Supporting Information for

Enantioselectivity in Organocatalytic Cascade Double Michael Addition Reaction: A Theoretical Study

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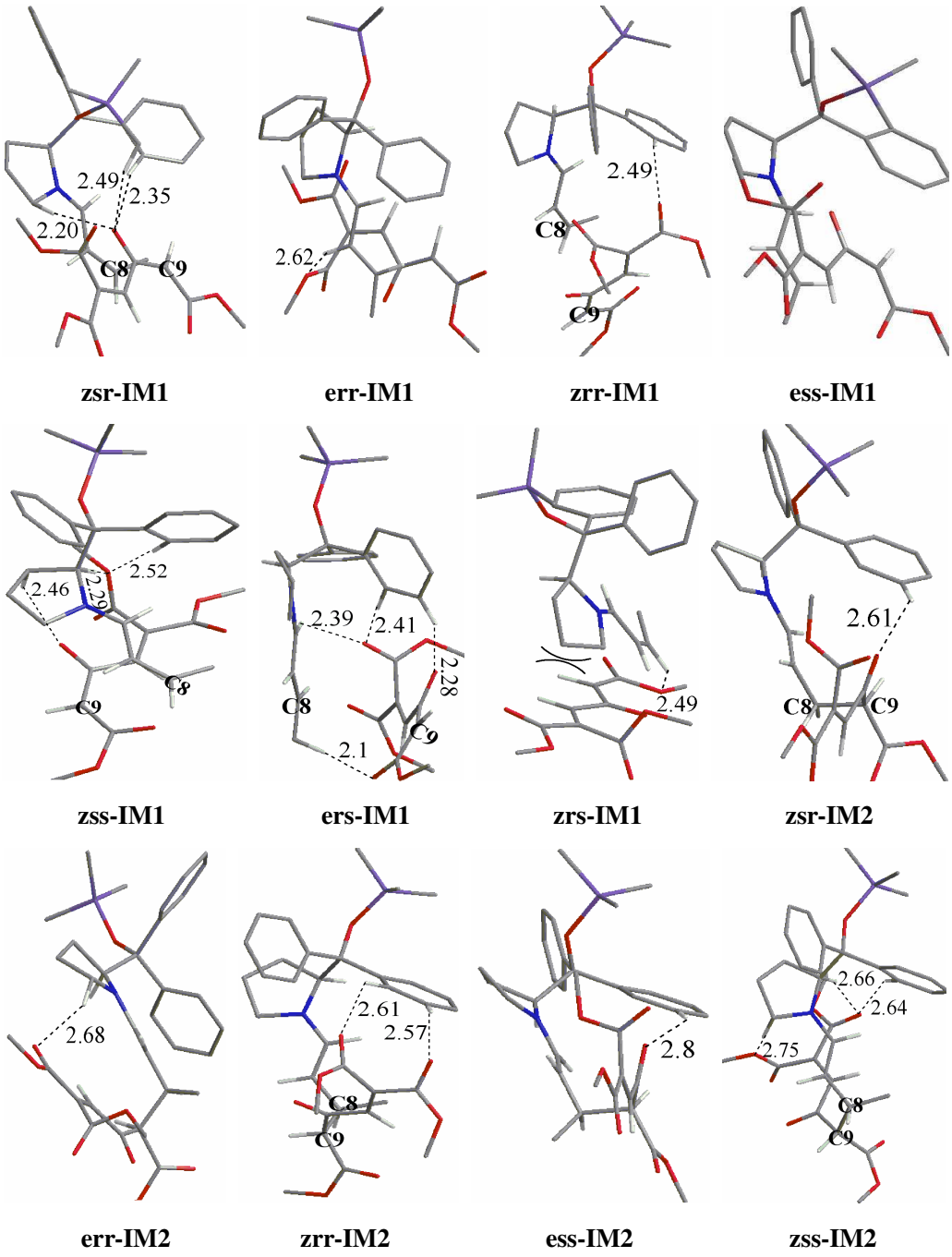

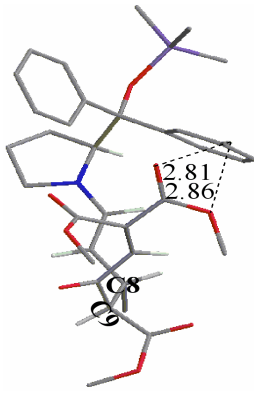

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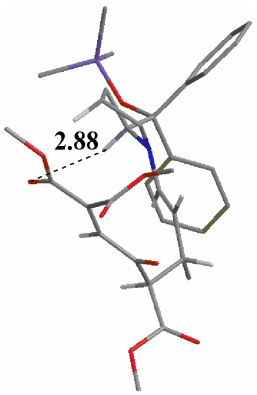

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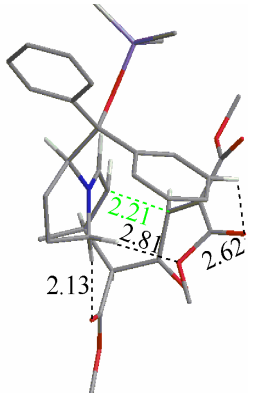

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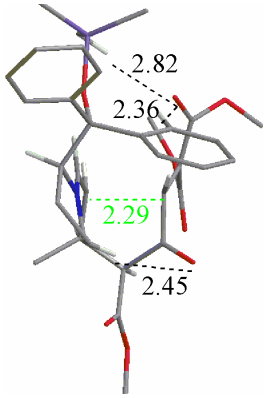

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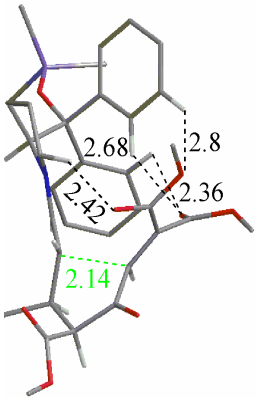

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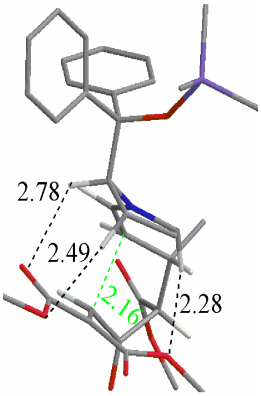

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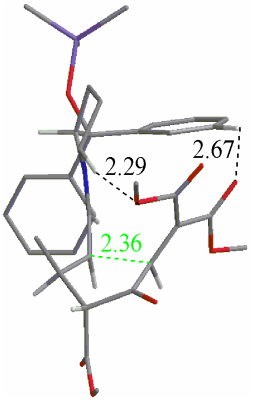

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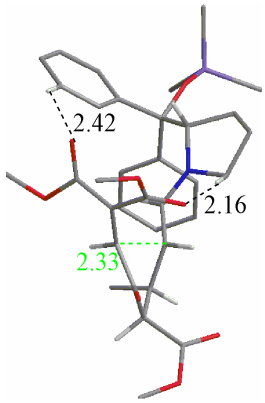

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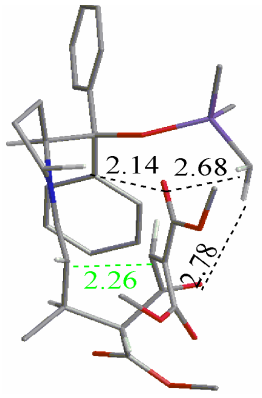

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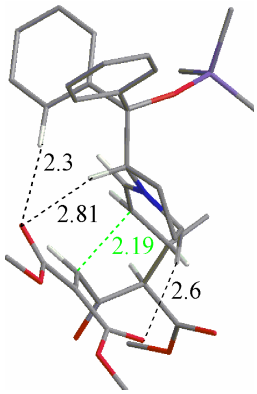

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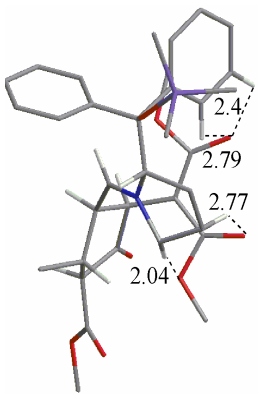

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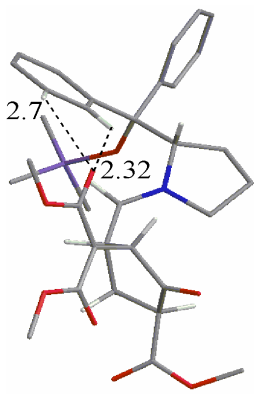

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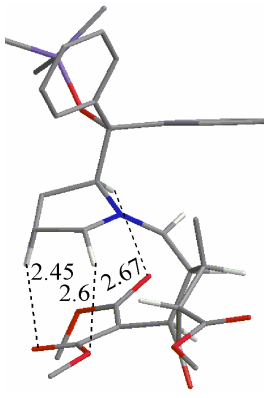

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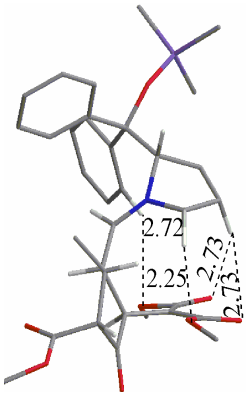

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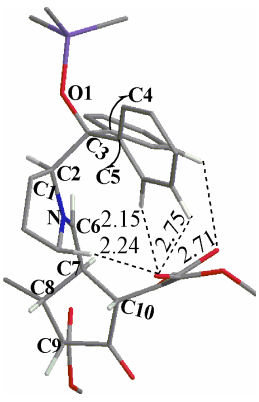

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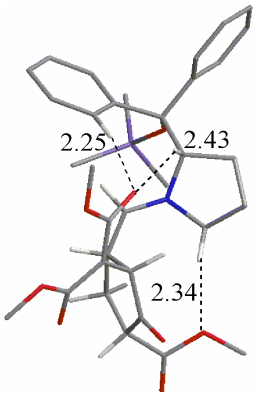

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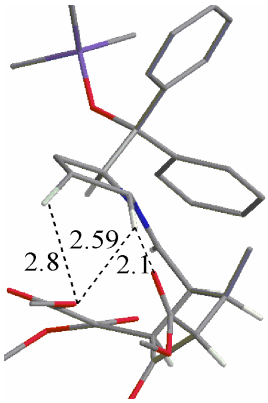

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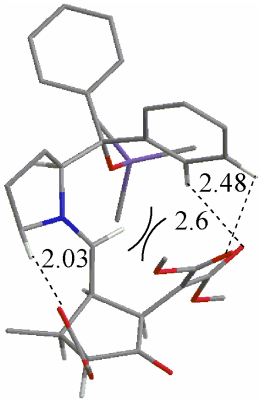

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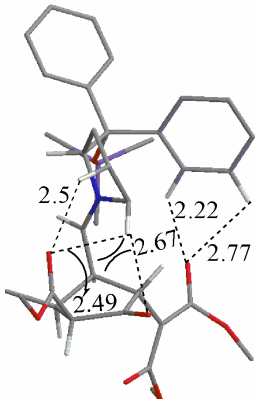

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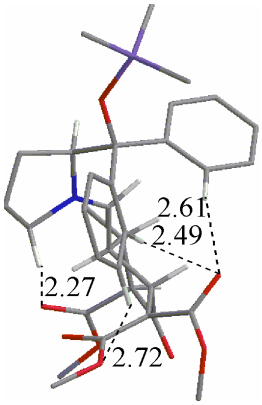

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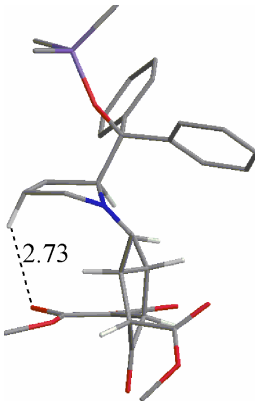

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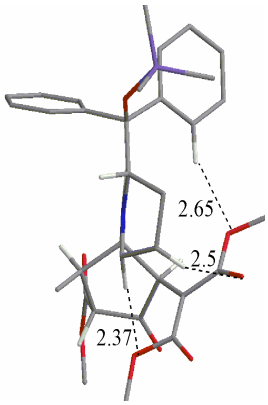

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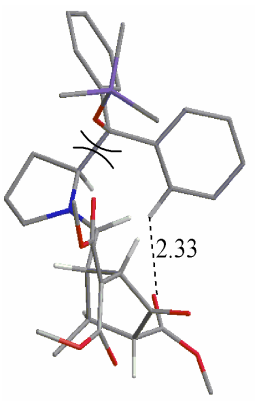

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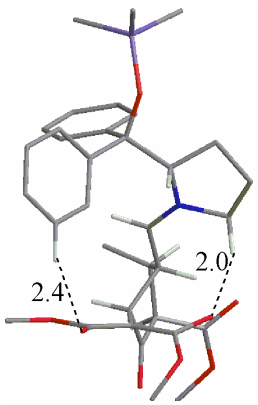

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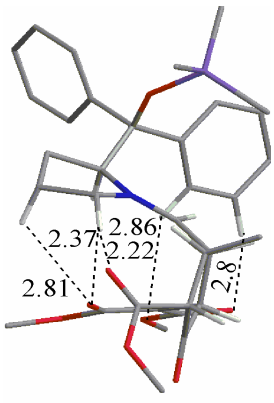

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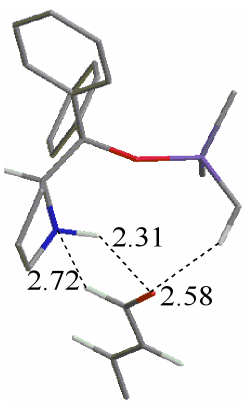
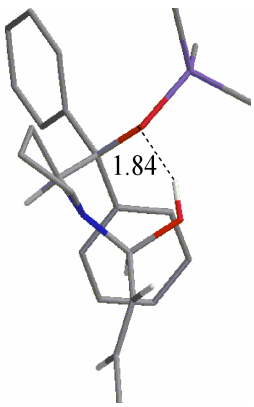
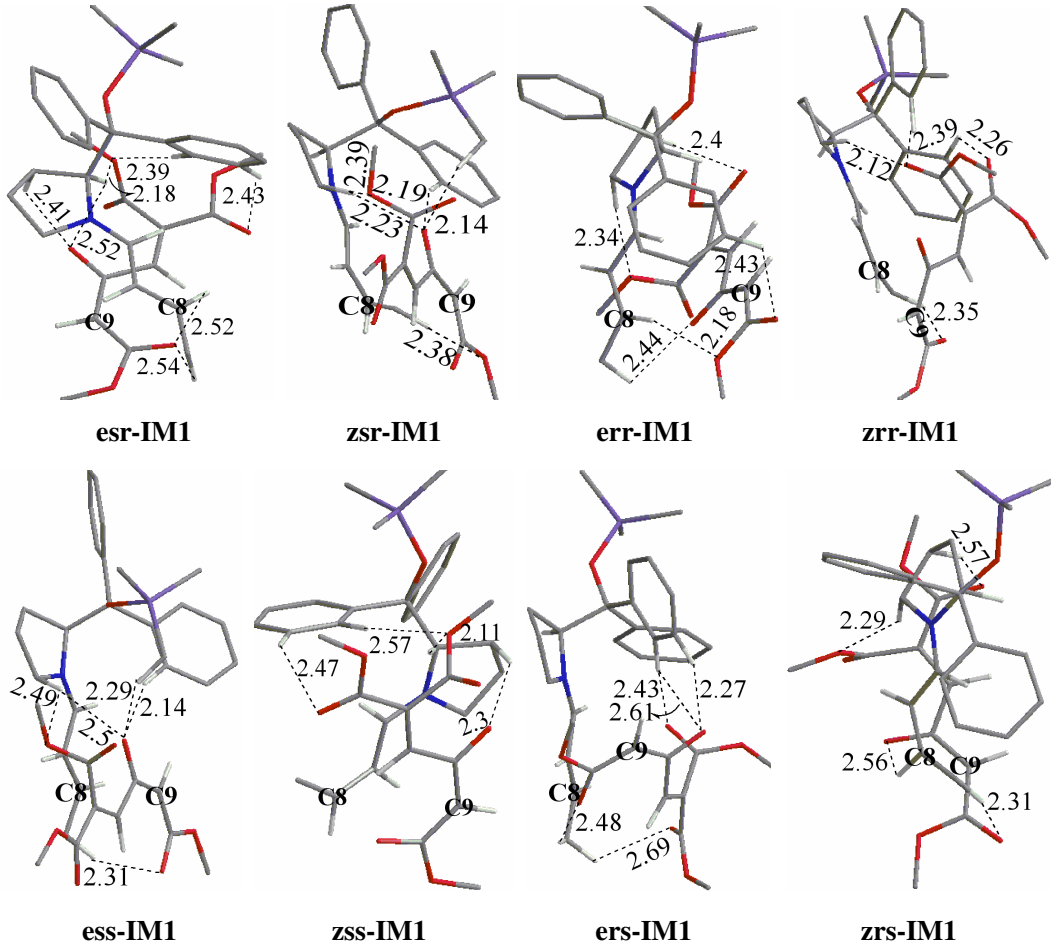


IM0-1



IM0-2

Figure S2. The structures (bond length in Å) of **IM1** optimized by M06-2x in *O*-TMS-protected diphenylprolinol-catalyzed cascade double Michael addition reaction. (Only key hydrogen atoms are left for clarity).



esr-IM1 **zsr-IM1** **err-IM1** **zrr-IM1**

ess-IM1 **zss-IM1** **ers-IM1** **zrs-IM1**

Table S1. Relative energy properties (kcal mol^{-1}) of species in *O*-TMS-protected diphenylprolinol-catalyzed cascade double Michael addition (italic values are real energies (a.u.)).

	ΔE^{CP+ZPE}_{gas}	ΔE^{298}_{PCM}	ΔG^{298}_{PCM}
cat+1+2-H_2O	*-2266.693241*	*-2266.974299*	*-2267.06025*
	0	0	0
ess(zss)-IM2	-9.44(-9.63)	-9.82(-10.02)	-9.36(-9.55)
ssrr(ssrs)-TS2	7.68(11.62)	7.05(10.96)	8.76(12.61)
sssr(ssss)-TS2	3.42(4.74)	3.14(4.41)	5.41(6.19)
ers(zrs)-IM2	-6.64(-6.74)	-6.91(-7.01)	-7.14(-7.24)
rsrr(rsrs)-TS2	15.04(11.86)	14.24(11.19)	16.13(12.9)
rssr(rsss)-TS2	8.93(4.39)	8.57(4.11)	8.83(7.14)
srrr(srrs)-IM3	-6.31(-10.79)	-6.06(-10.53)	-3.17(-6.31)
srsr(srss)-IM3	-4.14(-3.19)	-3.94(-3.04)	-2.42(-2.13)
rrrr(rrrs)-IM3	-4.20(-11.38)	-3.98(-10.8)	-2.88(-5.17)
rrsr(rrss)-IM3	-9.85(-2.26)	-9.56(-2.14)	-3.06(-1.68)
ssrr(ssrs)-IM3	0.92(0.31)	0.97(0.34)	1.29(0.53)
sssr(ssss)-IM3	-1.42(-0.36)	-1.33(-0.32)	-0.64(-0.16)
rsrr(rsrs)-IM3	1.15(0.78)	1.21(0.86)	1.5(1.18)
rssr(rsss)-IM3	0.23(-1.21)	0.28(-1.12)	0.44(-0.55)

Table S2. The selected dihedral angles (°) of **IM1**, **TS1**, **IM2** and **TS2** in pathways of *O*-TMS-protected diphenylprolinol-catalyzed cascade double Michael addition.

	D1 C1-C2-C3-C4	D2 C1-C2-C3-O1	D3 O1-C3-C4-C5	D4 C2-N-C6-C7
esr-IM1	57.36	-58.78	-123.15	-175.94
esr-TS1	58.72	-57.16	-122.92	-175.64
zsr-IM1	-64.55	51.96	123.96	-173.83
zsr-TS1	-63.16	53.6	123.67	-173.49
err-IM1	-177.96	-65.96	120.6	-175.91
err-TS1	-176.11	-64.02	120.15	-176.6
zrr-IM1	51.67	-65.03	-124.67	-173.52
zrr-TS1	53.56	-63.05	-124.14	-172.57
ess-IM1	-60.56	56.03	123.72	-167.39
ess-TS1	-52.12	64.71	122.05	-172.22
zss-IM1	57.76	-58.83	-122.84	-176.87
zss-TS1	69.62	-46.91	-121.03	-171.86
ers-IM1	65.46	-51.28	-122.43	-168.68
ers-TS1	53.65	-63.14	-124.19	-173.65
zrs-IM1	-166.86	-57.98	120.91	-173.23
zrs-TS1	-178.74	-69.93	119.07	-178.28
esr-IM2	-68.53	48.25	122.63	-177.07
srrr-TS2	-42.56	-56.86	120.4	-170.28
srrs-TS2	-67.05	51.48	122.66	-176.41

zsr-IM2	-68.62	48.12	122.6	-177.15
srsr-TS2	-59.32	67.21	122.09	-171.7
srss-TS2	-167.89	-64.02	120.2	-164.37
err-IM2	-174.63	-62.63	119.74	-177.51
rrrr-TS2	-154.24	-35.48	118.52	-170.75
rrrs-IM2	-177.54	-66.48	119.84	-176.53
zrr-IM2	-174.91	-63.19	119.69	-177.68
rrsr-TS2	-167.99	-53.36	120.01	-173.45
rrss-IM2	-66.38	68.16	124.62	-162.51

Cartesian coordinates, energy, and imaginary frequency (transition structures) for all the calculated structures

Structure **IM0-1**

E(RB3LYP) **=** -1428.727826a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.452902	0.027440	-0.939094
2	6	0	0.562749	-0.687585	0.449432
3	7	0	1.768081	-0.143734	1.127187
4	6	0	2.652647	0.394837	0.063543
5	6	0	1.669702	0.984613	-0.985562
6	6	0	3.712940	1.408607	0.608418
7	6	0	4.811357	0.741989	1.464968
8	6	0	4.624922	-0.505873	2.085724
9	6	0	5.627652	-1.056831	2.893640
10	6	0	6.828968	-0.372193	3.104028
11	6	0	7.026023	0.871327	2.491063
12	6	0	6.029378	1.417379	1.676474
13	8	0	2.951713	2.365024	1.399585
14	14	0	3.148808	3.311546	2.861612
15	6	0	1.399032	4.015305	3.104176
16	6	0	4.418498	4.720955	2.603350
17	6	0	3.655301	2.277465	4.384652
18	6	0	0.066913	-0.960151	5.470763
19	6	0	0.405732	-2.187642	5.914383
20	6	0	-0.039386	-2.802212	7.204439
21	6	0	4.342023	2.117869	-0.609524
22	6	0	4.001432	3.435326	-0.943788
23	6	0	4.540478	4.045776	-2.083446
24	6	0	5.421294	3.343070	-2.911573
25	6	0	5.762103	2.023121	-2.589722
26	6	0	5.228652	1.417467	-1.448227

27	1	0	-0.491560	0.571492	-1.044541
28	1	0	0.496974	-0.705266	-1.753798
29	1	0	0.669571	-1.770637	0.310528
30	1	0	-0.313044	-0.517917	1.082927
31	1	0	3.204320	-0.441818	-0.390080
32	1	0	1.383424	1.991082	-0.662325
33	1	0	2.107087	1.059949	-1.984777
34	1	0	3.678688	-1.019473	1.951076
35	1	0	5.466364	-2.024279	3.360531
36	1	0	7.603907	-0.801916	3.731535
37	1	0	7.957026	1.410630	2.637642
38	1	0	6.205196	2.368099	1.184973
39	1	0	1.072755	4.564680	2.215099
40	1	0	1.370155	4.697295	3.962451
41	1	0	0.697008	3.195209	3.284785
42	1	0	5.431590	4.331504	2.462966
43	1	0	4.424339	5.370552	3.487622
44	1	0	4.163349	5.333122	1.732398
45	1	0	3.618969	2.920626	5.273325
46	1	0	4.665540	1.870559	4.292707
47	1	0	2.956677	1.450039	4.534931
48	1	0	-0.582495	-0.303221	6.044487
49	1	0	1.062532	-2.798768	5.291783
50	1	0	-0.577353	-3.742879	7.023914
51	1	0	-0.694444	-2.133945	7.770972
52	1	0	0.824480	-3.054990	7.834330
53	1	0	3.306873	3.970389	-0.309535
54	1	0	4.267426	5.068988	-2.323965
55	1	0	5.838139	3.815560	-3.795631
56	1	0	6.446091	1.467080	-3.223819
57	1	0	5.513823	0.400094	-1.199155
58	6	0	0.563218	-0.455536	4.194962
59	1	0	1.218108	-1.127460	3.614877
60	8	0	0.286497	0.674892	3.740602
61	1	0	1.519020	0.604588	1.776747

Structure **TS0**

Imaginary Frequency: -1597

E(RB3LYP) = -1428.701053a.u.

Standard orientation:

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

1	6	0	0.006716	0.026628	0.009770
2	6	0	0.005082	0.016451	1.556647
3	7	0	1.458630	0.004311	1.929131
4	6	0	2.130317	-0.859447	0.893433
5	6	0	1.468878	-0.309281	-0.394503
6	6	0	3.699591	-0.807846	0.880818
7	6	0	4.380836	-1.722588	1.929859
8	6	0	3.695533	-2.644558	2.737393
9	6	0	4.388199	-3.485679	3.620392
10	6	0	5.780246	-3.422951	3.711043
11	6	0	6.478852	-2.521948	2.897276
12	6	0	5.785958	-1.692919	2.012906
13	8	0	4.061443	0.573229	1.018950
14	14	0	5.013307	1.734184	1.935105
15	6	0	4.102864	3.374169	1.626398
16	6	0	6.754311	1.832416	1.136550
17	6	0	5.148880	1.372954	3.798762
18	6	0	0.664427	-0.439563	4.371779
19	6	0	0.748460	-1.540022	5.135541
20	6	0	-0.317687	-2.024171	6.078056
21	6	0	4.161100	-1.309774	-0.517090
22	6	0	4.661529	-0.414009	-1.471138
23	6	0	5.047444	-0.866613	-2.739064
24	6	0	4.928372	-2.219415	-3.073213
25	6	0	4.426662	-3.120520	-2.125772
26	6	0	4.050711	-2.669942	-0.856517
27	1	0	-0.294932	1.001919	-0.383475
28	1	0	-0.698956	-0.713617	-0.380667
29	1	0	-0.482172	-0.879287	1.958426
30	1	0	-0.456677	0.897081	2.008012
31	1	0	1.808512	-1.899563	1.036399
32	1	0	2.005452	0.593854	-0.698117
33	1	0	1.522681	-1.026651	-1.215109
34	1	0	2.615851	-2.721803	2.697134
35	1	0	3.833374	-4.188894	4.233957
36	1	0	6.315432	-4.072173	4.396360
37	1	0	7.562272	-2.473867	2.942465
38	1	0	6.339999	-1.028822	1.360027
39	1	0	3.910416	3.522335	0.558550
40	1	0	4.704027	4.217004	1.988570
41	1	0	3.152105	3.365348	2.166288
42	1	0	7.367042	0.950397	1.348516
43	1	0	7.280471	2.707695	1.538115
44	1	0	6.685584	1.949063	0.049636

45	1	0	5.781425	2.142888	4.259378
46	1	0	5.586824	0.394897	4.015125
47	1	0	4.141801	1.440003	4.224021
48	1	0	-0.219682	0.194453	4.414291
49	1	0	1.664655	-2.132520	5.104371
50	1	0	-0.639512	-3.044984	5.828936
51	1	0	-1.199549	-1.375126	6.055205
52	1	0	0.052584	-2.055458	7.112002
53	1	0	4.741690	0.632501	-1.208128
54	1	0	5.439062	-0.159761	-3.464388
55	1	0	5.226765	-2.569816	-4.056302
56	1	0	4.337090	-4.174538	-2.370490
57	1	0	3.689772	-3.384403	-0.123074
58	6	0	1.768910	0.056334	3.496371
59	1	0	2.685575	-0.522489	3.647199
60	8	0	1.949678	1.464158	3.491243
61	1	0	1.846820	1.165240	2.167575

Structure **IM0-2**

E(RB3LYP) **=** -1428.721197a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.135828	0.595235	0.447434
2	6	0	0.054126	0.877172	1.940682
3	7	0	1.392603	0.317401	2.216476
4	6	0	2.219062	0.218243	0.978344
5	6	0	1.282977	0.817839	-0.101921
6	6	0	3.677565	0.870545	1.001588
7	6	0	4.590477	0.110535	1.997668
8	6	0	4.620574	-1.300093	2.025593
9	6	0	5.454649	-1.991557	2.909653
10	6	0	6.282210	-1.291081	3.793896
11	6	0	6.260259	0.105517	3.781650
12	6	0	5.424213	0.794712	2.895068
13	8	0	3.502673	2.247857	1.444263
14	14	0	4.242605	3.839875	1.304583
15	6	0	3.110128	4.958458	0.249508
16	6	0	6.020382	3.801638	0.606441
17	6	0	4.232675	4.507598	3.091144
18	6	0	0.905464	-0.004927	4.614175
19	6	0	0.863362	-1.219478	5.174770

20	6	0	-0.125439	-1.654442	6.221767
21	6	0	4.287309	0.831742	-0.430892
22	6	0	3.899133	1.787716	-1.391048
23	6	0	4.415345	1.772622	-2.689766
24	6	0	5.339211	0.793439	-3.071148
25	6	0	5.737930	-0.161497	-2.133382
26	6	0	5.221718	-0.140494	-0.831360
27	1	0	-0.876168	1.252076	-0.020702
28	1	0	-0.454868	-0.443118	0.295059
29	1	0	-0.697584	0.380687	2.562762
30	1	0	0.005411	1.958954	2.150162
31	1	0	2.393654	-0.840624	0.736818
32	1	0	1.460809	1.895235	-0.171958
33	1	0	1.444775	0.374679	-1.087273
34	1	0	3.985467	-1.873158	1.359809
35	1	0	5.451288	-3.077158	2.908772
36	1	0	6.926496	-1.825725	4.484274
37	1	0	6.885429	0.666171	4.469433
38	1	0	5.410151	1.873544	2.928984
39	1	0	3.178517	4.745980	-0.821266
40	1	0	3.397496	6.005676	0.404373
41	1	0	2.066197	4.845937	0.561035
42	1	0	6.650055	3.090065	1.149381
43	1	0	6.462612	4.799792	0.714543
44	1	0	6.033988	3.528432	-0.451745
45	1	0	4.526480	5.564203	3.091522
46	1	0	4.923160	3.962871	3.742534
47	1	0	3.234190	4.427314	3.533262
48	1	0	0.205519	0.771578	4.917895
49	1	0	1.594467	-1.969238	4.866432
50	1	0	-0.718635	-2.514613	5.880655
51	1	0	-0.819353	-0.846015	6.477128
52	1	0	0.382068	-1.968359	7.144582
53	1	0	3.183138	2.551424	-1.125398
54	1	0	4.092766	2.525680	-3.402380
55	1	0	5.741788	0.778934	-4.078891
56	1	0	6.460133	-0.924940	-2.405764
57	1	0	5.572353	-0.881552	-0.126581
58	6	0	1.909867	0.411659	3.567175
59	1	0	2.786898	-0.236376	3.634590
60	8	0	2.293342	1.787154	3.919851
61	1	0	2.776212	2.140604	3.134836

Structure **esr-IM1**

E(RB3LYP) = -2266.974761a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.187440	0.272459	0.245709
2	6	0	0.021447	0.153548	1.762880
3	7	0	1.502455	0.065560	1.941345
4	6	0	2.232386	-0.034054	0.629320
5	6	0	1.095031	-0.333356	-0.367775
6	6	0	3.109092	1.248291	0.287564
7	6	0	4.290685	1.400822	1.275827
8	6	0	5.047601	0.265525	1.636613
9	6	0	6.132312	0.364594	2.515027
10	6	0	6.510387	1.612779	3.025162
11	6	0	5.799947	2.754052	2.641653
12	6	0	4.700981	2.649086	1.778831
13	6	0	2.215147	2.498733	0.192876
14	6	0	1.683469	3.115556	1.343662
15	6	0	0.814432	4.206892	1.238433
16	6	0	0.455672	4.706212	-0.019343
17	6	0	0.976428	4.102853	-1.168157
18	6	0	1.845104	3.009697	-1.061301
19	8	0	3.615250	0.910043	-1.031557
20	14	0	5.089855	1.248226	-1.935086
21	6	0	4.522158	0.916001	-3.723647
22	6	0	6.495311	0.050942	-1.455513
23	6	0	5.649363	3.066132	-1.750745
24	6	0	2.065308	-0.101900	3.121580
25	6	0	1.409260	-0.016812	4.379705
26	6	0	2.093790	-0.293465	5.529874
27	6	0	0.952850	-3.351096	3.479418
28	6	0	1.911246	-3.307244	2.434701
29	6	0	3.367463	-3.366978	2.752329
30	6	0	4.301959	-3.595413	1.803656
31	6	0	3.966847	-3.909717	0.376309
32	8	0	3.730404	-5.023114	-0.086626
33	8	0	4.062144	-2.772748	-0.410350
34	6	0	3.642380	-2.934924	-1.810116
35	6	0	5.733312	-3.569955	2.169444
36	8	0	6.211572	-3.110788	3.220139
37	8	0	6.523279	-4.099157	1.174663
38	6	0	7.968250	-4.139282	1.424798

39	8	0	1.570201	-3.225768	1.197085
40	6	0	1.199024	-3.246171	4.872677
41	8	0	2.273214	-2.915257	5.452011
42	8	0	0.110530	-3.425129	5.757061
43	6	0	-1.138111	-4.013900	5.298978
44	1	0	-0.307091	1.319814	-0.043092
45	1	0	-1.082595	-0.270517	-0.070210
46	1	0	-0.404435	-0.771122	2.170045
47	1	0	-0.372040	1.009072	2.319019
48	1	0	2.903819	-0.889788	0.668886
49	1	0	1.325759	0.062749	-1.356704
50	1	0	0.997264	-1.421086	-0.428639
51	1	0	4.803122	-0.705900	1.222730
52	1	0	6.663675	-0.536006	2.805125
53	1	0	7.349668	1.692514	3.708524
54	1	0	6.092566	3.730211	3.015907
55	1	0	4.165254	3.547456	1.500109
56	1	0	1.957801	2.755475	2.328584
57	1	0	0.423586	4.669706	2.139503
58	1	0	-0.216719	5.554220	-0.100438
59	1	0	0.706283	4.478592	-2.150216
60	1	0	2.232400	2.532166	-1.951330
61	1	0	3.713304	1.595780	-4.011416
62	1	0	4.157303	-0.110183	-3.834427
63	1	0	5.354631	1.059379	-4.422608
64	1	0	6.105677	-0.957869	-1.285562
65	1	0	7.006381	0.374305	-0.544317
66	1	0	7.230778	0.008118	-2.268271
67	1	0	6.474342	3.261048	-2.447164
68	1	0	6.001463	3.278173	-0.737169
69	1	0	4.834275	3.758591	-1.984542
70	1	0	3.131291	-0.300958	3.120031
71	1	0	0.349663	0.211722	4.423085
72	1	0	-0.064493	-3.479249	3.131481
73	1	0	3.671482	-3.220193	3.784351
74	1	0	3.635709	-1.924736	-2.213972
75	1	0	2.646628	-3.381123	-1.840177
76	1	0	4.347938	-3.575907	-2.343580
77	1	0	8.385195	-4.644795	0.556238
78	1	0	8.176105	-4.693311	2.342479
79	1	0	8.364356	-3.125106	1.517353
80	1	0	-1.708438	-4.219409	6.205687
81	1	0	-0.961880	-4.945607	4.751724
82	1	0	-1.703591	-3.321863	4.663211

83	6	0	1.500141	-0.276130	6.895923
84	1	0	0.456783	0.052133	6.893266
85	1	0	1.546520	-1.294890	7.299675
86	1	0	2.077418	0.371735	7.568994
87	1	0	3.150384	-0.539472	5.465098

Structure **esr-TS1**

Imaginary Frequency: -235

E(RB3LYP) **=** -2266.972737a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.074349	0.108267	-0.057369
2	6	0	-0.096764	0.046398	1.478208
3	7	0	1.336056	0.039433	1.870762
4	6	0	2.259052	-0.123426	0.710974
5	6	0	1.298801	-0.486815	-0.445143
6	6	0	3.198706	1.119215	0.407589
7	6	0	4.227868	1.359582	1.537986
8	6	0	4.920176	0.270538	2.110261
9	6	0	5.893671	0.472213	3.095415
10	6	0	6.216112	1.766771	3.518397
11	6	0	5.561044	2.857111	2.938700
12	6	0	4.579805	2.655248	1.959965
13	6	0	2.347933	2.357721	0.080434
14	6	0	1.625201	3.030365	1.086823
15	6	0	0.799669	4.115056	0.773478
16	6	0	0.678390	4.552084	-0.551496
17	6	0	1.392692	3.893852	-1.557067
18	6	0	2.217867	2.806486	-1.242813
19	8	0	3.887354	0.669730	-0.792412
20	14	0	5.500645	0.798871	-1.475552
21	6	0	5.173676	0.339914	-3.295899
22	6	0	6.697871	-0.466027	-0.695757
23	6	0	6.192385	2.574696	-1.346672
24	6	0	1.717047	-0.137337	3.144040
25	6	0	0.902870	-0.153635	4.270032
26	6	0	1.455559	-0.519360	5.514266
27	6	0	1.425137	-2.782761	5.675541
28	6	0	1.320512	-3.124852	4.282098
29	6	0	2.539468	-3.332351	3.452509
30	6	0	2.489571	-3.892966	2.225821

31	6	0	1.264519	-4.557534	1.670899
32	8	0	0.827535	-5.653180	2.020718
33	8	0	0.719942	-3.821568	0.642196
34	6	0	-0.501946	-4.377296	0.039780
35	6	0	3.707675	-3.910615	1.383968
36	8	0	4.669269	-3.129180	1.486460
37	8	0	3.658218	-4.896190	0.434529
38	6	0	4.804975	-5.010270	-0.477307
39	8	0	0.190041	-3.129242	3.699617
40	6	0	2.640643	-2.913923	6.461727
41	8	0	3.800488	-2.716577	6.048757
42	8	0	2.509655	-3.163486	7.835133
43	6	0	1.294935	-3.759472	8.388370
44	1	0	-0.160223	1.142945	-0.399960
45	1	0	-0.903667	-0.459202	-0.490239
46	1	0	-0.550490	-0.879675	1.856669
47	1	0	-0.610269	0.900941	1.931239
48	1	0	2.926940	-0.962115	0.914673
49	1	0	1.675027	-0.115882	-1.398353
50	1	0	1.229181	-1.577728	-0.499499
51	1	0	4.726289	-0.748881	1.793986
52	1	0	6.395112	-0.387150	3.528335
53	1	0	6.968839	1.921428	4.284689
54	1	0	5.808402	3.868655	3.245736
55	1	0	4.089686	3.516295	1.523897
56	1	0	1.712946	2.712923	2.119340
57	1	0	0.255645	4.620838	1.565405
58	1	0	0.038865	5.395024	-0.793580
59	1	0	1.308696	4.222524	-2.588495
60	1	0	2.758147	2.287524	-2.023500
61	1	0	4.504948	1.064891	-3.771730
62	1	0	4.704857	-0.647418	-3.361991
63	1	0	6.111604	0.315120	-3.863134
64	1	0	6.190253	-1.416793	-0.500898
65	1	0	7.102918	-0.106119	0.253920
66	1	0	7.533830	-0.651497	-1.381481
67	1	0	7.125473	2.646921	-1.918929
68	1	0	6.404201	2.847466	-0.308898
69	1	0	5.482942	3.301960	-1.755204
70	1	0	2.781634	-0.291144	3.286076
71	1	0	-0.166530	0.007062	4.187119
72	1	0	0.473120	-2.845272	6.187439
73	1	0	3.487362	-2.978782	3.846509
74	1	0	-0.760619	-3.683716	-0.758166

75	1	0	-1.290314	-4.427185	0.793511
76	1	0	-0.307112	-5.377184	-0.353144
77	1	0	4.580911	-5.878184	-1.093490
78	1	0	5.724294	-5.155218	0.093226
79	1	0	4.890534	-4.106502	-1.084908
80	1	0	1.577357	-4.097361	9.385421
81	1	0	0.961778	-4.610501	7.787216
82	1	0	0.486999	-3.024903	8.468550
83	6	0	0.743132	-0.201330	6.805178
84	1	0	-0.328090	-0.420400	6.740593
85	1	0	1.171199	-0.747398	7.649353
86	1	0	0.846192	0.872559	7.021851
87	1	0	2.542223	-0.558116	5.573251

Structure **esr-IM2**

E(RB3LYP) **=** -2266.994872a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.349019	0.520341	0.180250
2	6	0	-0.396261	0.059524	1.646733
3	7	0	1.013837	-0.218800	1.992188
4	6	0	1.918709	-0.204952	0.820296
5	6	0	0.938965	-0.126757	-0.376156
6	6	0	3.015670	0.945045	0.819849
7	6	0	4.071148	0.734086	1.931616
8	6	0	4.623478	-0.547193	2.144402
9	6	0	5.625829	-0.752002	3.098774
10	6	0	6.114234	0.319905	3.855041
11	6	0	5.592987	1.598713	3.640501
12	6	0	4.585632	1.802374	2.688687
13	6	0	2.335414	2.321312	0.870496
14	6	0	1.707896	2.775741	2.048787
15	6	0	1.029116	3.998441	2.073762
16	6	0	0.960716	4.794183	0.923476
17	6	0	1.578187	4.353224	-0.250672
18	6	0	2.256108	3.127680	-0.275831
19	8	0	3.651218	0.749375	-0.477855
20	14	0	5.234443	1.031131	-1.178825
21	6	0	4.823656	1.217447	-3.030994
22	6	0	6.364830	-0.486650	-0.935311
23	6	0	6.075716	2.615394	-0.520411

24	6	0	1.342740	-0.789870	3.194948
25	6	0	0.498721	-1.050149	4.231932
26	6	0	0.965013	-1.758605	5.486074
27	6	0	0.167284	-3.089792	5.662957
28	6	0	-0.158318	-3.745996	4.306731
29	6	0	0.917400	-3.820412	3.299368
30	6	0	0.730383	-4.218243	2.019516
31	6	0	-0.584453	-4.689127	1.477146
32	8	0	-0.910207	-5.866696	1.333934
33	8	0	-1.374177	-3.627843	1.109189
34	6	0	-2.729452	-3.963428	0.641977
35	6	0	1.881308	-4.162524	1.094633
36	8	0	2.997756	-3.687081	1.368505
37	8	0	1.572278	-4.659312	-0.143337
38	6	0	2.641878	-4.655249	-1.151984
39	8	0	-1.296491	-4.220494	4.097176
40	6	0	0.937013	-4.089630	6.538202
41	8	0	2.168483	-4.117669	6.579766
42	8	0	0.234060	-5.014574	7.272745
43	6	0	-1.237173	-5.055892	7.318121
44	1	0	-0.287586	1.610475	0.122932
45	1	0	-1.239962	0.204001	-0.370941
46	1	0	-0.984513	-0.862198	1.768087
47	1	0	-0.812481	0.823172	2.315079
48	1	0	2.476914	-1.143602	0.778183
49	1	0	1.374127	0.421898	-1.211540
50	1	0	0.723883	-1.146498	-0.718315
51	1	0	4.280100	-1.401971	1.572902
52	1	0	6.020395	-1.751741	3.249793
53	1	0	6.889347	0.159103	4.597460
54	1	0	5.966391	2.443137	4.211662
55	1	0	4.201369	2.803091	2.538038
56	1	0	1.748892	2.172681	2.947888
57	1	0	0.555678	4.329231	2.993224
58	1	0	0.434878	5.743596	0.944416
59	1	0	1.531066	4.958484	-1.150982
60	1	0	2.714026	2.780529	-1.192713
61	1	0	4.206750	2.103565	-3.214205
62	1	0	4.272780	0.341222	-3.388433
63	1	0	5.742172	1.311837	-3.622259
64	1	0	5.852442	-1.401934	-1.250738
65	1	0	6.667317	-0.606742	0.108461
66	1	0	7.268337	-0.373272	-1.547136
67	1	0	6.980810	2.813129	-1.107911

