612322	-2.210537	-0.146365
39	6	0	-7.052022	-1.310403	-1.135117
40	1	0	-5.980029	0.460326	-1.730888
41	6	0	-5.745276	-3.010252	-0.034880
42	1	0	-3.654458	-2.567706	0.232998
43	6	0	-6.969925	-2.560990	-0.528145
44	1	0	-8.001242	-0.955405	-1.526603
45	1	0	-5.672169	-3.988071	0.433436
46	1	0	-7.854126	-3.186467	-0.444509
47	6	0	4.716056	-1.764356	0.294255
48	6	0	4.604603	-2.774429	-0.669688
49	6	0	5.941877	-1.587887	0.942652
50	6	0	5.692200	-3.587540	-0.972793
51	1	0	3.651494	-2.916246	-1.175320
52	6	0	7.032636	-2.401521	0.639839
53	1	0	6.037837	-0.808998	1.697209
54	6	0	6.910439	-3.403055	-0.319628
55	1	0	5.589378	-4.369973	-1.719958
56	1	0	7.977479	-2.252322	1.155533
57	1	0	7.759258	-4.038269	-0.556821
58	17	0	-0.320092	0.791973	-2.323149
59	6	0	-0.112505	-1.399537	-0.000127
60	6	0	0.245371	-2.036753	-1.289501
61	6	0	-0.586683	-2.332397	0.990986
62	8	0	1.395284	-2.206181	-1.660810
63	8	0	-0.839039	-2.401016	-1.987709
64	6	0	-0.439089	-3.734195	0.825449
65	6	0	-1.272868	-1.871109	2.140248
66	6	0	-0.573145	-2.887473	-3.314472
67	6	0	-0.943181	-4.619484	1.762238
68	1	0	0.093548	-4.118448	-0.041313
69	6	0	-1.806311	-2.762656	3.057373
70	1	0	-1.391641	-0.802603	2.276384
71	1	0	-1.546547	-3.105168	-3.748103
72	1	0	-0.056987	-2.122070	-3.897809
73	1	0	0.039601	-3.790017	-3.273257
74	6	0	-1.637629	-4.135870	2.874283
75	1	0	-0.811499	-5.688129	1.626009
76	1	0	-2.352245	-2.391385	3.919084

77	1	0	-2.050497	-4.833147	3.597335
78	17	0	0.690344	0.676467	2.447559

19-ax

1	6	0	-1.075561	2.902007	-0.042838
2	6	0	0.081735	2.157865	-0.279770
3	6	0	1.298698	2.783259	-0.557209
4	6	0	1.368549	4.181686	-0.547286
5	6	0	0.224363	4.940577	-0.265076
6	6	0	-1.004191	4.294403	-0.029392
7	1	0	2.306463	4.687389	-0.766352
8	1	0	-1.895903	4.890718	0.151702
9	6	0	-2.216378	2.016856	0.097543
10	8	0	-3.464160	2.437349	0.235015
11	7	0	-2.039118	0.720505	0.041316
12	77	0	-0.018391	0.202545	-0.382953
13	6	0	2.301195	1.793413	-0.887725
14	8	0	3.561170	2.058702	-1.194686
15	7	0	1.955581	0.530058	-0.899330
16	6	0	0.300677	6.436257	-0.213741
17	1	0	-0.543497	6.900525	-0.730854
18	1	0	0.276604	6.797709	0.820095
19	1	0	1.222307	6.806746	-0.667529
20	6	0	3.452533	-1.261965	-0.086324
21	1	0	2.549126	-1.851554	0.114658
22	1	0	3.666587	-0.675177	0.812990
23	6	0	-4.302916	1.239457	0.310223
24	1	0	-4.775734	1.242928	1.293019
25	1	0	-5.068986	1.331437	-0.463312
26	6	0	4.195824	0.770953	-1.490229
27	1	0	4.531802	0.812667	-2.526795
28	1	0	5.061751	0.680214	-0.829584
29	6	0	3.116051	-0.296189	-1.225397
30	1	0	2.891472	-0.870449	-2.133538
31	6	0	-3.343415	0.056578	0.085685
32	1	0	-3.372081	-0.623726	0.945792
33	6	0	-3.584716	-0.745480	-1.195184
34	1	0	-2.699509	-1.375807	-1.354083
35	1	0	-3.624741	-0.047445	-2.039627
36	6	0	-4.832601	-1.574870	-1.108502
37	6	0	-6.033361	-1.139091	-1.677195
38	6	0	-4.824554	-2.788835	-0.410449
39	6	0	-7.197370	-1.895016	-1.553512
40	1	0	-6.049942	-0.204774	-2.235884
41	6	0	-5.984407	-3.547208	-0.286585
42	1	0	-3.892510	-3.146113	0.026428
43	6	0	-7.175916	-3.100413	-0.856701
44	1	0	-8.120483	-1.543223	-2.005929
45	1	0	-5.958634	-4.490616	0.252102
46	1	0	-8.081270	-3.693490	-0.763145
47	6	0	4.607415	-2.154476	-0.438269
48	6	0	4.451453	-3.174486	-1.385235
49	6	0	5.866537	-1.965411	0.139211
50	6	0	5.524850	-3.985057	-1.741024

51	1	0	3.474425	-3.335162	-1.838405
52	6	0	6.943708	-2.775995	-0.214258
53	1	0	5.997963	-1.179461	0.880905
54	6	0	6.775412	-3.787511	-1.156171
55	1	0	5.385657	-4.775109	-2.473810
56	1	0	7.914066	-2.617415	0.248132
57	1	0	7.613366	-4.421254	-1.432383
58	17	0	-0.617949	0.566094	-2.822419
59	6	0	0.374363	-0.038026	1.488640
60	6	0	1.224319	1.022246	2.112820
61	6	0	-0.094480	-1.057787	2.385326
62	8	0	2.436970	1.082836	2.039527
63	8	0	0.450512	1.932885	2.719160
64	6	0	-1.151018	-1.930159	2.032915
65	6	0	0.476515	-1.185393	3.677004
66	6	0	1.143086	3.100018	3.202977
67	6	0	-1.623626	-2.868876	2.933988
68	1	0	-1.589395	-1.846111	1.046201
69	6	0	0.020651	-2.147788	4.561059
70	1	0	1.297006	-0.535331	3.970359
71	1	0	0.375369	3.737138	3.635604
72	1	0	1.882031	2.818787	3.954794
73	1	0	1.639368	3.608232	2.372350
74	6	0	-1.035453	-2.985383	4.194879
75	1	0	-2.450226	-3.515609	2.656377
76	1	0	0.477611	-2.243545	5.540501
77	1	0	-1.403751	-3.727400	4.897065
78	17	0	-0.000826	-2.317905	-0.924736

19_ax_a2:

1	6	0	-1.076455	2.940953	0.071385
2	6	0	0.062321	2.187375	-0.215803
3	6	0	1.288711	2.801302	-0.474006
4	6	0	1.388886	4.195326	-0.386825
5	6	0	0.262651	4.961450	-0.058102
6	6	0	-0.977436	4.328961	0.152503
7	1	0	2.336953	4.692181	-0.581973
8	1	0	-1.855034	4.932686	0.372878
9	6	0	-2.230256	2.071123	0.196153
10	8	0	-3.467479	2.506963	0.372190
11	7	0	-2.076527	0.774947	0.087704
12	77	0	-0.072523	0.238960	-0.374194
13	6	0	2.271926	1.808069	-0.847211
14	8	0	3.539603	2.066076	-1.132002
15	7	0	1.906934	0.551876	-0.907577
16	6	0	0.367558	6.451437	0.063670
17	1	0	-0.451790	6.955651	-0.456050
18	1	0	0.319880	6.767670	1.111074
19	1	0	1.308573	6.822169	-0.347939
20	6	0	3.364164	-1.314079	-0.180501
21	1	0	2.450418	-1.900704	-0.023362
22	1	0	3.581173	-0.785995	0.753962
23	6	0	-4.326040	1.322022	0.415684
24	1	0	-4.786194	1.298168	1.404097