68	1	0	6.362504	2.512046	0.529763
69	1	0	5.412558	3.481708	-0.611609
70	1	0	2.385937	-1.074699	3.283770
71	1	0	-0.546800	-0.752367	4.190880
72	1	0	-0.803517	-2.865169	6.114665
73	1	0	1.921169	-3.553131	3.607926
74	1	0	-3.164186	-3.011650	0.343559
75	1	0	-3.292695	-4.416428	1.460454
76	1	0	-2.676922	-4.658225	-0.198375
77	1	0	2.198024	-5.129372	-2.024407
78	1	0	3.500793	-5.221761	-0.787029
79	1	0	2.946548	-3.629365	-1.370415
80	1	0	-1.461415	-5.982429	7.843949
81	1	0	-1.666829	-5.070598	6.315400
82	1	0	-1.622898	-4.205761	7.889191
83	6	0	0.839005	-0.888538	6.754996
84	1	0	-0.202159	-0.581144	6.918177
85	1	0	1.185383	-1.427749	7.644915
86	1	0	1.443530	0.018267	6.650503
87	1	0	2.021837	-2.029218	5.372117

Structure **zsr-IM1**

E(RB3LYP) **=** -2266.972419a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.296101	-0.616257	0.355969
2	6	0	0.526252	-0.762478	1.868657
3	7	0	1.994777	-0.549677	2.043258
4	6	0	2.683932	-0.229677	0.758658
5	6	0	1.692263	-0.817636	-0.274307
6	6	0	3.029817	1.305867	0.488965
7	6	0	3.874562	1.949207	1.617583
8	6	0	3.259586	2.223989	2.859646
9	6	0	3.971909	2.860701	3.883949
10	6	0	5.307117	3.235364	3.699351
11	6	0	5.922956	2.978303	2.471596
12	6	0	5.213166	2.348916	1.441589
13	8	0	1.762518	1.982018	0.374789
14	14	0	1.219822	3.670598	0.495314
15	6	0	-0.205971	3.699358	-0.773235
16	6	0	2.603067	4.891465	-0.015010

17	6	0	0.555360	4.118040	2.218214
18	6	0	2.610758	-0.707854	3.198963
19	6	0	1.972764	-1.133828	4.391648
20	6	0	3.761795	1.279251	-0.878989
21	6	0	3.218434	1.925892	-1.998752
22	6	0	3.848863	1.862139	-3.247693
23	6	0	5.031901	1.135298	-3.407092
24	6	0	5.575824	0.466196	-2.305028
25	6	0	4.945416	0.534179	-1.058471
26	6	0	2.565684	-1.139907	5.625047
27	6	0	3.964842	-0.755140	5.988783
28	6	0	1.277321	1.399840	6.347231
29	6	0	1.306394	1.328351	7.777022
30	8	0	0.383964	1.138157	8.601444
31	8	0	2.636210	1.476390	8.245811
32	6	0	2.795135	1.461297	9.699301
33	6	0	0.161578	1.275603	5.499104
34	8	0	0.280235	1.326011	4.205427
35	6	0	-1.178510	1.023391	6.080347
36	6	0	-2.328616	1.042348	5.372732
37	6	0	-2.455379	1.438586	3.935343
38	8	0	-2.524458	2.591511	3.505338
39	8	0	-2.622382	0.333250	3.120195
40	6	0	-3.004606	0.621653	1.732760
41	6	0	-3.593420	0.723570	6.073908
42	8	0	-3.704189	0.321578	7.239725
43	8	0	-4.690982	0.930089	5.261158
44	6	0	-6.003339	0.659174	5.856444
45	1	0	-0.062120	0.386246	0.123425
46	1	0	-0.428457	-1.348895	-0.011504
47	1	0	0.285035	-1.773123	2.219218
48	1	0	-0.001730	-0.038708	2.498494
49	1	0	3.633928	-0.769184	0.759934
50	1	0	1.782946	-0.334707	-1.246450
51	1	0	1.905558	-1.886100	-0.404890
52	1	0	2.221376	1.963745	3.043297
53	1	0	3.471147	3.074594	4.822160
54	1	0	5.852521	3.732292	4.495315
55	1	0	6.951845	3.280380	2.301835
56	1	0	5.707978	2.201103	0.491671
57	1	0	-0.672364	4.691352	-0.790626
58	1	0	-0.976462	2.971853	-0.496331
59	1	0	0.138017	3.464378	-1.785934
60	1	0	2.183728	5.905388	-0.026977

61	1	0	3.005993	4.675902	-1.008954
62	1	0	3.429747	4.876928	0.701793
63	1	0	-0.147493	4.954119	2.113963
64	1	0	1.361811	4.429324	2.888125
65	1	0	0.023212	3.290246	2.696633
66	1	0	3.677254	-0.513735	3.197951
67	1	0	0.922111	-1.387100	4.337385
68	1	0	2.286098	2.462436	-1.895809
69	1	0	3.406982	2.375462	-4.095990
70	1	0	5.519712	1.083891	-4.375002
71	1	0	6.489287	-0.110246	-2.413022
72	1	0	5.394437	0.009579	-0.220929
73	1	0	1.961634	-1.502793	6.452637
74	1	0	3.931932	-0.017587	6.801584
75	1	0	4.536487	-0.325214	5.162582
76	1	0	4.510549	-1.628826	6.373319
77	1	0	2.218914	1.629822	5.870861
78	1	0	3.859706	1.621752	9.869164
79	1	0	2.473280	0.503549	10.116951
80	1	0	2.203798	2.257101	10.158828
81	1	0	-1.229482	0.810559	7.144751
82	1	0	-3.125387	-0.354915	1.266283
83	1	0	-2.226949	1.204268	1.233802
84	1	0	-3.941392	1.183422	1.713251
85	1	0	-6.719756	0.902138	5.073991
86	1	0	-6.154208	1.286186	6.737919
87	1	0	-6.076824	-0.391538	6.146543

Structure **zsr-TS1**

Imaginary Frequency: -217

E(RB3LYP) = -2266.97057 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.537969
3	7	0	1.437389	0.000000	1.910190
4	6	0	2.341146	0.020307	0.734417
5	6	0	1.406606	-0.511885	-0.382296
6	6	0	3.017922	1.419186	0.362306
7	6	0	3.851815	2.022600	1.521270
8	6	0	3.177396	2.541729	2.646880

9	6	0	3.884089	3.145166	3.693630
10	6	0	5.278709	3.246968	3.646642
11	6	0	5.958725	2.747855	2.532375
12	6	0	5.253702	2.149382	1.480470
13	8	0	1.927955	2.310511	0.032729
14	14	0	1.730933	4.067206	-0.065641
15	6	0	0.437890	4.225444	-1.461420
16	6	0	3.359505	4.945323	-0.551069
17	6	0	1.040385	4.844663	1.529723
18	6	0	1.839425	-0.120577	3.183956
19	6	0	0.987175	-0.266541	4.273349
20	6	0	3.868588	1.108789	-0.895068
21	6	0	3.585160	1.709774	-2.130795
22	6	0	4.321552	1.389244	-3.278079
23	6	0	5.350882	0.445689	-3.217957
24	6	0	5.631336	-0.180860	-1.998682
25	6	0	4.896229	0.143720	-0.853995
26	6	0	1.399772	-0.214527	5.617075
27	6	0	2.838808	-0.335583	6.059213
28	6	0	0.992680	1.951081	6.241975
29	6	0	0.847644	1.803976	7.676527
30	8	0	-0.174333	1.519688	8.336193
31	8	0	2.082123	1.949395	8.319376
32	6	0	2.064830	1.812878	9.779631
33	6	0	-0.073345	2.279799	5.336408
34	8	0	0.181204	2.529825	4.108348
35	6	0	-1.484386	2.229152	5.787711
36	6	0	-2.532027	2.579948	5.011798
37	6	0	-2.436123	3.159793	3.633699
38	8	0	-2.271465	4.351287	3.368678
39	8	0	-2.678534	2.204043	2.669339
40	6	0	-2.803529	2.704265	1.292782
41	6	0	-3.898959	2.456303	5.576583
42	8	0	-4.189378	1.983690	6.682920
43	8	0	-4.850531	2.942419	4.707303
44	6	0	-6.244464	2.888773	5.163410
45	1	0	-0.132067	1.013408	-0.380035
46	1	0	-0.793251	-0.637036	-0.403068
47	1	0	-0.466688	-0.908291	1.941767
48	1	0	-0.494619	0.865108	1.990722
49	1	0	3.161453	-0.676167	0.930180
50	1	0	1.714708	-0.180470	-1.373240
51	1	0	1.430568	-1.608832	-0.369291
52	1	0	2.098577	2.493496	2.724185

53	1	0	3.332019	3.547618	4.536576
54	1	0	5.823481	3.718568	4.458385
55	1	0	7.039065	2.834338	2.467526
56	1	0	5.809106	1.807034	0.618289
57	1	0	0.181142	5.279171	-1.621608
58	1	0	-0.480300	3.689675	-1.197058
59	1	0	0.807594	3.814910	-2.406860
60	1	0	3.161416	6.019220	-0.657639
61	1	0	3.764113	4.575127	-1.497342
62	1	0	4.123822	4.817345	0.221458
63	1	0	0.523919	5.776888	1.268106
64	1	0	1.843183	5.085325	2.232181
65	1	0	0.327222	4.203306	2.055489
66	1	0	2.912800	-0.103174	3.332243
67	1	0	-0.079452	-0.302708	4.088720
68	1	0	2.767605	2.413186	-2.200617
69	1	0	4.081219	1.873066	-4.219754
70	1	0	5.920809	0.195681	-4.106938
71	1	0	6.420542	-0.923651	-1.935905
72	1	0	5.139290	-0.355992	0.078215
73	1	0	0.667184	-0.536567	6.352816
74	1	0	2.977776	0.074835	7.061620
75	1	0	3.529446	0.187644	5.391277
76	1	0	3.129369	-1.396210	6.085266
77	1	0	1.978039	2.249849	5.909690
78	1	0	3.101442	1.948176	10.084550
79	1	0	1.693774	0.827424	10.071021
80	1	0	1.423552	2.577277	10.224375
81	1	0	-1.680721	1.887426	6.799562
82	1	0	-3.046491	1.825642	0.697722
83	1	0	-1.864274	3.155790	0.966457
84	1	0	-3.600646	3.449100	1.238963
85	1	0	-6.819703	3.326351	4.350029
86	1	0	-6.360693	3.464841	6.083920
87	1	0	-6.541055	1.853465	5.345773

Structure **zsr-IM2**

E(RB3LYP) **=** -2266.994984a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000

2	6	0	0.000000	0.000000	1.545162
3	7	0	1.422966	0.000000	1.918217
4	6	0	2.329472	0.062045	0.767729
5	6	0	1.430952	-0.438291	-0.391803
6	6	0	3.003475	1.476443	0.449009
7	6	0	3.642163	2.132343	1.695888
8	6	0	2.803788	2.526761	2.759555
9	6	0	3.316711	3.156021	3.898294
10	6	0	4.688098	3.421770	3.995913
11	6	0	5.531540	3.056801	2.942629
12	6	0	5.014857	2.421031	1.805797
13	8	0	1.928039	2.326240	-0.037928
14	14	0	1.686193	4.059448	-0.190666
15	6	0	0.752504	4.232001	-1.847243
16	6	0	3.317026	5.052675	-0.231009
17	6	0	0.544105	4.688311	1.203669
18	6	0	1.840002	-0.346661	3.188348
19	6	0	1.051270	-0.476384	4.281130
20	6	0	4.018033	1.197595	-0.681289
21	6	0	3.858409	1.750517	-1.960932
22	6	0	4.755240	1.455419	-2.995315
23	6	0	5.828507	0.587671	-2.774902
24	6	0	5.991964	0.012393	-1.509567
25	6	0	5.095783	0.310831	-0.478309
26	6	0	1.557658	-0.839015	5.658328
27	6	0	2.875597	-1.638725	5.663444
28	6	0	1.737232	0.470487	6.556392
29	6	0	2.114618	0.085544	7.968776
30	8	0	1.456695	-0.648687	8.720296
31	8	0	3.317092	0.632723	8.337741
32	6	0	3.801182	0.315492	9.692841
33	6	0	0.471860	1.321705	6.513632
34	8	0	0.466102	2.401845	5.887484
35	6	0	-0.747936	0.798886	7.173241
36	6	0	-1.983409	1.289875	6.945566
37	6	0	-2.273904	2.450285	6.041518
38	8	0	-2.519168	3.591905	6.431040
39	8	0	-2.283477	2.065564	4.727857
40	6	0	-2.493947	3.137366	3.741124
41	6	0	-3.133505	0.674160	7.663447
42	8	0	-3.047563	-0.210523	8.523671
43	8	0	-4.326978	1.194377	7.238152
44	6	0	-5.543615	0.676124	7.880808
45	1	0	-0.189195	1.004605	-0.381550

46	1	0	-0.762143	-0.675319	-0.402148
47	1	0	-0.476984	-0.899598	1.963080
48	1	0	-0.526202	0.869191	1.963230
49	1	0	3.160755	-0.628997	0.946730
50	1	0	1.734271	-0.040327	-1.360686
51	1	0	1.495258	-1.532479	-0.437625
52	1	0	1.742590	2.332403	2.701472
53	1	0	2.638150	3.420386	4.702879
54	1	0	5.090451	3.910669	4.877702
55	1	0	6.594856	3.270712	2.995565
56	1	0	5.690580	2.170901	0.998748
57	1	0	0.442090	5.272724	-1.999612
58	1	0	-0.144948	3.604152	-1.846440
59	1	0	1.371840	3.934577	-2.699825
60	1	0	3.094746	6.096626	-0.484674
61	1	0	4.005387	4.656564	-0.984115
62	1	0	3.823257	5.033364	0.737853
63	1	0	0.187094	5.696311	0.959690
64	1	0	1.062471	4.728161	2.165115
65	1	0	-0.327533	4.033006	1.307482
66	1	0	2.910335	-0.515023	3.261293
67	1	0	-0.007118	-0.238783	4.210623
68	1	0	3.012804	2.395934	-2.153112
69	1	0	4.606929	1.899666	-3.974899
70	1	0	6.523381	0.357204	-3.576097
71	1	0	6.815729	-0.669776	-1.323025
72	1	0	5.249902	-0.143186	0.495330
73	1	0	0.796753	-1.447470	6.166776
74	1	0	3.125877	-1.981091	6.673036
75	1	0	3.715463	-1.037182	5.297055
76	1	0	2.779225	-2.520508	5.022064
77	1	0	2.538731	1.072604	6.126213
78	1	0	4.738967	0.859034	9.784419
79	1	0	3.955950	-0.760828	9.793540
80	1	0	3.075321	0.648250	10.437342
81	1	0	-0.634187	-0.023212	7.873713
82	1	0	-2.566600	2.623212	2.784831
83	1	0	-1.641776	3.819833	3.759764
84	1	0	-3.410778	3.684387	3.968975
85	1	0	-6.357869	1.221536	7.409251
86	1	0	-5.507563	0.868392	8.955009
87	1	0	-5.629812	-0.398292	7.705603

Structure **esr-IM1** (M06-2x)

E(RB3LYP) = -2265.704653 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.062855	-0.104847	0.062199
2	6	0	-0.033275	-0.129124	1.589144
3	7	0	1.408226	-0.115069	1.935212
4	6	0	2.283193	-0.308064	0.741237
5	6	0	1.286859	-0.714041	-0.347271
6	6	0	3.170033	0.947181	0.409338
7	6	0	4.135873	1.224396	1.569564
8	6	0	4.970087	0.174770	1.997246
9	6	0	5.844350	0.343524	3.069975
10	6	0	5.921725	1.577723	3.720583
11	6	0	5.134249	2.637831	3.277159
12	6	0	4.249235	2.463047	2.210534
13	6	0	2.288562	2.134262	0.030693
14	6	0	1.466946	2.774379	0.975160
15	6	0	0.593836	3.791055	0.591743
16	6	0	0.521643	4.191231	-0.743504
17	6	0	1.334189	3.567397	-1.687866
18	6	0	2.207316	2.548440	-1.302735
19	8	0	3.907615	0.496320	-0.735390
20	14	0	5.537466	0.844102	-1.276706
21	6	0	5.360005	0.652279	-3.150124
22	6	0	6.797229	-0.415387	-0.624840
23	6	0	6.045936	2.613488	-0.822769
24	6	0	1.843454	-0.129527	3.175926
25	6	0	1.065114	0.055256	4.344196
26	6	0	1.670552	-0.043365	5.561618
27	6	0	0.943533	-3.181586	3.603695
28	6	0	2.019450	-3.261138	2.691096
29	6	0	3.423985	-3.214995	3.178501
30	6	0	4.460359	-3.402180	2.339683
31	6	0	4.293565	-3.777163	0.905608
32	8	0	4.241070	-4.915177	0.458355
33	8	0	4.312137	-2.656526	0.113377
34	6	0	3.956401	-2.851905	-1.281967
35	6	0	5.833846	-3.206172	2.820660
36	8	0	6.173439	-2.857783	3.956604
37	8	0	6.738908	-3.388301	1.811571
38	6	0	8.130745	-3.118394	2.118841

39	8	0	1.830244	-3.336297	1.427968
40	6	0	1.021988	-2.914962	4.991134
41	8	0	2.036771	-2.620090	5.670204
42	8	0	-0.177929	-2.844338	5.710887
43	6	0	-1.431208	-3.214660	5.113256
44	1	0	-0.162663	0.923766	-0.304123
45	1	0	-0.905974	-0.684058	-0.325899
46	1	0	-0.449833	-1.061902	2.001841
47	1	0	-0.539618	0.728396	2.048232
48	1	0	2.967410	-1.139287	0.933381
49	1	0	1.624591	-0.391365	-1.335806
50	1	0	1.218243	-1.808879	-0.328882
51	1	0	4.929520	-0.781638	1.477292
52	1	0	6.445802	-0.494992	3.414625
53	1	0	6.596563	1.709023	4.561408
54	1	0	5.204744	3.608864	3.759537
55	1	0	3.657756	3.307841	1.873062
56	1	0	1.501910	2.479659	2.021549
57	1	0	-0.030272	4.273302	1.339398
58	1	0	-0.159808	4.982771	-1.041759
59	1	0	1.286719	3.867875	-2.730903
60	1	0	2.820279	2.039604	-2.040190
61	1	0	4.653620	1.384214	-3.558193
62	1	0	4.995294	-0.350582	-3.400559
63	1	0	6.328733	0.796955	-3.643800
64	1	0	6.322720	-1.386207	-0.431871
65	1	0	7.257751	-0.070416	0.308591
66	1	0	7.587569	-0.553522	-1.373832
67	1	0	6.914301	2.905235	-1.427121
68	1	0	6.319616	2.689959	0.236263
69	1	0	5.234692	3.324083	-1.022713
70	1	0	2.917749	-0.265851	3.307127
71	1	0	-0.013841	0.184448	4.277520
72	1	0	-0.023548	-3.344885	3.138430
73	1	0	3.603857	-2.998110	4.231747
74	1	0	3.794693	-1.843438	-1.667829
75	1	0	3.043243	-3.452745	-1.336223
76	1	0	4.765157	-3.364069	-1.812181
77	1	0	8.682083	-3.420290	1.230100
78	1	0	8.446150	-3.689128	2.995715
79	1	0	8.267104	-2.049122	2.313813
80	1	0	-2.168114	-3.156114	5.915551
81	1	0	-1.402156	-4.235895	4.716290
82	1	0	-1.714732	-2.523119	4.307405

83	6	0	0.965333	0.023697	6.859113
84	1	0	-0.100308	0.242435	6.739440
85	1	0	1.062318	-0.960736	7.337236
86	1	0	1.418905	0.765365	7.528452
87	1	0	2.750202	-0.195714	5.594240

Structure **zsr-IM1** (M06-2x)

E(RB3LYP) **=** -2265.7011 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.136719	0.015282	0.120195
2	6	0	-0.088608	0.137445	1.645719
3	7	0	1.354104	0.045934	1.978693
4	6	0	2.211281	0.019879	0.773364
5	6	0	1.241236	-0.540182	-0.277479
6	6	0	2.837260	1.404916	0.359615
7	6	0	3.646370	2.053862	1.495614
8	6	0	2.942794	2.626014	2.571629
9	6	0	3.619294	3.299416	3.588712
10	6	0	5.010205	3.406258	3.566568
11	6	0	5.716952	2.842650	2.506010
12	6	0	5.042390	2.180631	1.478223
13	8	0	1.738648	2.242412	0.014205
14	14	0	1.563993	3.991313	-0.101914
15	6	0	0.461932	4.155351	-1.636929
16	6	0	3.243889	4.827117	-0.385001
17	6	0	0.694201	4.721945	1.403315
18	6	0	1.806462	-0.007633	3.214196
19	6	0	0.982209	-0.091507	4.354167
20	6	0	3.687771	1.082143	-0.878869
21	6	0	3.390716	1.656634	-2.118031
22	6	0	4.129657	1.331134	-3.256440
23	6	0	5.171747	0.409665	-3.180263
24	6	0	5.464099	-0.190565	-1.955359
25	6	0	4.726622	0.139050	-0.819628
26	6	0	1.438475	0.055073	5.634391
27	6	0	2.842896	0.286009	6.071182
28	6	0	0.606881	2.648038	5.931712
29	6	0	0.375831	2.573947	7.339169
30	8	0	-0.684680	2.387307	7.967528
31	8	0	1.581252	2.681006	8.039674

32	6	0	1.467202	2.668051	9.483004
33	6	0	-0.349696	2.556675	4.914236
34	8	0	-0.019696	2.562106	3.666708
35	6	0	-1.773735	2.342003	5.246787
36	6	0	-2.758274	2.504160	4.343273
37	6	0	-2.551996	3.079740	2.986316
38	8	0	-2.421016	4.274126	2.734578
39	8	0	-2.623753	2.122334	2.008137
40	6	0	-2.494524	2.615574	0.648405
41	6	0	-4.145510	2.216537	4.741891
42	8	0	-4.505039	1.674676	5.789415
43	8	0	-5.034423	2.632929	3.788890
44	6	0	-6.439701	2.412677	4.076458
45	1	0	-0.272104	1.000453	-0.332993
46	1	0	-0.951522	-0.640560	-0.203447
47	1	0	-0.614575	-0.690638	2.139253
48	1	0	-0.474917	1.083489	2.057203
49	1	0	3.042512	-0.667040	0.974132
50	1	0	1.529898	-0.254131	-1.291799
51	1	0	1.246999	-1.636617	-0.217899
52	1	0	1.856399	2.578685	2.638928
53	1	0	3.041473	3.759113	4.387311
54	1	0	5.534052	3.935452	4.357484
55	1	0	6.798816	2.933698	2.460790
56	1	0	5.618588	1.798177	0.642851
57	1	0	0.094495	5.184538	-1.730111
58	1	0	-0.406664	3.490187	-1.553697
59	1	0	0.997922	3.897687	-2.557819
60	1	0	3.069886	5.873838	-0.666464
61	1	0	3.820152	4.347160	-1.184286
62	1	0	3.847241	4.816326	0.530401
63	1	0	-0.040869	5.473679	1.089152
64	1	0	1.418921	5.199309	2.074208
65	1	0	0.161627	3.969843	2.000641
66	1	0	2.889622	-0.019896	3.324766
67	1	0	-0.088921	-0.187548	4.199003
68	1	0	2.552626	2.341678	-2.192314
69	1	0	3.880310	1.793655	-4.207367
70	1	0	5.745408	0.153938	-4.066313
71	1	0	6.266311	-0.919655	-1.882134
72	1	0	4.978534	-0.339497	0.124922
73	1	0	0.711843	-0.079562	6.435360
74	1	0	2.857838	1.053572	6.856510
75	1	0	3.500200	0.620707	5.261520

76	1	0	3.263852	-0.630305	6.509892
77	1	0	1.626802	2.847430	5.620281
78	1	0	2.487744	2.762391	9.853754
79	1	0	1.008212	1.738122	9.831302
80	1	0	0.851839	3.505005	9.825493
81	1	0	-2.030229	2.041896	6.262687
82	1	0	-2.662148	1.748236	0.009575
83	1	0	-1.490589	3.031815	0.495050
84	1	0	-3.235590	3.395817	0.454475
85	1	0	-6.971125	2.780271	3.200422
86	1	0	-6.732097	2.964948	4.973644
87	1	0	-6.630229	1.348042	4.236774

Structure **srrr-TS2**

Imaginary Frequency: -213

E(RB3LYP) = -2266.970442 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.013190	0.004521	0.008482
2	6	0	-0.009084	0.000807	1.539397
3	7	0	1.432782	0.007796	1.919413
4	6	0	2.271423	-0.617584	0.821350
5	6	0	1.311440	-0.676835	-0.402545
6	6	0	1.099505	3.423668	3.228727
7	6	0	-0.070885	3.534683	2.384480
8	8	0	-0.215367	4.120578	1.297691
9	8	0	-1.143482	2.784543	2.924008
10	6	0	-2.468379	3.002277	2.332188
11	6	0	2.305171	4.149117	2.859679
12	8	0	2.425915	5.064053	2.031194
13	8	0	3.425848	3.734909	3.613786
14	6	0	4.629665	4.551573	3.433971
15	6	0	3.713495	-0.050851	0.467512
16	6	0	4.703623	-0.295014	1.630790
17	6	0	5.209840	-1.589214	1.845112
18	6	0	6.083042	-1.849424	2.906384
19	6	0	6.465420	-0.819699	3.774468
20	6	0	5.964463	0.470523	3.572040
21	6	0	5.092840	0.733563	2.507468
22	6	0	3.788455	1.392815	-0.040709
23	6	0	5.039552	1.874750	-0.479112

24	6	0	5.171573	3.164456	-0.998819
25	6	0	4.057626	4.012857	-1.068237
26	6	0	2.820332	3.563816	-0.601422
27	6	0	2.690265	2.262399	-0.096856
28	8	0	4.078455	-1.005769	-0.582539
29	14	0	4.672572	-1.077325	-2.226552
30	6	0	4.272051	-2.881248	-2.690734
31	6	0	6.564339	-0.812071	-2.305758
32	6	0	3.782575	0.124243	-3.415390
33	6	0	-0.273528	0.262024	4.710135
34	6	0	-0.691068	1.310938	5.757136
35	6	0	-0.156229	2.682396	5.320593
36	6	0	1.076908	2.674261	4.428177
37	6	0	1.177033	0.578643	4.338981
38	8	0	-0.608509	3.744425	5.759219
39	6	0	-2.181495	1.358800	5.997153
40	8	0	-3.055829	1.173842	5.140524
41	8	0	-2.468278	1.644431	7.303803
42	6	0	-3.886111	1.834495	7.649877
43	6	0	1.868997	0.190928	3.177067
44	6	0	-0.427802	-1.177002	5.243553
45	1	0	-0.058975	1.031634	-0.365707
46	1	0	-0.886481	-0.522989	-0.385814
47	1	0	-0.478078	-0.910150	1.936945
48	1	0	-0.507753	0.868997	1.967574
49	1	0	2.494235	-1.639794	1.146243
50	1	0	1.756340	-0.185653	-1.267242
51	1	0	1.145712	-1.722693	-0.676229
52	1	0	-3.133359	2.376728	2.924519
53	1	0	-2.468673	2.712981	1.278514
54	1	0	-2.742119	4.056928	2.411588
55	1	0	4.973094	4.505963	2.398171
56	1	0	5.366041	4.120433	4.111916
57	1	0	4.425195	5.593234	3.693228
58	1	0	4.930522	-2.379927	1.159757
59	1	0	6.468098	-2.854203	3.051319
60	1	0	7.145507	-1.020255	4.596369
61	1	0	6.250069	1.277570	4.239447
62	1	0	4.700790	1.735124	2.377066
63	1	0	5.914067	1.239316	-0.394337
64	1	0	6.144306	3.512671	-1.333310
65	1	0	4.160980	5.022134	-1.452543
66	1	0	1.962503	4.224282	-0.572302
67	1	0	1.728507	1.962368	0.289840

68	1	0	4.594195	-3.098984	-3.715827
69	1	0	3.195497	-3.068447	-2.621292
70	1	0	4.782072	-3.575529	-2.014892
71	1	0	6.945017	-1.213087	-3.253272
72	1	0	7.064303	-1.340971	-1.487492
73	1	0	6.836252	0.245663	-2.252758
74	1	0	4.202350	0.001530	-4.421741
75	1	0	3.913857	1.166963	-3.114389
76	1	0	2.709802	-0.087612	-3.472377
77	1	0	-0.941697	0.396016	3.861124
78	1	0	-0.208300	1.092309	6.722071
79	1	0	1.992851	2.779052	5.006221
80	1	0	1.832048	0.488465	5.208842
81	1	0	-3.885065	2.033832	8.719217
82	1	0	-4.455489	0.932921	7.414264
83	1	0	-4.292510	2.680588	7.092431
84	1	0	2.942773	0.105618	3.277761
85	1	0	-0.148512	-1.908231	4.476479
86	1	0	-1.464893	-1.376239	5.538386
87	1	0	0.216539	-1.345381	6.116091

Structure **srrr-IM3**

E(RB3LYP) **=** -2266.983956a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.579299	0.896183	-0.063321
2	6	0	0.173602	0.372178	1.315844
3	7	0	1.489363	0.033122	1.951752
4	6	0	2.348857	-0.602271	0.850881
5	6	0	1.809450	0.043010	-0.459858
6	6	0	1.048780	3.084245	3.372372
7	6	0	-0.032935	3.435081	2.518003
8	8	0	-0.083765	4.166861	1.510225
9	8	0	-1.230213	2.719617	2.912363
10	6	0	-2.483092	3.189346	2.320254
11	6	0	2.346360	3.633951	3.145730
12	8	0	2.725092	4.482488	2.311301
13	8	0	3.314334	3.041833	4.036455
14	6	0	4.623599	3.680766	4.102380
15	6	0	3.922096	-0.706034	0.941080
16	6	0	4.362580	-1.508627	2.189041

17	6	0	4.093321	-2.887780	2.244053
18	6	0	4.451518	-3.641926	3.365661
19	6	0	5.088766	-3.031473	4.453087
20	6	0	5.367718	-1.661941	4.406395
21	6	0	5.010532	-0.905595	3.282146
22	6	0	4.709657	0.597688	0.788693
23	6	0	6.108162	0.505416	0.627121
24	6	0	6.884431	1.648496	0.428251
25	6	0	6.279174	2.913513	0.404538
26	6	0	4.901213	3.022940	0.604915
27	6	0	4.123983	1.870759	0.797676
28	8	0	4.141942	-1.596235	-0.199816
29	14	0	4.922776	-1.666840	-1.770291
30	6	0	3.868185	-2.978605	-2.662728
31	6	0	6.712177	-2.308891	-1.585804
32	6	0	4.898101	-0.025022	-2.745394
33	6	0	-0.541597	0.042681	4.465166
34	6	0	-1.155260	0.978067	5.519222
35	6	0	-0.453013	2.351802	5.326760
36	6	0	0.861687	2.181392	4.547259
37	6	0	0.928354	0.555011	4.345656
38	8	0	-0.827698	3.401798	5.841873
39	6	0	-2.656652	1.062975	5.457029
40	8	0	-3.361426	0.784193	4.477127
41	8	0	-3.173687	1.498429	6.646315
42	6	0	-4.622958	1.744389	6.696414
43	6	0	1.775891	0.104856	3.223916
44	6	0	-0.626848	-1.444657	4.835891
45	1	0	0.827062	1.959903	0.011758
46	1	0	-0.241615	0.799765	-0.778695
47	1	0	-0.401499	-0.560889	1.239488
48	1	0	-0.376689	1.093845	1.912068
49	1	0	2.039574	-1.652872	0.874331
50	1	0	2.575187	0.650564	-0.941400
51	1	0	1.534627	-0.752542	-1.156944
52	1	0	-3.212843	2.412903	2.544886
53	1	0	-2.359798	3.338864	1.245704
54	1	0	-2.776606	4.137996	2.779521
55	1	0	5.374819	3.014775	3.668804
56	1	0	4.846969	3.861468	5.156953
57	1	0	4.604351	4.617739	3.542004
58	1	0	3.632736	-3.368331	1.389154
59	1	0	4.240825	-4.706623	3.386881
60	1	0	5.369900	-3.617591	5.322093

61	1	0	5.868832	-1.178086	5.238673
62	1	0	5.236690	0.154530	3.259052
63	1	0	6.586700	-0.466671	0.670959
64	1	0	7.958744	1.554482	0.302239
65	1	0	6.880689	3.803799	0.251700
66	1	0	4.409973	3.987044	0.657165
67	1	0	3.064276	2.000652	0.972722
68	1	0	4.272502	-3.184330	-3.660798
69	1	0	2.833556	-2.638302	-2.776783
70	1	0	3.858766	-3.915319	-2.096062
71	1	0	7.065085	-2.686310	-2.553394
72	1	0	6.753445	-3.131573	-0.864353
73	1	0	7.400981	-1.525124	-1.258236
74	1	0	5.378493	-0.194176	-3.717503
75	1	0	5.442983	0.770458	-2.230335
76	1	0	3.876663	0.319333	-2.934017
77	1	0	-1.095457	0.213513	3.542108
78	1	0	-0.885620	0.651496	6.535284
79	1	0	1.672655	2.410027	5.243458
80	1	0	1.450912	0.196685	5.243421
81	1	0	-4.811861	2.071505	7.716475
82	1	0	-5.169880	0.827699	6.465289
83	1	0	-4.892800	2.521988	5.979159
84	1	0	2.791107	-0.171442	3.478150
85	1	0	-0.165071	-2.075327	4.065758
86	1	0	-1.672042	-1.756967	4.937598
87	1	0	-0.115162	-1.647734	5.785808

Structure **srrs-TS2**

Imaginary Frequency: -286

E(RB3LYP) = -2266.974012 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.346163	-0.102599	0.064137
2	6	0	0.083596	-0.124204	1.572494
3	7	0	1.418759	-0.421010	2.179867
4	6	0	2.435974	-0.777481	1.130094
5	6	0	1.521905	-1.081861	-0.084163
6	6	0	1.325824	2.152200	6.257207
7	6	0	0.396139	2.342303	7.354055
8	8	0	-0.842892	2.513208	7.203260

9	8	0	0.935731	2.301661	8.616312
10	6	0	0.015375	2.561526	9.727594
11	6	0	2.781153	2.161242	6.360225
12	8	0	3.531602	1.724584	5.451595
13	8	0	3.312493	2.713041	7.500372
14	6	0	4.775458	2.712783	7.595341
15	6	0	3.552677	0.328166	0.862617
16	6	0	4.167605	0.061420	-0.538297
17	6	0	5.063406	-1.005677	-0.731182
18	6	0	5.585311	-1.281670	-1.998933
19	6	0	5.228138	-0.490057	-3.096825
20	6	0	4.339878	0.574733	-2.913957
21	6	0	3.809657	0.843606	-1.646356
22	6	0	4.729125	0.289903	1.876182
23	6	0	4.968025	-0.755447	2.784012
24	6	0	6.097959	-0.754142	3.614109
25	6	0	7.026164	0.284702	3.541910
26	6	0	6.823146	1.315839	2.617303
27	6	0	5.696689	1.309313	1.794160
28	8	0	2.853581	1.583546	0.868284
29	14	0	2.979525	3.314159	1.134893
30	6	0	3.942074	4.146392	-0.298921
31	6	0	3.783612	3.809330	2.793918
32	6	0	1.167418	3.884776	1.066556
33	6	0	-0.696243	-0.524824	4.656243
34	6	0	-1.493774	0.796361	4.905259
35	6	0	-0.595149	1.973478	4.533655
36	6	0	0.842183	1.868567	4.961925
37	6	0	0.814980	-0.270743	4.604528
38	8	0	-0.960231	2.904568	3.794010
39	6	0	-2.820974	0.800253	4.142071
40	8	0	-3.063951	-0.007764	3.238014
41	8	0	-3.799506	1.682732	4.500182
42	6	0	-3.598622	2.830758	5.402509
43	6	0	-1.034515	-1.581622	5.727999
44	6	0	1.669046	-0.445120	3.503806
45	1	0	0.641733	0.896402	-0.261666
46	1	0	-0.536864	-0.413215	-0.501148
47	1	0	-0.627096	-0.917370	1.819338
48	1	0	-0.303621	0.819589	1.960523
49	1	0	2.944604	-1.695440	1.434541
50	1	0	2.039212	-0.994120	-1.037077
51	1	0	1.158985	-2.114162	0.004775
52	1	0	0.647738	2.548659	10.613453

53	1	0	-0.750796	1.784294	9.780716
54	1	0	-0.469127	3.532557	9.603304
55	1	0	4.985928	3.153094	8.568428
56	1	0	5.210557	3.309255	6.790016
57	1	0	5.163212	1.693475	7.531621
58	1	0	5.372666	-1.612712	0.113263
59	1	0	6.276913	-2.108824	-2.125781
60	1	0	5.638696	-0.699385	-4.079434
61	1	0	4.055143	1.196946	-3.756942
62	1	0	3.110605	1.657523	-1.510442
63	1	0	4.292285	-1.599009	2.858519
64	1	0	6.246247	-1.572004	4.312093
65	1	0	7.900308	0.286751	4.184700
66	1	0	7.547196	2.119841	2.529741
67	1	0	5.584038	2.094078	1.055859
68	1	0	4.051154	5.213993	-0.069847
69	1	0	3.402022	4.058992	-1.247274
70	1	0	4.943778	3.728253	-0.441817
71	1	0	3.294226	4.722626	3.155359
72	1	0	4.850625	4.019644	2.672363
73	1	0	3.685125	3.038464	3.564187
74	1	0	1.132061	4.980359	1.016603
75	1	0	0.595842	3.574450	1.947362
76	1	0	0.667986	3.490999	0.175047
77	1	0	-1.050636	-0.913125	3.703369
78	1	0	-1.692668	0.898369	5.978432
79	1	0	1.536279	2.088613	4.159762
80	1	0	1.330525	-0.465575	5.539838
81	1	0	-4.590178	3.039175	5.802537
82	1	0	-3.235666	3.673005	4.812892
83	1	0	-2.894851	2.616248	6.207769
84	1	0	-0.530275	-2.529915	5.510904
85	1	0	-2.113693	-1.770526	5.755284
86	1	0	-0.717760	-1.248799	6.724745
87	1	0	2.720174	-0.531944	3.750363

Structure **srrs-IM3**

E(RB3LYP) **=** -2266.99108 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.349509	-1.135095	0.139115

2	6	0	0.060446	-0.297875	1.384151
3	7	0	1.380329	-0.265952	2.095100
4	6	0	2.513513	-0.480270	1.088919
5	6	0	1.761752	-0.677998	-0.248106
6	6	0	2.128838	0.742245	6.504554
7	6	0	1.520540	-0.165968	7.409444
8	8	0	0.297082	-0.526840	7.296055
9	8	0	2.293494	-0.712808	8.419382
10	6	0	1.603208	-1.622818	9.329993
11	6	0	3.444928	1.294283	6.508083
12	8	0	3.900587	2.073140	5.619185
13	8	0	4.255014	0.936544	7.577697
14	6	0	5.564985	1.577682	7.627750
15	6	0	3.567080	0.696567	1.022669
16	6	0	4.327524	0.538873	-0.327279
17	6	0	5.267226	-0.494330	-0.496348
18	6	0	5.927514	-0.665229	-1.716780
19	6	0	5.668553	0.200509	-2.786519
20	6	0	4.740991	1.233885	-2.623772
21	6	0	4.070870	1.397336	-1.404906
22	6	0	4.639340	0.669407	2.136766
23	6	0	4.900797	-0.448628	2.947270
24	6	0	5.971713	-0.451282	3.851324
25	6	0	6.807742	0.660881	3.953303
26	6	0	6.568847	1.775695	3.141660
27	6	0	5.504958	1.772789	2.240548
28	8	0	2.765857	1.881098	1.014937
29	14	0	2.582662	3.580816	1.438169
30	6	0	3.391150	4.636153	0.060811
31	6	0	3.300528	4.103570	3.121671
32	6	0	0.695177	3.817890	1.372901
33	6	0	-0.911842	0.362136	4.276530
34	6	0	-1.333111	1.361097	5.384168
35	6	0	-0.036142	1.944628	5.970187
36	6	0	1.204129	1.234387	5.432664
37	6	0	0.601636	0.077847	4.498780
38	8	0	-0.007384	2.888672	6.765303
39	6	0	-2.257120	2.448094	4.841204
40	8	0	-2.272125	2.769089	3.646402
41	8	0	-3.103299	3.095678	5.698472
42	6	0	-3.126986	2.834114	7.148644
43	6	0	-1.769040	-0.916312	4.348284
44	6	0	1.555016	-0.125389	3.385467
45	1	0	-0.383417	-0.953853	-0.651418

46	1	0	0.325496	-2.203985	0.384206
47	1	0	-0.700882	-0.727770	2.024877
48	1	0	-0.210734	0.730282	1.125594
49	1	0	3.012057	-1.410995	1.371573
50	1	0	1.707857	0.277924	-0.774273
51	1	0	2.283786	-1.387393	-0.892211
52	1	0	2.363288	-1.912358	10.055157
53	1	0	1.221053	-2.497349	8.796149
54	1	0	0.766443	-1.120924	9.822706
55	1	0	6.031156	1.179378	8.528910
56	1	0	5.463472	2.664574	7.691191
57	1	0	6.154404	1.333760	6.740598
58	1	0	5.506310	-1.152896	0.332286
59	1	0	6.651627	-1.466344	-1.827334
60	1	0	6.187821	0.073251	-3.730919
61	1	0	4.535239	1.915170	-3.443570
62	1	0	3.348124	2.192268	-1.283044
63	1	0	4.290216	-1.343528	2.886034
64	1	0	6.143527	-1.323760	4.473070
65	1	0	7.637723	0.659520	4.651851
66	1	0	7.214514	2.645122	3.207183
67	1	0	5.360742	2.628472	1.591427
68	1	0	3.306574	5.695078	0.335048
69	1	0	2.892663	4.498237	-0.904454
70	1	0	4.454407	4.406818	-0.067898
71	1	0	2.660697	4.895310	3.532469
72	1	0	4.307644	4.517423	3.003392
73	1	0	3.368065	3.305286	3.868848
74	1	0	0.456959	4.886093	1.446711
75	1	0	0.168629	3.312672	2.189416
76	1	0	0.291600	3.450486	0.423004
77	1	0	-1.076526	0.882208	3.330121
78	1	0	-1.806492	0.823792	6.213328
79	1	0	1.752367	1.969925	4.830657
80	1	0	0.670235	-0.807880	5.150131
81	1	0	-3.799348	3.593685	7.544072
82	1	0	-2.127264	2.947369	7.568495
83	1	0	-3.534972	1.838982	7.351146
84	1	0	-1.483296	-1.662412	3.595745
85	1	0	-2.829795	-0.684454	4.198327
86	1	0	-1.647594	-1.382182	5.332801
87	1	0	2.590273	-0.161540	3.717175