25	1	0	-5.100524	1.455366	-0.343447
26	6	0	4.161024	0.779761	-1.458046
27	1	0	4.530628	0.853670	-2.481206
28	1	0	5.005426	0.649225	-0.775149
29	6	0	3.056409	-0.277917	-1.264879
30	1	0	2.832828	-0.796875	-2.206195
31	6	0	-3.390883	0.131186	0.135711
32	1	0	-3.414855	-0.574911	0.974879
33	6	0	-3.672401	-0.627360	-1.163163
34	1	0	-2.799047	-1.262501	-1.363316
35	1	0	-3.726657	0.096386	-1.984721
36	6	0	-4.927345	-1.445268	-1.068001
37	6	0	-6.137163	-0.982675	-1.594497
38	6	0	-4.915262	-2.675981	-0.399990
39	6	0	-7.306365	-1.728492	-1.458088
40	1	0	-6.157560	-0.034702	-2.129592
41	6	0	-6.080204	-3.424153	-0.263411
42	1	0	-3.976516	-3.053551	0.004043
43	6	0	-7.280954	-2.950327	-0.790715
44	1	0	-8.236785	-1.355581	-1.877162
45	1	0	-6.051343	-4.380594	0.251640
46	1	0	-8.190643	-3.535049	-0.686838
47	6	0	4.513515	-2.199253	-0.566843
48	6	0	4.351538	-3.190958	-1.542225
49	6	0	5.775124	-2.029451	0.011573
50	6	0	5.422008	-3.993916	-1.923759
51	1	0	3.372388	-3.336104	-1.995962
52	6	0	6.849379	-2.831375	-0.368466
53	1	0	5.909950	-1.266113	0.776353
54	6	0	6.674918	-3.815921	-1.337685
55	1	0	5.278437	-4.763256	-2.677316
56	1	0	7.821606	-2.688413	0.094966
57	1	0	7.510030	-4.444382	-1.633757
58	17	0	-0.682758	0.672338	-2.800151
59	6	0	0.344072	-0.049049	1.488768
60	6	0	1.110225	1.029150	2.185120
61	6	0	-0.126710	-1.095365	2.357566
62	8	0	0.527048	1.895408	2.810887
63	8	0	2.432741	0.968466	2.015785
64	6	0	-1.194988	-1.946932	1.992890
65	6	0	0.479686	-1.288750	3.624460
66	6	0	3.180533	2.048723	2.610902
67	6	0	-1.639569	-2.934399	2.855459
68	1	0	-1.664067	-1.811648	1.026503
69	6	0	0.050141	-2.296607	4.470063
70	1	0	1.306562	-0.652782	3.930690
71	1	0	4.221128	1.849258	2.363624
72	1	0	2.859692	3.004205	2.189751
73	1	0	3.033541	2.059378	3.692027
74	6	0	-1.014773	-3.116776	4.090454
75	1	0	-2.473494	-3.567291	2.568235
76	1	0	0.534552	-2.441405	5.430151
77	1	0	-1.361217	-3.896746	4.762168
78	17	0	-0.112526	-2.267715	-0.981426

19-ax-b1:

1	6	0	-1.077140	2.802128	-0.598748
2	6	0	0.097598	2.054481	-0.556173
3	6	0	1.316682	2.609083	-0.942777
4	6	0	1.373459	3.955265	-1.313937
5	6	0	0.208200	4.736366	-1.305947
6	6	0	-1.022965	4.147923	-0.966508
7	1	0	2.315480	4.400607	-1.626620
8	1	0	-1.931258	4.744767	-1.009831
9	6	0	-2.225710	1.950673	-0.354840
10	8	0	-3.476081	2.364880	-0.491516
11	7	0	-2.052316	0.684004	-0.066851
12	77	0	0.005245	0.122494	-0.167788
13	6	0	2.337887	1.587039	-0.974243
14	8	0	3.557760	1.767160	-1.459822
15	7	0	2.039668	0.371598	-0.578836
16	6	0	0.270199	6.189747	-1.665014
17	1	0	-0.620273	6.507362	-2.213313
18	1	0	0.332294	6.815894	-0.768257
19	1	0	1.146168	6.415155	-2.277285
20	6	0	3.572428	-1.428500	0.229822
21	1	0	2.684082	-1.976355	0.565716
22	1	0	3.901171	-0.800848	1.064786
23	6	0	-4.327501	1.206361	-0.222052
24	1	0	-4.875898	1.420577	0.696763
25	1	0	-5.029941	1.117436	-1.054347
26	6	0	4.236711	0.475118	-1.354789
27	1	0	4.687538	0.265593	-2.324204
28	1	0	5.023790	0.586829	-0.601622
29	6	0	3.149344	-0.523251	-0.922663
30	1	0	2.819345	-1.145106	-1.767557
31	6	0	-3.360017	0.017810	-0.101693
32	1	0	-3.527084	-0.508970	0.844113
33	6	0	-3.427444	-0.983509	-1.256216
34	1	0	-2.542424	-1.628676	-1.181166
35	1	0	-3.330895	-0.436382	-2.201290
36	6	0	-4.691232	-1.792344	-1.222981
37	6	0	-5.718263	-1.569736	-2.144644
38	6	0	-4.874036	-2.776110	-0.242799
39	6	0	-6.895558	-2.314135	-2.096149
40	1	0	-5.585224	-0.812875	-2.915552
41	6	0	-6.048677	-3.519482	-0.189607
42	1	0	-4.077510	-2.968080	0.476026
43	6	0	-7.063833	-3.290806	-1.118181
44	1	0	-7.679708	-2.132438	-2.825979
45	1	0	-6.170695	-4.283819	0.572823
46	1	0	-7.978967	-3.874909	-1.080903
47	6	0	4.663634	-2.370977	-0.192046
48	6	0	4.369008	-3.498365	-0.968456
49	6	0	5.997778	-2.118735	0.141811
50	6	0	5.381732	-4.351934	-1.395166
51	1	0	3.332937	-3.707257	-1.230627
52	6	0	7.014456	-2.969819	-0.285745
53	1	0	6.238170	-1.250336	0.752944
54	6	0	6.708506	-4.088976	-1.056038

55	1	0	5.135337	-5.226207	-1.991296
56	1	0	8.045197	-2.759788	-0.013719
57	1	0	7.498932	-4.756109	-1.388308
58	17	0	-0.317688	-0.061995	-2.687400
59	6	0	0.246067	0.320685	1.728852
60	6	0	1.531141	0.907056	2.212033
61	6	0	-0.648763	-0.084351	2.785329
62	8	0	2.393209	0.203976	2.705927
63	8	0	1.636042	2.223379	2.022871
64	6	0	-1.683372	-1.022485	2.571598
65	6	0	-0.509369	0.477588	4.078024
66	6	0	2.906609	2.790702	2.395458
67	6	0	-2.543648	-1.370279	3.599645
68	1	0	-1.753606	-1.503605	1.601066
69	6	0	-1.388522	0.145181	5.094389
70	1	0	0.279724	1.199723	4.271150
71	1	0	2.841163	3.846152	2.141476
72	1	0	3.082324	2.658425	3.464457
73	1	0	3.711838	2.308548	1.835544
74	6	0	-2.406598	-0.780279	4.858100
75	1	0	-3.323631	-2.105542	3.426135
76	1	0	-1.280779	0.599412	6.073882
77	1	0	-3.089182	-1.048549	5.659179
78	17	0	-0.052544	-2.430465	-0.091439

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1	6	0	-1.127482	2.844703	-0.541260
2	6	0	0.056513	2.110124	-0.512592
3	6	0	1.271896	2.690343	-0.873816
4	6	0	1.313330	4.047322	-1.207754
5	6	0	0.139176	4.813404	-1.183631
6	6	0	-1.087182	4.200772	-0.868197
7	1	0	2.251360	4.513209	-1.501770
8	1	0	-2.001820	4.788747	-0.897627
9	6	0	-2.265929	1.974646	-0.316520
10	8	0	-3.521894	2.375290	-0.438846
11	7	0	-2.076379	0.704472	-0.055046
12	77	0	-0.014081	0.172913	-0.167169
13	6	0	2.303952	1.680853	-0.931840
14	8	0	3.521199	1.880661	-1.418276
15	7	0	2.013972	0.450884	-0.574827
16	6	0	0.184768	6.277263	-1.499940
17	1	0	-0.700312	6.596930	-2.055855
18	1	0	0.219915	6.878084	-0.584623
19	1	0	1.068324	6.533492	-2.088676
20	6	0	3.548537	-1.399977	0.126232
21	1	0	2.659265	-1.956830	0.444323
22	1	0	3.901972	-0.827157	0.988956
23	6	0	-4.357877	1.200867	-0.189601
24	1	0	-4.908611	1.391912	0.732820
25	1	0	-5.059346	1.117742	-1.023328
26	6	0	4.204618	0.588570	-1.357667
27	1	0	4.660709	0.416265	-2.331873
28	1	0	4.988343	0.674199	-0.597485
29	6	0	3.118854	-0.427936	-0.968409

30	1	0	2.778583	-1.002977	-1.842389
31	6	0	-3.375050	0.022423	-0.090476
32	1	0	-3.529426	-0.519352	0.849545
33	6	0	-3.436434	-0.963486	-1.258550
34	1	0	-2.544637	-1.600579	-1.195222
35	1	0	-3.347313	-0.401809	-2.195768
36	6	0	-4.692001	-1.785274	-1.234375
37	6	0	-5.721112	-1.562806	-2.153742
38	6	0	-4.864818	-2.781838	-0.265447
39	6	0	-6.890558	-2.319977	-2.114145
40	1	0	-5.595708	-0.795916	-2.915946
41	6	0	-6.031781	-3.537787	-0.220900
42	1	0	-4.066284	-2.973798	0.451127
43	6	0	-7.049055	-3.309113	-1.147146
44	1	0	-7.676376	-2.138175	-2.842155
45	1	0	-6.146251	-4.311670	0.533049
46	1	0	-7.958163	-3.902867	-1.116655
47	6	0	4.625975	-2.326188	-0.361946
48	6	0	4.312181	-3.413556	-1.186020
49	6	0	5.966631	-2.096081	-0.038372
50	6	0	5.313200	-4.251071	-1.668776
51	1	0	3.270799	-3.604048	-1.441087
52	6	0	6.971448	-2.930640	-0.522430
53	1	0	6.221113	-1.258128	0.609297
54	6	0	6.646645	-4.010929	-1.339182
55	1	0	5.052401	-5.095527	-2.300734
56	1	0	8.007695	-2.738579	-0.258053
57	1	0	7.427590	-4.666047	-1.714887
58	17	0	-0.330430	0.005809	-2.686082
59	6	0	0.228493	0.358019	1.731684
60	6	0	1.360483	1.225885	2.178347
61	6	0	-0.590329	-0.156505	2.799104
62	8	0	1.298638	2.439972	2.214046
63	8	0	2.432487	0.506495	2.523351
64	6	0	-1.607915	-1.110778	2.564535
65	6	0	-0.387253	0.289262	4.129871
66	6	0	3.589781	1.282640	2.889004
67	6	0	-2.387982	-1.583582	3.605848
68	1	0	-1.729585	-1.503762	1.560905
69	6	0	-1.181116	-0.175968	5.163600
70	1	0	0.384097	1.024366	4.343318
71	1	0	4.380385	0.559602	3.077740
72	1	0	3.866985	1.954153	2.072948
73	1	0	3.383330	1.870326	3.785137
74	6	0	-2.183719	-1.112397	4.904517
75	1	0	-3.157624	-2.324262	3.411432
76	1	0	-1.021702	0.187108	6.173747
77	1	0	-2.803053	-1.479686	5.717589
78	17	0	-0.029119	-2.390123	-0.128560

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1	6	0	-1.115224	2.920492	-0.359491
2	6	0	0.037396	2.139873	-0.495803
3	6	0	1.222045	2.703883	-0.986760
4	6	0	1.281429	4.078436	-1.240819

5	6	0	0.154296	4.882431	-1.025787
6	6	0	-1.054350	4.290183	-0.613339
7	1	0	2.195019	4.526729	-1.625044
8	1	0	-1.946196	4.906362	-0.521075
9	6	0	-2.265412	2.070839	-0.113113
10	8	0	-3.510146	2.511207	-0.012765
11	7	0	-2.099571	0.776037	-0.047488
12	77	0	-0.093863	0.191259	-0.354798
13	6	0	2.197550	1.664668	-1.222020
14	8	0	3.410705	1.844367	-1.720669
15	7	0	1.870778	0.426460	-0.931005
16	6	0	0.221570	6.361503	-1.254595
17	1	0	-0.683291	6.734943	-1.741570
18	1	0	0.318502	6.904181	-0.307816
19	1	0	1.078983	6.633391	-1.873919
20	6	0	3.404010	-1.282651	-0.038328
21	1	0	2.514265	-1.811763	0.326252
22	1	0	3.721213	-0.589133	0.750995
23	6	0	-4.358405	1.325617	0.152922
24	1	0	-4.875333	1.437432	1.106581
25	1	0	-5.087556	1.337832	-0.661223
26	6	0	4.041344	0.521244	-1.773737
27	1	0	4.345196	0.353086	-2.806728
28	1	0	4.928104	0.563868	-1.134901
29	6	0	2.976835	-0.466821	-1.259215
30	1	0	2.645194	-1.149573	-2.052711
31	6	0	-3.399693	0.121578	0.096159
32	1	0	-3.396601	-0.430115	1.040807
33	6	0	-3.653721	-0.857037	-1.050948
34	1	0	-2.738088	-1.450582	-1.172742
35	1	0	-3.794259	-0.293937	-1.981080
36	6	0	-4.828606	-1.748072	-0.768079
37	6	0	-6.048902	-1.587826	-1.429381
38	6	0	-4.720437	-2.747154	0.208153
39	6	0	-7.136054	-2.406998	-1.128044
40	1	0	-6.143628	-0.817476	-2.192605
41	6	0	-5.803324	-3.565964	0.511035
42	1	0	-3.772150	-2.879071	0.729115
43	6	0	-7.015954	-3.397627	-0.157022
44	1	0	-8.077121	-2.270683	-1.654229
45	1	0	-5.701031	-4.339971	1.266759
46	1	0	-7.861916	-4.037512	0.077663
47	6	0	4.505872	-2.246098	-0.374199
48	6	0	4.230593	-3.397071	-1.122764
49	6	0	5.827674	-1.992087	0.003011
50	6	0	5.251535	-4.270535	-1.483363
51	1	0	3.203614	-3.607605	-1.417448
52	6	0	6.852372	-2.865215	-0.356748
53	1	0	6.052451	-1.104746	0.592366
54	6	0	6.566635	-4.005711	-1.102579
55	1	0	5.020740	-5.161319	-2.060959
56	1	0	7.873807	-2.653745	-0.052662
57	1	0	7.363984	-4.687897	-1.383910
58	17	0	-0.630130	0.300618	-2.837352
59	6	0	0.159534	-0.009759	1.544702
60	6	0	-0.476585	-1.233795	2.138275

61	6	0	0.748513	0.853459	2.540197
62	8	0	-1.676473	-1.364356	2.291267
63	8	0	0.448713	-2.105954	2.545482
64	6	0	1.726433	1.816851	2.210125
65	6	0	0.371929	0.730566	3.902176
66	6	0	-0.077348	-3.349664	3.042612
67	6	0	2.301919	2.612774	3.186648
68	1	0	2.062948	1.890220	1.186552
69	6	0	0.921005	1.556163	4.868026
70	1	0	-0.383041	0.004107	4.190372
71	1	0	0.789366	-3.966327	3.267654
72	1	0	-0.671648	-3.177228	3.942065
73	1	0	-0.698501	-3.819842	2.277003
74	6	0	1.891175	2.495779	4.514725
75	1	0	3.071045	3.328565	2.914513
76	1	0	0.601519	1.464520	5.901128
77	1	0	2.331286	3.132254	5.276589
78	17	0	-0.220820	-2.388446	-0.588482

19-ax-c2:

1	6	0	-1.123181	2.779879	-0.470823
2	6	0	0.044564	2.021491	-0.602163
3	6	0	1.185423	2.573480	-1.199617
4	6	0	1.188386	3.921962	-1.572436
5	6	0	0.047172	4.709789	-1.370817
6	6	0	-1.118943	4.123866	-0.843876
7	1	0	2.067515	4.361575	-2.038488
8	1	0	-2.024224	4.720950	-0.756668
9	6	0	-2.233595	1.928979	-0.089038
10	8	0	-3.485116	2.347963	0.026287
11	7	0	-2.031889	0.647266	0.087158
12	77	0	-0.022994	0.090993	-0.293666
13	6	0	2.181821	1.544050	-1.385797
14	8	0	3.374397	1.710927	-1.935232
15	7	0	1.898244	0.326598	-0.983743
16	6	0	0.051860	6.162508	-1.737854
17	1	0	-0.860580	6.445748	-2.269966
18	1	0	0.107648	6.796614	-0.846573
19	1	0	0.905544	6.413354	-2.370883
20	6	0	3.510031	-1.243601	0.015928
21	1	0	2.645167	-1.745075	0.469547
22	1	0	3.845467	-0.470711	0.719197
23	6	0	-4.266537	1.180038	0.443324
24	1	0	-4.555165	1.349087	1.482480
25	1	0	-5.159501	1.143613	-0.183876
26	6	0	4.034152	0.400457	-1.910453
27	1	0	4.289493	0.153107	-2.940597
28	1	0	4.950397	0.514650	-1.324499
29	6	0	3.020093	-0.562997	-1.263584
30	1	0	2.685212	-1.330058	-1.974292
31	6	0	-3.324887	-0.018666	0.255785
32	1	0	-3.294606	-0.639386	1.155197
33	6	0	-3.635595	-0.894985	-0.961811
34	1	0	-2.773300	-1.555657	-1.112778
35	1	0	-3.697586	-0.251288	-1.847447

36	6	0	-4.899500	-1.680855	-0.774256
37	6	0	-6.104633	-1.255259	-1.341954
38	6	0	-4.903725	-2.838345	0.014170
39	6	0	-7.284417	-1.965328	-1.129989
40	1	0	-6.112052	-0.364731	-1.968179
41	6	0	-6.079554	-3.551092	0.226739
42	1	0	-3.968524	-3.185349	0.452422
43	6	0	-7.274968	-3.114698	-0.343758
44	1	0	-8.210652	-1.622017	-1.582687
45	1	0	-6.063675	-4.451275	0.834935
46	1	0	-8.193008	-3.671999	-0.179643
47	6	0	4.612710	-2.223905	-0.263890
48	6	0	4.323887	-3.449734	-0.875630
49	6	0	5.944565	-1.919423	0.031503
50	6	0	5.341115	-4.347772	-1.182175
51	1	0	3.289149	-3.699422	-1.104781
52	6	0	6.965749	-2.817216	-0.274282
53	1	0	6.179693	-0.972865	0.515455
54	6	0	6.666365	-4.032812	-0.883336
55	1	0	5.100170	-5.297313	-1.652367
56	1	0	7.995118	-2.566354	-0.033808
57	1	0	7.460863	-4.734753	-1.120619
58	17	0	-0.682839	0.012823	-2.752445
59	6	0	0.332458	0.066388	1.600060
60	6	0	-0.050704	-1.188159	2.326824
61	6	0	0.895136	1.063649	2.482071
62	8	0	0.799532	-1.920602	2.795517
63	8	0	-1.368631	-1.362899	2.438148
64	6	0	1.784378	2.062384	2.030746
65	6	0	0.548822	1.056640	3.856821
66	6	0	-1.760225	-2.602812	3.054872
67	6	0	2.297207	3.008005	2.903829
68	1	0	2.105587	2.056100	0.999807
69	6	0	1.032836	2.027374	4.717380
70	1	0	-0.131522	0.299785	4.237581
71	1	0	-2.841653	-2.549449	3.163341
72	1	0	-1.477648	-3.433670	2.404382
73	1	0	-1.278317	-2.715394	4.027577
74	6	0	1.911776	3.003202	4.244721
75	1	0	2.998835	3.751807	2.540201
76	1	0	0.735067	2.020854	5.760716
77	1	0	2.302975	3.754344	4.924321
78	17	0	-0.142897	-2.489902	-0.332958

19-ax-d1:

1	6	0	-1.273995	2.937013	0.084527
2	6	0	-0.093576	2.240159	-0.180527
3	6	0	1.087105	2.902334	-0.517488
4	6	0	1.099601	4.302373	-0.537515
5	6	0	-0.065033	5.018777	-0.228671
6	6	0	-1.257912	4.330982	0.069490
7	1	0	2.004645	4.842855	-0.805047
8	1	0	-2.165195	4.897126	0.268730
9	6	0	-2.379107	2.004941	0.243661
10	8	0	-3.628721	2.352548	0.511366

11	7	0	-2.156928	0.725380	0.087603
12	77	0	-0.153152	0.278676	-0.321925
13	6	0	2.118884	1.941660	-0.854332
14	8	0	3.349346	2.254787	-1.240838
15	7	0	1.843192	0.663211	-0.773188
16	6	0	-0.054529	6.517000	-0.227217
17	1	0	-0.889492	6.923892	-0.804844
18	1	0	-0.151894	6.913231	0.788961
19	1	0	0.872562	6.911986	-0.647469
20	6	0	3.367298	-1.228655	-0.257402
21	1	0	2.482967	-1.868558	-0.142649
22	1	0	3.579879	-0.785945	0.722190
23	6	0	-4.375647	1.099972	0.671100
24	1	0	-4.635602	1.022437	1.728545
25	1	0	-5.283727	1.183160	0.070784
26	6	0	4.071398	0.986638	-1.362931
27	1	0	4.592050	0.997818	-2.319664
28	1	0	4.802915	0.956793	-0.547379
29	6	0	2.999449	-0.108180	-1.228411
30	1	0	2.748111	-0.546779	-2.205152
31	6	0	-3.415637	-0.003355	0.196844
32	1	0	-3.308310	-0.780145	0.963911
33	6	0	-3.783671	-0.672688	-1.129675
34	1	0	-2.887739	-1.198992	-1.482707
35	1	0	-4.014003	0.104069	-1.868382
36	6	0	-4.933632	-1.621429	-0.955779
37	6	0	-6.231643	-1.274041	-1.339797
38	6	0	-4.725147	-2.863789	-0.343542
39	6	0	-7.296642	-2.146348	-1.121517
40	1	0	-6.405293	-0.314361	-1.823552
41	6	0	-5.785841	-3.736558	-0.123782
42	1	0	-3.714818	-3.147097	-0.048570
43	6	0	-7.076801	-3.378430	-0.511329
44	1	0	-8.299038	-1.862323	-1.430143
45	1	0	-5.605704	-4.699474	0.346329
46	1	0	-7.905773	-4.059815	-0.341903
47	6	0	4.553014	-2.019981	-0.729924
48	6	0	4.443452	-2.896091	-1.816401
49	6	0	5.797275	-1.875067	-0.109021
50	6	0	5.549117	-3.611486	-2.265765
51	1	0	3.478137	-3.023836	-2.304109
52	6	0	6.906311	-2.589726	-0.556714
53	1	0	5.889830	-1.201262	0.742207
54	6	0	6.784629	-3.459641	-1.637089
55	1	0	5.446123	-4.293217	-3.105585
56	1	0	7.864804	-2.468061	-0.059639
57	1	0	7.646819	-4.020910	-1.985962
58	17	0	-0.619376	0.757672	-2.775011
59	6	0	0.153355	-0.197618	1.509750
60	6	0	-1.005991	-0.735727	2.285466
61	6	0	1.371242	-0.101187	2.289831
62	8	0	-1.684597	0.036559	2.941163
63	8	0	-1.208525	-2.047267	2.196929
64	6	0	2.229211	1.015042	2.228180
65	6	0	1.738095	-1.195418	3.105054
66	6	0	-2.301109	-2.552949	2.993033

67	6	0	3.421560	1.025436	2.936037
68	1	0	1.917796	1.887542	1.665821
69	6	0	2.958774	-1.200846	3.763075
70	1	0	1.082971	-2.059999	3.167006
71	1	0	-2.327839	-3.622441	2.800349
72	1	0	-2.121479	-2.351319	4.050171
73	1	0	-3.242170	-2.086953	2.691124
74	6	0	3.801530	-0.091730	3.682717
75	1	0	4.061915	1.901247	2.900390
76	1	0	3.249343	-2.065031	4.351614
77	1	0	4.748691	-0.091550	4.213996
78	17	0	-0.234445	-2.199648	-0.952911

19-ax-d2:

1	6	0	-1.310289	2.899844	-0.098543
2	6	0	-0.109101	2.212951	-0.277026
3	6	0	1.081278	2.880095	-0.565932
4	6	0	1.079168	4.278769	-0.623076
5	6	0	-0.109922	4.988085	-0.400180
6	6	0	-1.309802	4.293571	-0.152841
7	1	0	1.991334	4.823651	-0.854973
8	1	0	-2.234007	4.852692	-0.023637
9	6	0	-2.413737	1.960423	0.022311
10	8	0	-3.678959	2.309751	0.201979
11	7	0	-2.172730	0.678633	-0.073567
12	77	0	-0.134846	0.245154	-0.366363
13	6	0	2.139243	1.924125	-0.831718
14	8	0	3.378315	2.244302	-1.181950
15	7	0	1.876038	0.644834	-0.731568
16	6	0	-0.114646	6.485907	-0.435584
17	1	0	-0.951847	6.870106	-1.024894
18	1	0	-0.218667	6.905057	0.570811
19	1	0	0.810253	6.880458	-0.861233
20	6	0	3.406694	-1.225823	-0.147112
21	1	0	2.520899	-1.863652	-0.032941
22	1	0	3.607435	-0.767423	0.827722
23	6	0	-4.452435	1.065712	0.243885
24	1	0	-4.963816	1.040242	1.207196
25	1	0	-5.191660	1.119068	-0.559192
26	6	0	4.116450	0.981637	-1.262348
27	1	0	4.664893	0.983407	-2.203452
28	1	0	4.823500	0.972751	-0.425242
29	6	0	3.052046	-0.122023	-1.141301
30	1	0	2.830186	-0.575580	-2.118423
31	6	0	-3.423163	-0.063211	0.042417
32	1	0	-3.363562	-0.706267	0.930893
33	6	0	-3.675082	-0.960529	-1.168082
34	1	0	-2.747008	-1.515557	-1.357309
35	1	0	-3.862967	-0.335873	-2.048821
36	6	0	-4.819222	-1.898442	-0.907180
37	6	0	-6.046651	-1.757144	-1.558957
38	6	0	-4.678503	-2.913760	0.048057
39	6	0	-7.109132	-2.612109	-1.269808
40	1	0	-6.166854	-0.972063	-2.303111
41	6	0	-5.737234	-3.767460	0.339451

42	1	0	-3.724725	-3.033779	0.562506
43	6	0	-6.957399	-3.618058	-0.319318
44	1	0	-8.056660	-2.489935	-1.787577
45	1	0	-5.610487	-4.552618	1.079647
46	1	0	-7.784921	-4.284419	-0.092652
47	6	0	4.596229	-2.026640	-0.593960
48	6	0	4.500406	-2.904178	-1.680739
49	6	0	5.828830	-1.892679	0.051791
50	6	0	5.607842	-3.631250	-2.106258
51	1	0	3.544284	-3.024333	-2.188063
52	6	0	6.939611	-2.619512	-0.371729
53	1	0	5.910601	-1.217736	0.903138
54	6	0	6.831659	-3.490333	-1.452809
55	1	0	5.515117	-4.313407	-2.946942
56	1	0	7.888949	-2.506275	0.144667
57	1	0	7.695192	-4.060678	-1.782962
58	17	0	-0.484019	0.653246	-2.851785
59	6	0	0.087380	-0.171526	1.486337
60	6	0	-1.076177	-0.769848	2.218652
61	6	0	1.295029	-0.108878	2.287577
62	8	0	-1.344236	-1.953380	2.262978
63	8	0	-1.766375	0.194898	2.845028
64	6	0	2.144068	1.015368	2.268731
65	6	0	1.649289	-1.217272	3.087825
66	6	0	-2.867450	-0.265655	3.654604
67	6	0	3.315956	1.022588	3.010797
68	1	0	1.840791	1.896708	1.714518
69	6	0	2.852738	-1.224045	3.777402
70	1	0	0.999560	-2.087323	3.110871
71	1	0	-3.388820	0.632730	3.976190
72	1	0	-3.531146	-0.911233	3.074348
73	1	0	-2.490756	-0.821924	4.514502
74	6	0	3.686811	-0.105887	3.744219
75	1	0	3.948313	1.904885	3.009195
76	1	0	3.136866	-2.099041	4.353165
77	1	0	4.619722	-0.108850	4.299994
78	17	0	-0.122725	-2.241268	-0.934315

trans-20:

1	6	0	-7.267728	-3.367939	-0.007952
2	6	0	-6.063002	-3.848698	0.503762
3	6	0	-4.885194	-3.135200	0.305023
4	6	0	-4.888690	-1.932006	-0.411072
5	6	0	-6.103605	-1.461117	-0.919252
6	6	0	-7.285266	-2.171838	-0.720570
7	6	0	-3.624096	-1.142787	-0.588171
8	6	0	-3.237606	-0.374407	0.680699
9	7	0	-1.997620	0.372324	0.473864
10	6	0	-2.259723	1.653642	0.527401
11	8	0	-3.514836	1.992577	0.807121
12	6	0	-4.223311	0.741615	1.069894
13	6	0	-1.188911	2.588868	0.276971
14	6	0	-0.001461	1.897752	0.001101
15	6	0	1.187395	2.589012	-0.278235
16	6	0	1.181033	3.984718	-0.282004

17	6	0	-0.001728	4.691406	-0.004457
18	6	0	-1.181792	3.987477	0.274745
19	6	0	2.258609	1.652727	-0.527202
20	8	0	3.512688	1.991847	-0.810022
21	6	0	4.223560	0.740465	-1.064596
22	6	0	3.236116	-0.375406	-0.678349
23	7	0	1.996850	0.371998	-0.469018
24	77	0	-0.000476	-0.017904	0.002777
25	6	0	0.007634	6.190625	-0.006753
26	6	0	3.622274	-1.148336	0.587719
27	6	0	4.888031	-1.935184	0.408046
28	6	0	6.101915	-1.464691	0.919078
29	6	0	7.284775	-2.172665	0.717849
30	6	0	7.269503	-3.365540	-0.000225
31	6	0	6.065815	-3.845897	-0.514744
32	6	0	4.886778	-3.135130	-0.313457
33	17	0	0.508765	-0.201302	2.351820
34	17	0	-0.508523	-0.202307	-2.346322
35	1	0	-2.095544	4.537593	0.489267
36	1	0	2.095048	4.533388	-0.500012
37	1	0	0.687966	6.588961	0.752870
38	1	0	0.344486	6.588505	-0.969161
39	1	0	-0.986083	6.597496	0.192311
40	1	0	-2.782411	-1.794118	-0.851439
41	1	0	-3.728155	-0.421570	-1.407772
42	1	0	4.496006	0.735103	-2.121422
43	1	0	5.131685	0.749106	-0.457004
44	1	0	-4.488332	0.738846	2.128713
45	1	0	-5.135595	0.747969	0.468631
46	1	0	-3.099600	-1.082742	1.506477
47	1	0	3.096401	-1.081003	-1.506218
48	1	0	2.781214	-1.801736	0.847849
49	1	0	3.725057	-0.430283	1.410230
50	1	0	6.113790	-0.539200	1.492373
51	1	0	3.948604	-3.516403	-0.712708
52	1	0	8.217512	-1.793460	1.125849
53	1	0	6.046056	-4.778181	-1.072589
54	1	0	8.189896	-3.921210	-0.156246
55	1	0	-3.946202	-3.516823	0.702012
56	1	0	-6.117210	-0.533101	-1.488439
57	1	0	-6.041475	-4.783492	1.057355
58	1	0	-8.218801	-1.792268	-1.126393
59	1	0	-8.187138	-3.925818	0.145992

cis-20:

1	6	0	-7.043059	-3.459015	0.337827
2	6	0	-5.750207	-3.797642	0.735486
3	6	0	-4.672770	-3.004154	0.354672
4	6	0	-4.866520	-1.861578	-0.431168
5	6	0	-6.167045	-1.533395	-0.824714
6	6	0	-7.248894	-2.325975	-0.444494
7	6	0	-3.696601	-0.988858	-0.785791
8	6	0	-3.256243	-0.132561	0.403253
9	7	0	-2.030229	0.606657	0.113049
10	6	0	-2.245652	1.888939	0.289462