Structure **srsr-TS2**

Imaginary Frequency: -237

E(RB3LYP) = -2266.97108 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.118279	-0.038718	0.241669
2	6	0	0.051193	0.164825	1.759587
3	7	0	1.470620	0.119651	2.184924
4	6	0	2.397026	0.402948	1.024084
5	6	0	1.415721	0.691940	-0.138221
6	6	0	2.419041	-3.810249	3.885003
7	6	0	2.418970	-4.353228	5.240230
8	8	0	1.598148	-3.969474	6.107708
9	8	0	3.364839	-5.301578	5.525968
10	6	0	3.352594	-5.828407	6.896844
11	6	0	3.526044	-3.754161	2.948389
12	8	0	3.534657	-3.007383	1.929345
13	8	0	4.604251	-4.553958	3.235782
14	6	0	5.712602	-4.531099	2.278064
15	6	0	3.429774	1.581226	1.218592
16	6	0	4.002042	1.916892	-0.188116
17	6	0	4.782859	0.972652	-0.878848
18	6	0	5.285229	1.259300	-2.151510
19	6	0	5.025877	2.498695	-2.749844
20	6	0	4.258831	3.445046	-2.063466
21	6	0	3.746461	3.154904	-0.792652
22	6	0	4.651094	1.263838	2.116700
23	6	0	5.108534	-0.039207	2.381680
24	6	0	6.272550	-0.246436	3.136719
25	6	0	7.011326	0.835391	3.620335
26	6	0	6.585372	2.137204	3.328733
27	6	0	5.424973	2.344642	2.579844
28	8	0	2.705495	2.733462	1.677779
29	14	0	2.252674	3.638792	3.099949
30	6	0	2.716274	2.826645	4.763979
31	6	0	0.363727	3.873072	2.985929
32	6	0	3.080773	5.353502	2.947395
33	6	0	-0.092441	-1.090283	5.029004
34	6	0	-0.978750	-2.210116	4.421660
35	6	0	-0.094563	-3.400646	4.033839
36	6	0	1.287207	-3.071819	3.521936
37	6	0	1.313738	-1.082580	4.413529

38	8	0	-0.524503	-4.562200	3.979833
39	6	0	-2.113809	-2.596287	5.379579
40	8	0	-2.069988	-2.351151	6.584012
41	8	0	-3.252264	-3.182169	4.877441
42	6	0	-3.416152	-3.586371	3.477567
43	6	0	-0.811932	0.271828	5.099248
44	6	0	1.920537	-0.417878	3.339714
45	1	0	-0.760124	0.364372	-0.270731
46	1	0	0.189601	-1.107493	0.005342
47	1	0	-0.516854	-0.611266	2.271261
48	1	0	-0.388858	1.137011	2.007583
49	1	0	2.948259	-0.521722	0.822554
50	1	0	1.238314	1.769964	-0.199659
51	1	0	1.824221	0.361796	-1.094493
52	1	0	4.170273	-6.546420	6.919956
53	1	0	2.395780	-6.310463	7.108238
54	1	0	3.512738	-5.022362	7.616506
55	1	0	6.406753	-5.283915	2.647113
56	1	0	6.184077	-3.545082	2.254767
57	1	0	5.357768	-4.779165	1.275352
58	1	0	5.017488	0.017564	-0.420154
59	1	0	5.885326	0.518493	-2.670763
60	1	0	5.421357	2.723310	-3.735373
61	1	0	4.055227	4.411236	-2.515293
62	1	0	3.147118	3.879722	-0.257982
63	1	0	4.582041	-0.913878	2.013572
64	1	0	6.595373	-1.262109	3.343766
65	1	0	7.910525	0.669927	4.204809
66	1	0	7.161831	2.989708	3.674412
67	1	0	5.125503	3.354767	2.327776
68	1	0	2.326085	3.453256	5.576070
69	1	0	3.798785	2.738732	4.887645
70	1	0	2.276866	1.829887	4.865230
71	1	0	0.042338	4.658903	3.679963
72	1	0	-0.172738	2.955580	3.245499
73	1	0	0.073065	4.172434	1.973613
74	1	0	2.703573	6.017167	3.734863
75	1	0	2.849394	5.809358	1.978872
76	1	0	4.169261	5.297805	3.046864
77	1	0	0.065043	-1.411115	6.064036
78	1	0	-1.435185	-1.859379	3.481432
79	1	0	1.288460	-2.729090	2.488083
80	1	0	2.059062	-1.339131	5.160068
81	1	0	-4.396165	-4.060242	3.448626

82	1	0	-2.641030	-4.298730	3.195369
83	1	0	-3.416823	-2.714733	2.813533
84	1	0	-0.150949	1.027071	5.537395
85	1	0	-1.695306	0.189837	5.740612
86	1	0	-1.135962	0.633630	4.118151
87	1	0	3.001281	-0.427361	3.385690

Structure **srsr-IM3**

E(RB3LYP) **=** -2266.980578 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.030981	-1.349467	0.559069
2	6	0	-0.214292	-0.397629	1.748775
3	7	0	1.182293	-0.078109	2.202140
4	6	0	2.194606	-0.766982	1.298339
5	6	0	1.364131	-0.994071	0.021776
6	6	0	0.256508	-0.126609	6.488270
7	6	0	-0.563062	0.623108	7.376743
8	8	0	-1.549730	1.309732	6.955440
9	8	0	-0.270251	0.598970	8.721905
10	6	0	-1.164767	1.377133	9.583141
11	6	0	1.462518	-0.838767	6.713652
12	8	0	2.184919	-1.305104	5.770741
13	8	0	1.854765	-1.009026	8.032467
14	6	0	3.101451	-1.730267	8.256258
15	6	0	3.577020	-0.041295	1.085981
16	6	0	4.189209	-0.640184	-0.206560
17	6	0	4.782764	-1.915050	-0.181407
18	6	0	5.289092	-2.487300	-1.352742
19	6	0	5.216760	-1.791450	-2.565858
20	6	0	4.629847	-0.522303	-2.597537
21	6	0	4.113635	0.046498	-1.426637
22	6	0	4.573532	-0.249967	2.251584
23	6	0	4.236560	-0.849820	3.475875
24	6	0	5.186304	-0.977683	4.499967
25	6	0	6.493422	-0.525717	4.312696
26	6	0	6.852594	0.048351	3.084953
27	6	0	5.905223	0.177479	2.067576
28	8	0	3.243051	1.350342	0.877429
29	14	0	3.961567	2.949154	1.034187
30	6	0	4.169899	3.421736	2.870269

31	6	0	2.648396	4.030533	0.182316
32	6	0	5.627460	3.156273	0.116658
33	6	0	-0.557491	2.259393	4.027123
34	6	0	-1.907875	1.516523	4.047980
35	6	0	-1.641219	0.198151	4.814721
36	6	0	-0.140408	-0.020504	5.054286
37	6	0	0.589498	1.207337	4.292337
38	8	0	-2.473701	-0.707822	4.967264
39	6	0	-3.011995	2.432533	4.598100
40	8	0	-2.767302	3.532030	5.093050
41	8	0	-4.328277	2.065251	4.459756
42	6	0	-4.774168	0.862997	3.739798
43	6	0	-0.353466	3.187815	2.824438
44	6	0	1.475294	0.695924	3.220637
45	1	0	-0.819663	-1.219026	-0.186253
46	1	0	-0.058348	-2.392276	0.895251
47	1	0	-0.787178	-0.838083	2.564258
48	1	0	-0.688274	0.538723	1.443027
49	1	0	2.400010	-1.739880	1.762666
50	1	0	1.336312	-0.069890	-0.565131
51	1	0	1.788541	-1.782491	-0.599833
52	1	0	-0.769041	1.232499	10.587648
53	1	0	-2.189598	1.006354	9.507078
54	1	0	-1.150805	2.432835	9.302013
55	1	0	3.149539	-1.869308	9.335973
56	1	0	3.959814	-1.144858	7.911024
57	1	0	3.095757	-2.692946	7.738888
58	1	0	4.866747	-2.454280	0.756669
59	1	0	5.746580	-3.470814	-1.315367
60	1	0	5.615919	-2.232912	-3.473270
61	1	0	4.569395	0.025890	-3.532595
62	1	0	3.643749	1.021346	-1.453811
63	1	0	3.243029	-1.218645	3.698110
64	1	0	4.866060	-1.419979	5.435576
65	1	0	7.227849	-0.624055	5.105608
66	1	0	7.871276	0.383639	2.916424
67	1	0	6.208111	0.583362	1.109474
68	1	0	4.587114	4.434048	2.937079
69	1	0	4.851936	2.740138	3.387652
70	1	0	3.211042	3.423260	3.399257
71	1	0	2.912506	5.091239	0.265725
72	1	0	1.665377	3.884508	0.638720
73	1	0	2.570946	3.781193	-0.881362
74	1	0	5.790065	4.227439	-0.057377

75	1	0	5.625543	2.654355	-0.855883
76	1	0	6.472658	2.779857	0.698839
77	1	0	-0.571691	2.884248	4.924892
78	1	0	-2.214049	1.222143	3.031747
79	1	0	0.143847	-0.957939	4.566394
80	1	0	1.273062	1.663833	5.010635
81	1	0	-5.842162	0.809898	3.946948
82	1	0	-4.261431	-0.024326	4.110449
83	1	0	-4.620180	0.991893	2.661618
84	1	0	0.599068	3.724999	2.903144
85	1	0	-1.151952	3.936553	2.799298
86	1	0	-0.356139	2.649256	1.867810
87	1	0	2.531401	0.877404	3.356265

Structure **srss-TS2**

Imaginary Frequency: -207

E(RB3LYP) **=** -2266.968084 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.022542	0.110872	0.055553
2	6	0	0.021357	0.060894	1.600880
3	7	0	1.454213	0.051159	1.972139
4	6	0	2.309719	0.661397	0.906861
5	6	0	1.428260	0.628601	-0.368010
6	6	0	1.266346	-3.359272	1.602400
7	6	0	0.048112	-3.398015	0.825618
8	8	0	-0.086148	-3.258374	-0.411165
9	8	0	-1.081480	-3.589238	1.623668
10	6	0	-2.373375	-3.740507	0.950805
11	6	0	2.577968	-3.195384	0.960208
12	8	0	3.511126	-2.589701	1.534088
13	8	0	2.849892	-3.694305	-0.296405
14	6	0	2.195781	-4.885817	-0.847844
15	6	0	3.000035	2.056545	1.234320
16	6	0	3.891621	1.875533	2.481367
17	6	0	5.187303	1.352095	2.343605
18	6	0	5.985212	1.119699	3.469666
19	6	0	5.499190	1.404177	4.751105
20	6	0	4.207497	1.922084	4.898486
21	6	0	3.409339	2.154151	3.772664
22	6	0	2.125047	3.317635	1.383285

23	6	0	2.773542	4.508353	1.777938
24	6	0	2.081265	5.715888	1.885369
25	6	0	0.708868	5.767283	1.609072
26	6	0	0.048472	4.597988	1.227254
27	6	0	0.749919	3.388875	1.112600
28	8	0	3.870586	2.183451	0.072439
29	14	0	4.311123	3.312960	-1.187229
30	6	0	5.208631	2.180325	-2.424404
31	6	0	5.513487	4.646389	-0.530399
32	6	0	2.801352	4.140381	-2.016612
33	6	0	0.196006	-1.389016	4.821210
34	6	0	-0.767849	-2.494391	4.313173
35	6	0	0.107045	-3.683484	3.893985
36	6	0	1.290373	-3.321716	3.021736
37	6	0	1.510050	-1.423098	4.016757
38	8	0	-0.036904	-4.830446	4.333282
39	6	0	2.025371	-0.613965	2.989067
40	6	0	-0.489605	-0.016609	4.970345
41	1	0	-0.781391	0.755885	-0.315739
42	1	0	-0.144417	-0.888828	-0.351612
43	1	0	-0.462913	-0.836891	1.985365
44	1	0	-0.476492	0.932344	2.039831
45	1	0	3.168012	-0.003280	0.781245
46	1	0	1.380764	1.612041	-0.837246
47	1	0	1.874493	-0.051396	-1.097652
48	1	0	-3.093201	-3.805885	1.765018
49	1	0	-2.377162	-4.651933	0.348501
50	1	0	-2.575256	-2.883629	0.304288
51	1	0	2.983180	-5.419896	-1.381538
52	1	0	1.393509	-4.584362	-1.518018
53	1	0	1.793638	-5.514594	-0.047605
54	1	0	5.558259	1.131864	1.350696
55	1	0	6.984157	0.714117	3.344325
56	1	0	6.118918	1.224369	5.623864
57	1	0	3.820044	2.147262	5.887321
58	1	0	2.411925	2.560240	3.900197
59	1	0	3.830127	4.478489	2.017588
60	1	0	2.609723	6.612777	2.193042
61	1	0	0.165446	6.702559	1.695785
62	1	0	-1.015537	4.618241	1.012772
63	1	0	0.201776	2.514644	0.799790
64	1	0	5.562438	2.751877	-3.290549
65	1	0	4.537934	1.391622	-2.779947
66	1	0	6.071384	1.700279	-1.951543

67	1	0	6.018361	5.131473	-1.374832
68	1	0	6.278571	4.194054	0.109358
69	1	0	4.993165	5.418145	0.043873
70	1	0	2.251949	4.784709	-1.324527
71	1	0	2.109275	3.393448	-2.419443
72	1	0	3.152212	4.757802	-2.853173
73	1	0	0.476224	-1.696021	5.837002
74	1	0	2.236438	-3.644035	3.447307
75	1	0	2.335331	-1.752049	4.645083
76	1	0	3.103972	-0.627839	2.913202
77	1	0	0.237155	0.741676	5.281260
78	1	0	-1.266047	-0.074257	5.740960
79	1	0	-0.960491	0.321622	4.043698
80	6	0	-1.794346	-2.905925	5.340332
81	8	0	-1.674940	-2.801224	6.565424
82	8	0	-2.914389	-3.431562	4.743504
83	6	0	-3.939827	-3.984312	5.643476
84	1	0	-4.303435	-3.209599	6.321782
85	1	0	-4.730658	-4.334213	4.983255
86	1	0	-3.517539	-4.807626	6.222755
87	1	0	-1.295505	-2.165193	3.414159

Structure **srss-IM3**

E(RB3LYP) = -2266.979143a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.003871	0.011239	-0.003651
2	6	0	-0.003966	0.013255	1.539623
3	7	0	1.439553	0.008893	1.907189
4	6	0	2.243601	0.721573	0.850352
5	6	0	1.385815	0.570701	-0.434731
6	6	0	0.721362	-3.170515	1.702597
7	6	0	-0.548127	-3.282662	1.058986
8	8	0	-0.820866	-3.351991	-0.166009
9	8	0	-1.612169	-3.197614	1.979231
10	6	0	-2.960234	-3.435620	1.468091
11	6	0	1.931133	-2.940604	1.006962
12	8	0	2.927314	-2.376979	1.605543
13	8	0	2.145913	-3.204070	-0.330446
14	6	0	1.681725	-4.456584	-0.948668
15	6	0	2.779199	2.172939	1.210975

16	6	0	3.762746	2.002732	2.391682
17	6	0	5.079520	1.581988	2.137299
18	6	0	5.968281	1.331872	3.188857
19	6	0	5.555144	1.492566	4.516495
20	6	0	4.244436	1.903630	4.782495
21	6	0	3.355741	2.153588	3.729507
22	6	0	1.768030	3.311782	1.462686
23	6	0	2.213394	4.479963	2.118821
24	6	0	1.379621	5.588969	2.287845
25	6	0	0.067384	5.565193	1.802725
26	6	0	-0.389851	4.422677	1.141665
27	6	0	0.451844	3.316390	0.967511
28	8	0	3.536188	2.452304	-0.004178
29	14	0	4.137998	3.853497	-0.874237
30	6	0	5.189358	3.027460	-2.227657
31	6	0	5.230852	4.980129	0.219173
32	6	0	2.713795	4.855710	-1.655183
33	6	0	0.406320	-1.194412	4.869346
34	6	0	-0.872032	-2.028075	4.625754
35	6	0	-0.322982	-3.368178	4.091181
36	6	0	0.900126	-3.084130	3.213622
37	6	0	1.474371	-1.704536	3.808759
38	8	0	-0.683285	-4.484511	4.465064
39	6	0	2.057803	-0.772082	2.782123
40	6	0	0.166370	0.315785	4.987008
41	1	0	-0.833355	0.612428	-0.392357
42	1	0	-0.137377	-1.006102	-0.378713
43	1	0	-0.513400	-0.845698	1.966617
44	1	0	-0.451743	0.928390	1.940470
45	1	0	3.159904	0.142551	0.731679
46	1	0	1.323384	1.515900	-0.974520
47	1	0	1.878315	-0.144164	-1.098161
48	1	0	-3.604636	-3.333181	2.340573
49	1	0	-3.034225	-4.440474	1.045645
50	1	0	-3.214368	-2.705103	0.696553
51	1	0	2.417290	-4.674663	-1.723884
52	1	0	0.683238	-4.318054	-1.356388
53	1	0	1.668329	-5.258727	-0.204162
54	1	0	5.396328	1.447133	1.110279
55	1	0	6.980435	1.007198	2.969555
56	1	0	6.244141	1.298702	5.332152
57	1	0	3.911215	2.032839	5.807649
58	1	0	2.345724	2.476612	3.952652
59	1	0	3.221725	4.519383	2.511676

60	1	0	1.755777	6.468028	2.801724
61	1	0	-0.584607	6.422236	1.936203
62	1	0	-1.401735	4.387636	0.750269
63	1	0	0.064447	2.470543	0.422751
64	1	0	5.601095	3.778194	-2.912373
65	1	0	4.581325	2.326328	-2.808028
66	1	0	6.021952	2.468631	-1.788145
67	1	0	5.844762	5.621298	-0.425233
68	1	0	5.901350	4.385123	0.847390
69	1	0	4.630959	5.625610	0.866740
70	1	0	2.083819	5.330193	-0.897563
71	1	0	2.081041	4.212857	-2.276115
72	1	0	3.131959	5.641358	-2.296613
73	1	0	0.789118	-1.523162	5.844001
74	1	0	1.645434	-3.843287	3.479806
75	1	0	2.355858	-1.994782	4.385994
76	1	0	3.109231	-0.557385	2.893805
77	1	0	1.107512	0.849561	5.155103
78	1	0	-0.483988	0.514592	5.846026
79	1	0	-0.312692	0.738309	4.099336
80	6	0	-1.719873	-2.206920	5.855150
81	8	0	-1.322929	-2.139661	7.024614
82	8	0	-3.023619	-2.477768	5.524701
83	6	0	-3.931867	-2.801263	6.636054
84	1	0	-3.959010	-1.978266	7.353323
85	1	0	-4.902614	-2.949638	6.167634
86	1	0	-3.593951	-3.710569	7.136992
87	1	0	-1.493945	-1.605549	3.830451

Structure **err-IM1**

E(RB3LYP) **=** -2266.96947 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.002180	-0.002076	-0.000719
2	6	0	0.001620	-0.001519	1.535970
3	7	0	1.456303	-0.000899	1.876566
4	6	0	2.305377	0.470090	0.720130
5	6	0	1.268254	0.794046	-0.381591
6	6	0	1.947844	-0.614536	2.950496
7	6	0	1.202868	-1.145527	4.016838
8	6	0	1.831928	-1.879225	5.002462

9	6	0	2.530965	-4.630672	3.574838
10	6	0	3.385589	-4.959976	4.682334
11	8	0	4.638564	-4.892825	4.653447
12	8	0	2.731571	-5.376312	5.842304
13	6	0	3.598661	-5.801357	6.939969
14	6	0	1.129429	-4.612627	3.485098
15	8	0	0.261672	-4.778374	4.431134
16	6	0	0.611515	-4.270235	2.133403
17	6	0	-0.689799	-4.010670	1.870615
18	6	0	-1.764881	-4.072822	2.912107
19	8	0	-2.551642	-4.998139	3.093896
20	8	0	-1.866101	-2.858249	3.583465
21	6	0	-2.835065	-2.841929	4.688629
22	6	0	-1.085332	-3.667484	0.494108
23	8	0	-0.309714	-3.457775	-0.458711
24	8	0	-2.449945	-3.563312	0.354328
25	6	0	-2.961965	-3.281812	-0.990389
26	6	0	3.380831	1.608818	0.984092
27	6	0	4.381155	1.140482	2.064305
28	6	0	5.340588	0.166716	1.733091
29	6	0	6.202850	-0.344859	2.707819
30	6	0	6.126819	0.115259	4.029186
31	6	0	5.187421	1.095873	4.363699
32	6	0	4.319589	1.605456	3.388859
33	6	0	2.852333	3.011449	1.320590
34	6	0	1.553821	3.278688	1.778704
35	6	0	1.156812	4.584414	2.100499
36	6	0	2.056159	5.645831	1.978066
37	6	0	3.364486	5.389847	1.546277
38	6	0	3.756720	4.087928	1.228872
39	8	0	4.109836	1.609756	-0.270609
40	14	0	4.283913	2.422885	-1.810584
41	6	0	4.366595	1.001551	-3.075339
42	6	0	5.943346	3.362986	-1.783656
43	6	0	2.858263	3.618931	-2.250655
44	1	0	-0.908423	0.447535	-0.407171
45	1	0	0.066557	-1.031739	-0.367391
46	1	0	-0.476567	-0.884691	1.964783
47	1	0	-0.484795	0.888991	1.952524
48	1	0	2.917548	-0.382311	0.409711
49	1	0	1.058254	1.866871	-0.405687
50	1	0	1.647615	0.505722	-1.363307
51	1	0	3.025735	-0.725878	2.976632
52	1	0	0.122470	-1.056620	4.037575

53	1	0	3.094003	-4.409574	2.674512
54	1	0	4.238748	-4.980086	7.274916
55	1	0	4.235808	-6.633012	6.628372
56	1	0	2.914660	-6.110945	7.729358
57	1	0	1.312394	-4.223464	1.303514
58	1	0	-2.825711	-1.818191	5.061067
59	1	0	-2.514425	-3.546677	5.458751
60	1	0	-3.827332	-3.121101	4.328409
61	1	0	-2.594696	-4.028423	-1.697409
62	1	0	-2.644919	-2.288661	-1.318612
63	1	0	-4.044158	-3.333661	-0.890105
64	1	0	5.411088	-0.173219	0.707162
65	1	0	6.931189	-1.102563	2.438409
66	1	0	6.793106	-0.286298	4.785338
67	1	0	5.125869	1.466759	5.381920
68	1	0	3.594955	2.362447	3.665469
69	1	0	0.841645	2.475685	1.903490
70	1	0	0.144816	4.764722	2.449006
71	1	0	1.748576	6.656468	2.225589
72	1	0	4.080277	6.201892	1.467273
73	1	0	4.778130	3.892912	0.923220
74	1	0	3.426193	0.441692	-3.110531
75	1	0	5.167636	0.301727	-2.816296
76	1	0	4.566019	1.394424	-4.079351
77	1	0	6.206006	3.684184	-2.798811
78	1	0	6.743903	2.715085	-1.412370
79	1	0	5.899693	4.253287	-1.148555
80	1	0	3.075134	4.068035	-3.228136
81	1	0	2.761466	4.425966	-1.519311
82	1	0	1.896930	3.102061	-2.326524
83	6	0	1.115890	-2.554909	6.093251
84	1	0	0.196152	-2.030229	6.373540
85	1	0	0.791711	-3.567519	5.711092
86	1	0	1.742698	-2.730140	6.969689
87	1	0	2.914612	-1.990180	4.956133

Structure **err-TS1**

Imaginary Frequency: -204

E(RB3LYP) = -2266.966681 a.u.

Standard orientation:

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

1	6	0	-0.059450	0.034466	0.071718
2	6	0	-0.034044	0.038296	1.608089
3	7	0	1.415831	0.029141	1.933869
4	6	0	2.263188	0.446119	0.769023
5	6	0	1.225814	0.787826	-0.329531
6	6	0	1.899923	-0.607962	3.024199
7	6	0	1.163444	-1.073914	4.098676
8	6	0	1.776442	-1.798558	5.151937
9	6	0	2.092594	-3.979255	4.564549
10	6	0	2.979279	-4.322942	5.689991
11	8	0	4.012402	-3.657462	5.906046
12	8	0	2.720994	-5.366706	6.553973
13	6	0	1.872815	-6.516467	6.213143
14	6	0	0.716304	-4.300215	4.359894
15	8	0	-0.114451	-4.637633	5.270768
16	6	0	0.207524	-4.062769	2.981803
17	6	0	-1.066066	-4.284163	2.597716
18	6	0	-2.106059	-4.892741	3.492435
19	8	0	-2.324807	-6.099104	3.604249
20	8	0	-2.842011	-3.917544	4.113344
21	6	0	-3.821599	-4.384258	5.104967
22	6	0	-1.456813	-3.944905	1.210896
23	8	0	-0.751581	-3.330476	0.391276
24	8	0	-2.722631	-4.375166	0.915224
25	6	0	-3.223761	-4.104863	-0.438620
26	6	0	3.367307	1.562444	0.997264
27	6	0	4.411543	1.060940	2.018969
28	6	0	5.357621	0.100503	1.618930
29	6	0	6.263785	-0.434337	2.540010
30	6	0	6.242696	-0.016145	3.876609
31	6	0	5.314569	0.949087	4.280198
32	6	0	4.406216	1.485121	3.358557
33	6	0	2.881673	2.968850	1.380333
34	6	0	1.591913	3.262550	1.847319
35	6	0	1.233512	4.572009	2.198486
36	6	0	2.161818	5.610488	2.097382
37	6	0	3.461687	5.327376	1.656873
38	6	0	3.815680	4.022071	1.310080
39	8	0	4.038855	1.575877	-0.294758
40	14	0	4.184322	2.459296	-1.794259
41	6	0	4.247194	1.090178	-3.118081
42	6	0	5.839693	3.409359	-1.778902
43	6	0	2.745317	3.664820	-2.159060
44	1	0	-0.961254	0.509203	-0.326580

45	1	0	-0.037795	-1.001655	-0.280420
46	1	0	-0.506351	-0.852610	2.028588
47	1	0	-0.528021	0.921249	2.035634
48	1	0	2.852604	-0.423496	0.456264
49	1	0	1.045612	1.866188	-0.360304
50	1	0	1.589307	0.483414	-1.312698
51	1	0	2.973737	-0.759673	3.030502
52	1	0	0.090654	-0.910636	4.143091
53	1	0	2.656838	-3.688987	3.684772
54	1	0	2.031767	-6.818607	5.173216
55	1	0	0.824016	-6.268199	6.365446
56	1	0	2.205046	-7.307947	6.884748
57	1	0	0.895464	-3.669300	2.239176
58	1	0	-4.331081	-3.482683	5.439963
59	1	0	-3.294275	-4.869369	5.929079
60	1	0	-4.519896	-5.088246	4.647645
61	1	0	-2.572410	-4.573239	-1.179326
62	1	0	-3.262379	-3.027916	-0.616752
63	1	0	-4.219090	-4.543067	-0.456119
64	1	0	5.383669	-0.208153	0.581073
65	1	0	6.985549	-1.177249	2.215476
66	1	0	6.937866	-0.439875	4.593501
67	1	0	5.292076	1.284129	5.312214
68	1	0	3.689590	2.227944	3.689126
69	1	0	0.860134	2.475998	1.958821
70	1	0	0.227933	4.772813	2.554611
71	1	0	1.883566	6.623607	2.368913
72	1	0	4.200407	6.120290	1.594634
73	1	0	4.830932	3.805177	0.998232
74	1	0	3.309369	0.525699	-3.149942
75	1	0	5.058919	0.387361	-2.904100
76	1	0	4.419449	1.522718	-4.110766
77	1	0	6.078280	3.755673	-2.791857
78	1	0	6.652126	2.758357	-1.439986
79	1	0	5.803481	4.284222	-1.122501
80	1	0	2.951752	4.173571	-3.109174
81	1	0	2.644925	4.425364	-1.379991
82	1	0	1.789618	3.141751	-2.259536
83	6	0	1.049237	-1.998644	6.452600
84	1	0	0.183209	-2.665789	6.331687
85	1	0	1.703487	-2.430524	7.212016
86	1	0	0.676135	-1.033201	6.821431
87	1	0	2.864026	-1.817803	5.196903

Structure **err-IM2**

E(RB3LYP) **=** -2266.993199 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.020319	0.116320	0.090350
2	6	0	-0.006988	0.115772	1.628870
3	7	0	1.430368	0.095599	1.970530
4	6	0	2.299523	0.457895	0.820954
5	6	0	1.288880	0.835588	-0.292885
6	6	0	1.894042	-0.609947	3.069013
7	6	0	1.170679	-1.024774	4.137517
8	6	0	1.789263	-1.804302	5.281296
9	6	0	1.673983	-3.378671	5.072543
10	6	0	2.666227	-4.133079	5.961565
11	8	0	3.388286	-3.586103	6.792709
12	8	0	2.841766	-5.489088	5.758497
13	6	0	2.005323	-6.309109	4.881996
14	6	0	0.239482	-3.836246	5.265591
15	8	0	-0.134813	-4.410052	6.310267
16	6	0	-0.710452	-3.524003	4.170778
17	6	0	-2.051971	-3.592142	4.295538
18	6	0	-2.747477	-4.063132	5.538258
19	8	0	-3.237910	-5.184295	5.673088
20	8	0	-2.793502	-3.075820	6.480180
21	6	0	-3.333470	-3.452729	7.798394
22	6	0	-2.883652	-3.205621	3.124867
23	8	0	-2.437225	-2.805785	2.038540
24	8	0	-4.218257	-3.312732	3.391432
25	6	0	-5.149775	-2.958218	2.309248
26	6	0	3.432496	1.546381	1.047198
27	6	0	4.464102	1.027800	2.073348
28	6	0	5.421645	0.080608	1.670415
29	6	0	6.327825	-0.454929	2.591560
30	6	0	6.294188	-0.051324	3.932064
31	6	0	5.349978	0.896777	4.340378
32	6	0	4.443109	1.433403	3.418189
33	6	0	2.978077	2.964707	1.427244
34	6	0	1.704072	3.275760	1.927342
35	6	0	1.369518	4.592746	2.273426
36	6	0	2.305277	5.620908	2.137478
37	6	0	3.590534	5.319345	1.667947

38	6	0	3.921368	4.006601	1.324969
39	8	0	4.120774	1.549659	-0.239363
40	14	0	4.277316	2.399299	-1.751102
41	6	0	4.322471	1.013213	-3.059737
42	6	0	5.949678	3.321471	-1.753638
43	6	0	2.865527	3.628071	-2.146344
44	1	0	-0.906813	0.607737	-0.322199
45	1	0	-0.012478	-0.917210	-0.275250
46	1	0	-0.503381	-0.768467	2.042910
47	1	0	-0.514209	1.001246	2.042452
48	1	0	2.872403	-0.427103	0.509087
49	1	0	1.134581	1.918560	-0.313169
50	1	0	1.655189	0.533102	-1.276025
51	1	0	2.956235	-0.832402	3.034963
52	1	0	0.123264	-0.751070	4.238891
53	1	0	1.956781	-3.559432	4.025553
54	1	0	1.838553	-5.834337	3.909404
55	1	0	1.052215	-6.526073	5.367115
56	1	0	2.572428	-7.228348	4.741223
57	1	0	-0.301620	-3.196808	3.221516
58	1	0	-3.360318	-2.522818	8.362063
59	1	0	-2.663740	-4.178542	8.263827
60	1	0	-4.330831	-3.882161	7.687715
61	1	0	-4.969999	-3.594766	1.440730
62	1	0	-5.015050	-1.911172	2.030168
63	1	0	-6.137312	-3.132753	2.729619
64	1	0	5.457412	-0.214578	0.629178
65	1	0	7.062589	-1.183310	2.261880
66	1	0	6.995297	-0.468428	4.647853
67	1	0	5.316658	1.220873	5.375781
68	1	0	3.714023	2.162332	3.751720
69	1	0	0.975314	2.492064	2.073066
70	1	0	0.376058	4.807636	2.654970
71	1	0	2.044635	6.639771	2.405775
72	1	0	4.336417	6.103360	1.580239
73	1	0	4.926568	3.775773	0.991401
74	1	0	3.377127	0.461253	-3.085353
75	1	0	5.124664	0.302258	-2.836442
76	1	0	4.501341	1.432156	-4.057164
77	1	0	6.192787	3.649360	-2.771712
78	1	0	6.751225	2.661789	-1.405547
79	1	0	5.928698	4.205782	-1.109266
80	1	0	3.092437	4.122837	-3.099236
81	1	0	2.771855	4.397932	-1.375522

82	1	0	1.901090	3.122343	-2.250718
83	6	0	1.210191	-1.361654	6.640636
84	1	0	0.122212	-1.498458	6.678305
85	1	0	1.662484	-1.922623	7.461335
86	1	0	1.417115	-0.296873	6.791998
87	1	0	2.870739	-1.619721	5.295556

Structure **zrr-IM1**

E(RB3LYP) **=** -2266.96751 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.538837
3	7	0	1.453564	0.000000	1.918936
4	6	0	2.359286	-0.030316	0.719327
5	6	0	1.411805	-0.485455	-0.408271
6	6	0	3.142734	1.323312	0.413664
7	6	0	4.066592	1.678894	1.603060
8	6	0	5.032994	0.727262	2.001456
9	6	0	5.901450	0.977936	3.067901
10	6	0	5.824144	2.191231	3.766525
11	6	0	4.882037	3.145552	3.376534
12	6	0	4.017014	2.896822	2.300202
13	6	0	2.168401	2.431553	-0.017528
14	6	0	1.284389	3.024569	0.903863
15	6	0	0.356015	3.986757	0.491540
16	6	0	0.286516	4.372077	-0.851422
17	6	0	1.149753	3.780257	-1.779419
18	6	0	2.077873	2.816938	-1.366379
19	8	0	3.957005	0.885650	-0.710241
20	14	0	5.426101	1.495234	-1.475963
21	6	0	5.103934	1.242562	-3.338295
22	6	0	6.897216	0.395321	-0.959472
23	6	0	5.767722	3.328572	-1.072042
24	6	0	1.883492	-0.103116	3.157749
25	6	0	1.049973	-0.209752	4.308153
26	6	0	1.540775	-0.422314	5.564839
27	6	0	-0.338281	1.151609	8.182621
28	6	0	-0.541227	1.978925	7.057788
29	6	0	0.550515	2.882816	6.601767
30	6	0	0.451279	3.568206	5.442322

31	6	0	-0.622802	3.273812	4.413771
32	8	0	-0.455326	2.401693	3.548924
33	8	0	-1.675427	4.135177	4.276150
34	6	0	-2.127555	4.934496	5.420664
35	6	0	1.530730	4.456803	4.940190
36	8	0	1.742160	4.624576	3.729937
37	8	0	2.374449	5.112306	5.817209
38	6	0	2.078709	5.417154	7.223473
39	8	0	-1.653453	2.050144	6.408520
40	6	0	0.898400	0.972810	8.872006
41	8	0	2.042297	1.382774	8.523879
42	8	0	0.894060	0.228711	10.067753
43	6	0	-0.351009	-0.206378	10.681339
44	1	0	-0.184299	1.007462	-0.377564
45	1	0	-0.782606	-0.654526	-0.394046
46	1	0	-0.448598	-0.911350	1.951030
47	1	0	-0.483222	0.870384	1.988785
48	1	0	3.133996	-0.774934	0.908219
49	1	0	1.739129	-0.086417	-1.368337
50	1	0	1.434953	-1.579769	-0.475116
51	1	0	5.122842	-0.207618	1.457992
52	1	0	6.637872	0.231351	3.349734
53	1	0	6.489543	2.385071	4.601473
54	1	0	4.793099	4.085412	3.910462
55	1	0	3.300388	3.661216	2.039310
56	1	0	1.295288	2.758584	1.951584
57	1	0	-0.304367	4.423585	1.231924
58	1	0	-0.432139	5.120296	-1.170505
59	1	0	1.100971	4.061452	-2.827147
60	1	0	2.719107	2.345978	-2.098430
61	1	0	6.019172	1.440419	-3.908919
62	1	0	4.320923	1.909470	-3.712920
63	1	0	4.795480	0.210315	-3.534596
64	1	0	7.767627	0.629276	-1.584571
65	1	0	6.655980	-0.664190	-1.098810
66	1	0	7.174370	0.554401	0.086238
67	1	0	6.630903	3.669341	-1.657007
68	1	0	5.993625	3.472673	-0.011672
69	1	0	4.910398	3.959061	-1.326374
70	1	0	2.960324	-0.146143	3.277812
71	1	0	-0.019273	-0.093576	4.186997
72	1	0	-1.222193	0.627823	8.521128
73	1	0	1.429832	2.943623	7.230441
74	1	0	-2.997832	5.475991	5.052862

75	1	0	-1.355912	5.643602	5.736987
76	1	0	-2.393582	4.255274	6.231720
77	1	0	2.510367	6.403792	7.394695
78	1	0	2.558003	4.682170	7.872824
79	1	0	1.003307	5.435126	7.411611
80	1	0	-0.060079	-0.636429	11.640360
81	1	0	-0.853877	-0.970391	10.077179
82	1	0	-1.033234	0.634773	10.843328
83	6	0	2.952812	-0.489962	6.034753
84	1	0	3.705071	-0.302310	5.264929
85	1	0	3.064345	0.244447	6.848404
86	1	0	3.152375	-1.468470	6.494548
87	1	0	0.801220	-0.512642	6.358071

Structure **zrr-TS1**

Imaginary Frequency: -188

E(RB3LYP) **=** -2266.964626 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.008187	0.015833	0.019224
2	6	0	0.012524	0.008707	1.556502
3	7	0	1.450059	0.011928	1.927662
4	6	0	2.354885	-0.164962	0.752611
5	6	0	1.378677	-0.581084	-0.370867
6	6	0	3.256959	1.091975	0.386865
7	6	0	4.328871	1.335961	1.475909
8	6	0	5.150418	0.257333	1.873899
9	6	0	6.154080	0.427293	2.832114
10	6	0	6.365939	1.684945	3.414449
11	6	0	5.575169	2.766731	3.017409
12	6	0	4.572618	2.593922	2.050766
13	6	0	2.367422	2.305297	0.070925
14	6	0	1.677975	2.992611	1.089946
15	6	0	0.825075	4.058793	0.784986
16	6	0	0.629479	4.451584	-0.543570
17	6	0	1.297163	3.768271	-1.565076
18	6	0	2.156810	2.706068	-1.259574
19	8	0	3.917628	0.609711	-0.819437
20	14	0	5.390597	1.041679	-1.683078
21	6	0	4.908626	0.767201	-3.507793
22	6	0	6.781843	-0.181796	-1.223855

23	6	0	5.939795	2.844241	-1.383842
24	6	0	1.858545	0.050578	3.206003
25	6	0	1.022190	-0.023481	4.315141
26	6	0	1.472470	0.049658	5.650389
27	6	0	2.929044	0.090646	6.041802
28	6	0	0.647857	1.997720	6.396907
29	6	0	1.331570	2.949010	5.553934
30	6	0	2.542556	3.641522	6.055414
31	6	0	3.101468	4.730096	5.483573
32	6	0	2.653313	5.351352	4.182140
33	8	0	3.287093	5.207499	3.140121
34	8	0	1.573139	6.207388	4.177429
35	6	0	0.686441	6.367938	5.328860
36	6	0	4.403609	5.251946	6.026298
37	8	0	5.355031	5.540433	5.298828
38	8	0	4.571348	5.360722	7.391070
39	6	0	3.484237	5.403755	8.383230
40	8	0	0.906642	3.179156	4.374955
41	6	0	0.872342	1.841724	7.822215
42	8	0	1.911780	2.139337	8.450023
43	8	0	-0.118498	1.200507	8.574218
44	6	0	-1.467233	0.976337	8.062207
45	1	0	-0.084279	1.038402	-0.353795
46	1	0	-0.825355	-0.567677	-0.382908
47	1	0	-0.463040	-0.895331	1.962582
48	1	0	-0.476693	0.884924	1.993910
49	1	0	3.049027	-0.979455	0.969655
50	1	0	1.738335	-0.237753	-1.340278
51	1	0	1.319187	-1.675770	-0.404771
52	1	0	5.025149	-0.718577	1.416606
53	1	0	6.771597	-0.418797	3.119159
54	1	0	7.140842	1.818602	4.162683
55	1	0	5.713786	3.748746	3.457404
56	1	0	3.985465	3.457276	1.775286
57	1	0	1.803446	2.731058	2.132801
58	1	0	0.338940	4.586719	1.597891
59	1	0	-0.027043	5.283618	-0.778366
60	1	0	1.154184	4.060401	-2.601269
61	1	0	2.655942	2.172746	-2.057594
62	1	0	5.789261	0.865999	-4.153550
63	1	0	4.160232	1.493873	-3.840419
64	1	0	4.493804	-0.236984	-3.644822
65	1	0	7.630671	-0.045757	-1.905253
66	1	0	6.432695	-1.215872	-1.318529

67	1	0	7.134430	-0.027228	-0.200356
68	1	0	6.779133	3.079704	-2.049922
69	1	0	6.265365	3.001122	-0.351785
70	1	0	5.127691	3.547068	-1.593436
71	1	0	2.932587	0.096448	3.341196
72	1	0	-0.044895	-0.138231	4.157216
73	1	0	0.824139	-0.406264	6.395211
74	1	0	3.050578	0.482378	7.055434
75	1	0	3.532408	0.702750	5.365742
76	1	0	3.342437	-0.928261	6.033729
77	1	0	-0.336061	1.757517	6.016893
78	1	0	2.979932	3.224437	6.953345
79	1	0	0.031113	7.193950	5.056044
80	1	0	1.243459	6.625051	6.234242
81	1	0	0.102079	5.459538	5.483214
82	1	0	3.895123	5.984878	9.208194
83	1	0	3.224959	4.398873	8.720127
84	1	0	2.598261	5.900441	7.980543
85	1	0	-2.028300	0.596584	8.915517
86	1	0	-1.478467	0.230995	7.259826
87	1	0	-1.919116	1.908172	7.708142

Structure **zrr-IM2**

E(RB3LYP) **=** -2266.994378 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.131208	0.132408	-0.093098
2	6	0	0.055492	-0.341961	1.370335
3	7	0	1.454970	-0.369567	1.826084
4	6	0	2.434137	-0.116157	0.750616
5	6	0	1.574678	-0.206001	-0.532722
6	6	0	3.246826	1.248031	0.880922
7	6	0	4.208275	1.190822	2.093559
8	6	0	5.130468	0.123145	2.162149
9	6	0	6.040231	0.015888	3.217642
10	6	0	6.054789	0.980179	4.234768
11	6	0	5.161287	2.053182	4.173295
12	6	0	4.253811	2.160430	3.108745
13	6	0	2.276929	2.438725	0.877721
14	6	0	1.450866	2.715153	1.986147
15	6	0	0.528291	3.766404	1.950353

16	6	0	0.394377	4.553409	0.801249
17	6	0	1.195430	4.279251	-0.311763
18	6	0	2.125115	3.232992	-0.271890
19	8	0	4.046867	1.232830	-0.341940
20	14	0	5.504999	2.069419	-0.858695
21	6	0	5.198491	2.376520	-2.716853
22	6	0	7.018603	0.919168	-0.679985
23	6	0	5.795134	3.712224	0.069740
24	6	0	1.791344	-0.830711	3.077937
25	6	0	0.921259	-1.215355	4.046786
26	6	0	1.327524	-1.747850	5.398786
27	6	0	2.842117	-1.741032	5.669444
28	6	0	0.473749	-1.000706	6.544498
29	6	0	0.747812	0.495255	6.615558
30	6	0	1.980788	1.002758	7.255247
31	6	0	2.361661	2.297631	7.214553
32	6	0	1.717284	3.346847	6.330962
33	8	0	2.057452	3.488755	5.160448
34	8	0	0.825591	4.223951	6.890786
35	6	0	0.226759	3.962963	8.202270
36	6	0	3.643969	2.733911	7.864743
37	8	0	4.412270	3.523446	7.311891
38	8	0	3.996560	2.219391	9.090523
39	6	0	3.081831	1.570116	10.046323
40	8	0	-0.091133	1.287391	6.133656
41	6	0	0.643888	-1.716285	7.872754
42	8	0	1.527844	-1.459439	8.699826
43	8	0	-0.198859	-2.768064	8.159779
44	6	0	-1.360087	-3.128233	7.337701
45	1	0	-0.043467	1.209699	-0.151977
46	1	0	-0.617514	-0.363359	-0.719069
47	1	0	-0.380528	-1.351125	1.455816
48	1	0	-0.542736	0.331662	1.996866
49	1	0	3.192105	-0.905569	0.746922
50	1	0	1.955328	0.455328	-1.311306
51	1	0	1.621053	-1.232745	-0.916190
52	1	0	5.151946	-0.618408	1.371179
53	1	0	6.738472	-0.815705	3.243269
54	1	0	6.757556	0.898769	5.058207
55	1	0	5.151424	2.807573	4.952946
56	1	0	3.578542	3.003046	3.097381
57	1	0	1.528751	2.128641	2.891601
58	1	0	-0.067540	3.973759	2.832753
59	1	0	-0.319690	5.370794	0.776336

60	1	0	1.100053	4.877064	-1.213494
61	1	0	2.725493	3.016138	-1.145148
62	1	0	6.096085	2.794949	-3.187787
63	1	0	4.371351	3.075054	-2.879883
64	1	0	4.953623	1.435474	-3.220745
65	1	0	7.882355	1.369998	-1.184113
66	1	0	6.821754	-0.052363	-1.146398
67	1	0	7.279450	0.753663	0.368878
68	1	0	6.653318	4.232365	-0.373586
69	1	0	6.006394	3.539833	1.128837
70	1	0	4.921246	4.366705	-0.001161
71	1	0	2.859438	-0.877524	3.253218
72	1	0	-0.149353	-1.162888	3.865470
73	1	0	0.991908	-2.796068	5.489331
74	1	0	3.069905	-2.085275	6.682462
75	1	0	3.277922	-0.745964	5.534091
76	1	0	3.343555	-2.415879	4.967959
77	1	0	-0.566553	-1.066164	6.217503
78	1	0	2.570908	0.278096	7.796680
79	1	0	-0.450186	4.799581	8.365242
80	1	0	0.985566	3.948608	8.990612
81	1	0	-0.332382	3.025377	8.179474
82	1	0	3.502020	1.802911	11.023950
83	1	0	3.064638	0.490745	9.890339
84	1	0	2.069103	1.970557	9.965239
85	1	0	-1.777067	-4.004281	7.831454
86	1	0	-1.065143	-3.384515	6.317288
87	1	0	-2.098362	-2.321639	7.330689

Structure **err-IM1** (M06-2x)

E(RB3LYP) **=** -2265.697817 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.126933	0.324429	-0.215677
2	6	0	-0.315873	0.333187	1.301383
3	7	0	1.070836	0.159172	1.811035
4	6	0	2.093585	0.441150	0.757576
5	6	0	1.261241	0.936861	-0.431720
6	6	0	1.344163	-0.475480	2.943827
7	6	0	0.423418	-0.779830	3.958798
8	6	0	0.799510	-1.679829	4.920547

9	6	0	2.772762	-3.634815	2.742463
10	6	0	3.614902	-3.870015	3.876784
11	8	0	4.851672	-4.031468	3.830293
12	8	0	2.966484	-3.899901	5.105266
13	6	0	3.777873	-4.293385	6.237205
14	6	0	1.375590	-3.640324	2.667713
15	8	0	0.520424	-3.720231	3.626663
16	6	0	0.842839	-3.448613	1.298769
17	6	0	-0.474790	-3.357543	1.031169
18	6	0	-1.537302	-3.564593	2.053749
19	8	0	-2.100214	-4.628049	2.283764
20	8	0	-1.929686	-2.380224	2.630401
21	6	0	-2.917378	-2.518310	3.685196
22	6	0	-0.904987	-3.112180	-0.347929
23	8	0	-0.165062	-2.990506	-1.333442
24	8	0	-2.259964	-2.965268	-0.436180
25	6	0	-2.801217	-2.701707	-1.757231
26	6	0	3.301954	1.362399	1.145552
27	6	0	4.075770	0.711868	2.293076
28	6	0	4.836391	-0.435692	2.032234
29	6	0	5.418342	-1.152462	3.074962
30	6	0	5.254464	-0.722549	4.394535
31	6	0	4.527026	0.436768	4.661197
32	6	0	3.939386	1.151812	3.615077
33	6	0	2.986537	2.815409	1.479313
34	6	0	1.708398	3.321592	1.725163
35	6	0	1.519433	4.677271	2.008337
36	6	0	2.608354	5.543434	2.062894
37	6	0	3.896291	5.041109	1.858743
38	6	0	4.079945	3.690722	1.580033
39	8	0	4.121340	1.282058	-0.030885
40	14	0	4.519754	2.258475	-1.415291
41	6	0	4.672755	0.983719	-2.800343
42	6	0	6.192796	3.102861	-1.129878
43	6	0	3.223607	3.571268	-1.867506
44	1	0	-0.918986	0.874079	-0.733274
45	1	0	-0.129356	-0.707664	-0.587679
46	1	0	-0.936554	-0.498489	1.660160
47	1	0	-0.741717	1.279377	1.664755
48	1	0	2.565499	-0.519863	0.501274
49	1	0	1.208867	2.032348	-0.436514
50	1	0	1.710015	0.617142	-1.376415
51	1	0	2.369062	-0.822876	3.067688
52	1	0	-0.601342	-0.420521	3.908200

53	1	0	3.335023	-3.565255	1.814246
54	1	0	4.574563	-3.567052	6.424037
55	1	0	4.235929	-5.270574	6.060210
56	1	0	3.087599	-4.337484	7.080016
57	1	0	1.539019	-3.361002	0.463548
58	1	0	-3.067439	-1.512588	4.079856
59	1	0	-2.534025	-3.195652	4.454783
60	1	0	-3.850722	-2.923466	3.284761
61	1	0	-2.524962	-3.503350	-2.446736
62	1	0	-2.414122	-1.752479	-2.141090
63	1	0	-3.879861	-2.657486	-1.618696
64	1	0	4.956447	-0.765581	1.004349
65	1	0	5.952026	-2.076435	2.875994
66	1	0	5.694833	-1.299760	5.202504
67	1	0	4.406536	0.784703	5.683640
68	1	0	3.352353	2.040794	3.833392
69	1	0	0.844839	2.666162	1.709112
70	1	0	0.515839	5.052190	2.188568
71	1	0	2.459195	6.597492	2.278081
72	1	0	4.757155	5.700521	1.927136
73	1	0	5.082977	3.290698	1.448487
74	1	0	3.714055	0.489446	-2.994065
75	1	0	5.400988	0.212658	-2.527043
76	1	0	5.006977	1.462900	-3.728635
77	1	0	6.673659	3.295596	-2.097151
78	1	0	6.854322	2.455443	-0.543239
79	1	0	6.083371	4.059484	-0.606539
80	1	0	3.614552	4.146354	-2.717428
81	1	0	3.036713	4.267900	-1.042229
82	1	0	2.271923	3.123215	-2.173422
83	6	0	-0.055658	-2.155160	6.027544
84	1	0	-1.053954	-1.704956	6.018191
85	1	0	-0.141120	-3.244756	5.928125
86	1	0	0.416370	-1.954070	6.998737
87	1	0	1.826111	-2.046859	4.929353

Structure **zrr-IM1** (M06-2x)

E(RB3LYP) **=** -2265.696303 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.022702	-0.121598	0.092032

2	6	0	0.060458	-0.061854	1.620689
3	7	0	1.513469	-0.008719	1.958948
4	6	0	2.385305	-0.091771	0.750866
5	6	0	1.426762	-0.585022	-0.334631
6	6	0	3.129207	1.252979	0.407298
7	6	0	4.050624	1.626326	1.577556
8	6	0	5.075467	0.721213	1.914419
9	6	0	5.938343	0.974603	2.978431
10	6	0	5.785190	2.136243	3.742716
11	6	0	4.777050	3.040840	3.417288
12	6	0	3.928146	2.795590	2.333190
13	6	0	2.114584	2.317528	0.002003
14	6	0	1.221035	2.860671	0.936835
15	6	0	0.235974	3.765528	0.545474
16	6	0	0.120174	4.139205	-0.793677
17	6	0	0.993838	3.596169	-1.735511
18	6	0	1.979301	2.690074	-1.341350
19	8	0	3.931067	0.849682	-0.711937
20	14	0	5.369014	1.589894	-1.394057
21	6	0	5.048233	1.635636	-3.258230
22	6	0	6.834891	0.443380	-1.043439
23	6	0	5.677538	3.330030	-0.713548
24	6	0	1.981730	0.010876	3.184594
25	6	0	1.195777	0.010805	4.364769
26	6	0	1.757139	-0.050547	5.604099
27	6	0	-0.523540	1.169562	8.113129
28	6	0	-0.645566	1.998516	6.984725
29	6	0	0.530008	2.783370	6.528707
30	6	0	0.489181	3.458189	5.366206
31	6	0	-0.605772	3.254128	4.350746
32	8	0	-0.547604	2.343566	3.520243
33	8	0	-1.533010	4.230248	4.193456
34	6	0	-1.807711	5.139143	5.289799
35	6	0	1.619212	4.249137	4.843723
36	8	0	1.772118	4.448770	3.633942
37	8	0	2.561078	4.767247	5.692712
38	6	0	2.348209	5.083167	7.095316
39	8	0	-1.731967	2.179041	6.330012
40	6	0	0.681582	0.917362	8.830386
41	8	0	1.850687	1.254311	8.508612
42	8	0	0.599085	0.191178	10.014447
43	6	0	-0.670651	-0.214890	10.556052
44	1	0	-0.202262	0.866966	-0.320459
45	1	0	-0.752989	-0.809919	-0.257047

46	1	0	-0.352933	-0.967244	2.084876
47	1	0	-0.437185	0.816708	2.046823
48	1	0	3.175135	-0.824568	0.949582
49	1	0	1.727849	-0.197621	-1.311269
50	1	0	1.470087	-1.680471	-0.381034
51	1	0	5.210699	-0.181653	1.321816
52	1	0	6.728674	0.265949	3.212635
53	1	0	6.447149	2.329637	4.581985
54	1	0	4.627397	3.945789	4.000895
55	1	0	3.167984	3.534281	2.110469
56	1	0	1.264014	2.590914	1.986649
57	1	0	-0.436743	4.165684	1.298908
58	1	0	-0.647070	4.844166	-1.100997
59	1	0	0.906248	3.871031	-2.783338
60	1	0	2.632241	2.243074	-2.084523
61	1	0	5.989107	1.800465	-3.797473
62	1	0	4.356164	2.440957	-3.528919
63	1	0	4.621117	0.684469	-3.595312
64	1	0	7.683693	0.718808	-1.681421
65	1	0	6.568516	-0.597740	-1.259636
66	1	0	7.153940	0.513010	0.002530
67	1	0	6.390133	3.847316	-1.368547
68	1	0	6.094488	3.299790	0.299595
69	1	0	4.751344	3.915989	-0.685794
70	1	0	3.067183	-0.009961	3.272598
71	1	0	0.116237	0.093048	4.281867
72	1	0	-1.454220	0.718121	8.437177
73	1	0	1.408457	2.769325	7.166489
74	1	0	-2.616296	5.777213	4.935841
75	1	0	-0.929588	5.753240	5.524770
76	1	0	-2.122103	4.557038	6.159971
77	1	0	2.898080	6.009016	7.270059
78	1	0	2.749432	4.288117	7.729668
79	1	0	1.285927	5.229766	7.314318
80	1	0	-0.439659	-0.692489	11.509119
81	1	0	-1.176183	-0.934627	9.900713
82	1	0	-1.328917	0.645428	10.724098
83	6	0	3.187347	-0.053321	5.985868
84	1	0	3.892086	0.101220	5.162939
85	1	0	3.325544	0.722712	6.751885
86	1	0	3.434891	-0.994473	6.496987
87	1	0	1.067044	-0.076140	6.448847

Structure **rrrr-TS2**

Imaginary Frequency: -223
E(RB3LYP) =-2266.969757 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.034025	-0.074546	0.067404
2	6	0	-0.004327	-0.059491	1.625696
3	7	0	1.445474	-0.048960	1.947125
4	6	0	2.057497	-0.976048	0.936095
5	6	0	1.410980	-0.468767	-0.374484
6	6	0	0.303573	3.385557	1.664489
7	6	0	-1.125827	3.186827	1.498308
8	8	0	-1.823422	3.329156	0.484069
9	8	0	-1.734659	2.784422	2.712617
10	6	0	-3.200972	2.781096	2.717212
11	6	0	1.094479	3.599956	0.459512
12	8	0	0.772274	3.363200	-0.718076
13	8	0	2.362336	4.140277	0.739980
14	6	0	3.099395	4.633771	-0.425542
15	6	0	3.576551	-1.376053	0.991676
16	6	0	3.822227	-2.117558	2.334043
17	6	0	3.325247	-3.424512	2.483507
18	6	0	3.478482	-4.115718	3.688590
19	6	0	4.133565	-3.513548	4.769662
20	6	0	4.641285	-2.218877	4.629123
21	6	0	4.489424	-1.528005	3.420321
22	6	0	4.654351	-0.317263	0.732576
23	6	0	5.995377	-0.757932	0.742619
24	6	0	7.048133	0.119907	0.483414
25	6	0	6.783970	1.470277	0.218253
26	6	0	5.463345	1.922904	0.219952
27	6	0	4.403519	1.037828	0.470261
28	8	0	3.633412	-2.406818	-0.047307
29	14	0	4.247627	-2.600863	-1.680585
30	6	0	2.951812	-3.745153	-2.481977
31	6	0	5.932324	-3.495833	-1.618946
32	6	0	4.394834	-0.968869	-2.661409
33	6	0	0.290583	1.369973	4.664922
34	6	0	-0.090727	2.759162	5.252742
35	6	0	0.139420	3.827481	4.174113
36	6	0	0.918211	3.432295	2.931752
37	6	0	1.557825	1.572649	3.833912

38	8	0	-0.210629	5.002333	4.334532
39	6	0	0.730979	3.115151	6.477033
40	8	0	1.957884	3.287112	6.496949
41	8	0	-0.048241	3.214276	7.600292
42	6	0	0.637252	3.580400	8.851661
43	6	0	2.073880	0.717606	2.852051
44	6	0	0.473533	0.282268	5.745022
45	1	0	-0.301099	0.910060	-0.323867
46	1	0	-0.774637	-0.795121	-0.292662
47	1	0	-0.453976	-0.971479	2.042210
48	1	0	-0.501065	0.803701	2.051651
49	1	0	1.582077	-1.944749	1.146113
50	1	0	1.934764	0.402726	-0.774961
51	1	0	1.408217	-1.249018	-1.136569
52	1	0	-3.480740	2.413143	3.703701
53	1	0	-3.581343	2.128538	1.929018
54	1	0	-3.580163	3.793073	2.558446
55	1	0	4.014690	5.060866	-0.017246
56	1	0	2.515167	5.398025	-0.943684
57	1	0	3.315530	3.823758	-1.125580
58	1	0	2.844665	-3.900538	1.637575
59	1	0	3.092893	-5.126449	3.780688
60	1	0	4.253555	-4.049998	5.705571
61	1	0	5.161609	-1.743560	5.454686
62	1	0	4.914338	-0.535159	3.327158
63	1	0	6.205644	-1.797415	0.967697
64	1	0	8.070572	-0.244169	0.498295
65	1	0	7.598733	2.159781	0.022410
66	1	0	5.249160	2.967104	0.029078
67	1	0	3.393969	1.427763	0.466550
68	1	0	3.267465	-4.035521	-3.491051
69	1	0	1.978203	-3.249925	-2.558788
70	1	0	2.824168	-4.655235	-1.886809
71	1	0	6.207977	-3.834197	-2.625190
72	1	0	5.877080	-4.373727	-0.966670
73	1	0	6.727034	-2.840515	-1.250934
74	1	0	4.663963	-1.207538	-3.698030
75	1	0	5.166359	-0.312455	-2.250244
76	1	0	3.448669	-0.419891	-2.677285
77	1	0	-0.549725	1.085113	4.029789
78	1	0	-1.143255	2.789715	5.540557
79	1	0	1.923245	3.844030	2.924328
80	1	0	2.353970	2.014093	4.432550
81	1	0	-0.154358	3.627763	9.596251

82	1	0	1.130962	4.547136	8.736038
83	1	0	1.379122	2.821729	9.109707
84	1	0	3.150481	0.718468	2.738824
85	1	0	0.648807	-0.692236	5.277068
86	1	0	-0.417313	0.204024	6.380362
87	1	0	1.335323	0.502416	6.385119

Structure **rrrr-IM3**

E(RB3LYP) **=** -2266.980641 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.022569	0.050220	-0.027714
2	6	0	0.009594	0.044259	1.523288
3	7	0	1.469435	0.037966	1.865070
4	6	0	2.047853	-0.979099	0.896570
5	6	0	1.428545	-0.501171	-0.438461
6	6	0	0.538560	3.258430	1.645890
7	6	0	-0.861731	3.133658	1.434520
8	8	0	-1.549391	3.246228	0.402720
9	8	0	-1.529037	2.758153	2.674112
10	6	0	-2.974208	2.968845	2.718568
11	6	0	1.384797	3.513128	0.523659
12	8	0	1.127075	3.479295	-0.698874
13	8	0	2.733754	3.815197	0.927576
14	6	0	3.521916	4.519656	-0.079297
15	6	0	3.538731	-1.466554	0.990007
16	6	0	3.768323	-2.052695	2.409082
17	6	0	3.139009	-3.262907	2.751548
18	6	0	3.275222	-3.802385	4.033823
19	6	0	4.047007	-3.143576	4.999005
20	6	0	4.689868	-1.948016	4.665496
21	6	0	4.554645	-1.408996	3.379568
22	6	0	4.669083	-0.520207	0.578078
23	6	0	5.972041	-1.063517	0.549866
24	6	0	7.064198	-0.299833	0.139235
25	6	0	6.878451	1.034186	-0.248717
26	6	0	5.599046	1.589908	-0.202337
27	6	0	4.498864	0.822845	0.212742
28	8	0	3.487665	-2.615780	0.088465
29	14	0	4.008728	-3.072126	-1.529255
30	6	0	2.563020	-4.147536	-2.147208

31	6	0	5.584978	-4.136357	-1.382483
32	6	0	4.302721	-1.600504	-2.710126
33	6	0	0.407917	1.377241	4.610730
34	6	0	-0.014402	2.729231	5.246449
35	6	0	0.261748	3.789453	4.140083
36	6	0	1.142318	3.217141	3.016773
37	6	0	1.585735	1.786227	3.664685
38	8	0	-0.096326	4.963126	4.220269
39	6	0	0.785290	3.097723	6.474000
40	8	0	2.023233	3.069061	6.562202
41	8	0	-0.019275	3.498956	7.506771
42	6	0	0.653169	3.967112	8.730467
43	6	0	2.112295	0.784447	2.718894
44	6	0	0.780306	0.260496	5.596824
45	1	0	-0.121802	1.066820	-0.401445
46	1	0	-0.788263	-0.572954	-0.414802
47	1	0	-0.411237	-0.886945	1.923590
48	1	0	-0.501424	0.889865	1.963644
49	1	0	1.511111	-1.895149	1.171388
50	1	0	2.022215	0.286365	-0.906735
51	1	0	1.355713	-1.336056	-1.136189
52	1	0	-3.411624	2.121101	3.250269
53	1	0	-3.359473	3.028602	1.698518
54	1	0	-3.181630	3.899064	3.256022
55	1	0	4.522686	4.606151	0.345163
56	1	0	3.103934	5.514667	-0.260546
57	1	0	3.532063	3.971116	-1.023990
58	1	0	2.571434	-3.792073	1.995515
59	1	0	2.786717	-4.740953	4.276316
60	1	0	4.153585	-3.562686	5.994301
61	1	0	5.303323	-1.434636	5.398923
62	1	0	5.086564	-0.496707	3.132474
63	1	0	6.121708	-2.091673	0.859860
64	1	0	8.056267	-0.739939	0.126052
65	1	0	7.723243	1.632743	-0.573480
66	1	0	5.444483	2.621278	-0.492399
67	1	0	3.528978	1.302040	0.249264
68	1	0	2.809733	-4.600179	-3.114830
69	1	0	1.650433	-3.555397	-2.272985
70	1	0	2.351865	-4.952561	-1.435857
71	1	0	5.783915	-4.639191	-2.336652
72	1	0	5.460392	-4.903857	-0.611529
73	1	0	6.460200	-3.530862	-1.129493
74	1	0	4.544569	-1.998695	-3.703727

75	1	0	5.136288	-0.973703	-2.382288
76	1	0	3.415664	-0.967593	-2.810353
77	1	0	-0.447730	1.057552	4.012822
78	1	0	-1.074695	2.758386	5.497439
79	1	0	2.052346	3.821322	2.980222
80	1	0	2.424095	2.034153	4.325587
81	1	0	-0.157257	4.232876	9.405618
82	1	0	1.278086	4.833065	8.503557
83	1	0	1.272448	3.170326	9.147681
84	1	0	3.188325	0.662722	2.699483
85	1	0	1.032821	-0.663544	5.062718
86	1	0	-0.059364	0.037543	6.266088
87	1	0	1.642309	0.540252	6.210656

Structure **rrrs-TS2**

Imaginary Frequency: -261

E(RB3LYP) **=** -2266.972546 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.003257	-0.011259	-0.004301
2	6	0	-0.006217	-0.011337	1.531197
3	7	0	1.436193	-0.001338	1.877589
4	6	0	2.226141	0.706437	0.807151
5	6	0	1.214874	0.880312	-0.356344
6	6	0	2.363458	-0.224738	6.379406
7	6	0	3.542068	-0.987589	6.758250
8	8	0	4.608549	-0.573496	7.253954
9	8	0	3.406878	-2.327272	6.396127
10	6	0	4.533707	-3.216533	6.681402
11	6	0	2.325341	1.243298	6.391558
12	8	0	1.626402	1.891244	5.583080
13	8	0	3.036286	1.975514	7.318542
14	6	0	3.305717	1.494805	8.683249
15	6	0	2.938110	2.068187	1.212731
16	6	0	4.038525	1.814406	2.269975
17	6	0	5.057321	0.885708	1.960818
18	6	0	6.072368	0.590541	2.875201
19	6	0	6.095571	1.219360	4.127078
20	6	0	5.109995	2.159402	4.436986
21	6	0	4.097041	2.460841	3.514998
22	6	0	1.893839	3.130481	1.594529

23	6	0	1.600815	4.194745	0.724170
24	6	0	0.617546	5.139574	1.042711
25	6	0	-0.099349	5.035572	2.238664
26	6	0	0.172086	3.972081	3.106330
27	6	0	1.150576	3.023498	2.785712
28	8	0	3.570926	2.412771	-0.057786
29	14	0	4.915904	3.447588	-0.525544
30	6	0	6.452085	2.375437	-0.892025
31	6	0	5.320059	4.786663	0.774001
32	6	0	4.325091	4.235574	-2.159154
33	6	0	0.287998	-2.464764	3.774226
34	6	0	0.183112	-3.138535	5.168746
35	6	0	0.708312	-2.159077	6.238338
36	6	0	1.273755	-0.847586	5.754216
37	6	0	1.604747	-1.701579	3.743380
38	8	0	0.583390	-2.396674	7.445466
39	6	0	0.939416	-4.451693	5.295560
40	8	0	2.052755	-4.714372	4.823015
41	8	0	0.220453	-5.349044	6.040655
42	6	0	0.864036	-6.638966	6.337856
43	6	0	2.050478	-0.745699	2.826900
44	6	0	0.121438	-3.473826	2.615201
45	1	0	-0.932016	0.368872	-0.425701
46	1	0	0.148847	-1.034502	-0.372449
47	1	0	-0.504823	-0.878012	1.957839
48	1	0	-0.475949	0.895706	1.929462
49	1	0	3.032960	0.034903	0.503387
50	1	0	0.905793	1.925197	-0.427923
51	1	0	1.673183	0.611226	-1.309477
52	1	0	5.453670	-2.810380	6.255284
53	1	0	4.258063	-4.157951	6.210147
54	1	0	4.659583	-3.332576	7.760934
55	1	0	3.158852	2.366567	9.322519
56	1	0	4.323806	1.118880	8.741039
57	1	0	2.603819	0.702766	8.959096
58	1	0	5.062136	0.397177	0.992348
59	1	0	6.838059	-0.133437	2.613157
60	1	0	6.863885	0.973675	4.852247
61	1	0	5.099677	2.642173	5.407778
62	1	0	3.345069	3.183694	3.795524
63	1	0	2.131882	4.271142	-0.214625
64	1	0	0.413872	5.953270	0.352954
65	1	0	-0.855553	5.772285	2.491663
66	1	0	-0.357971	3.877675	4.048384

67	1	0	1.343023	2.232398	3.498502
68	1	0	7.214946	2.986728	-1.389668
69	1	0	6.194806	1.545308	-1.558924
70	1	0	6.885114	1.964587	0.023971
71	1	0	6.094486	5.453005	0.374383
72	1	0	5.691152	4.345941	1.703647
73	1	0	4.437529	5.388915	1.010537
74	1	0	5.145155	4.790069	-2.630882
75	1	0	3.494580	4.930438	-1.998107
76	1	0	3.990126	3.460211	-2.856115
77	1	0	-0.554672	-1.759068	3.733591
78	1	0	-0.857933	-3.360371	5.423227
79	1	0	0.510879	-0.153196	5.398634
80	1	0	2.432511	-2.276128	4.151697
81	1	0	0.111607	-7.202750	6.884733
82	1	0	1.754019	-6.477220	6.949479
83	1	0	1.143768	-7.143313	5.410709
84	1	0	3.116482	-0.546970	2.867261
85	1	0	0.104174	-2.961458	1.647681
86	1	0	-0.815894	-4.035961	2.716338
87	1	0	0.953648	-4.182450	2.602334

Structure **rrrs-IM3**

E(RB3LYP) **=** -2266.99151 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.596466	1.434520	-0.397900
2	6	0	0.775555	1.724905	1.097969
3	7	0	1.521191	0.519977	1.584820
4	6	0	2.352826	-0.091493	0.458834
5	6	0	1.868712	0.652945	-0.806191
6	6	0	1.972914	2.277198	5.056807
7	6	0	2.558977	1.573387	6.143881
8	8	0	3.724824	1.611238	6.615084
9	8	0	1.637194	0.635653	6.694099
10	6	0	2.121419	-0.185960	7.796182
11	6	0	2.596880	3.320022	4.307583
12	8	0	2.226859	3.637728	3.129019
13	8	0	3.660225	4.067856	4.796944
14	6	0	3.763163	4.438974	6.212368
15	6	0	3.946419	-0.095013	0.640380

16	6	0	4.313942	-0.725068	2.003297
17	6	0	4.043950	-2.098332	2.194626
18	6	0	4.275200	-2.715268	3.427673
19	6	0	4.762427	-1.966508	4.508246
20	6	0	5.029520	-0.605728	4.336906
21	6	0	4.821396	0.005603	3.090688
22	6	0	4.550889	1.297639	0.394274
23	6	0	5.436484	1.535449	-0.670003
24	6	0	5.969105	2.811693	-0.891755
25	6	0	5.613469	3.882384	-0.064994
26	6	0	4.707731	3.667300	0.978811
27	6	0	4.184576	2.389067	1.200334
28	8	0	4.287433	-1.004241	-0.441668
29	14	0	5.677799	-2.004430	-0.868940
30	6	0	5.188266	-3.840182	-0.677729
31	6	0	7.227634	-1.599920	0.167500
32	6	0	5.962279	-1.674292	-2.726156
33	6	0	-0.955397	0.052286	3.810246
34	6	0	-1.507369	0.646244	5.132176
35	6	0	-0.545645	1.847071	5.438904
36	6	0	0.661607	1.803343	4.491663
37	6	0	0.589931	0.330497	3.939874
38	8	0	-0.791954	2.721440	6.262808
39	6	0	-1.536683	-0.301637	6.310083
40	8	0	-0.821032	-1.297757	6.484780
41	8	0	-2.479861	0.102656	7.217478
42	6	0	-2.547988	-0.635501	8.488016
43	6	0	1.405567	-0.045271	2.753651
44	6	0	-1.332722	-1.401063	3.492637
45	1	0	0.480109	2.357469	-0.971569
46	1	0	-0.301907	0.825876	-0.556768
47	1	0	-0.166158	1.809757	1.638047
48	1	0	1.379651	2.608952	1.327033
49	1	0	2.083198	-1.148815	0.426724
50	1	0	2.645353	1.340613	-1.146223
51	1	0	1.678178	-0.053091	-1.616473
52	1	0	3.080083	-0.645921	7.544070
53	1	0	1.348166	-0.940210	7.939280
54	1	0	2.251976	0.419748	8.697759
55	1	0	4.260971	5.410393	6.213633
56	1	0	4.336991	3.690109	6.755191
57	1	0	2.765282	4.526520	6.653982
58	1	0	3.645433	-2.682635	1.373116
59	1	0	4.063449	-3.773376	3.548377

60	1	0	4.921630	-2.437756	5.472498
61	1	0	5.358110	0.002112	5.172490
62	1	0	5.049180	1.057209	2.990041
63	1	0	5.692023	0.735233	-1.348287
64	1	0	6.654706	2.965915	-1.719687
65	1	0	6.027002	4.870661	-0.239154
66	1	0	4.385694	4.468276	1.634640
67	1	0	3.477006	2.288701	2.011074
68	1	0	5.916757	-4.465532	-1.208013
69	1	0	4.202196	-4.026461	-1.117218
70	1	0	5.169962	-4.156644	0.368808
71	1	0	8.077059	-2.179109	-0.215063
72	1	0	7.082293	-1.858725	1.220120
73	1	0	7.483238	-0.537802	0.109206
74	1	0	6.688769	-2.393648	-3.122819
75	1	0	6.343661	-0.667374	-2.920509
76	1	0	5.025134	-1.794932	-3.279767
77	1	0	-1.349479	0.690541	3.005615
78	1	0	-2.514839	1.055880	5.018315
79	1	0	0.421978	2.503522	3.678191
80	1	0	0.945794	-0.312468	4.750520
81	1	0	-3.376148	-0.180224	9.026575
82	1	0	-1.611641	-0.516186	9.036863
83	1	0	-2.730487	-1.695636	8.300110
84	1	0	1.996527	-0.949108	2.863676
85	1	0	-0.960928	-1.689376	2.501416
86	1	0	-2.422496	-1.523051	3.480194
87	1	0	-0.921970	-2.086658	4.236784

Structure **rrsr-TS2**

Imaginary Frequency: -244

E(RB3LYP) = -2266.971478 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.028777	-0.041600	-0.008831
2	6	0	0.016531	-0.015350	1.523992
3	7	0	1.457408	-0.007104	1.884139
4	6	0	2.307087	0.457643	0.724660
5	6	0	1.255324	0.817537	-0.352452
6	6	0	2.462172	-4.158957	2.946395
7	6	0	2.366504	-5.029281	4.114403

8	8	0	1.440644	-4.922549	4.955558
9	8	0	3.336482	-5.985152	4.253168
10	6	0	3.215802	-6.862879	5.424037
11	6	0	3.617265	-3.950621	2.081166
12	8	0	3.683636	-3.024846	1.229482
13	8	0	4.665096	-4.819412	2.249384
14	6	0	5.820086	-4.630619	1.367467
15	6	0	3.291276	1.657716	1.011717
16	6	0	3.762974	2.201347	-0.367091
17	6	0	4.564743	1.407680	-1.207100
18	6	0	4.973431	1.881778	-2.457189
19	6	0	4.597203	3.161322	-2.883849
20	6	0	3.808009	3.958585	-2.049187
21	6	0	3.390106	3.480841	-0.800864
22	6	0	4.577336	1.294622	1.796231
23	6	0	5.114649	-0.003642	1.858066
24	6	0	6.333427	-0.241038	2.510826
25	6	0	7.046287	0.807788	3.095401
26	6	0	6.537304	2.109568	3.008767
27	6	0	5.323620	2.346872	2.359737
28	8	0	2.546454	2.704605	1.652942
29	14	0	2.115442	3.385698	3.198908
30	6	0	2.727769	2.412396	4.722551
31	6	0	0.213102	3.513175	3.215730
32	6	0	2.834328	5.155943	3.222718
33	6	0	0.147074	-1.571479	4.701815
34	6	0	-0.685631	-2.846408	4.262487
35	6	0	-0.038573	-3.628502	3.124863
36	6	0	1.375143	-3.322586	2.693744
37	6	0	1.487543	-1.459372	3.961605
38	8	0	-0.666979	-4.493836	2.497104
39	6	0	-0.682675	-0.272894	4.809840
40	6	0	1.999618	-0.662832	2.936455
41	1	0	-0.897382	0.352093	-0.438059
42	1	0	0.157968	-1.069998	-0.367682
43	1	0	-0.490052	-0.875652	1.960393
44	1	0	-0.468077	0.896773	1.890344
45	1	0	2.894987	-0.402832	0.387427
46	1	0	1.007239	1.880785	-0.274445
47	1	0	1.637467	0.633717	-1.357950
48	1	0	4.063811	-7.540360	5.344013
49	1	0	2.269662	-7.407462	5.393491
50	1	0	3.262409	-6.278364	6.345671
51	1	0	6.491386	-5.449535	1.619109

52	1	0	6.295035	-3.664403	1.556718
53	1	0	5.513981	-4.678008	0.320152
54	1	0	4.888087	0.423882	-0.882946
55	1	0	5.591450	1.255152	-3.092793
56	1	0	4.919590	3.531665	-3.851918
57	1	0	3.513768	4.954206	-2.367630
58	1	0	2.774485	4.089683	-0.152272
59	1	0	4.610358	-0.852724	1.408771
60	1	0	6.719989	-1.254589	2.556295
61	1	0	7.988532	0.619014	3.599659
62	1	0	7.090709	2.940762	3.434879
63	1	0	4.959732	3.362723	2.263470
64	1	0	2.338282	2.900037	5.625321
65	1	0	3.819224	2.399285	4.782489
66	1	0	2.372475	1.377874	4.714012
67	1	0	-0.109083	4.169094	4.033541
68	1	0	-0.256627	2.536176	3.360700
69	1	0	-0.151651	3.937659	2.274616
70	1	0	2.462755	5.696732	4.101571
71	1	0	2.527894	5.708659	2.328319
72	1	0	3.928050	5.155766	3.264657
73	1	0	0.448458	-1.797861	5.730986
74	1	0	1.428386	-2.790494	1.747786
75	1	0	2.299977	-1.830653	4.579907
76	1	0	-0.049307	0.538851	5.182148
77	1	0	-1.501991	-0.412976	5.524578
78	1	0	-1.121532	0.037761	3.861689
79	1	0	3.081049	-0.647938	2.905646
80	6	0	-2.150483	-2.584924	3.981258
81	8	0	-3.081942	-2.820329	4.753833
82	8	0	-2.350332	-2.002777	2.745495
83	6	0	-3.748115	-1.780194	2.341137
84	1	0	-4.239750	-1.100486	3.040207
85	1	0	-3.685010	-1.346120	1.345339
86	1	0	-4.281656	-2.732119	2.321491
87	1	0	-0.680247	-3.547894	5.103203

Structure **rrsr-IM3**

E(RB3LYP) = -2266.989534 a.u.

Standard orientation:

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

1	6	0	0.618766	-1.755058	1.117447
2	6	0	0.342958	-0.393770	1.757421
3	7	0	1.638248	-0.056943	2.419941
4	6	0	2.786157	-0.819965	1.758888
5	6	0	2.070706	-1.603611	0.634434
6	6	0	0.956885	-1.009979	6.376092
7	6	0	0.513044	-0.434782	7.607303
8	8	0	-0.387227	0.458343	7.652234
9	8	0	1.116764	-0.868413	8.770649
10	6	0	0.639997	-0.247144	10.006653
11	6	0	2.150401	-1.707493	6.082988
12	8	0	2.601807	-1.844424	4.886423
13	8	0	2.873669	-2.226327	7.144301
14	6	0	4.111474	-2.923684	6.816500
15	6	0	3.987672	0.049425	1.232237
16	6	0	4.796189	-0.843472	0.250564
17	6	0	5.513804	-1.951639	0.735444
18	6	0	6.227891	-2.773714	-0.140897
19	6	0	6.245694	-2.494651	-1.513355
20	6	0	5.540748	-1.389429	-1.999519
21	6	0	4.815864	-0.571194	-1.123601
22	6	0	4.987286	0.529065	2.313382
23	6	0	5.043101	0.011722	3.619810
24	6	0	6.029975	0.451503	4.516543
25	6	0	6.983988	1.391973	4.124130
26	6	0	6.960864	1.882552	2.811839
27	6	0	5.980738	1.446558	1.918459
28	8	0	3.409372	1.135707	0.483817
29	14	0	3.195115	2.869030	0.460675
30	6	0	3.281379	3.687166	2.184187
31	6	0	1.471210	3.093316	-0.316902
32	6	0	4.490627	3.655298	-0.702878
33	6	0	-0.477953	1.852607	4.444220
34	6	0	-1.741504	1.080111	4.959453
35	6	0	-1.291045	-0.337474	5.352428
36	6	0	0.213093	-0.538806	5.173360
37	6	0	0.765865	0.876466	4.615156
38	8	0	-2.073697	-1.237584	5.658689
39	6	0	-0.637622	2.565997	3.091500
40	6	0	1.774250	0.551876	3.574279
41	1	0	-0.077405	-1.973178	0.303013
42	1	0	0.532853	-2.550856	1.866011
43	1	0	-0.482786	-0.381932	2.465917
44	1	0	0.158036	0.362568	0.986608

45	1	0	3.130253	-1.513367	2.531233
46	1	0	2.102959	-1.024202	-0.293453
47	1	0	2.560572	-2.561320	0.453168
48	1	0	1.207491	-0.737838	10.796503
49	1	0	-0.432459	-0.413847	10.131834
50	1	0	0.830527	0.829417	9.999965
51	1	0	4.446795	-3.346883	7.762860
52	1	0	4.863629	-2.232318	6.422398
53	1	0	3.935357	-3.709916	6.078260
54	1	0	5.531891	-2.165653	1.799404
55	1	0	6.776356	-3.625418	0.248969
56	1	0	6.805877	-3.129486	-2.192387
57	1	0	5.550676	-1.161909	-3.061131
58	1	0	4.261474	0.280914	-1.494522
59	1	0	4.337392	-0.735740	3.972203
60	1	0	6.044260	0.047924	5.524154
61	1	0	7.744056	1.727961	4.821880
62	1	0	7.714072	2.590811	2.480937
63	1	0	6.003579	1.795154	0.892462
64	1	0	2.989150	4.740672	2.091871
65	1	0	4.291646	3.645336	2.599139
66	1	0	2.600340	3.212246	2.896876
67	1	0	1.263056	4.157241	-0.480674
68	1	0	0.683942	2.688369	0.325778
69	1	0	1.421011	2.583001	-1.284476
70	1	0	4.200410	4.690056	-0.922545
71	1	0	4.541855	3.110356	-1.651367
72	1	0	5.492373	3.673871	-0.263647
73	1	0	-0.295563	2.641225	5.180596
74	1	0	0.338010	-1.294236	4.390042
75	1	0	1.350276	1.296875	5.434817
76	1	0	0.285237	3.089903	2.822387
77	1	0	-1.432397	3.317810	3.163912
78	1	0	-0.904726	1.887231	2.280596
79	1	0	2.802312	0.690816	3.878281
80	6	0	-2.920483	1.041131	4.017871
81	8	0	-3.974798	1.664994	4.148479
82	8	0	-2.696010	0.202473	2.936991
83	6	0	-3.828984	0.003492	2.017793
84	1	0	-4.119360	0.953386	1.564148
85	1	0	-3.463583	-0.697298	1.269614
86	1	0	-4.676956	-0.413423	2.563878
87	1	0	-2.103497	1.549670	5.877366

Structure **rrss-TS2**

Imaginary Frequency: -204

E(RB3LYP) = -2266.967478 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.104342	0.227818	0.140646
2	6	0	-0.067563	0.181542	1.676657
3	7	0	1.385752	0.135940	1.981279
4	6	0	2.210486	0.674332	0.839283
5	6	0	1.156554	1.033306	-0.236225
6	6	0	1.124140	-3.470415	1.732515
7	6	0	-0.034721	-3.349613	0.874864
8	8	0	-0.036912	-3.288326	-0.374198
9	8	0	-1.225294	-3.258198	1.594776
10	6	0	-2.478890	-3.155213	0.837832
11	6	0	2.482404	-3.509913	1.148678
12	8	0	3.433285	-2.899759	1.678920
13	8	0	2.763808	-4.233363	0.013338
14	6	0	1.939665	-5.353188	-0.454357
15	6	0	3.257487	1.832422	1.135776
16	6	0	4.289405	1.373516	2.191598
17	6	0	5.314949	0.489964	1.812819
18	6	0	6.236671	0.022425	2.754233
19	6	0	6.152946	0.434077	4.090019
20	6	0	5.138454	1.316117	4.475297
21	6	0	4.213096	1.782555	3.533527
22	6	0	2.694617	3.210327	1.523193
23	6	0	3.539096	4.329186	1.385815
24	6	0	3.112844	5.606619	1.756123
25	6	0	1.830462	5.794921	2.288286
26	6	0	0.992988	4.689992	2.457676
27	6	0	1.424189	3.409341	2.083640
28	8	0	3.989834	1.914758	-0.116646
29	14	0	4.081073	2.684260	-1.677251
30	6	0	4.150490	1.257281	-2.938326
31	6	0	5.725967	3.651026	-1.715332
32	6	0	2.632169	3.862856	-2.092936
33	6	0	0.252944	-1.220278	4.947567
34	6	0	-0.770257	-2.399328	4.763475
35	6	0	-0.139969	-3.582075	3.983115
36	6	0	1.081897	-3.333656	3.127114