11	8	0	-3.477087	2.237072	0.640664
12	6	0	-4.240385	0.995046	0.769825
13	6	0	-1.142328	2.811114	0.118345
14	6	0	0.026208	2.095145	-0.167230
15	6	0	1.252459	2.756072	-0.320425
16	6	0	1.303647	4.146944	-0.210837
17	6	0	0.133471	4.876824	0.061445
18	6	0	-1.086696	4.204001	0.230469
19	6	0	2.304791	1.790543	-0.560752
20	8	0	3.591048	2.089400	-0.694214
21	6	0	4.278271	0.827182	-0.974184
22	6	0	3.220339	-0.267034	-0.752205
23	7	0	1.990923	0.518838	-0.644419
24	77	0	-0.032132	0.154469	-0.275913
25	6	0	0.192867	6.371772	0.160698
26	6	0	3.426474	-1.107773	0.511593
27	6	0	4.655343	-1.965556	0.430795
28	6	0	5.812772	-1.630067	1.139988
29	6	0	6.961246	-2.413173	1.045871
30	6	0	6.968408	-3.545168	0.235049
31	6	0	5.821906	-3.888324	-0.481043
32	6	0	4.676765	-3.104077	-0.384400
33	17	0	0.354270	0.077612	2.015033
34	17	0	-0.093156	-2.342562	-0.760285
35	1	0	-1.984326	4.775513	0.457001
36	1	0	2.248693	4.673970	-0.326834
37	1	0	1.056569	6.702330	0.744384
38	1	0	0.284477	6.834377	-0.828070
39	1	0	-0.706690	6.778669	0.628196
40	1	0	-2.833816	-1.594951	-1.088393
41	1	0	-3.942960	-0.326162	-1.624342
42	1	0	4.638980	0.883065	-2.002888
43	1	0	5.129883	0.761143	-0.293175
44	1	0	-4.609636	0.950934	1.794941
45	1	0	-5.088615	1.063697	0.082789
46	1	0	-3.065315	-0.790050	1.262352
47	1	0	3.151742	-0.931728	-1.620897
48	1	0	2.523866	-1.717153	0.644122
49	1	0	3.481474	-0.430492	1.372711
50	1	0	5.806015	-0.751019	1.782095
51	1	0	3.781009	-3.379755	-0.939163
52	1	0	7.848873	-2.140224	1.609787
53	1	0	5.819013	-4.772581	-1.112276
54	1	0	7.861020	-4.160050	0.163055
55	1	0	-3.663258	-3.272692	0.662942
56	1	0	-6.331001	-0.652565	-1.443406
57	1	0	-5.580967	-4.683938	1.340906
58	1	0	-8.252791	-2.057528	-0.762008
59	1	0	-7.884954	-4.078429	0.633567

TS1:

1	6	0	-7.004159	-3.542569	0.310571
2	6	0	-5.703592	-3.876642	0.686581
3	6	0	-4.640121	-3.057429	0.321717
4	6	0	-4.855072	-1.892856	-0.425457

5	6	0	-6.162964	-1.570301	-0.798675
6	6	0	-7.231115	-2.388788	-0.434631
7	6	0	-3.698527	-0.994271	-0.757427
8	6	0	-3.256913	-0.177561	0.460667
9	7	0	-2.025214	0.561932	0.191567
10	6	0	-2.262946	1.847147	0.303254
11	8	0	-3.506202	2.193124	0.616703
12	6	0	-4.233952	0.946207	0.853747
13	6	0	-1.175470	2.776994	0.091108
14	6	0	0.010949	2.072256	-0.147900
15	6	0	1.223607	2.745277	-0.349362
16	6	0	1.242335	4.141888	-0.327755
17	6	0	0.058099	4.861713	-0.098008
18	6	0	-1.147441	4.174355	0.116021
19	6	0	2.291031	1.789300	-0.547689
20	8	0	3.570085	2.099815	-0.719698
21	6	0	4.283294	0.833832	-0.896722
22	6	0	3.225563	-0.266370	-0.688413
23	7	0	1.994915	0.511445	-0.563147
24	77	0	-0.011958	0.133166	-0.167080
25	6	0	0.079696	6.360857	-0.101046
26	6	0	3.440884	-1.133964	0.554182
27	6	0	4.671075	-1.986842	0.443627
28	6	0	5.835143	-1.659484	1.145441
29	6	0	6.987382	-2.432093	1.018284
30	6	0	6.991134	-3.545630	0.182304
31	6	0	5.837280	-3.881185	-0.525505
32	6	0	4.688387	-3.107286	-0.396288
33	17	0	0.381813	0.308365	2.137852
34	17	0	-0.137157	-2.155389	-1.204005
35	1	0	-2.057878	4.738558	0.307583
36	1	0	2.175203	4.680461	-0.482138
37	1	0	1.026867	6.750394	0.280497
38	1	0	-0.044181	6.759301	-1.114285
39	1	0	-0.727621	6.775845	0.507376
40	1	0	-2.832239	-1.577304	-1.091687
41	1	0	-3.958985	-0.302511	-1.568029
42	1	0	4.711806	0.846645	-1.899861
43	1	0	5.089161	0.808548	-0.158481
44	1	0	-4.518081	0.937766	1.907147
45	1	0	-5.135077	0.972175	0.236065
46	1	0	-3.076398	-0.859205	1.301687
47	1	0	3.151823	-0.914934	-1.569393
48	1	0	2.540945	-1.749222	0.679922
49	1	0	3.500727	-0.477252	1.430477
50	1	0	5.831393	-0.794797	1.806825
51	1	0	3.786730	-3.376474	-0.944937
52	1	0	7.880752	-2.165441	1.576107
53	1	0	5.831725	-4.751524	-1.175822
54	1	0	7.886974	-4.152224	0.084085
55	1	0	-3.624442	-3.322269	0.612596
56	1	0	-6.343773	-0.672952	-1.388194
57	1	0	-5.517599	-4.779070	1.262523
58	1	0	-8.241052	-2.124007	-0.735489
59	1	0	-7.835651	-4.181386	0.594431

trans-TS2:

1	6	0	3.126308	-3.831638	-2.251177
2	6	0	2.658547	-4.345161	-1.041271
3	6	0	1.717013	-3.640406	-0.303497
4	6	0	1.239962	-2.391754	-0.749379
5	6	0	1.709131	-1.897840	-1.978878
6	6	0	2.645776	-2.609228	-2.719714
7	6	0	0.177585	-1.650179	-0.018350
8	6	0	-0.136201	-2.082787	1.380875
9	8	0	0.994465	-2.169886	2.096557
10	6	0	0.805834	-2.309535	3.514014
11	77	0	-0.184893	0.555464	-0.180714
12	17	0	-0.870852	0.407803	-2.501167
13	6	0	-0.397902	2.528779	-0.224964
14	6	0	0.696929	3.342062	-0.511890
15	6	0	0.569048	4.734055	-0.471196
16	6	0	-0.660017	5.315518	-0.124919
17	6	0	-1.747832	4.491386	0.206430
18	6	0	-1.614125	3.101797	0.152088
19	6	0	1.871332	2.526876	-0.716422
20	8	0	3.091462	3.031534	-0.870209
21	6	0	3.978988	1.888165	-1.050922
22	6	0	3.139198	0.674306	-0.638852
23	7	0	1.774644	1.218265	-0.673727
24	6	0	-2.548215	2.061692	0.516840
25	8	0	-3.753782	2.283899	1.039327
26	6	0	-4.199021	0.977669	1.529937
27	6	0	-3.384192	-0.009973	0.701538
28	7	0	-2.204461	0.804723	0.372151
29	6	0	-0.813001	6.806517	-0.107817
30	6	0	-4.130439	-0.418626	-0.576855
31	6	0	-5.196686	-1.441658	-0.307969
32	6	0	-4.857838	-2.700699	0.204942
33	6	0	-5.840172	-3.651441	0.463248
34	6	0	-7.181063	-3.358093	0.217644
35	6	0	-7.531276	-2.107340	-0.283410
36	6	0	-6.544847	-1.157268	-0.541340
37	6	0	3.461650	0.127528	0.755046
38	6	0	4.822166	-0.501788	0.799754
39	6	0	5.903145	0.134708	1.415987
40	6	0	7.168597	-0.449613	1.413532
41	6	0	7.370378	-1.679203	0.791026
42	6	0	6.299290	-2.322409	0.170658
43	6	0	5.038543	-1.735803	0.175977
44	17	0	0.339890	0.888836	2.181709
45	8	0	-1.253104	-2.257897	1.834339
46	1	0	-2.688028	4.944232	0.514931
47	1	0	1.421305	5.373740	-0.690787
48	1	0	-1.528739	7.128746	0.652895
49	1	0	0.139079	7.306375	0.086712
50	1	0	-1.180910	7.179445	-1.070175
51	1	0	-3.403347	-0.783079	-1.307987
52	1	0	-4.569472	0.482162	-1.024337
53	1	0	4.274345	1.872545	-2.102468
54	1	0	4.859951	2.050306	-0.426109