37	6	0	1.483560	-1.330212	4.034176
38	8	0	-0.537774	-4.739019	4.160073
39	6	0	-2.136880	-2.044667	4.202418
40	8	0	-2.419371	-1.177038	3.365984
41	8	0	-3.095208	-2.831118	4.791092
42	6	0	-4.484968	-2.657245	4.343435
43	6	0	1.970516	-0.592480	2.953279
44	6	0	-0.377522	0.184512	5.067851
45	1	0	-1.022294	0.692941	-0.231454
46	1	0	-0.048115	-0.785574	-0.268890
47	1	0	-0.572266	-0.684988	2.099029
48	1	0	-0.534209	1.075301	2.108739
49	1	0	2.843218	-0.148714	0.490391
50	1	0	0.943821	2.106321	-0.218962
51	1	0	1.516936	0.778826	-1.234702
52	1	0	-3.011551	-2.291823	1.235404
53	1	0	-3.045197	-4.074028	1.007761
54	1	0	-2.255551	-3.035318	-0.222679
55	1	0	2.648185	-6.064979	-0.879321
56	1	0	1.234838	-4.997912	-1.203422
57	1	0	1.398794	-5.813506	0.378087
58	1	0	5.385318	0.178482	0.778847
59	1	0	7.016105	-0.665891	2.443948
60	1	0	6.870048	0.071896	4.820068
61	1	0	5.065602	1.646611	5.507019
62	1	0	3.435085	2.468329	3.847994
63	1	0	4.542598	4.185735	1.002712
64	1	0	3.783445	6.452388	1.639613
65	1	0	1.496219	6.786532	2.576073
66	1	0	0.002469	4.816521	2.883705
67	1	0	0.766873	2.568796	2.250025
68	1	0	4.313955	1.649447	-3.949326
69	1	0	3.220893	0.679118	-2.943285
70	1	0	4.970612	0.572980	-2.698063
71	1	0	5.942616	3.986390	-2.736777
72	1	0	6.549925	3.012231	-1.381327
73	1	0	5.693360	4.533520	-1.068306
74	1	0	2.535708	4.663147	-1.354015
75	1	0	1.677029	3.333604	-2.156447
76	1	0	2.829514	4.320808	-3.070533
77	1	0	0.670407	-1.418017	5.945012
78	1	0	-0.997787	-2.829679	5.744622
79	1	0	1.999968	-3.638937	3.622249
80	1	0	2.331635	-1.730965	4.585322

81	1	0	-5.071091	-3.275421	5.019956
82	1	0	-4.591363	-3.001847	3.312881
83	1	0	-4.775650	-1.606934	4.410849
84	1	0	3.032404	-0.718031	2.787620
85	1	0	0.406899	0.912547	5.299829
86	1	0	-1.105976	0.203258	5.888439
87	1	0	-0.896312	0.498408	4.164172

Structure **rrss-IM3**

E(RB3LYP) **=** -2266.977709 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.133269	0.826593	0.530126
2	6	0	0.137197	1.228293	1.994713
3	7	0	1.407518	0.520988	2.322819
4	6	0	2.260434	0.383536	1.083370
5	6	0	1.230002	0.363892	-0.069176
6	6	0	0.862928	-2.565256	3.536823
7	6	0	-0.036029	-2.481468	2.451971
8	8	0	0.045586	-2.934231	1.280241
9	8	0	-1.155873	-1.630988	2.772718
10	6	0	-2.365680	-1.824067	1.977991
11	6	0	2.176893	-3.165375	3.474509
12	8	0	3.134479	-2.721471	4.168956
13	8	0	2.471006	-4.235461	2.646509
14	6	0	1.460476	-5.230683	2.271888
15	6	0	3.495799	1.385637	0.995715
16	6	0	4.397493	1.063274	2.207641
17	6	0	5.289793	-0.019305	2.137549
18	6	0	6.034084	-0.408123	3.256183
19	6	0	5.900554	0.280287	4.466467
20	6	0	5.012219	1.357866	4.550929
21	6	0	4.260971	1.742180	3.433351
22	6	0	3.240400	2.901635	0.854591
23	6	0	4.291752	3.791672	1.163141
24	6	0	4.169325	5.168632	0.957577
25	6	0	2.985396	5.701041	0.435139
26	6	0	1.936064	4.836024	0.115287
27	6	0	2.066343	3.455425	0.314435
28	8	0	4.105772	0.879806	-0.224835
29	14	0	5.240011	1.444894	-1.442992

30	6	0	5.494801	-0.133298	-2.473054
31	6	0	6.897931	2.023438	-0.686563
32	6	0	4.478435	2.827412	-2.516849
33	6	0	0.117439	0.579547	5.566031
34	6	0	-1.220641	-0.215574	5.648455
35	6	0	-0.845877	-1.692796	5.280770
36	6	0	0.612764	-1.782898	4.826113
37	6	0	1.157145	-0.304408	4.792532
38	8	0	-1.586624	-2.650474	5.490279
39	6	0	-2.408602	0.282781	4.868612
40	8	0	-2.411563	0.958231	3.827650
41	8	0	-3.570141	-0.109175	5.481146
42	6	0	-4.834547	0.225609	4.809683
43	6	0	1.728400	-0.132873	3.403523
44	6	0	0.049211	2.082074	5.247955
45	1	0	-0.578594	1.658298	-0.025398
46	1	0	-0.841357	-0.003090	0.506794
47	1	0	-0.656561	0.914607	2.667003
48	1	0	0.310186	2.303164	2.100909
49	1	0	2.750669	-0.588206	1.147693
50	1	0	1.568620	0.971740	-0.908198
51	1	0	1.136071	-0.663953	-0.427557
52	1	0	-2.833941	-0.844559	1.874237
53	1	0	-3.034749	-2.509728	2.508537
54	1	0	-2.098184	-2.241245	1.004736
55	1	0	2.013325	-6.164778	2.159417
56	1	0	0.973248	-4.934695	1.344879
57	1	0	0.709911	-5.328415	3.062602
58	1	0	5.381236	-0.565237	1.206600
59	1	0	6.701496	-1.260035	3.185936
60	1	0	6.471950	-0.027320	5.335740
61	1	0	4.899396	1.899415	5.485203
62	1	0	3.577640	2.580697	3.515031
63	1	0	5.212421	3.402356	1.579205
64	1	0	4.997590	5.823260	1.209928
65	1	0	2.884471	6.770122	0.279185
66	1	0	1.012388	5.228943	-0.297891
67	1	0	1.241814	2.824458	0.024471
68	1	0	6.160439	0.060700	-3.322285
69	1	0	4.537510	-0.496433	-2.860236
70	1	0	5.935691	-0.929433	-1.864643
71	1	0	7.645322	2.107058	-1.485346
72	1	0	7.267255	1.304735	0.051680
73	1	0	6.810517	3.000837	-0.203166

74	1	0	4.310144	3.745783	-1.947234
75	1	0	3.522489	2.506652	-2.944043
76	1	0	5.159499	3.057318	-3.345697
77	1	0	0.503406	0.527488	6.594565
78	1	0	-1.565074	-0.264719	6.687298
79	1	0	1.145664	-2.314385	5.625525
80	1	0	2.080803	-0.282293	5.385914
81	1	0	-5.607551	-0.131269	5.486661
82	1	0	-4.893065	-0.284973	3.846393
83	1	0	-4.906877	1.304453	4.656763
84	1	0	2.657270	-0.695218	3.337442
85	1	0	1.061506	2.502706	5.209201
86	1	0	-0.492515	2.608285	6.043049
87	1	0	-0.460670	2.298572	4.311439

Structure **ess-IM1**

E(RB3LYP) **=** -2266.968881a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.186670	-0.117940	-0.281696
2	6	0	0.059538	-0.148881	1.247577
3	7	0	1.468073	-0.077174	1.741510
4	6	0	2.462405	0.006491	0.626234
5	6	0	1.636102	-0.576034	-0.549736
6	6	0	3.086296	1.436955	0.297458
7	6	0	3.854314	2.063712	1.489847
8	6	0	3.122686	2.575926	2.583482
9	6	0	3.778404	3.221150	3.640189
10	6	0	5.169921	3.362987	3.638782
11	6	0	5.903953	2.861943	2.561047
12	6	0	5.253019	2.227354	1.496521
13	8	0	1.975954	2.275374	-0.075605
14	14	0	1.674890	4.023444	-0.159379
15	6	0	0.528739	4.139573	-1.681555
16	6	0	3.292365	5.001953	-0.455209
17	6	0	0.767134	4.690777	1.371619
18	6	0	1.764832	-0.201502	3.021880
19	6	0	0.829725	-0.532986	4.034924
20	6	0	4.005154	1.170438	-0.925047
21	6	0	3.772752	1.805613	-2.153667
22	6	0	4.572810	1.535081	-3.270977

23	6	0	5.615724	0.608544	-3.187152
24	6	0	5.847654	-0.050090	-1.974457
25	6	0	5.049654	0.225271	-0.859456
26	6	0	1.156306	-0.538399	5.363137
27	6	0	0.670377	2.364488	5.676766
28	6	0	0.578757	2.366075	7.102697
29	8	0	-0.388232	2.047216	7.842650
30	8	0	1.808715	2.717889	7.682353
31	6	0	1.843020	2.738267	9.143158
32	6	0	-0.371405	2.239470	4.739443
33	8	0	-0.131872	2.168133	3.465298
34	6	0	-1.777077	2.149266	5.201606
35	6	0	-2.846527	2.224270	4.380087
36	6	0	-2.790076	2.531797	2.916356
37	8	0	-2.708909	3.656210	2.419035
38	8	0	-2.975094	1.394609	2.149781
39	6	0	-3.174995	1.627236	0.713721
40	6	0	-4.199120	2.082920	4.966012
41	8	0	-4.461759	1.790740	6.140384
42	8	0	-5.185815	2.320915	4.029916
43	6	0	-6.570783	2.224413	4.502116
44	1	0	0.053083	0.897595	-0.653853
45	1	0	-0.546685	-0.774342	-0.759414
46	1	0	-0.378627	-1.093120	1.593044
47	1	0	-0.497197	0.678791	1.694886
48	1	0	3.297165	-0.646540	0.892073
49	1	0	2.008012	-0.240184	-1.516530
50	1	0	1.702775	-1.671168	-0.522617
51	1	0	2.040120	2.493163	2.619191
52	1	0	3.196286	3.624266	4.461655
53	1	0	5.670062	3.866394	4.459898
54	1	0	6.983143	2.977165	2.532764
55	1	0	5.847827	1.890120	0.659312
56	1	0	0.219540	5.179601	-1.838886
57	1	0	-0.374919	3.540620	-1.524472
58	1	0	1.017463	3.786086	-2.595433
59	1	0	3.041110	6.062660	-0.580266
60	1	0	3.823192	4.667654	-1.351474
61	1	0	3.970029	4.913042	0.399012
62	1	0	0.179060	5.568708	1.076487
63	1	0	1.469847	4.996784	2.152227
64	1	0	0.083620	3.957850	1.811238
65	1	0	2.810452	-0.083210	3.290107
66	1	0	-0.196456	-0.734289	3.751081

67	1	0	2.946988	2.496711	-2.242180
68	1	0	4.371580	2.044824	-4.208029
69	1	0	6.234533	0.396847	-4.053028
70	1	0	6.648411	-0.778572	-1.893737
71	1	0	5.259769	-0.295596	0.069368
72	1	0	1.658841	2.530904	5.275169
73	1	0	2.859038	3.040355	9.395964
74	1	0	1.617315	1.749955	9.553081
75	1	0	1.115616	3.452705	9.536783
76	1	0	-1.948387	2.010865	6.265603
77	1	0	-3.341871	0.638025	0.289951
78	1	0	-2.293748	2.101974	0.275941
79	1	0	-4.043344	2.271540	0.558270
80	1	0	-7.179177	2.455093	3.629710
81	1	0	-6.745927	2.942881	5.305914
82	1	0	-6.774605	1.216418	4.870658
83	6	0	0.229927	-0.988267	6.445938
84	1	0	-0.010757	-0.171696	7.141333
85	1	0	-0.712720	-1.365856	6.038515
86	1	0	0.696691	-1.784650	7.042332
87	1	0	2.168751	-0.268074	5.661644

Structure **ess-TS1**

Imaginary Frequency: -169

E(RB3LYP) = -2266.96265 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.198885	-0.059067	-0.268181
2	6	0	0.009239	0.028990	1.256006
3	7	0	1.387551	0.036526	1.809910
4	6	0	2.428583	0.044806	0.752039
5	6	0	1.648413	-0.565473	-0.441505
6	6	0	3.089984	1.455417	0.406761
7	6	0	3.828884	2.096041	1.609272
8	6	0	3.071492	2.618886	2.679015
9	6	0	3.696227	3.276811	3.745588
10	6	0	5.087073	3.422053	3.778722
11	6	0	5.848594	2.910493	2.725041
12	6	0	5.226528	2.262553	1.650844
13	8	0	1.998635	2.307081	-0.008317
14	14	0	1.732263	4.054418	-0.121723

15	6	0	0.618170	4.176951	-1.667426
16	6	0	3.365315	5.012968	-0.391682
17	6	0	0.802764	4.759012	1.382814
18	6	0	1.615453	-0.108173	3.122236
19	6	0	0.623501	-0.283537	4.083553
20	6	0	4.036866	1.162038	-0.783602
21	6	0	3.844214	1.772554	-2.031596
22	6	0	4.672376	1.471878	-3.120294
23	6	0	5.704876	0.539313	-2.987580
24	6	0	5.897270	-0.095051	-1.755135
25	6	0	5.071050	0.210103	-0.668816
26	6	0	0.885746	-0.317450	5.459756
27	6	0	0.984976	1.943827	6.008264
28	6	0	1.083997	1.889711	7.446735
29	8	0	0.172280	1.905843	8.303907
30	8	0	2.416321	1.718910	7.836708
31	6	0	2.657842	1.624555	9.278122
32	6	0	-0.145447	2.378580	5.244122
33	8	0	-0.043893	2.521627	3.974906
34	6	0	-1.463308	2.565628	5.894109
35	6	0	-2.592460	2.860099	5.215347
36	6	0	-2.675471	3.096020	3.737717
37	8	0	-2.590411	4.191864	3.181683
38	8	0	-2.989996	1.935184	3.061720
39	6	0	-3.271208	2.092504	1.629054
40	6	0	-3.855586	3.011911	5.977575
41	8	0	-3.985433	2.894795	7.203023
42	8	0	-4.915520	3.301779	5.146576
43	6	0	-6.220110	3.493707	5.790352
44	1	0	0.100481	0.926798	-0.722581
45	1	0	-0.529301	-0.735834	-0.725679
46	1	0	-0.518997	-0.849127	1.648519
47	1	0	-0.517800	0.924622	1.597323
48	1	0	3.240807	-0.612194	1.075718
49	1	0	2.074257	-0.285897	-1.404231
50	1	0	1.682980	-1.659321	-0.360979
51	1	0	1.991123	2.537923	2.692715
52	1	0	3.086016	3.683484	4.544757
53	1	0	5.566075	3.934002	4.607153
54	1	0	6.928105	3.026555	2.723606
55	1	0	5.843330	1.914943	0.833767
56	1	0	0.315388	5.217831	-1.831714
57	1	0	-0.289189	3.578069	-1.533461
58	1	0	1.127947	3.823063	-2.569618

59	1	0	3.129230	6.074207	-0.539492
60	1	0	3.911541	4.657670	-1.270471
61	1	0	4.023038	4.929283	0.478367
62	1	0	0.273399	5.669174	1.073826
63	1	0	1.490292	5.023276	2.191035
64	1	0	0.064508	4.068139	1.800203
65	1	0	2.658874	-0.094810	3.423820
66	1	0	-0.415043	-0.283744	3.773363
67	1	0	3.026732	2.467854	-2.157843
68	1	0	4.501511	1.962836	-4.073359
69	1	0	6.345889	0.304351	-3.831086
70	1	0	6.689140	-0.828193	-1.636912
71	1	0	5.248605	-0.293197	0.276294
72	1	0	1.933727	2.002943	5.494626
73	1	0	3.735430	1.498039	9.373369
74	1	0	2.124136	0.771583	9.704745
75	1	0	2.325533	2.535183	9.782276
76	1	0	-1.516147	2.455276	6.973200
77	1	0	-3.542348	1.095286	1.286063
78	1	0	-2.387142	2.464714	1.106219
79	1	0	-4.095024	2.795092	1.484393
80	1	0	-6.900021	3.731244	4.974706
81	1	0	-6.166366	4.312624	6.510911
82	1	0	-6.523911	2.579600	6.305434
83	1	0	1.921171	-0.371561	5.791715
84	6	0	-0.148705	-0.845227	6.419343
85	1	0	-0.011084	-1.930503	6.540807
86	1	0	-0.082389	-0.392820	7.411702
87	1	0	-1.162094	-0.680644	6.039315

Structure **ess-IM2**

E(RB3LYP) **=** -2266.989948 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.320672	-0.227976	-0.243414
2	6	0	0.148561	-0.118551	1.290364
3	7	0	1.519749	-0.061739	1.820451
4	6	0	2.541410	0.039739	0.774338
5	6	0	1.815598	-0.569182	-0.453078
6	6	0	3.120882	1.497680	0.479170
7	6	0	3.637249	2.212381	1.750439

8	6	0	2.720227	2.545029	2.768890
9	6	0	3.124177	3.232203	3.918311
10	6	0	4.461160	3.617425	4.073570
11	6	0	5.381168	3.311050	3.066827
12	6	0	4.973956	2.619081	1.918702
13	8	0	2.009533	2.248930	-0.079824
14	14	0	1.580335	3.945439	-0.227085
15	6	0	0.763390	4.046354	-1.949888
16	6	0	3.081075	5.123549	-0.132479
17	6	0	0.269789	4.404063	1.083215
18	6	0	1.802870	-0.373264	3.133230
19	6	0	0.908435	-0.490437	4.143934
20	6	0	4.219250	1.298002	-0.587092
21	6	0	4.100491	1.850700	-1.870962
22	6	0	5.077820	1.627468	-2.848890
23	6	0	6.192572	0.833199	-2.565885
24	6	0	6.317533	0.259581	-1.295332
25	6	0	5.341435	0.486820	-0.320049
26	6	0	1.312332	-0.869604	5.541774
27	6	0	1.533569	0.447230	6.463412
28	6	0	2.058872	0.039667	7.815622
29	8	0	1.412505	-0.167040	8.852640
30	8	0	3.420908	-0.144590	7.756751
31	6	0	4.082353	-0.601950	8.990007
32	6	0	0.302219	1.331914	6.469457
33	8	0	0.247415	2.283464	5.656856
34	6	0	-0.845090	1.027615	7.355800
35	6	0	-2.085792	1.517457	7.147520
36	6	0	-2.444959	2.443682	6.025103
37	8	0	-2.658850	3.648872	6.154712
38	8	0	-2.555889	1.766853	4.838254
39	6	0	-2.821067	2.589821	3.648060
40	6	0	-3.161705	1.146933	8.106097
41	8	0	-3.002552	0.486082	9.139994
42	8	0	-4.384216	1.609134	7.693894
43	6	0	-5.530884	1.319218	8.566388
44	1	0	0.092525	0.725909	-0.721061
45	1	0	-0.336645	-0.994656	-0.666432
46	1	0	-0.358015	-0.995221	1.719984
47	1	0	-0.432413	0.768869	1.576735
48	1	0	3.400113	-0.573098	1.070270
49	1	0	2.196881	-0.186970	-1.400509
50	1	0	1.964237	-1.655911	-0.441212
51	1	0	1.682620	2.261686	2.670393

52	1	0	2.385951	3.451465	4.682463
53	1	0	4.778382	4.153121	4.962918
54	1	0	6.418857	3.615785	3.164364
55	1	0	5.705813	2.417120	1.147993
56	1	0	0.339467	5.045091	-2.109448
57	1	0	-0.046665	3.314053	-2.033612
58	1	0	1.480818	3.850277	-2.753494
59	1	0	2.749734	6.142814	-0.366898
60	1	0	3.854213	4.841208	-0.854294
61	1	0	3.529216	5.127348	0.864706
62	1	0	-0.172859	5.376582	0.835424
63	1	0	0.700777	4.467200	2.085745
64	1	0	-0.532912	3.658406	1.097547
65	1	0	2.861595	-0.530641	3.331030
66	1	0	-0.142162	-0.262017	3.983847
67	1	0	3.224362	2.437011	-2.110501
68	1	0	4.960400	2.069454	-3.833668
69	1	0	6.949745	0.657757	-3.323397
70	1	0	7.173795	-0.365603	-1.061379
71	1	0	5.467652	0.038524	0.660262
72	1	0	2.317369	1.011546	5.954707
73	1	0	5.132713	-0.693280	8.721714
74	1	0	3.668954	-1.562072	9.305843
75	1	0	3.940274	0.132071	9.785704
76	1	0	-0.667859	0.392457	8.217160
77	1	0	-2.963461	1.873333	2.841359
78	1	0	-1.962469	3.237060	3.456412
79	1	0	-3.714673	3.198027	3.800993
80	1	0	-6.379517	1.784262	8.069855
81	1	0	-5.364949	1.751165	9.555375
82	1	0	-5.666711	0.239557	8.659065
83	1	0	2.312378	-1.322913	5.520266
84	6	0	0.327855	-1.873365	6.173817
85	1	0	-0.694868	-1.479587	6.174105
86	1	0	0.323774	-2.795380	5.582772
87	1	0	0.591868	-2.126625	7.205590

Structure **zss-IM1**

E(RB3LYP) = -2266.963702 a.u.

Standard orientation:

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

1	6	0	0.081061	-0.007001	0.451715
2	6	0	0.289990	0.063897	1.970736
3	7	0	1.770465	0.164783	2.151270
4	6	0	2.516603	-0.011613	0.857225
5	6	0	1.424896	-0.536249	-0.097707
6	6	0	3.263722	1.300834	0.363023
7	6	0	4.426300	1.678867	1.311716
8	6	0	5.291793	0.668966	1.785467
9	6	0	6.371078	0.976887	2.620804
10	6	0	6.635097	2.306136	2.973705
11	6	0	5.813766	3.321264	2.475741
12	6	0	4.720776	3.010816	1.655661
13	6	0	2.247932	2.434411	0.132712
14	6	0	1.670335	3.134824	1.211118
15	6	0	0.690723	4.110018	0.994654
16	6	0	0.263187	4.406118	-0.304944
17	6	0	0.824829	3.715071	-1.382978
18	6	0	1.803939	2.738142	-1.164498
19	8	0	3.815817	0.858363	-0.910040
20	14	0	5.177166	1.367235	-1.908653
21	6	0	4.667131	0.694126	-3.616280
22	6	0	6.803280	0.548967	-1.337826
23	6	0	5.385028	3.265707	-1.964133
24	6	0	2.342208	0.185505	3.340990
25	6	0	1.651836	0.287421	4.576275
26	6	0	2.262788	0.158338	5.796556
27	6	0	0.856046	-3.041384	4.102205
28	6	0	1.943442	-3.033386	3.191025
29	6	0	3.341235	-2.974519	3.704829
30	6	0	4.416772	-3.215147	2.924012
31	6	0	4.327221	-3.698991	1.508346
32	8	0	4.188533	-4.862353	1.140327
33	8	0	4.545787	-2.653266	0.621929
34	6	0	4.448261	-2.991780	-0.806206
35	6	0	5.771878	-3.023306	3.480194
36	8	0	6.061085	-2.351596	4.485246
37	8	0	6.729499	-3.662260	2.726330
38	6	0	8.119128	-3.554769	3.183535
39	8	0	1.775189	-3.075380	1.916296
40	6	0	0.904577	-2.801724	5.502233
41	8	0	1.877566	-2.364406	6.181883
42	8	0	-0.277133	-2.983156	6.251178
43	6	0	-1.429910	-3.661801	5.681334
44	1	0	-0.148708	0.982799	0.049160

45	1	0	-0.747195	-0.675865	0.202241
46	1	0	-0.031739	-0.853587	2.477843
47	1	0	-0.200184	0.925379	2.433071
48	1	0	3.269600	-0.784413	1.002104
49	1	0	1.619566	-0.227794	-1.124815
50	1	0	1.437660	-1.627630	-0.038726
51	1	0	5.140707	-0.364785	1.493208
52	1	0	6.994269	0.174682	3.002046
53	1	0	7.470905	2.544795	3.623367
54	1	0	6.015082	4.358124	2.726395
55	1	0	4.098785	3.815598	1.285105
56	1	0	1.990393	2.928491	2.225968
57	1	0	0.265909	4.639823	1.841743
58	1	0	-0.495212	5.163956	-0.472981
59	1	0	0.499551	3.930317	-2.396115
60	1	0	2.217859	2.190592	-2.000811
61	1	0	3.747002	1.171512	-3.969141
62	1	0	4.490457	-0.385372	-3.568624
63	1	0	5.454875	0.880138	-4.355641
64	1	0	6.671501	-0.526423	-1.181444
65	1	0	7.166628	0.985554	-0.403713
66	1	0	7.570861	0.691758	-2.108552
67	1	0	6.128689	3.520691	-2.729364
68	1	0	5.735842	3.658139	-1.005082
69	1	0	4.446167	3.766616	-2.218670
70	1	0	3.422788	0.120662	3.346571
71	1	0	0.572582	0.383617	4.557194
72	1	0	-0.097358	-3.262697	3.638878
73	1	0	3.483018	-2.718129	4.749515
74	1	0	4.448609	-2.030833	-1.317144
75	1	0	3.522593	-3.539587	-0.990893
76	1	0	5.301945	-3.605462	-1.103335
77	1	0	8.683948	-4.188884	2.503310
78	1	0	8.204854	-3.904778	4.214195
79	1	0	8.458361	-2.517440	3.125279
80	1	0	-2.108618	-3.824824	6.519299
81	1	0	-1.149223	-4.622992	5.238237
82	1	0	-1.929520	-3.045575	4.924025
83	6	0	3.715738	0.009060	6.105240
84	1	0	4.359018	-0.146403	5.237493
85	1	0	4.074862	0.892508	6.652829
86	1	0	3.838762	-0.855911	6.764683
87	1	0	1.617199	0.209565	6.668725

Structure **zss-TS1**

Imaginary Frequency: -146

E(RB3LYP) = -2266.952833 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.125334	0.059066	-0.103416
2	6	0	-0.225638	0.002892	1.427380
3	7	0	1.183007	0.067417	1.890709
4	6	0	2.167107	-0.141047	0.788220
5	6	0	1.268123	-0.533205	-0.409493
6	6	0	3.136923	1.077878	0.489786
7	6	0	4.121125	1.337772	1.655650
8	6	0	4.761776	0.257050	2.300012
9	6	0	5.700820	0.476592	3.314667
10	6	0	6.036633	1.780007	3.699369
11	6	0	5.428768	2.860309	3.053071
12	6	0	4.484400	2.640893	2.042257
13	6	0	2.323187	2.319502	0.090110
14	6	0	1.554479	3.023258	1.039493
15	6	0	0.767254	4.114225	0.657030
16	6	0	0.731835	4.526828	-0.680772
17	6	0	1.493497	3.838181	-1.629566
18	6	0	2.280277	2.744467	-1.246555
19	8	0	3.870770	0.594496	-0.669927
20	14	0	5.530603	0.525300	-1.232776
21	6	0	5.278454	0.121133	-3.077662
22	6	0	6.508561	-0.883917	-0.393567
23	6	0	6.424910	2.200797	-1.031942
24	6	0	1.497462	-0.022040	3.197190
25	6	0	0.600671	-0.087849	4.250752
26	6	0	1.023785	-0.336022	5.584094
27	6	0	0.973644	-2.564629	5.873636
28	6	0	0.832341	-3.000651	4.500442
29	6	0	2.028633	-3.275739	3.657682
30	6	0	1.945005	-3.861189	2.445132
31	6	0	0.692403	-4.483868	1.904212
32	8	0	0.218623	-5.562189	2.258250
33	8	0	0.166394	-3.726412	0.880498
34	6	0	-1.077549	-4.238780	0.283624
35	6	0	3.158466	-3.944221	1.598854
36	8	0	4.158615	-3.211371	1.691873

37	8	0	3.055272	-4.932914	0.657578
38	6	0	4.192998	-5.118150	-0.254075
39	8	0	-0.308793	-3.013510	3.947034
40	6	0	2.399984	0.039983	6.088695
41	6	0	2.170678	-2.810754	6.660532
42	8	0	3.323914	-2.961538	6.213702
43	8	0	2.060101	-2.779598	8.058665
44	6	0	0.767343	-2.819496	8.734211
45	1	0	-0.194372	1.092480	-0.454573
46	1	0	-0.928101	-0.513041	-0.578168
47	1	0	-0.658862	-0.942443	1.782852
48	1	0	-0.798961	0.834095	1.851295
49	1	0	2.812959	-0.980406	1.052072
50	1	0	1.691687	-0.179045	-1.349054
51	1	0	1.200874	-1.625265	-0.449170
52	1	0	4.547351	-0.769060	2.020087
53	1	0	6.167778	-0.374869	3.799289
54	1	0	6.763360	1.948815	4.487488
55	1	0	5.686349	3.877618	3.331196
56	1	0	4.031887	3.493620	1.552429
57	1	0	1.574722	2.725024	2.081037
58	1	0	0.185448	4.643622	1.405478
59	1	0	0.121718	5.374628	-0.976144
60	1	0	1.476761	4.148271	-2.670025
61	1	0	2.860174	2.202657	-1.981819
62	1	0	4.725771	0.920236	-3.582759
63	1	0	4.709935	-0.807872	-3.190791
64	1	0	6.243561	-0.001339	-3.583274
65	1	0	5.869354	-1.754281	-0.210173
66	1	0	6.925611	-0.570508	0.567354
67	1	0	7.335921	-1.191279	-1.045119
68	1	0	7.406000	2.153886	-1.520389
69	1	0	6.576434	2.451103	0.021795
70	1	0	5.849714	3.008305	-1.497282
71	1	0	2.559236	-0.067517	3.406712
72	1	0	-0.463475	-0.112345	4.049135
73	1	0	0.238663	-0.254874	6.331227
74	1	0	0.020438	-2.555727	6.386779
75	1	0	2.995693	-2.961119	4.033940
76	1	0	-1.318813	-3.532620	-0.508618
77	1	0	-1.862060	-4.267304	1.042396
78	1	0	-0.917627	-5.242245	-0.115924
79	1	0	3.923911	-5.982486	-0.857093
80	1	0	5.104803	-5.301242	0.317481

81	1	0	4.322646	-4.228883	-0.875114
82	1	0	2.533132	-0.255917	7.131253
83	1	0	2.521506	1.130015	6.026250
84	1	0	3.211654	-0.420963	5.518656
85	1	0	1.008647	-2.913647	9.792787
86	1	0	0.175814	-3.682563	8.413311
87	1	0	0.196530	-1.898650	8.572649

Structure **zss-IM2**

E(RB3LYP) = -2266.990267 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.319651	0.385242	0.108513
2	6	0	-0.402599	-0.133993	1.553629
3	7	0	1.002809	-0.387659	1.934282
4	6	0	1.941773	-0.319962	0.790647
5	6	0	0.996417	-0.217423	-0.431253
6	6	0	3.019928	0.845402	0.861061
7	6	0	4.043295	0.608525	1.998083
8	6	0	4.620745	-0.668720	2.166099
9	6	0	5.593652	-0.898284	3.145043
10	6	0	6.026219	0.144697	3.972969
11	6	0	5.479123	1.419733	3.804729
12	6	0	4.502202	1.648213	2.826878
13	6	0	2.319304	2.209873	0.936019
14	6	0	1.642135	2.613725	2.105168
15	6	0	0.947945	3.827231	2.148852
16	6	0	0.912987	4.664038	1.026593
17	6	0	1.578368	4.272621	-0.138951
18	6	0	2.271867	3.056420	-0.182796
19	8	0	3.699931	0.702989	-0.421353
20	14	0	5.303696	1.029580	-1.054057
21	6	0	4.955110	1.311825	-2.906832
22	6	0	6.433387	-0.495114	-0.854283
23	6	0	6.111211	2.579130	-0.281458
24	6	0	1.317315	-0.974731	3.134384
25	6	0	0.447341	-1.289752	4.132727
26	6	0	0.843982	-2.002782	5.412137
27	6	0	0.135447	-3.439064	5.428459
28	6	0	-0.132743	-3.982261	4.015859
29	6	0	0.970251	-4.040431	3.035904

30	6	0	0.802056	-4.352684	1.731255
31	6	0	-0.505844	-4.773395	1.133369
32	8	0	-0.855416	-5.936628	0.940489
33	8	0	-1.258283	-3.681826	0.770711
34	6	0	-2.606637	-3.973516	0.257073
35	6	0	1.973835	-4.263016	0.835219
36	8	0	3.088651	-3.811652	1.152712
37	8	0	1.686986	-4.696238	-0.432242
38	6	0	2.777098	-4.650921	-1.416882
39	8	0	-1.286438	-4.361882	3.727580
40	6	0	2.362090	-2.049136	5.677351
41	6	0	0.919658	-4.462734	6.233001
42	8	0	1.757977	-5.211269	5.727288
43	8	0	0.737821	-4.517828	7.602269
44	6	0	-0.332159	-3.787809	8.286828
45	1	0	-0.277032	1.477789	0.094989
46	1	0	-1.186976	0.074820	-0.482276
47	1	0	-0.971466	-1.072793	1.616986
48	1	0	-0.859062	0.593148	2.236719
49	1	0	2.516752	-1.247428	0.732697
50	1	0	1.444892	0.368228	-1.233932
51	1	0	0.810441	-1.228441	-0.813647
52	1	0	4.319370	-1.500531	1.539493
53	1	0	6.011075	-1.893992	3.256977
54	1	0	6.780177	-0.034647	4.732835
55	1	0	5.810407	2.242600	4.430759
56	1	0	4.099222	2.646215	2.711875
57	1	0	1.655619	1.977702	2.981899
58	1	0	0.435804	4.118515	3.060936
59	1	0	0.375106	5.606250	1.062062
60	1	0	1.556612	4.909435	-1.018218
61	1	0	2.766351	2.746905	-1.094050
62	1	0	4.345012	2.207257	-3.065741
63	1	0	4.416427	0.455853	-3.326517
64	1	0	5.892979	1.434073	-3.461441
65	1	0	5.930875	-1.396193	-1.222086
66	1	0	6.712826	-0.661874	0.189501
67	1	0	7.350095	-0.352466	-1.439771
68	1	0	7.025008	2.825173	-0.836391
69	1	0	6.378720	2.413698	0.765881
70	1	0	5.437930	3.440948	-0.331772
71	1	0	2.369329	-1.205743	3.245790
72	1	0	-0.609198	-1.054796	4.032936
73	1	0	0.399892	-1.457413	6.258959

74	1	0	-0.864281	-3.311258	5.851647
75	1	0	1.971358	-3.822047	3.380420
76	1	0	-3.014576	-3.003626	-0.020528
77	1	0	-3.200277	-4.441820	1.044868
78	1	0	-2.545488	-4.640954	-0.604617
79	1	0	2.344952	-5.066720	-2.324289
80	1	0	3.619722	-5.251357	-1.068448
81	1	0	3.101631	-3.619116	-1.569061
82	1	0	2.571306	-2.470032	6.666093
83	1	0	2.770689	-1.033970	5.648914
84	1	0	2.910216	-2.651903	4.947484
85	1	0	-0.181688	-4.009476	9.342225
86	1	0	-1.314670	-4.149816	7.970953
87	1	0	-0.253737	-2.709508	8.123339

Structure **ess-IM1** (M06-2x)

E(RB3LYP) **=** -2265.697275 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.065836	-0.056381	-0.056291
2	6	0	0.000763	0.213033	1.448863
3	7	0	1.401445	0.092323	1.917762
4	6	0	2.357366	0.021403	0.785534
5	6	0	1.472034	-0.635773	-0.288511
6	6	0	2.970287	1.389756	0.310311
7	6	0	3.789631	2.108881	1.394407
8	6	0	3.105036	2.675227	2.482328
9	6	0	3.777427	3.463905	3.416494
10	6	0	5.149549	3.685528	3.300440
11	6	0	5.841774	3.115520	2.234108
12	6	0	5.168163	2.343931	1.285723
13	8	0	1.857462	2.193290	-0.068530
14	14	0	1.580143	3.924422	-0.183185
15	6	0	0.446339	4.020870	-1.698358
16	6	0	3.209594	4.849745	-0.475585
17	6	0	0.650862	4.583609	1.318899
18	6	0	1.706858	-0.035967	3.194164
19	6	0	0.767436	-0.208978	4.229326
20	6	0	3.820691	1.032154	-0.916912
21	6	0	3.532431	1.579832	-2.169395
22	6	0	4.278126	1.226416	-3.295169

23	6	0	5.318065	0.305317	-3.189761
24	6	0	5.605582	-0.262460	-1.947862
25	6	0	4.862525	0.095563	-0.824668
26	6	0	1.142792	-0.264766	5.543282
27	6	0	1.300012	2.449014	5.869124
28	6	0	1.357955	2.396075	7.291797
29	8	0	0.426999	2.382103	8.128114
30	8	0	2.672167	2.259737	7.725304
31	6	0	2.857681	2.185059	9.158103
32	6	0	0.160958	2.563981	5.059133
33	8	0	0.238510	2.539466	3.773351
34	6	0	-1.184531	2.579301	5.667572
35	6	0	-2.305513	2.684304	4.930749
36	6	0	-2.340163	2.970444	3.470384
37	8	0	-2.317539	4.090936	2.969590
38	8	0	-2.553837	1.836469	2.727550
39	6	0	-2.807071	2.068912	1.315550
40	6	0	-3.609796	2.615137	5.610933
41	8	0	-3.796816	2.380244	6.806739
42	8	0	-4.640137	2.837450	4.738078
43	6	0	-5.978859	2.802016	5.297704
44	1	0	-0.044477	0.876187	-0.614423
45	1	0	-0.716208	-0.754727	-0.372698
46	1	0	-0.615990	-0.526228	1.974243
47	1	0	-0.352368	1.211371	1.735933
48	1	0	3.186990	-0.627814	1.091731
49	1	0	1.841374	-0.445073	-1.298504
50	1	0	1.469588	-1.721939	-0.126792
51	1	0	2.032035	2.543226	2.613068
52	1	0	3.211269	3.915890	4.227528
53	1	0	5.669793	4.302719	4.027234
54	1	0	6.908670	3.287764	2.120322
55	1	0	5.726589	1.959532	0.439317
56	1	0	0.128146	5.057290	-1.865193
57	1	0	-0.452855	3.415705	-1.526877
58	1	0	0.933016	3.658260	-2.610766
59	1	0	2.986550	5.891464	-0.739247
60	1	0	3.792981	4.405278	-1.290574
61	1	0	3.827017	4.848486	0.430174
62	1	0	-0.091794	5.328493	1.006395
63	1	0	1.329808	5.048077	2.043496
64	1	0	0.118141	3.792758	1.862174
65	1	0	2.770455	-0.054636	3.439182
66	1	0	-0.295300	-0.210770	3.992739

67	1	0	2.699704	2.269446	-2.261658
68	1	0	4.037398	1.668063	-4.258193
69	1	0	5.896914	0.027625	-4.065839
70	1	0	6.410335	-0.986139	-1.851924
71	1	0	5.115413	-0.347995	0.136747
72	1	0	2.257267	2.411168	5.358474
73	1	0	3.934420	2.100668	9.304026
74	1	0	2.338909	1.315363	9.573648
75	1	0	2.468380	3.083354	9.646047
76	1	0	-1.266567	2.473923	6.749426
77	1	0	-2.970204	1.080570	0.884164
78	1	0	-1.950791	2.568503	0.845132
79	1	0	-3.691537	2.700549	1.193842
80	1	0	-6.644540	2.992149	4.457654
81	1	0	-6.087171	3.571788	6.066476
82	1	0	-6.175399	1.823612	5.744544
83	6	0	0.194770	-0.575582	6.644244
84	1	0	0.202518	0.191166	7.432616
85	1	0	-0.832447	-0.662423	6.273896
86	1	0	0.471282	-1.523971	7.126510
87	1	0	2.200719	-0.182005	5.803581

Structure **zss-IM1** (M06-2x)

E(RB3LYP) = -2265.692765 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.005312	-0.069178	0.577981
2	6	0	0.219067	-0.028831	2.089482
3	7	0	1.689358	0.092772	2.252119
4	6	0	2.421599	-0.112020	0.968710
5	6	0	1.327829	-0.624818	0.028235
6	6	0	3.196109	1.151347	0.456858
7	6	0	4.268684	1.579204	1.468968
8	6	0	5.188769	0.615553	1.922095
9	6	0	6.178409	0.945429	2.847057
10	6	0	6.284444	2.254886	3.322125
11	6	0	5.402115	3.226012	2.855157
12	6	0	4.403526	2.890824	1.937807
13	6	0	2.217030	2.262206	0.091815
14	6	0	1.459735	2.918630	1.077674
15	6	0	0.502396	3.868908	0.727529

16	6	0	0.279564	4.180950	-0.615053
17	6	0	1.026436	3.537787	-1.599922
18	6	0	1.985834	2.586552	-1.247906
19	8	0	3.826724	0.638768	-0.724816
20	14	0	5.372070	0.972074	-1.472737
21	6	0	4.998793	0.679598	-3.303362
22	6	0	6.701692	-0.242766	-0.874283
23	6	0	5.898331	2.770997	-1.184005
24	6	0	2.285186	0.116384	3.426125
25	6	0	1.649813	0.200266	4.682768
26	6	0	2.351008	0.058806	5.849653
27	6	0	1.042047	-2.996329	4.031186
28	6	0	2.070306	-3.052289	3.062515
29	6	0	3.492055	-2.880131	3.460923
30	6	0	4.494000	-3.031782	2.573563
31	6	0	4.293868	-3.538667	1.183272
32	8	0	4.254546	-4.710965	0.836144
33	8	0	4.268395	-2.488569	0.299996
34	6	0	3.915588	-2.791714	-1.076112
35	6	0	5.863581	-2.672319	2.959958
36	8	0	6.201279	-2.088304	3.998238
37	8	0	6.758521	-3.006604	1.984593
38	6	0	8.152845	-2.672715	2.212316
39	8	0	1.822870	-3.179789	1.814742
40	6	0	1.183453	-2.703563	5.408672
41	8	0	2.239231	-2.449173	6.042522
42	8	0	0.020587	-2.564830	6.172644
43	6	0	-1.275754	-2.840533	5.617357
44	1	0	-0.189932	0.938383	0.190598
45	1	0	-0.844516	-0.705954	0.315418
46	1	0	-0.078644	-0.970361	2.581091
47	1	0	-0.284239	0.811515	2.582672
48	1	0	3.170247	-0.895367	1.114295
49	1	0	1.520608	-0.328631	-1.006331
50	1	0	1.327795	-1.719373	0.102238
51	1	0	5.126661	-0.405618	1.546159
52	1	0	6.840072	0.169261	3.223771
53	1	0	7.050136	2.511581	4.048420
54	1	0	5.484611	4.251689	3.203948
55	1	0	3.735967	3.667455	1.578756
56	1	0	1.614692	2.682148	2.128549
57	1	0	-0.070915	4.366697	1.504988
58	1	0	-0.468697	4.919447	-0.888091
59	1	0	0.859340	3.769833	-2.648178

60	1	0	2.550866	2.062941	-2.013229
61	1	0	4.261581	1.400863	-3.674681
62	1	0	4.600788	-0.328309	-3.465287
63	1	0	5.913269	0.786192	-3.899816
64	1	0	6.245393	-1.169638	-0.502532
65	1	0	7.297396	0.195726	-0.064692
66	1	0	7.373519	-0.493003	-1.704829
67	1	0	6.658148	3.052005	-1.924110
68	1	0	6.320418	2.907194	-0.181515
69	1	0	5.044494	3.451181	-1.292592
70	1	0	3.371843	0.067838	3.398794
71	1	0	0.563985	0.244326	4.728352
72	1	0	0.059510	-3.204741	3.619747
73	1	0	3.709298	-2.597479	4.491179
74	1	0	3.707506	-1.817533	-1.525596
75	1	0	3.030246	-3.434948	-1.090942
76	1	0	4.745937	-3.299185	-1.576607
77	1	0	8.705105	-3.221132	1.451292
78	1	0	8.456817	-2.972266	3.218159
79	1	0	8.301236	-1.594824	2.090938
80	1	0	-1.981383	-2.702907	6.437681
81	1	0	-1.344887	-3.869090	5.244305
82	1	0	-1.522167	-2.145249	4.802881
83	6	0	3.825193	-0.011038	6.030245
84	1	0	4.388126	-0.282264	5.130576
85	1	0	4.206378	0.956064	6.390552
86	1	0	4.052772	-0.763463	6.791072
87	1	0	1.767924	0.045569	6.769428

Structure **ssrr-TS2**

Imaginary Frequency: -181

E(RB3LYP) **=** -2266.963064 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.135451	0.007132	-0.159684
2	6	0	0.123367	0.336759	1.314366
3	6	0	1.433381	0.083703	2.085854
4	6	0	2.481475	-0.612758	1.154969
5	6	0	1.886729	-1.099139	-0.196846
6	6	0	1.790959	-2.429985	-0.683962
7	6	0	-1.021879	-0.484655	-0.799907

8	6	0	-2.016944	-1.258121	-0.082564
9	8	0	-3.210039	-1.441552	-0.376910
10	8	0	-1.486437	-1.796885	1.100731
11	6	0	-2.455895	-2.319660	2.064696
12	6	0	-1.206344	-0.237408	-2.216516
13	8	0	-1.948670	-0.846131	-3.013370
14	8	0	-0.379782	0.801145	-2.682547
15	6	0	-0.548229	1.186795	-4.082544
16	6	0	1.812329	-5.916720	0.406718
17	6	0	1.830871	-4.907319	-0.774718
18	7	0	1.435109	-3.599118	-0.135564
19	6	0	0.851031	-3.847813	1.202965
20	6	0	1.627717	-5.073801	1.692130
21	6	0	0.986879	-5.334736	-2.036195
22	6	0	1.522156	-6.679294	-2.594685
23	6	0	2.889195	-7.011126	-2.515973
24	6	0	3.391641	-8.173174	-3.110427
25	6	0	2.540740	-9.030560	-3.815657
26	6	0	1.184009	-8.709261	-3.919503
27	6	0	0.683113	-7.549383	-3.317235
28	6	0	-0.520828	-5.352376	-1.725226
29	6	0	-1.308735	-4.223353	-2.004880
30	6	0	-2.678196	-4.204267	-1.711500
31	6	0	-3.282431	-5.314726	-1.112710
32	6	0	-2.510178	-6.443190	-0.815381
33	6	0	-1.144507	-6.463397	-1.119742
34	8	0	1.292437	-4.281747	-3.005232
35	14	0	1.139186	-4.152526	-4.760307
36	6	0	-0.443776	-4.943446	-5.477496
37	6	0	2.691645	-4.900442	-5.582813
38	6	0	1.073093	-2.269340	-5.011140
39	6	0	1.124388	-0.581525	3.409576
40	8	0	0.829886	-1.770316	3.599572
41	8	0	1.192516	0.324544	4.434333
42	6	0	0.812382	-0.150887	5.774627
43	8	0	-0.832674	0.899721	1.859334
44	6	0	3.420764	-1.605681	1.869657
45	1	0	0.627892	0.792583	-0.733049
46	1	0	1.801880	1.080244	2.355709
47	1	0	3.134158	0.213903	0.843150
48	1	0	2.317451	-0.511808	-1.006529
49	1	0	2.015198	-2.556793	-1.739984
50	1	0	-1.857137	-2.614398	2.925660
51	1	0	-2.992377	-3.171077	1.640401

52	1	0	-3.172746	-1.540793	2.335842
53	1	0	0.006225	2.119411	-4.185282
54	1	0	-1.605940	1.331980	-4.312393
55	1	0	-0.140728	0.422824	-4.748895
56	1	0	2.727217	-6.514187	0.425579
57	1	0	0.975796	-6.608958	0.298399
58	1	0	2.847396	-4.755109	-1.141790
59	1	0	-0.209589	-4.079443	1.057892
60	1	0	0.908676	-2.976607	1.846818
61	1	0	2.598173	-4.769954	2.102584
62	1	0	1.090665	-5.619589	2.472799
63	1	0	3.585937	-6.361731	-2.000528
64	1	0	4.449258	-8.402835	-3.026209
65	1	0	2.929549	-9.931968	-4.278218
66	1	0	0.509840	-9.359924	-4.467622
67	1	0	-0.371686	-7.324197	-3.406353
68	1	0	-0.859828	-3.350079	-2.457682
69	1	0	-3.245901	-3.306652	-1.923638
70	1	0	-4.342833	-5.299653	-0.881754
71	1	0	-2.967917	-7.314248	-0.355846
72	1	0	-0.577768	-7.364380	-0.912595
73	1	0	-0.543738	-4.627161	-6.523543
74	1	0	-1.333215	-4.610469	-4.935093
75	1	0	-0.407787	-6.035546	-5.455219
76	1	0	2.661229	-4.718029	-6.664057
77	1	0	2.753745	-5.980081	-5.417151
78	1	0	3.601906	-4.439220	-5.184939
79	1	0	1.094323	-2.026563	-6.080323
80	1	0	1.923597	-1.774434	-4.530437
81	1	0	0.148319	-1.868368	-4.583199
82	1	0	0.944425	0.713994	6.420865
83	1	0	1.458767	-0.976779	6.078727
84	1	0	-0.227549	-0.482990	5.768705
85	1	0	4.180258	-1.967884	1.168697
86	1	0	2.894670	-2.463955	2.287978
87	1	0	3.940678	-1.104221	2.695863

Structure **ssrr-IM3**

E(RB3LYP) = -2266.972753 a.u.