55	1	0	-3.972330	0.943052	2.599349
56	1	0	-5.276575	0.913125	1.371615
57	1	0	-3.073162	-0.886700	1.276537
58	1	0	3.245480	-0.129816	-1.372835
59	1	0	2.682598	-0.600234	1.018890
60	1	0	3.377394	0.945415	1.480760
61	1	0	5.747293	1.092993	1.908615
62	1	0	4.200343	-2.237703	-0.303883
63	1	0	7.997326	0.056263	1.901139
64	1	0	6.444182	-3.284381	-0.315223
65	1	0	8.356416	-2.135456	0.790054
66	1	0	-3.814028	-2.934933	0.410147
67	1	0	-6.820296	-0.180138	-0.934249
68	1	0	-5.558874	-4.624204	0.857510
69	1	0	-8.573891	-1.868340	-0.474153
70	1	0	-7.947811	-4.100930	0.418289
71	1	0	1.349013	-4.059943	0.626993
72	1	0	1.314284	-0.954420	-2.347432
73	1	0	1.806261	-2.372985	3.936527
74	1	0	0.280682	-1.433899	3.900691
75	1	0	0.234817	-3.213211	3.734135
76	1	0	3.022655	-5.301051	-0.677489
77	1	0	3.001257	-2.209537	-3.664623
78	1	0	3.860836	-4.385347	-2.828983
79	7	0	-1.215356	-2.332084	-0.818035
80	7	0	-1.822951	-2.407846	-1.758057

***cis*-TS2:**

1	6	0	-0.931604	2.646690	-0.834668
2	6	0	0.243576	1.886233	-0.886472
3	6	0	1.494189	2.511505	-0.973756
4	6	0	1.567909	3.905067	-1.007910
5	6	0	0.395303	4.677259	-0.936667
6	6	0	-0.853092	4.042560	-0.847655
7	1	0	2.533462	4.402979	-1.077364
8	1	0	-1.757046	4.645597	-0.793582
9	6	0	-2.073108	1.764922	-0.727309
10	8	0	-3.333000	2.162661	-0.583774
11	7	0	-1.865599	0.469887	-0.710549
12	77	0	0.142576	-0.052876	-0.826335
13	6	0	2.543989	1.515444	-0.996360
14	8	0	3.838124	1.795519	-1.074874
15	7	0	2.219435	0.247656	-0.925402
16	6	0	0.489204	6.173265	-0.923773
17	1	0	-0.487479	6.638609	-1.073241
18	1	0	0.883458	6.538388	0.031591
19	1	0	1.162663	6.542406	-1.702591
20	6	0	3.561755	-1.406883	0.323132
21	1	0	2.648412	-2.009528	0.396635
22	1	0	3.577456	-0.730399	1.186239
23	6	0	-4.142164	0.943902	-0.553265
24	1	0	-4.822235	1.021927	0.295788
25	1	0	-4.718432	0.917212	-1.484215
26	6	0	4.538794	0.512052	-1.088940
27	1	0	5.092505	0.458482	-2.027151

28	1	0	5.243797	0.520624	-0.253006
29	6	0	3.440154	-0.558447	-0.943687
30	1	0	3.409569	-1.219229	-1.820023
31	6	0	-3.132491	-0.209297	-0.449978
32	1	0	-3.087445	-0.605945	0.574713
33	6	0	-3.408246	-1.364991	-1.405050
34	1	0	-2.534013	-2.027765	-1.384065
35	1	0	-3.499252	-0.978153	-2.427168
36	6	0	-4.654827	-2.099375	-0.997596
37	6	0	-5.806743	-2.070387	-1.787484
38	6	0	-4.694546	-2.792033	0.219569
39	6	0	-6.968692	-2.723165	-1.379223
40	1	0	-5.788683	-1.533711	-2.734408
41	6	0	-5.853860	-3.440346	0.632557
42	1	0	-3.802093	-2.826169	0.843743
43	6	0	-6.996090	-3.407955	-0.167433
44	1	0	-7.853490	-2.694461	-2.009061
45	1	0	-5.865188	-3.976404	1.578097
46	1	0	-7.901026	-3.916878	0.152501
47	6	0	4.781854	-2.280806	0.305526
48	6	0	4.820478	-3.426624	-0.498649
49	6	0	5.913169	-1.956221	1.060523
50	6	0	5.957388	-4.227487	-0.542312
51	1	0	3.943543	-3.694316	-1.086319
52	6	0	7.053732	-2.755681	1.019082
53	1	0	5.892120	-1.072526	1.695978
54	6	0	7.078645	-3.893555	0.216833
55	1	0	5.967934	-5.116883	-1.166205
56	1	0	7.921339	-2.490409	1.616798
57	1	0	7.965199	-4.520383	0.185568
58	17	0	0.023905	-0.084144	-3.155878
59	6	0	0.227025	0.351473	2.461465
60	6	0	1.167763	1.482536	2.361272
61	6	0	-1.229812	0.289130	2.689669
62	8	0	2.373058	1.341379	2.230448
63	8	0	0.550114	2.667510	2.457088
64	6	0	-1.829501	-0.924308	3.072564
65	6	0	-2.055003	1.413004	2.514327
66	6	0	1.427961	3.805641	2.459795
67	6	0	-3.200454	-1.008821	3.281167
68	1	0	-1.225747	-1.816928	3.211168
69	6	0	-3.426799	1.316087	2.728688
70	1	0	-1.626963	2.359341	2.206491
71	1	0	0.775799	4.674134	2.393691
72	1	0	2.006569	3.828733	3.385374
73	1	0	2.106066	3.769319	1.605558
74	6	0	-4.011522	0.111179	3.110642
75	1	0	-3.634699	-1.960562	3.574599
76	1	0	-4.042448	2.199856	2.581891
77	1	0	-5.084240	0.042307	3.265001
78	17	0	0.029126	-2.550171	-0.311286
79	7	0	0.890099	-0.794251	2.579765
80	7	0	1.425825	-1.789066	2.705281

cis-21:

1	6	0	-0.938495	2.692119	-0.971952
2	6	0	0.242004	1.974090	-0.738789
3	6	0	1.489770	2.593541	-0.869907
4	6	0	1.558548	3.953666	-1.188805
5	6	0	0.380265	4.693315	-1.371913
6	6	0	-0.867534	4.052992	-1.277235
7	1	0	2.523141	4.445362	-1.298569
8	1	0	-1.775545	4.626288	-1.453570
9	6	0	-2.077724	1.806785	-0.854501
10	8	0	-3.346677	2.172750	-1.009067
11	7	0	-1.866568	0.548469	-0.566449
12	77	0	0.157485	0.068955	-0.341291
13	6	0	2.542729	1.615350	-0.718996
14	8	0	3.826329	1.861767	-0.960437
15	7	0	2.230382	0.378829	-0.410205
16	6	0	0.451301	6.165188	-1.646087
17	1	0	-0.414422	6.512015	-2.215526
18	1	0	0.472516	6.739467	-0.712383
19	1	0	1.353554	6.429313	-2.203307
20	6	0	3.647641	-1.463710	0.520783
21	1	0	2.728994	-2.056792	0.609287
22	1	0	3.796198	-0.925361	1.465747
23	6	0	-4.152658	0.968482	-0.798568
24	1	0	-4.826812	1.175517	0.034671
25	1	0	-4.736067	0.805794	-1.709018
26	6	0	4.529937	0.608880	-0.700760
27	1	0	5.238478	0.453035	-1.513361
28	1	0	5.074473	0.733640	0.242447
29	6	0	3.426236	-0.450845	-0.594997
30	1	0	3.300599	-0.994149	-1.544410
31	6	0	-3.142050	-0.158763	-0.514152
32	1	0	-3.273004	-0.553104	0.502507
33	6	0	-3.185586	-1.325840	-1.501208
34	1	0	-2.243351	-1.876932	-1.388297
35	1	0	-3.209478	-0.932789	-2.524461
36	6	0	-4.363227	-2.218929	-1.234942
37	6	0	-5.470089	-2.251408	-2.086723
38	6	0	-4.383539	-3.012447	-0.080445
39	6	0	-6.569804	-3.057765	-1.796094
40	1	0	-5.465947	-1.642512	-2.989034
41	6	0	-5.480097	-3.815331	0.214605
42	1	0	-3.522685	-2.999731	0.587548
43	6	0	-6.578633	-3.840232	-0.644359
44	1	0	-7.420915	-3.073400	-2.471525
45	1	0	-5.476346	-4.426709	1.113007
46	1	0	-7.435437	-4.468168	-0.417042
47	6	0	4.820409	-2.356277	0.225870
48	6	0	4.703686	-3.361721	-0.741459
49	6	0	6.051151	-2.179650	0.864072
50	6	0	5.789590	-4.170245	-1.061746
51	1	0	3.747119	-3.511373	-1.240340
52	6	0	7.140706	-2.988308	0.545638
53	1	0	6.152710	-1.404958	1.621958
54	6	0	7.012760	-3.984652	-0.418794
55	1	0	5.680588	-4.948993	-1.811372
56	1	0	8.089795	-2.839941	1.053490

57	1	0	7.861018	-4.616213	-0.666832
58	17	0	0.244587	-0.345149	-2.742074
59	6	0	0.007344	0.438928	1.847606
60	6	0	0.819897	1.691376	2.160826
61	6	0	-1.404859	0.228061	2.362843
62	8	0	2.014783	1.650969	2.375428
63	8	0	0.086316	2.797064	2.113683
64	6	0	-1.836346	-1.051452	2.738392
65	6	0	-2.328100	1.282282	2.388299
66	6	0	0.819104	4.023408	2.313279
67	6	0	-3.150191	-1.268888	3.143061
68	1	0	-1.162122	-1.900974	2.693179
69	6	0	-3.642644	1.051840	2.784253
70	1	0	-2.033896	2.277908	2.084875
71	1	0	0.130761	4.817510	2.032245
72	1	0	1.109944	4.113263	3.360842
73	1	0	1.707851	4.037474	1.680583
74	6	0	-4.063402	-0.219455	3.165553
75	1	0	-3.456845	-2.271064	3.428189
76	1	0	-4.341193	1.884020	2.789298
77	1	0	-5.090646	-0.390252	3.472565
78	17	0	0.063411	-2.487213	0.064453
79	7	0	0.823033	-0.597302	2.349638
80	7	0	1.401725	-1.504742	2.663137

cis-TS3:

1	6	0	-1.078122	2.591142	-0.915427
2	6	0	0.115775	1.871791	-0.817229
3	6	0	1.338054	2.462832	-1.146863
4	6	0	1.375902	3.808790	-1.520109
5	6	0	0.189248	4.557856	-1.568838
6	6	0	-1.038955	3.939321	-1.280226
7	1	0	2.321666	4.284932	-1.772227
8	1	0	-1.957967	4.517235	-1.352215
9	6	0	-2.203132	1.722973	-0.638152
10	8	0	-3.477684	2.094643	-0.702912
11	7	0	-1.978719	0.470640	-0.329045
12	77	0	0.064304	-0.025529	-0.333099
13	6	0	2.399750	1.487817	-1.045531
14	8	0	3.671378	1.733275	-1.347786
15	7	0	2.114587	0.265138	-0.665020
16	6	0	0.237400	6.016247	-1.911872
17	1	0	-0.719111	6.370574	-2.302843
18	1	0	0.469390	6.621946	-1.028256
19	1	0	1.009590	6.230555	-2.655127
20	6	0	3.574096	-1.508389	0.330932
21	1	0	2.721172	-2.195467	0.392558
22	1	0	3.599549	-0.924925	1.258646
23	6	0	-4.254146	0.938229	-0.250813
24	1	0	-4.636937	1.181846	0.744369
25	1	0	-5.087217	0.810023	-0.944962
26	6	0	4.400219	0.515123	-1.002944
27	1	0	5.116635	0.320450	-1.799589
28	1	0	4.935146	0.712639	-0.065952
29	6	0	3.318864	-0.557014	-0.831537

30	1	0	3.192080	-1.144362	-1.753685
31	6	0	-3.259065	-0.230905	-0.246724
32	1	0	-3.305873	-0.775781	0.700824
33	6	0	-3.427310	-1.228093	-1.396314
34	1	0	-2.504057	-1.818356	-1.450488
35	1	0	-3.512925	-0.679658	-2.342239
36	6	0	-4.620638	-2.110389	-1.167784
37	6	0	-5.799916	-1.952703	-1.900455
38	6	0	-4.583060	-3.084290	-0.161026
39	6	0	-6.914123	-2.749302	-1.639422
40	1	0	-5.840862	-1.200994	-2.686921
41	6	0	-5.692529	-3.880786	0.101875
42	1	0	-3.668674	-3.217098	0.417138
43	6	0	-6.863371	-3.714421	-0.637243
44	1	0	-7.821955	-2.614647	-2.221362
45	1	0	-5.643483	-4.635223	0.882436
46	1	0	-7.730521	-4.336033	-0.432979
47	6	0	4.860947	-2.262837	0.145959
48	6	0	4.960560	-3.278964	-0.812284
49	6	0	5.996646	-1.933528	0.891947
50	6	0	6.163346	-3.948183	-1.016441
51	1	0	4.082783	-3.550103	-1.396572
52	6	0	7.202188	-2.602119	0.690303
53	1	0	5.929127	-1.149364	1.644078
54	6	0	7.288968	-3.610668	-0.265791
55	1	0	6.222715	-4.737326	-1.760998
56	1	0	8.073112	-2.335458	1.282448
57	1	0	8.227641	-4.134088	-0.424282
58	17	0	-0.158955	-0.437781	-2.779760
59	6	0	0.225209	0.424793	1.694355
60	6	0	1.304552	1.460705	1.980660
61	6	0	-1.071863	0.483540	2.462467
62	8	0	2.454358	1.173422	2.253040
63	8	0	0.863764	2.707486	1.816274
64	6	0	-1.794393	-0.701328	2.674531
65	6	0	-1.620912	1.692730	2.910505
66	6	0	1.867142	3.733615	1.945054
67	6	0	-3.018680	-0.681378	3.330059
68	1	0	-1.408806	-1.644009	2.291543
69	6	0	-2.864646	1.707626	3.537904
70	1	0	-1.095967	2.626139	2.754958
71	1	0	1.363575	4.660464	1.678910
72	1	0	2.237086	3.770066	2.970587
73	1	0	2.697533	3.537188	1.263499
74	6	0	-3.565021	0.526303	3.760663
75	1	0	-3.554809	-1.613834	3.484279
76	1	0	-3.278115	2.657043	3.865163
77	1	0	-4.527075	0.544809	4.263958
78	17	0	-0.071877	-2.544944	0.035355
79	7	0	0.987164	-0.856492	2.384099
80	7	0	1.174094	-1.961356	2.459216

Gaussian 09: complete reference.

Gaussian 09, Revision A.02, Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Mennucci, B., Petersson, G. A., Nakatsuji, H., Caricato, M., Li, X., Hratchian, H. P., Izmaylov, A. F., Bloino, J., Zheng, G., Sonnenberg, J. L., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Montgomery, Jr., J. A., Peralta, J. E., Ogliaro, F., Bearpark, M., Heyd, J. J., Brothers, E., Kudin, K. N., Staroverov, V. N., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J. C. Iyengar, S. S. Tomasi, J. Cossi, M. Rega, Millam, N. J., Klene, M. Knox, J. E., Cross, J. B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. Martin, R. L., Morokuma, K., Zakrzewski, V. G., Voth, G. A., Salvador, P., Dannenberg, J. J., Dapprich, S., Daniels, A. D., Farkas, O., Foresman, J. B., Ortiz, J. V., Cioslowski, J., and Fox, D. J., Gaussian, Inc., Wallingford CT, **2009**.