Standard orientation:

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

1	6	0	-0.052951	0.026970	-0.063028
2	6	0	-0.102071	0.035380	1.471135
3	6	0	1.346603	-0.032576	2.056613
4	6	0	2.238510	0.188197	0.812030
5	6	0	1.446580	-0.385091	-0.416148
6	6	0	1.492090	-1.720819	-1.109036
7	6	0	-1.183582	-0.717917	-0.709799
8	6	0	-1.594523	-1.949016	-0.123354
9	8	0	-2.644806	-2.607229	-0.212559
10	8	0	-0.523075	-2.463438	0.707964
11	6	0	-0.839217	-3.676925	1.454316
12	6	0	-1.865238	-0.177845	-1.829769
13	8	0	-2.733807	-0.703342	-2.569693
14	8	0	-1.384085	1.137672	-2.166947
15	6	0	-2.169216	1.854711	-3.165084
16	6	0	2.953543	-4.924836	-1.575084
17	6	0	2.528596	-3.670861	-2.347386
18	7	0	2.385824	-2.659168	-1.208318
19	6	0	3.517472	-2.923758	-0.258815
20	6	0	3.963786	-4.380206	-0.540202
21	6	0	1.423554	-3.779231	-3.450945
22	6	0	1.989004	-4.555792	-4.679571
23	6	0	3.359565	-4.655071	-4.979348
24	6	0	3.802080	-5.295010	-6.143961
25	6	0	2.883301	-5.838821	-7.045160
26	6	0	1.514937	-5.737681	-6.768726
27	6	0	1.076500	-5.108341	-5.600541
28	6	0	0.128466	-4.460960	-2.965902
29	6	0	-1.070752	-3.752996	-2.830000
30	6	0	-2.252743	-4.407333	-2.451417
31	6	0	-2.245747	-5.780214	-2.198269
32	6	0	-1.050998	-6.501449	-2.329490
33	6	0	0.122680	-5.850584	-2.715435
34	8	0	1.200529	-2.391486	-3.827149
35	14	0	0.765573	-1.441125	-5.253251
36	6	0	-1.054239	-1.706451	-5.750561
37	6	0	1.940838	-1.769988	-6.724011
38	6	0	1.064118	0.326799	-4.616220
39	6	0	1.567090	-1.295062	2.844058
40	8	0	2.137051	-2.331961	2.463325
41	8	0	1.045338	-1.171779	4.100002
42	6	0	1.082643	-2.354232	4.974431
43	8	0	-1.103965	0.180047	2.164587
44	6	0	3.747581	-0.016251	1.010300

45	1	0	-0.153716	1.078128	-0.367358
46	1	0	1.432482	0.795956	2.767342
47	1	0	2.130580	1.267707	0.620246
48	1	0	1.732768	0.236937	-1.288274
49	1	0	0.695580	-1.783795	-1.841681
50	1	0	0.100433	-3.978380	1.917943
51	1	0	-1.217044	-4.451281	0.783297
52	1	0	-1.599659	-3.470182	2.213597
53	1	0	-1.567865	2.722917	-3.438299
54	1	0	-3.125825	2.174385	-2.739740
55	1	0	-2.366304	1.224051	-4.034242
56	1	0	3.392009	-5.680821	-2.230302
57	1	0	2.083998	-5.362783	-1.078176
58	1	0	3.404134	-3.263194	-2.867459
59	1	0	3.134884	-2.785011	0.750902
60	1	0	4.318791	-2.208656	-0.457417
61	1	0	4.979957	-4.397259	-0.948707
62	1	0	3.967273	-4.974207	0.377158
63	1	0	4.112069	-4.239124	-4.320092
64	1	0	4.866880	-5.362827	-6.343704
65	1	0	3.226853	-6.334071	-7.947464
66	1	0	0.786588	-6.153897	-7.457295
67	1	0	0.014620	-5.053986	-5.394163
68	1	0	-1.112076	-2.689025	-3.013787
69	1	0	-3.148366	-3.814760	-2.321763
70	1	0	-3.159005	-6.285077	-1.900283
71	1	0	-1.035052	-7.571693	-2.145579
72	1	0	1.023926	-6.435471	-2.865235
73	1	0	-1.278136	-1.085580	-6.627385
74	1	0	-1.728849	-1.413683	-4.938391
75	1	0	-1.263642	-2.748188	-6.013345
76	1	0	1.729120	-1.032053	-7.508303
77	1	0	1.814518	-2.768350	-7.149801
78	1	0	2.987420	-1.653888	-6.424101
79	1	0	0.841148	1.053774	-5.406750
80	1	0	2.113864	0.454602	-4.328016
81	1	0	0.428011	0.556612	-3.754941
82	1	0	0.689092	-2.003472	5.925715
83	1	0	2.107541	-2.716780	5.076474
84	1	0	0.452209	-3.142506	4.558650
85	1	0	4.287907	0.086835	0.061573
86	1	0	3.994264	-0.978405	1.456226
87	1	0	4.127153	0.762935	1.682373

Structure **ssrs-TS2**

Imaginary Frequency: -148

E(RB3LYP) = -2266.956833 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.041052	0.122154	-0.028481
2	6	0	0.151137	0.100198	1.477870
3	6	0	1.536290	0.040509	2.109082
4	6	0	2.539130	-0.696046	1.132320
5	6	0	1.884607	-1.238343	-0.154239
6	6	0	1.348757	-2.466953	-0.549469
7	6	0	0.200799	1.246963	-0.841484
8	6	0	0.958540	2.405134	-0.351742
9	8	0	1.050292	2.704034	0.851578
10	8	0	1.638443	3.224695	-1.250234
11	6	0	2.126697	2.755137	-2.554752
12	6	0	-0.394311	1.153248	-2.182259
13	8	0	-0.537179	0.079721	-2.798637
14	8	0	-0.863708	2.299594	-2.810388
15	6	0	-1.293106	3.493584	-2.062709
16	6	0	0.004557	-5.710320	0.581826
17	6	0	0.420123	-4.781900	-0.589423
18	7	0	0.753313	-3.491324	0.104354
19	6	0	0.524771	-3.571333	1.567447
20	6	0	-0.413165	-4.770101	1.731818
21	6	0	-0.623320	-4.672486	-1.776664
22	6	0	-0.900675	-6.067085	-2.391139
23	6	0	0.066335	-7.090195	-2.378173
24	6	0	-0.158506	-8.308050	-3.028661
25	6	0	-1.352578	-8.528996	-3.722799
26	6	0	-2.318569	-7.518080	-3.758269
27	6	0	-2.093997	-6.303978	-3.100166
28	6	0	-1.909405	-3.956582	-1.330354
29	6	0	-2.084757	-2.588087	-1.586863
30	6	0	-3.236277	-1.919603	-1.150928
31	6	0	-4.228941	-2.603759	-0.443458
32	6	0	-4.065331	-3.968978	-0.181698
33	6	0	-2.919421	-4.638728	-0.623851
34	8	0	0.091323	-3.872267	-2.767781
35	14	0	0.011668	-3.614780	-4.511481
36	6	0	0.596667	-5.172225	-5.450804

37	6	0	1.255937	-2.196031	-4.742124
38	6	0	-1.720260	-3.075566	-5.105614
39	6	0	1.465817	-0.489751	3.525750
40	8	0	1.145352	-1.631159	3.879689
41	8	0	1.827501	0.479117	4.427546
42	6	0	1.753373	0.121304	5.852458
43	8	0	-0.896304	0.071378	2.141087
44	6	0	3.508625	-1.674812	1.831623
45	1	0	-0.657067	-0.623694	-0.391646
46	1	0	1.846922	1.087927	2.191752
47	1	0	3.175709	0.115409	0.758806
48	1	0	2.267331	-0.722939	-1.030949
49	1	0	1.317673	-2.627800	-1.621900
50	1	0	3.068064	3.281966	-2.712152
51	1	0	1.411766	3.006334	-3.339209
52	1	0	2.299986	1.675390	-2.545684
53	1	0	-2.115224	3.909506	-2.644978
54	1	0	-0.473138	4.209188	-1.991448
55	1	0	-1.639058	3.222091	-1.062158
56	1	0	0.868988	-6.312973	0.886310
57	1	0	-0.785938	-6.405876	0.295896
58	1	0	1.340555	-5.134127	-1.063146
59	1	0	0.107838	-2.640927	1.948664
60	1	0	1.470470	-3.748717	2.089967
61	1	0	-0.304495	-5.237241	2.714460
62	1	0	-1.454573	-4.458492	1.616112
63	1	0	1.009269	-6.950550	-1.864329
64	1	0	0.603304	-9.080648	-2.995869
65	1	0	-1.526608	-9.473256	-4.228584
66	1	0	-3.249459	-7.671645	-4.295101
67	1	0	-2.857164	-5.536090	-3.132748
68	1	0	-1.328093	-2.041889	-2.134348
69	1	0	-3.349672	-0.863180	-1.371894
70	1	0	-5.118978	-2.084018	-0.103743
71	1	0	-4.830994	-4.516475	0.359379
72	1	0	-2.826067	-5.702264	-0.433212
73	1	0	-0.102237	-6.006160	-5.343451
74	1	0	1.576748	-5.497008	-5.086076
75	1	0	0.691553	-4.935585	-6.518004
76	1	0	1.348632	-1.939238	-5.804197
77	1	0	2.246953	-2.481008	-4.372195
78	1	0	0.910259	-1.310422	-4.199388
79	1	0	-1.692897	-2.934255	-6.193390
80	1	0	-2.002993	-2.124867	-4.643984

81	1	0	-2.491556	-3.817665	-4.880413
82	1	0	2.066587	1.020116	6.379179
83	1	0	2.420636	-0.716508	6.066358
84	1	0	0.729638	-0.153998	6.113735
85	1	0	4.203730	-2.090732	1.094756
86	1	0	2.991426	-2.497236	2.326518
87	1	0	4.098313	-1.147521	2.592220

Structure **ssrs-IM3**

E(RB3LYP) = -2266.973757 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.127769	0.155045	0.224373
2	6	0	0.264006	0.141877	1.714434
3	6	0	1.814599	0.007784	1.869328
4	6	0	2.346524	0.054900	0.410836
5	6	0	1.130608	-0.400277	-0.505388
6	6	0	1.164925	-1.831581	-0.924454
7	6	0	-0.549480	1.516969	-0.313312
8	6	0	0.054493	2.644084	0.304025
9	8	0	0.719499	2.565695	1.377553
10	8	0	-0.014009	3.931129	-0.273563
11	6	0	0.292399	4.112126	-1.696637
12	6	0	-1.429895	1.445795	-1.434723
13	8	0	-1.536297	0.420903	-2.169823
14	8	0	-2.271068	2.517761	-1.775618
15	6	0	-2.899945	3.332646	-0.725844
16	6	0	0.105399	-5.238978	-0.287324
17	6	0	0.637567	-4.187577	-1.288786
18	7	0	0.452622	-2.865263	-0.580356
19	6	0	-0.507119	-3.032433	0.555884
20	6	0	-0.209548	-4.464753	1.017778
21	6	0	-0.045064	-4.169677	-2.717948
22	6	0	0.296110	-5.465387	-3.489850
23	6	0	1.436143	-6.238012	-3.204163
24	6	0	1.778509	-7.343307	-3.991921
25	6	0	0.994354	-7.695926	-5.093716
26	6	0	-0.138512	-6.933040	-5.397982
27	6	0	-0.481913	-5.833946	-4.605079
28	6	0	-1.559045	-3.910057	-2.585849
29	6	0	-2.034505	-2.588289	-2.540092

30	6	0	-3.394801	-2.319778	-2.343813
31	6	0	-4.306385	-3.369813	-2.190037
32	6	0	-3.845980	-4.691167	-2.232141
33	6	0	-2.485933	-4.959884	-2.427065
34	8	0	0.613922	-3.048713	-3.366587
35	14	0	0.664403	-2.344641	-4.988641
36	6	0	2.058591	-3.215890	-5.957355
37	6	0	1.089954	-0.529829	-4.612277
38	6	0	-0.980749	-2.437020	-5.953357
39	6	0	2.151297	-1.250034	2.619221
40	8	0	2.024730	-2.409228	2.179277
41	8	0	2.611767	-0.996622	3.878206
42	6	0	2.892549	-2.154729	4.741790
43	8	0	-0.529408	0.015859	2.651426
44	6	0	3.689755	-0.632307	0.137025
45	1	0	-0.983018	-0.511844	0.095331
46	1	0	2.156468	0.868531	2.443381
47	1	0	2.455457	1.121710	0.192948
48	1	0	1.237880	0.128773	-1.462022
49	1	0	1.863009	-2.049994	-1.725565
50	1	0	0.634678	5.144394	-1.785534
51	1	0	-0.590427	3.946138	-2.316641
52	1	0	1.093205	3.431611	-2.006234
53	1	0	-3.857512	3.647766	-1.143636
54	1	0	-2.279465	4.194818	-0.479968
55	1	0	-3.057275	2.733307	0.175506
56	1	0	0.841847	-6.029335	-0.121668
57	1	0	-0.799168	-5.709189	-0.676786
58	1	0	1.710934	-4.283988	-1.455513
59	1	0	-1.521526	-2.923532	0.162797
60	1	0	-0.322236	-2.295168	1.328430
61	1	0	0.658263	-4.442957	1.682365
62	1	0	-1.055612	-4.894817	1.560060
63	1	0	2.080288	-5.994772	-2.367997
64	1	0	2.661312	-7.923656	-3.743219
65	1	0	1.260634	-8.551676	-5.705379
66	1	0	-0.758919	-7.193389	-6.249650
67	1	0	-1.369425	-5.262936	-4.847817
68	1	0	-1.364094	-1.745311	-2.635191
69	1	0	-3.711012	-1.283054	-2.311553
70	1	0	-5.361488	-3.163731	-2.040355
71	1	0	-4.542606	-5.516071	-2.118073
72	1	0	-2.155464	-5.991860	-2.474738
73	1	0	1.827080	-4.272888	-6.121632

74	1	0	3.006483	-3.153320	-5.412590
75	1	0	2.193587	-2.736592	-6.934500
76	1	0	1.176335	0.042188	-5.543647
77	1	0	2.044647	-0.448522	-4.080150
78	1	0	0.302633	-0.074457	-3.999795
79	1	0	-0.887416	-1.799718	-6.841865
80	1	0	-1.815356	-2.062747	-5.354732
81	1	0	-1.215638	-3.450097	-6.291055
82	1	0	3.249250	-1.722151	5.673722
83	1	0	3.652220	-2.791474	4.283570
84	1	0	1.978540	-2.730591	4.900128
85	1	0	3.986072	-0.500361	-0.911047
86	1	0	3.657929	-1.704015	0.357449
87	1	0	4.476682	-0.185465	0.755401

Structure **sssr-TS2**

Imaginary Frequency: -193

E(RB3LYP) = -2266.969295 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.006971	-0.002577	-0.009097
2	6	0	0.001722	0.000812	1.524982
3	7	0	1.444536	-0.003376	1.900360
4	6	0	2.338452	-0.286878	0.734056
5	6	0	1.341344	-0.685736	-0.378976
6	6	0	0.439815	3.037817	4.452333
7	6	0	-0.881730	2.999464	3.866574
8	8	0	-1.609859	1.981534	3.811375
9	8	0	-1.262176	4.169916	3.213835
10	6	0	-2.549094	4.123975	2.511694
11	6	0	1.450125	4.074364	4.164858
12	8	0	2.625420	3.795752	3.858058
13	8	0	1.132113	5.410563	4.283384
14	6	0	0.014920	5.888075	5.108029
15	6	0	3.340356	0.872033	0.305944
16	6	0	4.397652	1.107941	1.410619
17	6	0	5.167482	0.003219	1.839953
18	6	0	6.157974	0.143204	2.815328
19	6	0	6.407244	1.397838	3.387975
20	6	0	5.663130	2.500616	2.964859
21	6	0	4.674477	2.359935	1.980923

22	6	0	2.552338	2.113322	-0.136363
23	6	0	2.405612	2.421825	-1.499353
24	6	0	1.619663	3.504494	-1.912534
25	6	0	0.957046	4.296487	-0.969254
26	6	0	1.086314	3.995611	0.391524
27	6	0	1.872701	2.912978	0.802382
28	8	0	3.997171	0.249337	-0.838190
29	14	0	5.503254	0.541587	-1.703498
30	6	0	6.810995	-0.739004	-1.162784
31	6	0	6.157796	2.320409	-1.475994
32	6	0	5.039500	0.207516	-3.522933
33	6	0	1.448253	-0.654928	5.622438
34	6	0	0.484312	-0.103434	6.709165
35	6	0	0.067492	1.319372	6.284101
36	6	0	0.894186	1.928846	5.185351
37	6	0	0.987390	-0.064167	4.291209
38	8	0	-0.839439	1.935428	6.857903
39	6	0	-0.768929	-0.936819	6.903290
40	8	0	-1.461075	-1.424004	6.002113
41	8	0	-1.065982	-1.081323	8.233081
42	6	0	-2.321569	-1.778223	8.557928
43	6	0	1.838984	-0.088145	3.185818
44	6	0	1.567414	-2.193570	5.613832
45	1	0	-0.021782	1.019807	-0.394365
46	1	0	-0.857472	-0.539217	-0.411052
47	1	0	-0.464402	-0.907460	1.933002
48	1	0	-0.512364	0.856480	1.969663
49	1	0	2.976260	-1.135442	0.992182
50	1	0	1.719389	-0.398391	-1.359643
51	1	0	1.220550	-1.775874	-0.374590
52	1	0	-2.702020	5.138149	2.145834
53	1	0	-3.345777	3.824916	3.195675
54	1	0	-2.504535	3.414541	1.682146
55	1	0	0.416298	6.721391	5.687274
56	1	0	-0.347649	5.100104	5.772977
57	1	0	-0.791160	6.219735	4.456747
58	1	0	5.009530	-0.970487	1.389064
59	1	0	6.735126	-0.723191	3.124427
60	1	0	7.170732	1.509596	4.151366
61	1	0	5.828874	3.477903	3.404335
62	1	0	4.113668	3.235632	1.691154
63	1	0	2.890578	1.799012	-2.238652
64	1	0	1.524015	3.723017	-2.971973
65	1	0	0.350367	5.138015	-1.289128

66	1	0	0.582759	4.598044	1.140693
67	1	0	1.970664	2.711052	1.859751
68	1	0	7.673197	-0.691133	-1.839260
69	1	0	6.399684	-1.753308	-1.208573
70	1	0	7.162103	-0.552862	-0.144112
71	1	0	7.032732	2.469555	-2.120681
72	1	0	6.456734	2.508097	-0.440877
73	1	0	5.398564	3.059062	-1.750553
74	1	0	5.937304	0.222702	-4.152280
75	1	0	4.341849	0.957926	-3.908561
76	1	0	4.569459	-0.776775	-3.620426
77	1	0	2.447085	-0.254261	5.854329
78	1	0	0.975484	-0.031433	7.685446
79	1	0	1.961169	1.951935	5.411403
80	1	0	-0.082172	-0.134075	4.107826
81	1	0	-2.364367	-1.778009	9.644906
82	1	0	-2.300706	-2.795617	8.161671
83	1	0	-3.166687	-1.236680	8.128667
84	1	0	2.910844	-0.189911	3.334044
85	1	0	2.342831	-2.505991	4.905808
86	1	0	0.623979	-2.658603	5.316202
87	1	0	1.845012	-2.571769	6.606294

Structure **sssr-IM3**

E(RB3LYP) = -2266.976418 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.341184	2.016985	0.482291
2	6	0	0.043383	1.356303	1.830457
3	7	0	1.226851	0.451882	2.065110
4	6	0	2.040024	0.260790	0.799558
5	6	0	1.186706	0.970088	-0.273997
6	6	0	1.566680	2.168385	5.520459
7	6	0	0.490214	3.000408	5.139649
8	8	0	-0.668271	2.592345	4.804603
9	8	0	0.776044	4.372983	5.012746
10	6	0	-0.331355	5.212886	4.562554
11	6	0	2.941178	2.548665	5.744867
12	8	0	3.909547	1.787972	5.473105
13	8	0	3.277990	3.792834	6.270402
14	6	0	2.452046	4.422111	7.305121

15	6	0	3.551971	0.761043	0.862576
16	6	0	4.350362	-0.088948	1.879627
17	6	0	4.369579	-1.491528	1.695666
18	6	0	5.066290	-2.327688	2.570858
19	6	0	5.764420	-1.780916	3.657498
20	6	0	5.763157	-0.398108	3.844834
21	6	0	5.072249	0.442532	2.959326
22	6	0	3.597048	2.283865	1.068432
23	6	0	3.859732	3.140073	-0.015129
24	6	0	3.819109	4.530861	0.140358
25	6	0	3.504064	5.094054	1.381380
26	6	0	3.228462	4.255788	2.467328
27	6	0	3.272334	2.865264	2.309075
28	8	0	3.983142	0.409970	-0.482740
29	14	0	5.565415	0.204658	-1.242349
30	6	0	5.944343	-1.657320	-1.411751
31	6	0	6.959072	1.101505	-0.297244
32	6	0	5.319012	0.937383	-2.985036
33	6	0	0.265016	-1.460603	5.027235
34	6	0	-0.320464	-1.070486	6.406837
35	6	0	0.436687	0.243869	6.769713
36	6	0	1.312736	0.696840	5.583986
37	6	0	0.588736	-0.074419	4.378959
38	8	0	0.365992	0.803473	7.859831
39	6	0	-1.813021	-0.812390	6.416138
40	8	0	-2.503758	-0.454571	5.454064
41	8	0	-2.325164	-1.001841	7.672317
42	6	0	-3.741691	-0.653317	7.870026
43	6	0	1.427209	-0.197066	3.182843
44	6	0	-0.583449	-2.400813	4.160204
45	1	0	0.907934	2.939927	0.626750
46	1	0	-0.582109	2.264462	-0.048753
47	1	0	-0.845463	0.715464	1.779824
48	1	0	-0.089103	2.043204	2.669470
49	1	0	2.091911	-0.812456	0.611535
50	1	0	1.825982	1.404564	-1.041514
51	1	0	0.534243	0.235036	-0.760428
52	1	0	0.029692	6.235310	4.675557
53	1	0	-1.222363	5.040645	5.169947
54	1	0	-0.576224	5.008847	3.516138
55	1	0	3.148108	4.756381	8.077974
56	1	0	1.741912	3.701128	7.720014
57	1	0	1.911398	5.264747	6.877838
58	1	0	3.856479	-1.930230	0.846335

59	1	0	5.066505	-3.400773	2.404846
60	1	0	6.296790	-2.428236	4.346969
61	1	0	6.271004	0.047120	4.692233
62	1	0	5.085701	1.503275	3.156079
63	1	0	4.075753	2.716638	-0.986468
64	1	0	4.029190	5.170426	-0.711731
65	1	0	3.474521	6.172338	1.501985
66	1	0	2.978361	4.664399	3.440341
67	1	0	3.071262	2.249093	3.173651
68	1	0	6.821318	-1.795088	-2.056031
69	1	0	5.100821	-2.184146	-1.871195
70	1	0	6.154401	-2.116802	-0.442172
71	1	0	7.901437	0.980147	-0.845415
72	1	0	7.090899	0.689509	0.707307
73	1	0	6.752562	2.171727	-0.201808
74	1	0	6.204383	0.746493	-3.603164
75	1	0	5.154973	2.019278	-2.954057
76	1	0	4.455064	0.475152	-3.474184
77	1	0	1.227185	-1.957868	5.229840
78	1	0	-0.106331	-1.807562	7.185840
79	1	0	2.296374	0.219399	5.726558
80	1	0	-0.338913	0.468418	4.184450
81	1	0	-3.926739	-0.842334	8.925115
82	1	0	-4.374834	-1.279525	7.237731
83	1	0	-3.903264	0.397369	7.621814
84	1	0	2.285447	-0.864458	3.207152
85	1	0	-0.037027	-2.682728	3.251238
86	1	0	-1.526578	-1.931279	3.873196
87	1	0	-0.812859	-3.325868	4.702878

Structure **ssss-TS2**

Imaginary Frequency: -186

E(RB3LYP) = -2266.967271 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.109744	-0.046227	0.260611
2	6	0	0.094311	0.360427	1.752734
3	7	0	1.455408	0.050428	2.248159
4	6	0	2.427693	-0.090942	1.135177
5	6	0	1.527853	-0.607182	-0.015230
6	6	0	0.441397	-2.950048	3.276061

7	6	0	-0.840830	-2.979976	2.578836
8	8	0	-1.163077	-3.583733	1.548178
9	8	0	-1.785219	-2.159431	3.235248
10	6	0	-3.166163	-2.265357	2.752727
11	6	0	1.689653	-3.390695	2.647736
12	8	0	2.820387	-3.196426	3.149265
13	8	0	1.553027	-4.027672	1.435559
14	6	0	2.785674	-4.550744	0.835883
15	6	0	3.219039	1.232476	0.786106
16	6	0	4.402786	0.948605	-0.170896
17	6	0	4.609002	-0.277184	-0.827135
18	6	0	5.683862	-0.451438	-1.709839
19	6	0	6.575255	0.595431	-1.956422
20	6	0	6.395200	1.817224	-1.295723
21	6	0	5.328314	1.984727	-0.410016
22	6	0	3.748334	1.880628	2.081040
23	6	0	4.879678	1.350556	2.728318
24	6	0	5.334251	1.895827	3.933036
25	6	0	4.668542	2.985218	4.508299
26	6	0	3.545444	3.520094	3.869307
27	6	0	3.085980	2.968484	2.666707
28	8	0	2.246238	2.124911	0.174503
29	14	0	2.139575	3.237504	-1.173355
30	6	0	0.321627	3.801205	-1.080892
31	6	0	2.485444	2.375556	-2.841732
32	6	0	3.262240	4.773301	-0.964143
33	6	0	-0.305630	0.222633	5.062492
34	6	0	-0.901835	-0.850956	6.020182
35	6	0	-0.569773	-2.272300	5.524777
36	6	0	0.573583	-2.456607	4.567393
37	6	0	1.122893	-0.160919	4.721068
38	8	0	-1.161160	-3.263209	5.985675
39	6	0	-0.401002	-0.729834	7.470395
40	8	0	0.737440	-0.353922	7.759534
41	8	0	-1.250727	-1.064613	8.496515
42	6	0	-2.607968	-1.595231	8.291865
43	6	0	1.837957	-0.093455	3.541486
44	6	0	-0.410197	1.655779	5.632922
45	1	0	-0.090765	0.821194	-0.369623
46	1	0	-0.650458	-0.805224	0.052863
47	1	0	-0.641471	-0.213872	2.313143
48	1	0	-0.115213	1.429268	1.878760
49	1	0	3.164435	-0.838583	1.446633
50	1	0	1.891783	-0.298139	-0.995515

51	1	0	1.505764	-1.701763	0.017047
52	1	0	-3.725339	-1.531931	3.332194
53	1	0	-3.549069	-3.273385	2.927870
54	1	0	-3.213349	-2.043917	1.684877
55	1	0	2.454308	-5.053588	-0.070604
56	1	0	3.273051	-5.249107	1.519654
57	1	0	3.479206	-3.738068	0.605508
58	1	0	3.946450	-1.115975	-0.659860
59	1	0	5.820550	-1.409976	-2.200501
60	1	0	7.406094	0.459156	-2.641079
61	1	0	7.092543	2.633065	-1.458687
62	1	0	5.221999	2.921281	0.124988
63	1	0	5.413637	0.514999	2.286480
64	1	0	6.207764	1.472631	4.418890
65	1	0	5.021433	3.409570	5.442703
66	1	0	3.021606	4.364031	4.307737
67	1	0	2.210274	3.371731	2.174331
68	1	0	0.117032	4.551007	-1.854356
69	1	0	0.105300	4.248696	-0.105111
70	1	0	-0.364684	2.961690	-1.229579
71	1	0	3.521801	2.034570	-2.916803
72	1	0	2.295964	3.081520	-3.659906
73	1	0	1.826848	1.512004	-2.982800
74	1	0	2.880336	5.582008	-1.599491
75	1	0	4.296610	4.573451	-1.255850
76	1	0	3.256751	5.125926	0.072645
77	1	0	-0.933657	0.172825	4.171533
78	1	0	-1.992872	-0.768477	6.015693
79	1	0	1.536522	-2.633892	5.038665
80	1	0	1.753225	-0.247341	5.601815
81	1	0	-2.924315	-1.907238	9.286059
82	1	0	-2.587940	-2.445672	7.609428
83	1	0	-3.274947	-0.807812	7.925888
84	1	0	2.897641	-0.299878	3.637507
85	1	0	-0.091175	2.379451	4.875474
86	1	0	0.231349	1.777422	6.509676
87	1	0	-1.443283	1.895460	5.919099

Structure **ssss-IM3**

E(RB3LYP) **=** -2266.974809 a.u.

Standard orientation:

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

1	6	0	0.491511	0.100959	-0.074666
2	6	0	0.188109	0.549614	1.366933
3	7	0	1.455531	0.248443	2.084341
4	6	0	2.613203	0.544427	1.168908
5	6	0	2.036287	0.217260	-0.235285
6	6	0	1.734950	-2.865165	2.954010
7	6	0	0.923076	-3.146517	1.817741
8	8	0	1.232085	-3.325313	0.620129
9	8	0	-0.475247	-3.116264	2.172054
10	6	0	-1.415976	-3.641512	1.187833
11	6	0	3.168382	-2.952282	2.955266
12	8	0	3.898175	-2.571019	3.916495
13	8	0	3.755614	-3.446214	1.798549
14	6	0	5.212779	-3.566447	1.824995
15	6	0	3.141654	2.016885	1.351716
16	6	0	4.503250	2.214001	0.648024
17	6	0	5.049803	1.298196	-0.267282
18	6	0	6.272370	1.558538	-0.901284
19	6	0	6.970402	2.739185	-0.635418
20	6	0	6.444759	3.654440	0.285524
21	6	0	5.230906	3.389112	0.923425
22	6	0	3.282844	2.313668	2.859517
23	6	0	4.313394	1.706651	3.601139
24	6	0	4.414617	1.911406	4.980771
25	6	0	3.491874	2.733665	5.639802
26	6	0	2.468798	3.345140	4.908216
27	6	0	2.361374	3.131682	3.527788
28	8	0	2.115869	2.876967	0.787854
29	14	0	2.003044	4.253838	-0.296254
30	6	0	0.120167	4.378900	-0.554409
31	6	0	2.881405	3.954037	-1.964037
32	6	0	2.639794	5.857257	0.525005
33	6	0	-0.826093	-0.901870	4.205934
34	6	0	-1.249853	-2.143556	5.045341
35	6	0	-0.131825	-3.189606	4.755696
36	6	0	1.125591	-2.464115	4.302102
37	6	0	0.728036	-0.944318	4.273452
38	8	0	-0.246752	-4.398587	4.971510
39	6	0	-1.285506	-1.900601	6.552843
40	8	0	-0.594070	-1.045202	7.115554
41	8	0	-2.100210	-2.689940	7.327925
42	6	0	-2.875163	-3.817545	6.781719
43	6	0	1.643238	-0.426750	3.191830

44	6	0	-1.453611	0.438716	4.611175
45	1	0	-0.045554	0.720447	-0.798096
46	1	0	0.190095	-0.940647	-0.213723
47	1	0	-0.641792	0.018107	1.819028
48	1	0	0.026888	1.628053	1.424780
49	1	0	3.413985	-0.142849	1.448229
50	1	0	2.304481	0.994126	-0.950766
51	1	0	2.438596	-0.738997	-0.581288
52	1	0	-2.257842	-2.946901	1.127613
53	1	0	-1.765703	-4.621751	1.524000
54	1	0	-0.917934	-3.730549	0.220146
55	1	0	5.470221	-3.983765	0.852159
56	1	0	5.531833	-4.230590	2.631780
57	1	0	5.685054	-2.590506	1.970053
58	1	0	4.543993	0.369864	-0.499145
59	1	0	6.674912	0.832665	-1.600431
60	1	0	7.916551	2.939226	-1.127527
61	1	0	6.986504	4.565830	0.517789
62	1	0	4.852220	4.087010	1.661702
63	1	0	5.042922	1.075635	3.102850
64	1	0	5.209958	1.427382	5.537680
65	1	0	3.569583	2.891962	6.710359
66	1	0	1.748950	3.983920	5.410415
67	1	0	1.564059	3.593862	2.960212
68	1	0	-0.120702	5.217789	-1.217770
69	1	0	-0.394733	4.539624	0.398611
70	1	0	-0.274236	3.462776	-1.006306
71	1	0	2.698843	4.814125	-2.620393
72	1	0	2.493028	3.061558	-2.465900
73	1	0	3.961865	3.839074	-1.844572
74	1	0	2.283978	6.721773	-0.048875
75	1	0	3.731852	5.899100	0.557211
76	1	0	2.260403	5.950272	1.547973
77	1	0	-1.139771	-1.163980	3.193285
78	1	0	-2.204336	-2.546209	4.699987
79	1	0	1.903441	-2.638946	5.054627
80	1	0	1.028396	-0.444953	5.206594
81	1	0	-3.237696	-4.344117	7.663191
82	1	0	-2.238910	-4.468004	6.179283
83	1	0	-3.725507	-3.448352	6.199186
84	1	0	2.686313	-0.561353	3.466211
85	1	0	-1.132192	1.238083	3.932479
86	1	0	-1.165601	0.718515	5.626924
87	1	0	-2.548645	0.388361	4.564606

Structure **ers-IM1**

E(RB3LYP) = -2266.966984 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.210997	-0.621140	0.355805
2	6	0	0.449707	-0.757905	1.862797
3	7	0	1.909653	-0.469458	2.040940
4	6	0	2.646367	-0.448455	0.721727
5	6	0	1.576890	-0.960083	-0.272397
6	6	0	3.304346	0.937119	0.307120
7	6	0	4.584237	1.248794	1.116428
8	6	0	5.473830	0.223359	1.497249
9	6	0	6.684089	0.513586	2.134543
10	6	0	7.044276	1.840537	2.390674
11	6	0	6.183998	2.869303	2.000123
12	6	0	4.970641	2.576377	1.370373
13	6	0	2.247109	2.053046	0.348678
14	6	0	1.885259	2.664771	1.564964
15	6	0	0.873950	3.632463	1.610524
16	6	0	0.203202	3.999055	0.437494
17	6	0	0.553932	3.398972	-0.777668
18	6	0	1.567406	2.433311	-0.821572
19	8	0	3.693568	0.645310	-1.069625
20	14	0	4.885014	1.314015	-2.185004
21	6	0	4.251530	0.633340	-3.847545
22	6	0	6.629888	0.632785	-1.827353
23	6	0	4.901963	3.223473	-2.199109
24	6	0	2.457345	-0.337551	3.233873
25	6	0	1.763346	-0.593878	4.451592
26	6	0	2.337518	-0.369292	5.670047
27	6	0	-0.397207	3.214026	5.982472
28	6	0	0.962907	3.489899	5.769780
29	6	0	1.963153	3.106532	6.805384
30	6	0	3.278538	3.006384	6.517967
31	6	0	3.809071	3.073438	5.104612
32	8	0	3.845575	2.070754	4.379340
33	8	0	4.441744	4.212480	4.683782
34	6	0	4.123247	5.502321	5.310288
35	6	0	4.262048	2.485089	7.511455
36	8	0	5.097807	1.622241	7.215294

37	8	0	4.239916	2.934016	8.816315
38	6	0	3.479843	4.093088	9.294551
39	8	0	1.426627	4.100846	4.725349
40	6	0	-0.911746	2.419170	7.048214
41	8	0	-0.256215	1.730404	7.880236
42	8	0	-2.307306	2.344592	7.214392
43	6	0	-3.201622	3.193888	6.444204
44	1	0	-0.082535	0.402026	0.110204
45	1	0	-0.581016	-1.293810	0.014795
46	1	0	0.247119	-1.775541	2.218904
47	1	0	-0.128711	-0.050548	2.461174
48	1	0	3.455928	-1.174364	0.792819
49	1	0	1.727948	-0.510419	-1.252003
50	1	0	1.682860	-2.045976	-0.383703
51	1	0	5.251435	-0.816305	1.282147
52	1	0	7.343757	-0.297151	2.427484
53	1	0	7.976607	2.066427	2.897333
54	1	0	6.435562	3.901791	2.213824
55	1	0	4.309089	3.389575	1.103007
56	1	0	2.406986	2.426877	2.485223
57	1	0	0.650427	4.087954	2.571036
58	1	0	-0.578245	4.752379	0.467952
59	1	0	0.043961	3.682416	-1.693880
60	1	0	1.833442	1.968860	-1.762941
61	1	0	4.939634	0.897100	-4.659224
62	1	0	3.264052	1.039344	-4.091044
63	1	0	4.170993	-0.457866	-3.806679
64	1	0	7.313815	0.950217	-2.624289
65	1	0	6.623460	-0.462009	-1.800568
66	1	0	7.019083	0.996568	-0.872750
67	1	0	5.494828	3.570221	-3.054606
68	1	0	5.350361	3.626817	-1.286910
69	1	0	3.890829	3.630494	-2.292298
70	1	0	3.495625	-0.024460	3.273946
71	1	0	0.753933	-0.991330	4.411664
72	1	0	-1.072137	3.619789	5.240839
73	1	0	1.587187	2.861940	7.792125
74	1	0	4.668348	6.237779	4.720091
75	1	0	4.470302	5.531047	6.347962
76	1	0	3.045353	5.659178	5.245784
77	1	0	4.092295	4.525761	10.085837
78	1	0	2.522639	3.763608	9.703896
79	1	0	3.311331	4.822377	8.499883
80	1	0	-4.189624	3.034091	6.877504

81	1	0	-3.217775	2.908197	5.385882
82	1	0	-2.924612	4.249943	6.530149
83	6	0	1.662604	-0.653333	6.961502
84	1	0	1.128428	0.248957	7.323765
85	1	0	0.903802	-1.437800	6.869561
86	1	0	2.384647	-0.928254	7.736882
87	1	0	3.327668	0.083686	5.704461

Structure **ers-TS1**

Imaginary Frequency: -152

E(RB3LYP) **=** -2266.954379 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.017014	0.006237	-0.006127
2	6	0	0.007375	0.006536	1.536326
3	7	0	1.445888	0.002214	1.929000
4	6	0	2.360008	0.059789	0.758392
5	6	0	1.454738	-0.412276	-0.400932
6	6	0	3.058736	1.461504	0.488778
7	6	0	3.958531	1.876856	1.674506
8	6	0	4.908862	0.956401	2.165883
9	6	0	5.774784	1.293526	3.208852
10	6	0	5.723094	2.569450	3.781020
11	6	0	4.807264	3.501958	3.289835
12	6	0	3.935999	3.160556	2.246170
13	6	0	2.017443	2.519267	0.090371
14	6	0	1.121331	3.048728	1.039122
15	6	0	0.140829	3.974091	0.667013
16	6	0	0.028078	4.381637	-0.667237
17	6	0	0.903234	3.854075	-1.622377
18	6	0	1.887567	2.931686	-1.246177
19	8	0	3.899982	1.122363	-0.655648
20	14	0	5.369392	1.787823	-1.354751
21	6	0	5.136005	1.472259	-3.220967
22	6	0	6.883548	0.797265	-0.747184
23	6	0	5.592696	3.650886	-1.003596
24	6	0	1.835031	-0.361982	3.168085
25	6	0	0.975939	-0.593268	4.230494
26	6	0	1.381638	-1.230199	5.435024
27	6	0	1.961400	0.126898	7.007109
28	6	0	1.071066	1.236032	6.734571

29	6	0	1.562190	2.453868	6.039861
30	6	0	0.741493	3.311022	5.397599
31	6	0	-0.689339	2.973384	5.025681
32	8	0	-0.939679	2.289610	4.031124
33	8	0	-1.713459	3.541798	5.728156
34	6	0	-1.475323	4.115516	7.057910
35	6	0	1.244243	4.560381	4.749692
36	8	0	0.729796	5.015722	3.723693
37	8	0	2.323290	5.239340	5.282254
38	6	0	2.792727	5.151751	6.670758
39	8	0	-0.154397	1.182045	7.069154
40	6	0	3.402812	0.202564	6.831058
41	8	0	4.015611	1.015262	6.111563
42	8	0	4.193852	-0.777346	7.443886
43	6	0	3.673626	-1.675864	8.469675
44	1	0	-0.214070	1.001439	-0.390837
45	1	0	-0.729787	-0.686826	-0.405674
46	1	0	-0.453561	-0.903214	1.943802
47	1	0	-0.504307	0.869231	1.970120
48	1	0	3.177727	-0.646368	0.918644
49	1	0	1.780006	0.010980	-1.351452
50	1	0	1.523729	-1.504182	-0.479063
51	1	0	4.989955	-0.028064	1.717085
52	1	0	6.479712	0.558793	3.583700
53	1	0	6.380649	2.822495	4.605413
54	1	0	4.749975	4.497374	3.718161
55	1	0	3.240800	3.906388	1.885298
56	1	0	1.174371	2.745100	2.076528
57	1	0	-0.512056	4.376455	1.432312
58	1	0	-0.730690	5.101853	-0.956900
59	1	0	0.822663	4.156834	-2.662273
60	1	0	2.547251	2.512882	-1.994332
61	1	0	6.041571	1.752072	-3.772390
62	1	0	4.298971	2.051206	-3.624843
63	1	0	4.935793	0.411638	-3.405855
64	1	0	7.767777	1.080526	-1.331389
65	1	0	6.718614	-0.277540	-0.880269
66	1	0	7.092727	0.987187	0.309203
67	1	0	6.451953	4.025266	-1.573711
68	1	0	5.774013	3.840376	0.058026
69	1	0	4.706823	4.218538	-1.304656
70	1	0	2.902538	-0.519289	3.294754
71	1	0	-0.064423	-0.297567	4.147856
72	1	0	1.591845	-0.510648	7.798542

73	1	0	2.631957	2.620234	6.057717
74	1	0	-2.459443	4.431032	7.400070
75	1	0	-0.811571	4.983881	6.999419
76	1	0	-1.065457	3.344454	7.712135
77	1	0	3.099782	6.165564	6.928714
78	1	0	3.648989	4.477287	6.729661
79	1	0	2.002079	4.813460	7.343693
80	1	0	4.543427	-2.230949	8.820065
81	1	0	2.937023	-2.375332	8.061903
82	1	0	3.234085	-1.118488	9.303152
83	6	0	0.302503	-1.958707	6.214097
84	1	0	0.696200	-2.467331	7.098330
85	1	0	-0.474563	-1.254716	6.534130
86	1	0	-0.167901	-2.713075	5.569957
87	1	0	2.367797	-1.693089	5.431377

Structure **ers-IM2**

E(RB3LYP) **=** -2266.985311 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.137632	0.536129	0.041231
2	6	0	0.040594	0.018274	1.488739
3	7	0	1.441796	-0.153763	1.921824
4	6	0	2.424015	0.085051	0.842226
5	6	0	1.545082	0.102501	-0.430562
6	6	0	3.329423	1.383531	1.003440
7	6	0	4.269167	1.252223	2.225714
8	6	0	5.089470	0.107177	2.323898
9	6	0	5.994867	-0.051395	3.376997
10	6	0	6.112169	0.940974	4.358488
11	6	0	5.321640	2.089701	4.266933
12	6	0	4.410589	2.243686	3.211443
13	6	0	2.456345	2.646582	0.997812
14	6	0	1.612818	2.957825	2.083634
15	6	0	0.766010	4.071247	2.043050
16	6	0	0.740313	4.896189	0.912752
17	6	0	1.564781	4.594552	-0.175613
18	6	0	2.410583	3.479387	-0.133174
19	8	0	4.140987	1.315697	-0.209137
20	14	0	5.678890	1.993509	-0.719268
21	6	0	5.416275	2.325234	-2.579300

22	6	0	7.057947	0.688031	-0.521054
23	6	0	6.142487	3.602044	0.199789
24	6	0	1.744001	-0.784852	3.102593
25	6	0	0.855710	-1.217916	4.039459
26	6	0	1.280658	-2.021504	5.252796
27	6	0	0.431959	-1.579222	6.480035
28	6	0	0.264589	-0.053475	6.539421
29	6	0	1.491656	0.764320	6.507548
30	6	0	1.492672	2.115631	6.507918
31	6	0	0.269941	2.947407	6.179438
32	8	0	-0.080913	3.117035	5.015036
33	8	0	-0.378509	3.604481	7.189781
34	6	0	-0.151633	3.238555	8.590905
35	6	0	2.772583	2.889492	6.563777
36	8	0	2.945542	3.913540	5.899088
37	8	0	3.805952	2.437572	7.357728
38	6	0	3.666875	1.524905	8.506079
39	8	0	-0.859912	0.454491	6.748683
40	6	0	1.064080	-2.019830	7.804417
41	8	0	2.283234	-1.971343	7.998680
42	8	0	0.253010	-2.413581	8.839757
43	6	0	-1.214657	-2.464570	8.728801
44	1	0	0.043565	1.624509	0.019900
45	1	0	-0.653717	0.119086	-0.589487
46	1	0	-0.477030	-0.952705	1.544747
47	1	0	-0.484291	0.716397	2.151462
48	1	0	3.126082	-0.752515	0.798424
49	1	0	1.965615	0.758359	-1.193129
50	1	0	1.507850	-0.911981	-0.846191
51	1	0	5.040289	-0.657194	1.556188
52	1	0	6.611029	-0.944300	3.426434
53	1	0	6.814201	0.822194	5.177770
54	1	0	5.397539	2.870124	5.015720
55	1	0	3.815049	3.145726	3.170622
56	1	0	1.599754	2.337268	2.970290
57	1	0	0.137747	4.277537	2.901648
58	1	0	0.085504	5.761605	0.881849
59	1	0	1.549619	5.221379	-1.062515
60	1	0	3.022694	3.238290	-0.991630
61	1	0	6.352482	2.658245	-3.043148
62	1	0	4.658814	3.097610	-2.748014
63	1	0	5.088381	1.411315	-3.085734
64	1	0	7.970078	1.036885	-1.020762
65	1	0	6.759445	-0.260072	-0.981587

66	1	0	7.290037	0.504027	0.531592
67	1	0	7.059503	4.014716	-0.238847
68	1	0	6.321459	3.419833	1.263250
69	1	0	5.351277	4.352769	0.111440
70	1	0	2.806733	-0.941589	3.266189
71	1	0	-0.213496	-1.089835	3.887281
72	1	0	-0.576313	-1.985300	6.371515
73	1	0	2.429200	0.224253	6.554088
74	1	0	-0.808963	3.896964	9.155773
75	1	0	0.886654	3.417665	8.886536
76	1	0	-0.431455	2.195546	8.753091
77	1	0	4.433027	1.849622	9.209312
78	1	0	3.850875	0.493184	8.202803
79	1	0	2.678017	1.604091	8.962485
80	1	0	-1.552439	-2.667977	9.743433
81	1	0	-1.520667	-3.279782	8.067480
82	1	0	-1.617089	-1.512717	8.376015
83	6	0	1.144736	-3.548184	5.040157
84	1	0	1.461600	-4.111764	5.927143
85	1	0	0.107233	-3.818109	4.805688
86	1	0	1.767793	-3.862605	4.196873
87	1	0	2.333469	-1.812521	5.481088

Structure **zrs-IM1**

E(RB3LYP) = -2266.962745 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.016133	-0.045218	-0.039874
2	6	0	0.004669	-0.040181	1.494838
3	7	0	1.457774	-0.025174	1.843807
4	6	0	2.300161	0.483932	0.698761
5	6	0	1.263252	0.784425	-0.411777
6	6	0	1.957450	-0.647840	2.909897
7	6	0	1.202727	-1.238186	3.941249
8	6	0	1.759363	-1.979532	4.964862
9	6	0	0.948482	-4.727523	4.380618
10	6	0	1.498202	-4.989527	5.674280
11	8	0	2.643433	-5.474985	5.876797
12	8	0	0.701234	-4.612071	6.756761
13	6	0	1.225073	-4.947435	8.080747
14	6	0	-0.280507	-4.119740	4.030286

15	8	0	-1.116325	-3.525466	4.800133
16	6	0	-0.547871	-4.089199	2.563190
17	6	0	-1.639969	-3.497440	2.029088
18	6	0	-2.731302	-2.907230	2.871417
19	8	0	-3.771635	-3.469141	3.204095
20	8	0	-2.484360	-1.564026	3.128450
21	6	0	-3.395404	-0.940511	4.099385
22	6	0	-1.793382	-3.455922	0.562681
23	8	0	-0.923255	-3.765586	-0.270625
24	8	0	-3.032622	-2.990695	0.184864
25	6	0	-3.314554	-2.950066	-1.253634
26	6	0	3.339694	1.650839	0.975455
27	6	0	4.461719	1.138200	1.908348
28	6	0	5.462776	0.302294	1.382653
29	6	0	6.466464	-0.215090	2.207873
30	6	0	6.488269	0.095315	3.573459
31	6	0	5.497419	0.927241	4.106038
32	6	0	4.490866	1.444539	3.280258
33	6	0	2.792082	2.994074	1.482717
34	6	0	1.452662	3.239130	1.817485
35	6	0	1.037110	4.504157	2.257643
36	6	0	1.955868	5.549078	2.374249
37	6	0	3.302170	5.315298	2.063114
38	6	0	3.712522	4.053186	1.630543
39	8	0	3.930474	1.789433	-0.349247
40	14	0	4.122503	2.942850	-1.655441
41	6	0	4.365783	1.801663	-3.159334
42	6	0	5.693926	3.993113	-1.383028
43	6	0	2.603994	4.073667	-1.910983
44	1	0	-0.904417	0.374670	-0.454657
45	1	0	0.108212	-1.075727	-0.401351
46	1	0	-0.483898	-0.911571	1.928537
47	1	0	-0.489157	0.848416	1.905415
48	1	0	2.935594	-0.348484	0.379738
49	1	0	1.024826	1.851066	-0.437870
50	1	0	1.664927	0.513733	-1.389163
51	1	0	3.038076	-0.698844	2.948522
52	1	0	0.119916	-1.183729	3.913822
53	1	0	1.566828	-5.113651	3.577965
54	1	0	2.188800	-4.461723	8.257096
55	1	0	1.356675	-6.027867	8.180562
56	1	0	0.469893	-4.583040	8.776133
57	1	0	0.171754	-4.539888	1.884447
58	1	0	-3.088399	0.103610	4.148359

59	1	0	-3.272349	-1.435499	5.064842
60	1	0	-4.430006	-1.032759	3.763431
61	1	0	-3.202577	-3.945993	-1.687282
62	1	0	-2.631542	-2.260924	-1.756473
63	1	0	-4.343981	-2.604691	-1.323807
64	1	0	5.457784	0.082758	0.322091
65	1	0	7.233431	-0.855500	1.784099
66	1	0	7.269354	-0.303376	4.212507
67	1	0	5.506882	1.179846	5.161515
68	1	0	3.733128	2.091629	3.707250
69	1	0	0.716533	2.452884	1.750291
70	1	0	-0.006174	4.664751	2.509916
71	1	0	1.633438	6.528078	2.713055
72	1	0	4.031940	6.111807	2.168013
73	1	0	4.761220	3.875105	1.422029
74	1	0	3.475775	1.188791	-3.336331
75	1	0	5.214128	1.128760	-2.998071
76	1	0	4.561367	2.390356	-4.063260
77	1	0	5.977641	4.477436	-2.325363
78	1	0	6.528390	3.361215	-1.061382
79	1	0	5.542527	4.775229	-0.633687
80	1	0	2.803677	4.741062	-2.758713
81	1	0	2.400472	4.692013	-1.032556
82	1	0	1.704762	3.495554	-2.145951
83	6	0	3.205289	-2.189514	5.271577
84	1	0	3.412965	-3.262981	5.384946
85	1	0	3.892950	-1.771212	4.533087
86	1	0	3.438789	-1.736464	6.246702
87	1	0	1.053837	-2.392815	5.682534

Structure **zrs-TS1**

Imaginary Frequency: -143

E(RB3LYP) = -2266.951463 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.018905	0.048665	0.056661
2	6	0	-0.005898	0.041659	1.592219
3	7	0	1.449467	0.038733	1.913427
4	6	0	2.278675	0.539957	0.762671
5	6	0	1.224051	0.880279	-0.319007
6	6	0	1.965220	-0.639734	2.954012

7	6	0	1.241266	-1.194873	4.007127
8	6	0	1.817981	-1.964793	5.025593
9	6	0	1.211080	-4.376205	4.604460
10	6	0	1.536878	-4.747088	5.956206
11	8	0	2.658964	-5.186454	6.313210
12	8	0	0.539504	-4.515293	6.893302
13	6	0	0.835723	-4.938190	8.264129
14	6	0	-0.068836	-4.047842	4.062026
15	8	0	-1.112618	-3.710924	4.706436
16	6	0	-0.122347	-4.024799	2.569688
17	6	0	-1.227166	-3.669425	1.879965
18	6	0	-2.523721	-3.319534	2.548632
19	8	0	-3.473545	-4.078993	2.722401
20	8	0	-2.560872	-1.970390	2.852953
21	6	0	-3.695763	-1.543341	3.684926
22	6	0	-1.177953	-3.642541	0.402518
23	8	0	-0.154238	-3.765464	-0.291569
24	8	0	-2.418015	-3.432632	-0.149259
25	6	0	-2.502845	-3.428795	-1.614349
26	6	0	3.342614	1.687373	1.026657
27	6	0	4.418810	1.195040	2.021570
28	6	0	5.409528	0.301811	1.576370
29	6	0	6.374013	-0.192394	2.460626
30	6	0	6.367862	0.201510	3.804844
31	6	0	5.388058	1.091977	4.255971
32	6	0	4.419467	1.584293	3.371860
33	6	0	2.809974	3.060729	1.464508
34	6	0	1.524551	3.283923	1.978772
35	6	0	1.122600	4.564703	2.384456
36	6	0	2.003459	5.644316	2.291152
37	6	0	3.299763	5.431135	1.803138
38	6	0	3.697063	4.154181	1.402003
39	8	0	4.004474	1.771611	-0.266151
40	14	0	4.089225	2.695896	-1.748221
41	6	0	4.174780	1.364075	-3.108227
42	6	0	5.714827	3.695224	-1.733882
43	6	0	2.606307	3.863252	-2.050526
44	1	0	-0.944740	0.468757	-0.346227
45	1	0	0.081344	-0.978076	-0.313329
46	1	0	-0.495388	-0.833716	2.020561
47	1	0	-0.492760	0.932176	2.010245
48	1	0	2.896732	-0.296412	0.417774
49	1	0	0.989393	1.948558	-0.300775
50	1	0	1.598228	0.636671	-1.314667

51	1	0	3.043289	-0.737932	2.940353
52	1	0	0.163429	-1.077146	4.035822
53	1	0	1.995854	-4.636887	3.903059
54	1	0	1.715788	-4.417460	8.650067
55	1	0	1.019495	-6.014741	8.301496
56	1	0	-0.056329	-4.676155	8.830929
57	1	0	0.766124	-4.295412	2.005359
58	1	0	-3.596677	-0.461897	3.765876
59	1	0	-3.613906	-2.023185	4.662312
60	1	0	-4.639518	-1.820269	3.211324
61	1	0	-2.109288	-4.364879	-2.015588
62	1	0	-1.932438	-2.592058	-2.024791
63	1	0	-3.564192	-3.323310	-1.828668
64	1	0	5.429628	0.020034	0.530917
65	1	0	7.134010	-0.877695	2.098658
66	1	0	7.119420	-0.178106	4.489489
67	1	0	5.376720	1.409975	5.293755
68	1	0	3.668864	2.275646	3.736792
69	1	0	0.829904	2.464050	2.085020
70	1	0	0.120858	4.710559	2.776076
71	1	0	1.691844	6.635390	2.604321
72	1	0	4.002415	6.256474	1.745531
73	1	0	4.710247	3.991586	1.052787
74	1	0	3.253908	0.772920	-3.149052
75	1	0	5.008485	0.679490	-2.921213
76	1	0	4.325402	1.828188	-4.090134
77	1	0	5.923097	4.078812	-2.740027
78	1	0	6.552744	3.058988	-1.430855
79	1	0	5.666764	4.548813	-1.050693
80	1	0	2.782694	4.412014	-2.984218
81	1	0	2.492774	4.591681	-1.243312
82	1	0	1.666462	3.313708	-2.157591
83	6	0	3.288950	-2.133978	5.269480
84	1	0	3.501358	-3.105912	5.726385
85	1	0	3.895550	-2.037470	4.365403
86	1	0	3.629704	-1.362699	5.977447
87	1	0	1.164507	-2.206231	5.858667

Structure **zrs-IM2**

E(RB3LYP) **=** -2266.98547 a.u.

Standard orientation:

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

1	6	0	-0.291074	0.019787	1.094687
2	6	0	0.082484	0.084575	2.585748
3	7	0	1.562238	0.042222	2.578585
4	6	0	2.127298	0.409903	1.252512
5	6	0	0.876307	0.748602	0.399279
6	6	0	2.251336	-0.783248	3.460265
7	6	0	1.777527	-1.295108	4.621690
8	6	0	2.543095	-2.246731	5.531029
9	6	0	2.023108	-3.719527	5.361404
10	6	0	2.430530	-4.613780	6.520679
11	8	0	2.944890	-4.259956	7.583500
12	8	0	2.145255	-5.927044	6.228597
13	6	0	2.414370	-6.916901	7.283753
14	6	0	0.499137	-3.739991	5.220451
15	8	0	-0.237368	-3.691157	6.225879
16	6	0	-0.059218	-3.780358	3.848129
17	6	0	-1.367840	-3.608769	3.564726
18	6	0	-2.413325	-3.358707	4.609902
19	8	0	-3.203297	-4.197928	5.038551
20	8	0	-2.398971	-2.042323	4.992381
21	6	0	-3.284327	-1.679771	6.111871
22	6	0	-1.796451	-3.657761	2.143848
23	8	0	-1.037524	-3.812206	1.174971
24	8	0	-3.146604	-3.481121	2.014365
25	6	0	-3.698321	-3.521170	0.652010
26	6	0	3.255517	1.524102	1.199124
27	6	0	4.495479	1.070031	2.002030
28	6	0	5.400390	0.162109	1.424842
29	6	0	6.520694	-0.279728	2.136599
30	6	0	6.759106	0.182548	3.436596
31	6	0	5.863568	1.085958	4.018953
32	6	0	4.739672	1.524575	3.308457
33	6	0	2.854991	2.947365	1.620749
34	6	0	1.761958	3.237736	2.451997
35	6	0	1.473178	4.558067	2.824834
36	6	0	2.279256	5.610982	2.385194
37	6	0	3.392192	5.331352	1.581518
38	6	0	3.677881	4.014892	1.211864
39	8	0	3.667497	1.501193	-0.198968
40	14	0	3.408856	2.212694	-1.765725
41	6	0	3.200501	0.724645	-2.941719
42	6	0	4.997299	3.159931	-2.239502
43	6	0	1.898268	3.376840	-1.906336

44	1	0	-1.260644	0.481977	0.882344
45	1	0	-0.336251	-1.027885	0.773231
46	1	0	-0.311028	-0.760859	3.155516
47	1	0	-0.298438	1.001781	3.058658
48	1	0	2.632679	-0.467852	0.825976
49	1	0	0.698011	1.828128	0.397632
50	1	0	1.006440	0.429145	-0.636792
51	1	0	3.263928	-1.005784	3.141950
52	1	0	0.790085	-1.009597	4.976228
53	1	0	2.459893	-4.138745	4.446644
54	1	0	1.819616	-6.687091	8.170092
55	1	0	3.474897	-6.909938	7.544318
56	1	0	2.121099	-7.870820	6.850496
57	1	0	0.621204	-3.960121	3.022517
58	1	0	-3.183580	-0.600694	6.207711
59	1	0	-2.944716	-2.190724	7.015051
60	1	0	-4.313470	-1.965822	5.886905
61	1	0	-3.471384	-4.482226	0.186390
62	1	0	-3.270725	-2.715159	0.051829
63	1	0	-4.769598	-3.390047	0.785686
64	1	0	5.228892	-0.170527	0.408900
65	1	0	7.212297	-0.976025	1.671749
66	1	0	7.632677	-0.153850	3.986231
67	1	0	6.039688	1.456498	5.024176
68	1	0	4.057867	2.227254	3.772615
69	1	0	1.147657	2.435225	2.833137
70	1	0	0.619080	4.756616	3.465066
71	1	0	2.054303	6.632702	2.674186
72	1	0	4.042591	6.136158	1.252718
73	1	0	4.557656	3.801963	0.615733
74	1	0	2.297390	0.150959	-2.708532
75	1	0	4.059774	0.051073	-2.858092
76	1	0	3.130294	1.064302	-3.982089
77	1	0	4.969431	3.427835	-3.302709
78	1	0	5.879232	2.534572	-2.066351
79	1	0	5.112752	4.081890	-1.660936
80	1	0	1.886901	3.806026	-2.916291
81	1	0	1.949337	4.198751	-1.186949
82	1	0	0.955356	2.843441	-1.756451
83	6	0	4.070935	-2.208831	5.348959
84	1	0	4.370343	-2.569281	4.356666
85	1	0	4.440603	-1.184644	5.454717
86	1	0	4.561114	-2.832306	6.101888
87	1	0	2.321896	-1.974089	6.571577

Structure **ers-IM1** (M06-2x)

E(RB3LYP) **=** -2265.695904 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.213901	0.945350	0.803816
2	6	0	0.088789	1.024307	2.297666
3	7	0	1.500398	0.555452	2.423251
4	6	0	2.071383	0.120654	1.110267
5	6	0	0.810539	-0.059040	0.254811
6	6	0	3.136476	1.079921	0.473479
7	6	0	4.420909	1.152778	1.307157
8	6	0	4.978451	-0.027707	1.826900
9	6	0	6.184138	-0.009769	2.524097
10	6	0	6.873338	1.191322	2.696305
11	6	0	6.350049	2.362642	2.157347
12	6	0	5.137387	2.343138	1.468905
13	6	0	2.495157	2.432993	0.185400
14	6	0	2.248872	3.351376	1.217224
15	6	0	1.587293	4.552502	0.956025
16	6	0	1.148470	4.847428	-0.335348
17	6	0	1.384891	3.938828	-1.367632
18	6	0	2.054315	2.742543	-1.108065
19	8	0	3.432351	0.380809	-0.751580
20	14	0	4.815404	0.501783	-1.819903
21	6	0	4.108988	-0.241562	-3.406695
22	6	0	6.275648	-0.531953	-1.201113
23	6	0	5.380027	2.288201	-2.098972
24	6	0	2.087834	0.402532	3.587380
25	6	0	1.424286	0.571969	4.833362
26	6	0	2.064017	0.308265	5.999015
27	6	0	-0.102349	4.087741	4.154104
28	6	0	1.193872	4.350121	4.617780
29	6	0	1.655401	3.821053	5.929919
30	6	0	2.956666	3.528008	6.106896
31	6	0	3.899563	3.424964	4.938695
32	8	0	3.873728	2.459959	4.175221
33	8	0	4.887089	4.346576	4.820133
34	6	0	4.731105	5.630993	5.483252
35	6	0	3.502426	2.970826	7.361283
36	8	0	4.342917	2.068970	7.368544

37	8	0	3.036431	3.427879	8.565013
38	6	0	2.329652	4.680029	8.756006
39	8	0	2.059891	5.042984	3.968949
40	6	0	-1.008196	3.184221	4.767698
41	8	0	-0.809775	2.488283	5.795105
42	8	0	-2.237024	2.963377	4.142773
43	6	0	-2.640746	3.740696	3.000745
44	1	0	-0.079902	1.926967	0.335728
45	1	0	-1.243683	0.622056	0.623483
46	1	0	-0.554492	0.363059	2.892703
47	1	0	0.021081	2.039033	2.713087
48	1	0	2.570293	-0.840906	1.265258
49	1	0	1.042205	0.087350	-0.802169
50	1	0	0.438260	-1.084234	0.379003
51	1	0	4.491273	-0.986150	1.657024
52	1	0	6.590032	-0.935309	2.923589
53	1	0	7.806371	1.211809	3.251548
54	1	0	6.862853	3.308373	2.303560
55	1	0	4.737665	3.275582	1.083005
56	1	0	2.582224	3.161572	2.237556
57	1	0	1.455679	5.242136	1.786926
58	1	0	0.636933	5.784545	-0.538509
59	1	0	1.050128	4.159388	-2.378060
60	1	0	2.223506	2.028721	-1.909848
61	1	0	4.883032	-0.318816	-4.179454
62	1	0	3.292244	0.377044	-3.796388
63	1	0	3.712657	-1.243758	-3.210370
64	1	0	6.999621	-0.652396	-2.017504
65	1	0	5.950686	-1.528503	-0.881294
66	1	0	6.780786	-0.047220	-0.357819
67	1	0	6.132587	2.298463	-2.898083
68	1	0	5.836122	2.704303	-1.193985
69	1	0	4.548728	2.936673	-2.394374
70	1	0	3.129675	0.084134	3.581280
71	1	0	0.393698	0.922128	4.876478
72	1	0	-0.367237	4.591118	3.231124
73	1	0	0.921350	3.677071	6.719652
74	1	0	5.580163	6.227718	5.152472
75	1	0	4.767999	5.515190	6.573600
76	1	0	3.784357	6.077013	5.160824
77	1	0	2.683979	5.073506	9.709574
78	1	0	1.253761	4.496081	8.811872
79	1	0	2.540424	5.391131	7.951297
80	1	0	-3.654690	3.412629	2.768350

81	1	0	-1.989159	3.560054	2.133823
82	1	0	-2.643758	4.813324	3.227257
83	6	0	1.389044	0.384787	7.316886
84	1	0	0.407794	0.863305	7.227639
85	1	0	1.256449	-0.624820	7.733602
86	1	0	2.004062	0.927191	8.046266
87	1	0	3.121992	0.033588	5.984419

Structure **zrs-IM1** (M06-2x)

E(RB3LYP) **=** -2265.691458 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.003666	-0.064834	-0.044368
2	6	0	-0.016358	-0.059933	1.482058
3	7	0	1.428221	-0.072280	1.827196
4	6	0	2.271776	0.430664	0.698515
5	6	0	1.251985	0.750945	-0.405632
6	6	0	1.922822	-0.719587	2.876467
7	6	0	1.172352	-1.283196	3.916651
8	6	0	1.745294	-2.033167	4.920734
9	6	0	1.006810	-4.706014	4.286044
10	6	0	1.585709	-4.986626	5.556979
11	8	0	2.724870	-5.483476	5.723109
12	8	0	0.843268	-4.587613	6.654824
13	6	0	1.429761	-4.870643	7.946991
14	6	0	-0.224469	-4.097073	3.974849
15	8	0	-1.073728	-3.565883	4.763958
16	6	0	-0.465514	-3.956904	2.513830
17	6	0	-1.514541	-3.260587	2.033975
18	6	0	-2.569873	-2.699101	2.927386
19	8	0	-3.643491	-3.230096	3.178487
20	8	0	-2.245226	-1.426496	3.340039
21	6	0	-3.050212	-0.915348	4.438107
22	6	0	-1.660495	-3.073494	0.588099
23	8	0	-0.882290	-3.477588	-0.285746
24	8	0	-2.767256	-2.328944	0.285894
25	6	0	-3.068612	-2.149853	-1.122741
26	6	0	3.296379	1.578413	1.001682
27	6	0	4.316446	1.083217	2.030962
28	6	0	5.327751	0.204960	1.623958
29	6	0	6.215006	-0.332909	2.555745

30	6	0	6.105732	0.003533	3.906633
31	6	0	5.103054	0.881688	4.319101
32	6	0	4.213831	1.418952	3.387329
33	6	0	2.742113	2.930816	1.433887
34	6	0	1.410297	3.187202	1.765000
35	6	0	0.997162	4.474349	2.121455
36	6	0	1.912848	5.522440	2.159591
37	6	0	3.255832	5.271472	1.866130
38	6	0	3.663533	3.987892	1.519430
39	8	0	3.974076	1.689295	-0.260268
40	14	0	4.059531	2.807143	-1.595210
41	6	0	4.361590	1.654078	-3.059582
42	6	0	5.537102	3.971218	-1.360293
43	6	0	2.486898	3.828992	-1.880277
44	1	0	-0.912595	0.359677	-0.466010
45	1	0	0.095129	-1.100334	-0.403014
46	1	0	-0.515694	-0.927470	1.920683
47	1	0	-0.505669	0.830094	1.900068
48	1	0	2.912670	-0.402224	0.375861
49	1	0	1.022093	1.823276	-0.414494
50	1	0	1.654912	0.490422	-1.388629
51	1	0	3.005827	-0.819506	2.888338
52	1	0	0.085989	-1.200799	3.909784
53	1	0	1.617831	-5.066012	3.462207
54	1	0	2.389219	-4.354447	8.063664
55	1	0	1.600989	-5.944003	8.068280
56	1	0	0.702015	-4.508847	8.672817
57	1	0	0.239383	-4.388624	1.803643
58	1	0	-2.678506	0.091662	4.627694
59	1	0	-2.898116	-1.565523	5.304660
60	1	0	-4.107807	-0.900971	4.163381
61	1	0	-3.206156	-3.122178	-1.603063
62	1	0	-2.254505	-1.619198	-1.625791
63	1	0	-3.989603	-1.570047	-1.144435
64	1	0	5.417054	-0.036686	0.569052
65	1	0	6.995885	-1.012440	2.226442
66	1	0	6.797989	-0.415067	4.631494
67	1	0	5.010845	1.150675	5.367752
68	1	0	3.431985	2.098188	3.719319
69	1	0	0.677525	2.389661	1.754968
70	1	0	-0.045311	4.651964	2.369707
71	1	0	1.589079	6.523071	2.430121
72	1	0	3.986199	6.074169	1.919377
73	1	0	4.713673	3.786025	1.319541

74	1	0	3.501930	0.993369	-3.219942
75	1	0	5.241237	1.027499	-2.877833
76	1	0	4.529112	2.229384	-3.978023
77	1	0	5.880681	4.329260	-2.338895
78	1	0	6.369539	3.445911	-0.878250
79	1	0	5.272676	4.842952	-0.751312
80	1	0	2.689075	4.524763	-2.705681
81	1	0	2.206680	4.420438	-1.001432
82	1	0	1.636771	3.203016	-2.172466
83	6	0	3.189082	-2.244633	5.189822
84	1	0	3.405673	-3.320132	5.289275
85	1	0	3.864168	-1.818173	4.441372
86	1	0	3.442925	-1.799913	6.163905
87	1	0	1.054524	-2.442812	5.661363

Structure **rsrr-TS2**

Imaginary Frequency: -87

E(RB3LYP) = -2266.951606 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.022655	0.020832	-0.005006
2	6	0	0.010655	0.011639	1.528479
3	7	0	1.452470	0.001943	1.873520
4	6	0	2.128831	-0.945642	0.901196
5	6	0	1.243727	-0.854223	-0.380375
6	6	0	0.806832	3.620502	2.264975
7	6	0	1.934633	4.134806	1.496973
8	8	0	1.966716	4.440417	0.292151
9	8	0	3.082303	4.266311	2.292803
10	6	0	4.250497	4.883328	1.663887
11	6	0	-0.496427	3.560248	1.632122
12	8	0	-0.873838	4.071197	0.569252
13	8	0	-1.404394	2.779456	2.403379
14	6	0	-2.822941	2.926753	2.065752
15	6	0	3.683282	-0.926373	0.618009
16	6	0	4.495612	-1.242592	1.896810
17	6	0	4.403590	-2.528945	2.457576
18	6	0	5.100790	-2.852589	3.625110
19	6	0	5.908212	-1.896862	4.253811
20	6	0	6.015692	-0.617711	3.700075
21	6	0	5.318160	-0.293846	2.529260

22	6	0	4.233178	0.291845	-0.130884
23	6	0	5.562940	0.234044	-0.598603
24	6	0	6.108930	1.277744	-1.347887
25	6	0	5.337359	2.412048	-1.637763
26	6	0	4.030964	2.500280	-1.149379
27	6	0	3.486965	1.448959	-0.395059
28	8	0	3.783304	-2.133339	-0.210225
29	14	0	4.201153	-2.690024	-1.815319
30	6	0	3.171109	-4.286278	-1.962902
31	6	0	6.058353	-3.130945	-1.898014
32	6	0	3.743123	-1.482097	-3.222625
33	6	0	0.322334	0.886416	5.042972
34	6	0	-0.134826	2.224970	5.688441
35	6	0	-0.054147	3.358209	4.652154
36	6	0	1.017819	3.237509	3.602924
37	6	0	1.506845	1.198675	4.102434
38	8	0	-0.754087	4.377345	4.756462
39	6	0	0.738174	2.601295	6.898211
40	8	0	1.903738	2.215864	7.019568
41	8	0	0.211251	3.406928	7.874250
42	6	0	-1.183630	3.884321	7.872410
43	6	0	2.019296	0.540529	2.968398
44	6	0	-0.896270	0.106656	4.528265
45	1	0	0.144056	1.047127	-0.367483
46	1	0	-0.912383	-0.367508	-0.418837
47	1	0	-0.466697	-0.904465	1.902376
48	1	0	-0.476474	0.878207	1.967420
49	1	0	1.987700	-1.940601	1.341695
50	1	0	1.797827	-0.424912	-1.215156
51	1	0	0.936138	-1.860933	-0.674821
52	1	0	4.710360	4.194370	0.952271
53	1	0	4.930129	5.099590	2.487574
54	1	0	3.961470	5.798717	1.142899
55	1	0	-3.313180	2.025402	2.434199
56	1	0	-2.941119	3.031201	0.986332
57	1	0	-3.223463	3.811268	2.568665
58	1	0	3.807672	-3.280803	1.954314
59	1	0	5.018828	-3.852435	4.040104
60	1	0	6.449126	-2.147640	5.160578
61	1	0	6.642984	0.130787	4.173558
62	1	0	5.418962	0.700776	2.109731
63	1	0	6.170639	-0.632450	-0.362639
64	1	0	7.133764	1.209656	-1.699906
65	1	0	5.756428	3.222533	-2.225636

66	1	0	3.426789	3.383916	-1.318372
67	1	0	2.479792	1.557273	-0.014748
68	1	0	3.382210	-4.795216	-2.910807
69	1	0	2.099121	-4.066012	-1.923920
70	1	0	3.407814	-4.972804	-1.143550
71	1	0	6.246475	-3.754369	-2.780811
72	1	0	6.358327	-3.697981	-1.010519
73	1	0	6.692257	-2.242670	-1.971727
74	1	0	4.027051	-1.939453	-4.178950
75	1	0	4.266437	-0.526512	-3.133222
76	1	0	2.666722	-1.287069	-3.252287
77	1	0	0.767304	0.282077	5.845524
78	1	0	-1.178132	2.157191	6.009067
79	1	0	1.989880	3.539228	3.986853
80	1	0	2.341240	1.489915	4.737932
81	1	0	-1.218444	4.602261	8.690119
82	1	0	-1.865148	3.053952	8.083340
83	1	0	-1.430496	4.363902	6.924835
84	1	0	3.100374	0.537953	2.909470
85	1	0	-0.598837	-0.848030	4.085221
86	1	0	-1.471065	0.678353	3.797305
87	1	0	-1.556738	-0.121153	5.374279

Structure **rsrr-IM3**

E(RB3LYP) **=** -2266.972371 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.380304	0.966108	0.586628
2	6	0	0.238929	0.351058	2.001409
3	7	0	1.662182	0.143637	2.423629
4	6	0	2.314636	-0.426899	1.172913
5	6	0	1.817415	0.577289	0.105147
6	6	0	0.587708	3.184586	3.422753
7	6	0	1.409620	3.850650	2.463429
8	8	0	1.121262	4.295085	1.330911
9	8	0	2.773428	3.970759	2.907989
10	6	0	3.563499	4.944908	2.157799
11	6	0	-0.819102	3.153492	3.216314
12	8	0	-1.526514	3.646466	2.319222
13	8	0	-1.464040	2.347277	4.243770
14	6	0	-2.907025	2.525952	4.383370

15	6	0	3.794145	-0.958028	1.175936
16	6	0	3.893645	-2.100743	2.223385
17	6	0	3.249760	-3.322095	1.955431
18	6	0	3.269017	-4.361325	2.889847
19	6	0	3.933924	-4.200659	4.111789
20	6	0	4.589432	-2.996540	4.383732
21	6	0	4.573038	-1.956647	3.445245
22	6	0	4.951672	0.035642	1.314803
23	6	0	6.255647	-0.487801	1.178749
24	6	0	7.377403	0.337497	1.256127
25	6	0	7.220946	1.711696	1.483228
26	6	0	5.938103	2.238350	1.641202
27	6	0	4.807937	1.409739	1.558052
28	8	0	3.833275	-1.609840	-0.130633
29	14	0	4.520363	-1.360470	-1.731702
30	6	0	3.180818	-2.096689	-2.868121
31	6	0	6.125769	-2.378587	-1.892338
32	6	0	4.841693	0.470240	-2.166693
33	6	0	0.749228	0.306009	5.706533
34	6	0	0.215352	1.399820	6.665330
35	6	0	0.376938	2.764688	5.938945
36	6	0	1.220474	2.640486	4.668177
37	6	0	1.748758	1.109395	4.771001
38	8	0	-0.035718	3.829477	6.407390
39	6	0	1.018746	1.430540	7.969792
40	8	0	2.179794	1.013250	8.035203
41	8	0	0.443069	1.945833	9.099973
42	6	0	-0.923063	2.498045	9.125968
43	6	0	2.258438	0.470019	3.534966
44	6	0	-0.371926	-0.520295	5.062613
45	1	0	0.261526	2.051489	0.628441
46	1	0	-0.391046	0.565019	-0.076492
47	1	0	-0.221095	-0.643715	1.967316
48	1	0	-0.290459	0.969164	2.710998
49	1	0	1.752619	-1.353991	1.009510
50	1	0	2.454468	1.462660	0.052531
51	1	0	1.809694	0.104062	-0.877139
52	1	0	4.502876	5.031295	2.705328
53	1	0	3.050701	5.909324	2.124518
54	1	0	3.734437	4.610527	1.131157
55	1	0	-3.333374	1.548228	4.618198
56	1	0	-3.314146	2.914074	3.447468
57	1	0	-3.105415	3.230457	5.197226
58	1	0	2.764787	-3.461031	0.996646

59	1	0	2.771923	-5.298681	2.660525
60	1	0	3.948697	-5.007184	4.837602
61	1	0	5.120598	-2.862842	5.320570
62	1	0	5.117315	-1.044275	3.663861
63	1	0	6.382308	-1.553252	1.023186
64	1	0	8.369595	-0.089135	1.148908
65	1	0	8.089653	2.358727	1.546406
66	1	0	5.804828	3.296556	1.829073
67	1	0	3.835554	1.863384	1.702376
68	1	0	3.512156	-2.078701	-3.913041
69	1	0	2.245479	-1.531470	-2.798394
70	1	0	2.972070	-3.135518	-2.592477
71	1	0	6.410418	-2.450711	-2.949159
72	1	0	5.977822	-3.393956	-1.509907
73	1	0	6.956673	-1.920437	-1.348155
74	1	0	5.214204	0.521320	-3.197600
75	1	0	5.592050	0.920815	-1.511691
76	1	0	3.929383	1.071785	-2.111050
77	1	0	1.378193	-0.380028	6.281784
78	1	0	-0.848961	1.263180	6.872187
79	1	0	2.115225	3.249990	4.834226
80	1	0	2.638740	1.195801	5.404423
81	1	0	-1.006388	2.954221	10.111054
82	1	0	-1.659027	1.693062	9.030665
83	1	0	-1.046217	3.246299	8.342310
84	1	0	3.321883	0.265988	3.530565
85	1	0	0.031287	-1.271067	4.373383
86	1	0	-1.090652	0.110205	4.538197
87	1	0	-0.906111	-1.067050	5.849828

Structure **rsrs-TS2**

Imaginary Frequency: -93

E(RB3LYP) = -2266.956467 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.039828	-0.038144	-0.022379
2	6	0	0.031835	-0.028153	1.514879
3	7	0	1.479171	-0.028487	1.902905
4	6	0	2.341941	-0.091252	0.670859
5	6	0	1.420996	0.528370	-0.400938
6	6	0	0.990022	-3.084380	4.393822

7	6	0	-0.252293	-3.377287	3.657115
8	8	0	-0.994188	-2.471664	3.227861
9	8	0	-0.646226	-4.672255	3.408507
10	6	0	-0.153240	-5.815303	4.180381
11	6	0	2.210676	-3.840545	4.170400
12	8	0	2.428600	-4.699218	3.289134
13	8	0	3.207116	-3.509400	5.103615
14	6	0	4.468999	-4.247565	5.051808
15	6	0	3.835288	0.449837	0.735279
16	6	0	4.790972	-0.751134	0.951569
17	6	0	6.105409	-0.695940	0.453871
18	6	0	6.971646	-1.786091	0.573430
19	6	0	6.534277	-2.971933	1.175741
20	6	0	5.232292	-3.043423	1.677541
21	6	0	4.378152	-1.936380	1.584020
22	6	0	4.068761	1.593256	1.746370
23	6	0	5.146285	1.578080	2.649368
24	6	0	5.379589	2.657857	3.511978
25	6	0	4.537279	3.773491	3.492166
26	6	0	3.454271	3.798861	2.603569
27	6	0	3.224987	2.722163	1.742731
28	8	0	4.084192	0.940461	-0.613947
29	14	0	4.800562	2.301974	-1.450547
30	6	0	5.413986	1.514509	-3.071063
31	6	0	6.250686	3.125863	-0.515907
32	6	0	3.462028	3.611764	-1.823915
33	6	0	1.167971	0.743585	5.610269
34	6	0	0.217704	0.000929	6.605369
35	6	0	-0.012490	-1.435273	6.077258
36	6	0	1.068164	-1.929351	5.181376
37	6	0	0.945668	0.070310	4.256150
38	8	0	-0.972899	-2.132969	6.441163
39	6	0	-1.114758	0.749530	6.747452
40	8	0	-1.523559	1.530218	5.885857
41	8	0	-1.868637	0.575170	7.879553
42	6	0	-1.521196	-0.367767	8.950173
43	6	0	1.850141	0.082315	3.192217
44	6	0	2.626583	0.829426	6.095731
45	1	0	-0.785481	0.548600	-0.434642
46	1	0	-0.065174	-1.063405	-0.395598
47	1	0	-0.471750	-0.894353	1.956526
48	1	0	-0.428947	0.882319	1.919090
49	1	0	2.428336	-1.150279	0.403398
50	1	0	1.422400	1.621249	-0.348270

51	1	0	1.746513	0.242482	-1.400550
52	1	0	-0.981398	-6.524217	4.194002
53	1	0	0.095945	-5.513210	5.202242
54	1	0	0.720623	-6.242049	3.689089
55	1	0	5.199054	-3.690939	4.459749
56	1	0	4.309913	-5.232686	4.609571
57	1	0	4.805080	-4.329979	6.085893
58	1	0	6.447223	0.197582	-0.051771
59	1	0	7.979211	-1.716418	0.175095
60	1	0	7.195000	-3.830652	1.239361
61	1	0	4.851271	-3.959285	2.115453
62	1	0	3.376993	-2.037726	1.987256
63	1	0	5.809345	0.722675	2.681483
64	1	0	6.222406	2.623310	4.195171
65	1	0	4.717372	4.609987	4.159504
66	1	0	2.785770	4.653690	2.584237
67	1	0	2.378308	2.761370	1.069265
68	1	0	5.852688	2.272100	-3.730986
69	1	0	4.584900	1.033619	-3.599830
70	1	0	6.170942	0.750002	-2.868592
71	1	0	6.668724	3.914523	-1.154347
72	1	0	7.054851	2.418019	-0.291083
73	1	0	5.926243	3.583011	0.422790
74	1	0	3.872163	4.375827	-2.495565
75	1	0	3.119639	4.111826	-0.912823
76	1	0	2.596600	3.157082	-2.317111
77	1	0	0.793261	1.771091	5.524996
78	1	0	0.683073	-0.090111	7.596395
79	1	0	2.057485	-1.738772	5.583386
80	1	0	-0.106651	0.036358	3.990553
81	1	0	-2.367092	-0.319104	9.634104
82	1	0	-0.612656	-0.047031	9.471090
83	1	0	-1.415218	-1.374898	8.546698
84	1	0	2.912624	0.168530	3.380633
85	1	0	3.227794	1.436833	5.410554
86	1	0	3.112241	-0.148677	6.186465
87	1	0	2.666503	1.312272	7.079237

Structure **rsrs-IM3**

E(RB3LYP) **=** -2266.972929 a.u.

Standard orientation:

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

1	6	0	-0.077510	-0.917483	0.758565
2	6	0	0.076624	0.177066	1.825443
3	7	0	1.573617	0.288464	2.045505
4	6	0	2.280609	-0.775800	1.225430
5	6	0	1.296243	-0.992959	0.062800
6	6	0	1.631639	0.328244	5.852102
7	6	0	0.402168	-0.389587	5.664831
8	8	0	-0.459507	-0.064266	4.791596
9	8	0	0.064675	-1.496245	6.429820
10	6	0	0.450622	-1.614779	7.838525
11	6	0	2.816370	-0.236498	6.400227
12	8	0	3.070314	-1.427650	6.726129
13	8	0	3.869931	0.726640	6.520505
14	6	0	5.126089	0.241012	7.074963
15	6	0	3.820446	-0.594619	0.871852
16	6	0	4.661907	-1.386223	1.904447
17	6	0	5.871660	-1.987359	1.515125
18	6	0	6.641863	-2.714579	2.427850
19	6	0	6.215546	-2.863806	3.752921
20	6	0	5.014886	-2.274861	4.159238
21	6	0	4.252364	-1.539358	3.241528
22	6	0	4.279378	0.874908	0.732929
23	6	0	5.424524	1.359639	1.388618
24	6	0	5.875922	2.668867	1.173488
25	6	0	5.189465	3.519689	0.301977
26	6	0	4.038049	3.054372	-0.347544
27	6	0	3.589827	1.747806	-0.132947
28	8	0	3.936459	-1.255495	-0.414252
29	14	0	4.777347	-1.104038	-1.947271
30	6	0	5.150264	-2.910108	-2.416601
31	6	0	6.384174	-0.073504	-1.865721
32	6	0	3.587388	-0.329808	-3.222814
33	6	0	1.425345	3.542293	3.656249
34	6	0	0.702731	4.003331	4.955336
35	6	0	0.910591	2.830704	5.969379
36	6	0	1.715643	1.720715	5.292433
37	6	0	1.307230	1.984078	3.786365
38	8	0	0.518060	2.845087	7.137011
39	6	0	-0.782912	4.275336	4.687521
40	8	0	-1.358004	3.850868	3.681740
41	8	0	-1.495153	5.027870	5.582278
42	6	0	-0.905848	5.614508	6.798435
43	6	0	2.101718	1.131157	2.884118

44	6	0	2.855197	4.095778	3.543639
45	1	0	-0.887144	-0.684266	0.062474
46	1	0	-0.315620	-1.875406	1.233646
47	1	0	-0.383649	-0.060781	2.793380
48	1	0	-0.280047	1.153212	1.484815
49	1	0	2.221458	-1.672906	1.852404
50	1	0	1.396701	-0.213769	-0.698616
51	1	0	1.482564	-1.951879	-0.418062
52	1	0	-0.373448	-2.149926	8.313876
53	1	0	0.562329	-0.621641	8.285445
54	1	0	1.387771	-2.162357	7.922891
55	1	0	5.706283	-0.297041	6.318352
56	1	0	4.940310	-0.428320	7.917208
57	1	0	5.663951	1.134307	7.396414
58	1	0	6.208722	-1.906156	0.490563
59	1	0	7.568158	-3.175007	2.098004
60	1	0	6.807071	-3.440415	4.456706
61	1	0	4.644285	-2.375980	5.174567
62	1	0	3.324904	-1.112135	3.607077
63	1	0	5.972195	0.712361	2.062147
64	1	0	6.766732	3.017172	1.686047
65	1	0	5.541605	4.531870	0.132319
66	1	0	3.491449	3.706828	-1.021088
67	1	0	2.703830	1.404582	-0.653338
68	1	0	5.626480	-2.963084	-3.402672
69	1	0	4.225350	-3.494792	-2.448723
70	1	0	5.816614	-3.377453	-1.684742
71	1	0	6.868095	-0.112542	-2.849861
72	1	0	7.093194	-0.462469	-1.128800
73	1	0	6.183659	0.974413	-1.626219
74	1	0	4.025603	-0.400262	-4.225757
75	1	0	3.398191	0.727164	-3.011281
76	1	0	2.628980	-0.859270	-3.235508
77	1	0	0.843797	3.865414	2.788868
78	1	0	1.166282	4.900607	5.381896
79	1	0	2.763402	2.032862	5.412758
80	1	0	0.251715	1.731595	3.703990
81	1	0	-1.759866	6.022452	7.336491
82	1	0	-0.218883	6.425082	6.532711
83	1	0	-0.407166	4.847811	7.391754
84	1	0	3.183259	1.143336	2.965803
85	1	0	3.342006	3.758893	2.622376
86	1	0	3.490001	3.802925	4.387719
87	1	0	2.829538	5.191607	3.516136

Structure **rssr-TS2**

Imaginary Frequency: -177

E(RB3LYP) = -2266.963829 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.325267	-0.184948	0.327244
2	6	0	-0.096146	-0.330746	1.833903
3	7	0	1.373464	-0.167509	1.967472
4	6	0	1.968921	0.554628	0.781372
5	6	0	0.712159	0.882965	-0.057418
6	6	0	-0.267275	0.531467	5.905795
7	6	0	-0.447951	-0.076499	7.231644
8	8	0	0.441391	-0.030653	8.106791
9	8	0	-1.583968	-0.787067	7.565455
10	6	0	-2.521343	-1.334744	6.588822
11	6	0	-1.307095	1.241907	5.194915
12	8	0	-1.210298	1.718143	4.034665
13	8	0	-2.462949	1.448352	5.936532
14	6	0	-3.501378	2.269358	5.308184
15	6	0	2.870848	1.819332	1.152430
16	6	0	3.301125	2.569658	-0.149721
17	6	0	4.616229	2.548430	-0.648834
18	6	0	4.966954	3.250875	-1.809069
19	6	0	4.014467	4.002883	-2.499688
20	6	0	2.705796	4.053922	-2.007523
21	6	0	2.359088	3.351617	-0.849989
22	6	0	4.101677	1.334011	1.954974
23	6	0	4.929895	0.306482	1.452504
24	6	0	5.982285	-0.212057	2.214415
25	6	0	6.231104	0.278656	3.502235
26	6	0	5.426952	1.303844	4.006756
27	6	0	4.377273	1.826177	3.238957
28	8	0	2.016065	2.651646	1.954790
29	14	0	1.911697	4.330121	2.481958
30	6	0	3.541590	5.283851	2.183424
31	6	0	1.452000	4.252855	4.325555
32	6	0	0.469250	5.173550	1.556833
33	6	0	2.516342	-1.841100	5.169929
34	6	0	2.716355	-0.984613	6.462899
35	6	0	2.299164	0.446266	6.129673

36	6	0	1.027806	0.592289	5.334393
37	6	0	1.524212	-1.160863	4.215608
38	8	0	3.004037	1.443710	6.359800
39	6	0	4.151878	-1.083363	6.986625
40	8	0	5.070256	-1.564144	6.313209
41	8	0	4.431509	-0.675092	8.260092
42	6	0	3.491542	0.060740	9.126714
43	6	0	2.049440	-0.632437	3.024691
44	6	0	2.112930	-3.287539	5.509169
45	1	0	-1.347263	0.125310	0.092001
46	1	0	-0.129911	-1.133140	-0.189051
47	1	0	-0.389700	-1.310766	2.223572
48	1	0	-0.605106	0.449983	2.415399
49	1	0	2.607192	-0.152553	0.238854
50	1	0	0.330831	1.858295	0.252582
51	1	0	0.931417	0.910533	-1.126036
52	1	0	-2.789951	-2.322544	6.966884
53	1	0	-2.060832	-1.424809	5.600087
54	1	0	-3.398555	-0.693153	6.527665
55	1	0	-4.301804	2.313584	6.044909
56	1	0	-3.846697	1.811697	4.377855
57	1	0	-3.114866	3.267521	5.091242
58	1	0	5.390310	2.004746	-0.126471
59	1	0	5.993068	3.213965	-2.161386
60	1	0	4.287118	4.548440	-3.397310
61	1	0	1.952761	4.645371	-2.519272
62	1	0	1.347138	3.430285	-0.481628
63	1	0	4.746547	-0.112514	0.468084
64	1	0	6.593958	-1.011681	1.808528
65	1	0	7.016706	-0.150465	4.113322
66	1	0	5.580479	1.673179	5.014139
67	1	0	3.740403	2.579041	3.677797
68	1	0	3.434296	6.302595	2.576096
69	1	0	3.777215	5.350620	1.117229
70	1	0	4.386980	4.811559	2.692705
71	1	0	1.390425	5.269456	4.733282
72	1	0	2.164956	3.684552	4.931080
73	1	0	0.470370	3.778677	4.430265
74	1	0	0.206603	6.103317	2.076457
75	1	0	-0.414598	4.526416	1.561673
76	1	0	0.720864	5.424162	0.522426
77	1	0	3.498539	-1.871969	4.685386
78	1	0	2.027890	-1.333012	7.242421
79	1	0	1.120388	1.304596	4.519517

80	1	0	0.500842	-1.520497	4.227248
81	1	0	3.912568	-0.045120	10.125378
82	1	0	2.481562	-0.347887	9.088692
83	1	0	3.475415	1.107466	8.822400
84	1	0	3.122030	-0.512350	2.974644
85	1	0	2.036240	-3.893584	4.599219
86	1	0	1.143155	-3.319399	6.022754
87	1	0	2.860065	-3.752387	6.161722

Structure **rssr-IM3**

E(RB3LYP) **=** -2266.973853 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.313193	1.258405	0.067775
2	6	0	0.430836	1.507358	1.572850
3	7	0	1.542609	0.595574	2.011631
4	6	0	2.268052	0.008127	0.807831
5	6	0	1.749930	0.898483	-0.340444
6	6	0	1.698040	2.238239	6.531914
7	6	0	0.699149	2.186121	7.541458
8	8	0	0.073742	1.104991	7.790916
9	8	0	0.317439	3.281681	8.313179
10	6	0	0.026837	4.583251	7.719100
11	6	0	2.655773	3.237916	6.215348
12	8	0	3.455585	3.170990	5.229956
13	8	0	2.725806	4.341881	7.065917
14	6	0	3.756604	5.327976	6.752719
15	6	0	3.841378	-0.058393	0.914056
16	6	0	4.360965	-0.240264	-0.539008
17	6	0	4.301787	-1.501993	-1.158093
18	6	0	4.716228	-1.665218	-2.483760
19	6	0	5.204311	-0.572003	-3.209715
20	6	0	5.268456	0.685142	-2.600012
21	6	0	4.842861	0.850432	-1.276459
22	6	0	4.363591	-1.244807	1.760496
23	6	0	3.535741	-2.199589	2.372607
24	6	0	4.079295	-3.258571	3.115421
25	6	0	5.462496	-3.394569	3.239249
26	6	0	6.302640	-2.467382	2.607354
27	6	0	5.758146	-1.411280	1.875063
28	8	0	4.213389	1.225300	1.441837

29	14	0	5.546785	2.104763	2.209360
30	6	0	7.119049	2.104453	1.108147
31	6	0	5.957779	1.442670	3.944464
32	6	0	4.845550	3.867962	2.300567
33	6	0	-0.258818	0.008955	4.689734
34	6	0	0.200075	-0.966028	5.798433
35	6	0	1.463967	-0.314432	6.458164
36	6	0	1.854715	0.969459	5.715168
37	6	0	1.011628	0.938950	4.397550
38	8	0	2.170059	-0.898059	7.287528
39	6	0	0.578361	-2.321084	5.223008
40	8	0	0.910923	-2.462853	4.032472
41	8	0	0.579774	-3.421094	6.024461
42	6	0	0.255329	-3.356053	7.465995
43	6	0	1.800872	0.376251	3.267049
44	6	0	-1.502780	0.824800	5.083647
45	1	0	-0.068442	2.136379	-0.459430
46	1	0	-0.369209	0.423473	-0.130246
47	1	0	-0.476517	1.276667	2.132067
48	1	0	0.737803	2.535248	1.794843
49	1	0	1.877821	-1.007788	0.681294
50	1	0	2.368590	1.798633	-0.402986
51	1	0	1.800131	0.380873	-1.298634
52	1	0	-0.980845	4.854131	8.047408
53	1	0	0.065347	4.538050	6.626638
54	1	0	0.755059	5.312291	8.069706
55	1	0	3.665117	6.082103	7.534248
56	1	0	3.592272	5.769004	5.765567
57	1	0	4.747778	4.868882	6.771417
58	1	0	3.951777	-2.363658	-0.599094
59	1	0	4.667370	-2.646925	-2.944246
60	1	0	5.534095	-0.700703	-4.235602
61	1	0	5.648316	1.539172	-3.152116
62	1	0	4.883686	1.825317	-0.809200
63	1	0	2.455969	-2.149488	2.316452
64	1	0	3.403067	-3.955270	3.597987
65	1	0	5.884117	-4.211214	3.815820
66	1	0	7.380664	-2.569220	2.681814
67	1	0	6.422574	-0.720232	1.369751
68	1	0	7.898837	2.662323	1.642436
69	1	0	6.944104	2.605883	0.151303
70	1	0	7.511532	1.104909	0.899097
71	1	0	6.873921	1.934545	4.296395
72	1	0	6.123576	0.362889	3.966096

73	1	0	5.150399	1.713195	4.631982
74	1	0	5.652037	4.579118	2.517975
75	1	0	4.113988	3.924810	3.112380
76	1	0	4.379001	4.159287	1.353494
77	1	0	-0.489880	-0.566315	3.787673
78	1	0	-0.551261	-1.060659	6.584560
79	1	0	2.917915	0.877705	5.469804
80	1	0	0.667948	1.948729	4.153632
81	1	0	0.487677	-4.354044	7.833363
82	1	0	-0.809814	-3.147857	7.602138
83	1	0	0.877187	-2.605311	7.953810
84	1	0	2.634148	-0.278089	3.489781
85	1	0	-1.737503	1.582607	4.325455
86	1	0	-1.364234	1.310840	6.051379
87	1	0	-2.368988	0.156616	5.164518

Structure **rsss-TS2**

Imaginary Frequency: -186

E(RB3LYP) **=** -2266.967749 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.180949	-0.701377	-0.034061
2	6	0	-0.045618	-0.146909	1.376807
3	7	0	1.332524	-0.034619	1.930860
4	6	0	2.371550	-0.044245	0.840343
5	6	0	1.514949	-0.062636	-0.448636
6	6	0	0.835969	-3.150944	3.104708
7	6	0	-0.497227	-3.428210	2.569602
8	8	0	-1.525851	-2.893608	3.049196
9	8	0	-0.581519	-4.308882	1.528419
10	6	0	-1.939194	-4.606115	1.043320
11	6	0	2.111743	-3.360584	2.428541
12	8	0	3.207720	-2.943160	2.876861
13	8	0	2.049455	-4.013857	1.221452
14	6	0	3.326518	-4.281069	0.549861
15	6	0	3.412919	1.145944	0.824623
16	6	0	4.135462	1.084255	-0.552225
17	6	0	4.997010	0.014871	-0.856206
18	6	0	5.628163	-0.059721	-2.101658
19	6	0	5.418795	0.939943	-3.059598
20	6	0	4.573441	2.012349	-2.758351

21	6	0	3.933490	2.082514	-1.514738
22	6	0	4.530146	1.087995	1.896776
23	6	0	4.906031	-0.086221	2.573393
24	6	0	5.993301	-0.081925	3.460288
25	6	0	6.732363	1.083298	3.675662
26	6	0	6.384701	2.250708	2.983925
27	6	0	5.302708	2.247161	2.100904
28	8	0	2.681245	2.379091	0.872565
29	14	0	2.109205	3.672241	1.890800
30	6	0	2.462709	3.472924	3.756171
31	6	0	0.230596	3.791222	1.591264
32	6	0	2.940460	5.262232	1.236007
33	6	0	-0.613275	-0.137870	4.652020
34	6	0	-0.965343	-1.248222	5.673821
35	6	0	-0.274593	-2.572963	5.318045
36	6	0	0.892676	-2.555254	4.359512
37	6	0	0.878904	-0.219761	4.384011
38	8	0	-0.542086	-3.637376	5.901153
39	6	0	-2.486526	-1.390794	5.839010
40	8	0	-3.278605	-1.002121	4.982747
41	8	0	-2.996245	-1.921006	7.001563
42	6	0	-2.172586	-2.337166	8.143328
43	6	0	1.646099	-0.022858	3.246355
44	6	0	-1.007865	1.257643	5.187752
45	1	0	-0.637434	-0.445214	-0.713206
46	1	0	0.266380	-1.793891	0.001946
47	1	0	-0.657028	-0.807503	1.987707
48	1	0	-0.516353	0.843740	1.348277
49	1	0	2.934871	-0.980232	0.924945
50	1	0	1.354569	0.967116	-0.782434
51	1	0	2.015338	-0.604309	-1.253130
52	1	0	-1.787109	-5.319780	0.236201
53	1	0	-2.421773	-3.695119	0.683477
54	1	0	-2.539852	-5.035533	1.847395
55	1	0	3.062170	-4.918235	-0.291982
56	1	0	4.015454	-4.787318	1.228879
57	1	0	3.782191	-3.350366	0.202509
58	1	0	5.199733	-0.749706	-0.112831
59	1	0	6.291162	-0.891673	-2.318689
60	1	0	5.913721	0.885354	-4.024075
61	1	0	4.408534	2.796976	-3.490682
62	1	0	3.275091	2.906954	-1.275509
63	1	0	4.369768	-1.019720	2.440043
64	1	0	6.254072	-0.999807	3.977514

65	1	0	7.573190	1.082062	4.361853
66	1	0	6.962801	3.159220	3.122293
67	1	0	5.066547	3.145035	1.541889
68	1	0	2.039221	4.339599	4.279739
69	1	0	3.534624	3.433807	3.966046
70	1	0	1.996694	2.571031	4.163052
71	1	0	-0.158597	4.725746	2.012934
72	1	0	-0.304838	2.959781	2.059976
73	1	0	0.009147	3.782365	0.519040
74	1	0	2.764699	5.374640	0.160978
75	1	0	4.022232	5.257482	1.404454
76	1	0	2.522455	6.139962	1.743529
77	1	0	-1.208254	-0.343211	3.763386
78	1	0	-0.538855	-0.961294	6.650605
79	1	0	1.873224	-2.520839	4.823763
80	1	0	1.469386	-0.105759	5.295768
81	1	0	-2.889018	-2.747960	8.853366
82	1	0	-1.670953	-1.473139	8.593189
83	1	0	-1.456003	-3.099392	7.838839
84	1	0	2.709006	0.064358	3.425335
85	1	0	-0.770071	2.030401	4.449035
86	1	0	-0.458241	1.496974	6.108250
87	1	0	-2.081172	1.305506	5.395526

Structure **rsss-IM3**

E(RB3LYP) **=** -2266.976084 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.891186	-0.985544	0.046930
2	6	0	0.443165	-0.281179	1.325737
3	7	0	1.740888	0.023520	2.026715
4	6	0	2.904358	0.017667	1.025540
5	6	0	2.204101	-0.278856	-0.320121
6	6	0	2.421937	-2.247192	4.353933
7	6	0	1.878094	-3.004446	3.283870
8	8	0	0.660031	-2.896215	2.921846
9	8	0	2.718194	-3.861345	2.591084
10	6	0	2.083672	-4.732982	1.602034
11	6	0	3.752642	-2.218430	4.870045
12	8	0	4.129190	-1.485547	5.831036
13	8	0	4.682725	-3.022072	4.209205

14	6	0	6.015174	-3.099851	4.803081
15	6	0	3.764122	1.338737	0.966872
16	6	0	4.642032	1.241803	-0.310901
17	6	0	5.668947	0.283980	-0.387568
18	6	0	6.454333	0.175463	-1.538730
19	6	0	6.233369	1.030009	-2.626110
20	6	0	5.220144	1.990611	-2.551022
21	6	0	4.425782	2.093204	-1.402143
22	6	0	4.728489	1.577082	2.153149
23	6	0	5.124993	0.581065	3.061101
24	6	0	6.004694	0.874444	4.114308
25	6	0	6.549131	2.153649	4.241553
26	6	0	6.218584	3.137251	3.300091
27	6	0	5.320174	2.849712	2.270505
28	8	0	2.829738	2.418036	0.795127
29	14	0	2.087209	3.812588	1.534820
30	6	0	2.111085	3.793099	3.443929
31	6	0	0.291087	3.772568	0.901396
32	6	0	2.932985	5.392503	0.873875
33	6	0	-0.527495	0.093287	4.430993
34	6	0	-1.131608	-1.245878	4.935651
35	6	0	0.059146	-2.161662	5.314927
36	6	0	1.392236	-1.438976	5.138417
37	6	0	1.028905	-0.040086	4.509948
38	8	0	-0.058877	-3.270283	5.846584
39	6	0	-2.116003	-1.848265	3.924638
40	8	0	-2.188919	-1.459677	2.755138
41	8	0	-2.995135	-2.810904	4.336417
42	6	0	-3.118087	-3.269496	5.731424
43	6	0	1.939787	0.077722	3.312805
44	6	0	-1.024019	1.291271	5.264806
45	1	0	0.137199	-0.905636	-0.740579
46	1	0	1.046904	-2.046490	0.263795
47	1	0	-0.189450	-0.912551	1.941515
48	1	0	-0.050256	0.672215	1.109206
49	1	0	3.536388	-0.827688	1.314485
50	1	0	1.996593	0.666655	-0.828871
51	1	0	2.844744	-0.879288	-0.968425
52	1	0	2.833374	-5.493797	1.385899
53	1	0	1.832527	-4.179671	0.691895
54	1	0	1.172194	-5.177478	2.005878
55	1	0	6.454039	-4.006892	4.387199
56	1	0	5.952506	-3.153552	5.891646
57	1	0	6.619270	-2.230248	4.524738

58	1	0	5.872694	-0.367640	0.456256
59	1	0	7.242259	-0.569759	-1.582263
60	1	0	6.847167	0.949245	-3.517498
61	1	0	5.043172	2.660953	-3.386540
62	1	0	3.635445	2.829715	-1.341147
63	1	0	4.764971	-0.438733	2.976977
64	1	0	6.222879	0.102593	4.843017
65	1	0	7.227228	2.381046	5.057371
66	1	0	6.660691	4.126539	3.366430
67	1	0	5.091791	3.610566	1.533739
68	1	0	1.591683	4.688027	3.809046
69	1	0	3.128460	3.800496	3.843237
70	1	0	1.588452	2.919050	3.844926
71	1	0	-0.223799	4.704509	1.163468
72	1	0	-0.273683	2.941365	1.335626
73	1	0	0.270473	3.666332	-0.188066
74	1	0	2.339670	6.268865	1.161969
75	1	0	2.993604	5.370184	-0.219351
76	1	0	3.944054	5.526627	1.269645
77	1	0	-0.862637	0.242173	3.405799
78	1	0	-1.683201	-1.077386	5.872364
79	1	0	1.817909	-1.279750	6.136682
80	1	0	1.398015	0.741612	5.188923
81	1	0	-3.803329	-4.113615	5.672032
82	1	0	-3.563039	-2.479983	6.347027
83	1	0	-2.149034	-3.581662	6.119876
84	1	0	2.960129	0.273641	3.611437
85	1	0	-0.610598	2.234544	4.888287
86	1	0	-0.729933	1.193888	6.318050
87	1	0	-2.116727	1.367297	5.224039

Structure **ksrrs-TS2**

Imaginary Frequency: -219

E(RB3LYP) = -2306.236729 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.045168	0.027591	-0.027502
2	6	0	-0.016201	0.015778	1.502569
3	7	0	1.418373	-0.015242	1.940899
4	6	0	2.340908	-0.184665	0.755764
5	6	0	1.357500	-0.719057	-0.313670

6	6	0	1.618958	2.636073	5.772971
7	6	0	0.920609	2.782755	7.032334
8	8	0	-0.326306	2.645517	7.165025
9	8	0	1.695724	3.069835	8.131061
10	6	0	0.981351	3.282124	9.392840
11	6	0	3.017941	2.947895	5.527420
12	8	0	3.624955	2.587174	4.484461
13	8	0	3.664236	3.698953	6.480612
14	6	0	5.071096	4.008272	6.211048
15	6	0	3.142124	1.123463	0.321584
16	6	0	3.617432	0.923365	-1.145352
17	6	0	4.697594	0.069993	-1.434602
18	6	0	5.100494	-0.152503	-2.755187
19	6	0	4.436635	0.481157	-3.812101
20	6	0	3.363026	1.333353	-3.534207
21	6	0	2.953565	1.546665	-2.212413
22	6	0	4.419521	1.387686	1.164316
23	6	0	5.027820	0.439204	2.003297
24	6	0	6.232784	0.717032	2.662966
25	6	0	6.867642	1.946217	2.484600
26	6	0	6.294621	2.889304	1.623763
27	6	0	5.095910	2.605949	0.968626
28	8	0	2.187700	2.194770	0.398029
29	14	0	1.939447	3.926941	0.561826
30	6	0	2.459271	4.832891	-1.045241
31	6	0	2.838748	4.728948	2.042633
32	6	0	0.055109	4.068686	0.771697
33	6	0	-0.275338	-0.451206	4.637785
34	6	0	-1.177160	0.726466	5.112964
35	6	0	-0.566828	2.010861	4.562150
36	6	0	0.933805	2.105956	4.645316
37	6	0	1.194867	0.008519	4.465459
38	8	0	-1.220997	2.863807	3.936110
39	6	0	-2.626079	0.521879	4.663994
40	8	0	-2.935173	-0.321476	3.813320
41	8	0	-3.623534	1.246514	5.249362
42	6	0	-3.401955	2.431449	6.098066
43	6	0	-0.442914	-1.680326	5.555556
44	6	0	1.861095	-0.024960	3.210513
45	1	0	0.102150	1.050136	-0.403083
46	1	0	-0.827255	-0.465654	-0.465041
47	1	0	-0.525052	-0.890098	1.841833
48	1	0	-0.525061	0.882963	1.926164
49	1	0	3.070176	-0.960777	0.997006

50	1	0	1.720277	-0.581395	-1.329731
51	1	0	1.217357	-1.795880	-0.151400
52	1	0	1.760732	3.546930	10.105264
53	1	0	0.462651	2.370606	9.699745
54	1	0	0.252335	4.089082	9.289536
55	1	0	5.408886	4.538593	7.099897
56	1	0	5.160711	4.636099	5.321194
57	1	0	5.643848	3.091253	6.055470
58	1	0	5.242168	-0.407591	-0.627109
59	1	0	5.938388	-0.812925	-2.956064
60	1	0	4.754236	0.314884	-4.836482
61	1	0	2.839948	1.832124	-4.344388
62	1	0	2.113849	2.194201	-2.001583
63	1	0	4.589857	-0.540713	2.151965
64	1	0	6.670624	-0.035285	3.311514
65	1	0	7.800596	2.162726	2.994797
66	1	0	6.786886	3.841616	1.452981
67	1	0	4.697626	3.334500	0.272992
68	1	0	2.357581	5.913003	-0.880431
69	1	0	1.816960	4.559499	-1.888558
70	1	0	3.496683	4.631205	-1.331432
71	1	0	2.161435	5.451918	2.513725
72	1	0	3.737068	5.264199	1.717611
73	1	0	3.140379	3.995419	2.795793
74	1	0	-0.238037	5.123412	0.695048
75	1	0	-0.280782	3.703315	1.747859
76	1	0	-0.475136	3.514942	-0.010190
77	1	0	-0.679455	-0.749497	3.675331
78	1	0	-1.131974	0.805664	6.204931
79	1	0	1.377153	2.384081	3.695221
80	1	0	-4.288500	2.485296	6.728878
81	1	0	-3.333776	3.307184	5.452078
82	1	0	-2.498642	2.353062	6.703578
83	1	0	0.151896	-2.526708	5.194083
84	1	0	-1.493361	-1.988639	5.556162
85	1	0	-0.145312	-1.469257	6.588134
86	1	0	2.940751	0.033011	3.278541
87	6	0	2.130151	-0.294917	5.634048
88	1	0	3.118607	0.137706	5.459010
89	1	0	1.753124	0.130785	6.569005
90	1	0	2.247964	-1.374907	5.786271

Structure **krssr-TS2**

Imaginary Frequency: -196

E(RB3LYP) = -2306.233287 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.008988	-0.387762	-0.025628
2	6	0	-0.086784	-0.029642	1.459977
3	7	0	1.322688	-0.157877	1.928085
4	6	0	2.292145	-0.164718	0.755739
5	6	0	1.361811	0.171800	-0.428241
6	6	0	-0.119866	2.631416	4.842202
7	6	0	-0.620246	2.786744	6.211531
8	8	0	0.153761	2.786248	7.194042
9	8	0	-1.963361	2.890908	6.518061
10	6	0	-3.059251	2.461011	5.655062
11	6	0	-0.713494	3.238554	3.671324
12	8	0	-0.394163	2.993375	2.479019
13	8	0	-1.656026	4.219062	3.948525
14	6	0	-2.218445	4.928191	2.796352
15	6	0	3.573157	0.780086	0.886952
16	6	0	4.331896	0.782988	-0.481408
17	6	0	5.530420	0.078309	-0.691876
18	6	0	6.178163	0.096981	-1.934174
19	6	0	5.648136	0.826400	-3.000016
20	6	0	4.466697	1.550328	-2.804422
21	6	0	3.825026	1.531739	-1.563295
22	6	0	4.487441	0.267999	2.027785
23	6	0	4.866265	-1.089147	2.111578
24	6	0	5.629629	-1.560455	3.185359
25	6	0	6.027591	-0.689521	4.206759
26	6	0	5.666227	0.658443	4.131479
27	6	0	4.909756	1.130231	3.050953
28	8	0	3.057541	2.082463	1.192278
29	14	0	3.404383	3.801927	1.038488
30	6	0	5.029145	4.176359	0.099767
31	6	0	3.576656	4.576923	2.772492
32	6	0	1.869042	4.509905	0.161452
33	6	0	1.848231	-0.573071	5.650168
34	6	0	2.083086	0.633798	6.607953
35	6	0	2.174742	1.875707	5.725224
36	6	0	1.134950	1.994036	4.638238
37	6	0	0.982532	-0.143306	4.432049
38	8	0	3.122107	2.678908	5.766194

39	6	0	3.335746	0.423616	7.464097
40	8	0	4.160542	-0.463655	7.215040
41	8	0	3.539364	1.198941	8.569543
42	6	0	2.759002	2.408176	8.892227
43	6	0	1.692237	-0.257250	3.208805
44	6	0	1.312417	-1.804375	6.406629
45	1	0	-0.827356	0.057253	-0.598561
46	1	0	-0.047949	-1.475276	-0.166878
47	1	0	-0.727718	-0.708831	2.021704
48	1	0	-0.413312	1.005842	1.619741
49	1	0	2.663151	-1.190838	0.645487
50	1	0	1.285243	1.258203	-0.519432
51	1	0	1.734356	-0.237799	-1.368000
52	1	0	-3.764656	1.951718	6.314556
53	1	0	-2.714308	1.775158	4.877166
54	1	0	-3.522613	3.333032	5.197316
55	1	0	-2.942405	5.619938	3.224058
56	1	0	-2.699911	4.229260	2.107875
57	1	0	-1.432587	5.468150	2.263848
58	1	0	5.986558	-0.476674	0.115551
59	1	0	7.104173	-0.455796	-2.057852
60	1	0	6.149812	0.841187	-3.962187
61	1	0	4.045929	2.137404	-3.615013
62	1	0	2.926716	2.119822	-1.436934
63	1	0	4.554855	-1.795602	1.348548
64	1	0	5.896782	-2.611612	3.231140
65	1	0	6.582504	-1.059099	5.061289
66	1	0	5.935028	1.340271	4.930374
67	1	0	4.600417	2.164231	3.041571
68	1	0	5.256016	5.242828	0.224074
69	1	0	4.967981	3.954515	-0.967551
70	1	0	5.864615	3.604541	0.518054
71	1	0	4.599423	4.485879	3.153919
72	1	0	2.911123	4.139601	3.519877
73	1	0	3.345639	5.647234	2.696771
74	1	0	0.972828	4.209363	0.715318
75	1	0	1.780815	4.148628	-0.868779
76	1	0	1.918332	5.604996	0.133076
77	1	0	2.843135	-0.845487	5.282531
78	1	0	1.210561	0.769459	7.258314
79	1	0	1.574436	2.199744	3.666403
80	1	0	3.019917	2.622890	9.927376
81	1	0	1.686052	2.250022	8.787139
82	1	0	3.072754	3.219862	8.235800

83	1	0	2.760463	-0.363312	3.326765
84	1	0	1.179259	-2.652757	5.725272
85	1	0	0.351712	-1.604203	6.894613
86	1	0	2.031909	-2.102372	7.175044
87	6	0	-0.515441	-0.347854	4.575085
88	1	0	-0.831872	-0.086426	5.589752
89	1	0	-1.088701	0.281985	3.893532
90	1	0	-0.803867	-1.394037	4.407835

Structure **msrrs-TS2**

Imaginary Frequency: -237

E(RB3LYP) **=** -2306.239071 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.052149	-0.389284	0.286197
2	6	0	0.060352	-0.492816	1.829575
3	7	0	1.486356	-0.189576	2.094649
4	6	0	2.239063	-0.904935	1.009203
5	6	0	1.406661	-0.532326	-0.242188
6	6	0	0.898163	4.474424	3.459080
7	6	0	0.100442	5.117782	4.493459
8	8	0	-1.093195	4.818919	4.750242
9	8	0	0.749266	6.075250	5.233188
10	6	0	-0.056954	6.793523	6.225615
11	6	0	2.141559	5.007665	2.907745
12	8	0	2.934491	4.323506	2.216561
13	8	0	2.381474	6.338727	3.140456
14	6	0	3.624852	6.883243	2.586242
15	6	0	3.784728	-0.715881	0.898674
16	6	0	4.226515	-1.561719	-0.328227
17	6	0	4.494193	-2.935295	-0.196837
18	6	0	4.830474	-3.708786	-1.313530
19	6	0	4.905796	-3.121677	-2.581137
20	6	0	4.634264	-1.756363	-2.723034
21	6	0	4.292263	-0.985281	-1.606582
22	6	0	4.542320	-1.209506	2.158332
23	6	0	3.910747	-1.817234	3.256744
24	6	0	4.653028	-2.270729	4.355887
25	6	0	6.042240	-2.128590	4.379233
26	6	0	6.687333	-1.540784	3.284268
27	6	0	5.944617	-1.096513	2.187972

28	8	0	4.001890	0.690166	0.654910
29	14	0	5.254793	1.904766	0.423397
30	6	0	6.778364	1.295522	-0.573962
31	6	0	5.823320	2.574751	2.113684
32	6	0	4.362241	3.238844	-0.593730
33	6	0	0.238203	1.177104	4.926099
34	6	0	-1.110173	1.869175	4.418322
35	6	0	-0.856175	2.618287	3.104893
36	6	0	0.493770	3.248359	2.911281
37	6	0	1.415913	1.489967	3.966575
38	8	0	-1.687419	2.650738	2.182109
39	6	0	-2.361018	1.001317	4.276712
40	8	0	-2.360047	-0.151884	3.837550
41	8	0	-3.569146	1.536055	4.651913
42	6	0	-3.749938	2.950864	5.008886
43	6	0	0.595107	1.854886	6.282045
44	6	0	1.989951	0.740560	2.932314
45	1	0	-0.480813	0.577004	0.004745
46	1	0	-0.711455	-1.168838	-0.106200
47	1	0	-0.166550	-1.509341	2.173003
48	1	0	-0.604535	0.178783	2.357205
49	1	0	2.085810	-1.976528	1.209021
50	1	0	1.775841	0.417002	-0.638651
51	1	0	1.492894	-1.289937	-1.023304
52	1	0	0.620578	7.537194	6.640926
53	1	0	-0.410725	6.108666	6.999923
54	1	0	-0.916609	7.267494	5.746659
55	1	0	3.628498	7.926303	2.897231
56	1	0	3.627619	6.797038	1.497188
57	1	0	4.488712	6.350057	2.989925
58	1	0	4.453610	-3.402343	0.781218
59	1	0	5.037833	-4.767106	-1.189753
60	1	0	5.171414	-3.720158	-3.446683
61	1	0	4.683332	-1.290562	-3.702444
62	1	0	4.064856	0.066400	-1.725677
63	1	0	2.835273	-1.937020	3.277121
64	1	0	4.137857	-2.733941	5.191550
65	1	0	6.615919	-2.477580	5.231707
66	1	0	7.768017	-1.438809	3.278268
67	1	0	6.463708	-0.681390	1.333549
68	1	0	7.430758	0.621963	-0.010400
69	1	0	7.369572	2.182447	-0.836845
70	1	0	6.489508	0.792561	-1.500741
71	1	0	6.628983	3.304316	1.962192

72	1	0	6.199285	1.780435	2.765576
73	1	0	4.988426	3.085066	2.602282
74	1	0	3.931529	2.819138	-1.509141
75	1	0	5.068076	4.028778	-0.878616
76	1	0	3.567678	3.687768	0.007658
77	1	0	-1.329250	2.670090	5.131003
78	1	0	0.953642	2.998059	1.962659
79	1	0	2.171965	2.115978	4.430852
80	1	0	-4.829865	3.091245	5.004945
81	1	0	-3.275752	3.610070	4.281766
82	1	0	-3.353031	3.151906	6.007878
83	1	0	1.514514	1.423464	6.693226
84	1	0	-0.209958	1.699342	7.009878
85	1	0	0.748555	2.932532	6.164751
86	1	0	3.018203	0.989619	2.698273
87	6	0	0.126520	-0.341346	5.218205
88	1	0	-0.145417	-0.935128	4.349630
89	1	0	1.093207	-0.687592	5.601727
90	1	0	-0.631907	-0.531468	5.985427

Structure **mrssr-TS2**

Imaginary Frequency: -168

E(RB3LYP) = -2306.231693a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.284110	0.090963	-0.443099
2	6	0	0.091352	0.199678	1.078680
3	7	0	1.473302	0.183771	1.641521
4	6	0	2.483753	-0.026619	0.551048
5	6	0	1.734505	0.554643	-0.666078
6	6	0	-0.966597	3.140044	4.093559
7	6	0	-1.397246	3.443096	5.468042
8	8	0	-0.583041	3.787953	6.349875
9	8	0	-2.708977	3.304338	5.875999
10	6	0	-3.710248	2.498894	5.178912
11	6	0	-1.732580	3.423030	2.891891
12	8	0	-1.423226	3.048146	1.735929
13	8	0	-2.835231	4.235081	3.095935
14	6	0	-3.575986	4.640982	1.896262
15	6	0	3.943214	0.514183	0.767490
16	6	0	4.631273	0.430186	-0.625176

17	6	0	5.186799	-0.780188	-1.076553
18	6	0	5.745938	-0.878492	-2.355530
19	6	0	5.762742	0.233362	-3.204700
20	6	0	5.207690	1.440597	-2.766089
21	6	0	4.640118	1.534677	-1.490680
22	6	0	4.767044	-0.338181	1.765549
23	6	0	4.272698	-1.483295	2.412022
24	6	0	5.083758	-2.233262	3.274930
25	6	0	6.408406	-1.856159	3.503851
26	6	0	6.921527	-0.728875	2.851446
27	6	0	6.111665	0.011505	1.988925
28	8	0	3.799829	1.881850	1.199522
29	14	0	4.768944	3.252716	1.764028
30	6	0	6.188942	3.700587	0.552406
31	6	0	5.527422	2.985311	3.490430
32	6	0	3.488884	4.657814	1.764926
33	6	0	0.911298	0.370007	5.416987
34	6	0	1.538136	1.719181	5.975793
35	6	0	1.435627	2.823142	4.912149
36	6	0	0.356737	2.720062	3.876566
37	6	0	0.660016	0.515084	3.899906
38	8	0	2.288047	3.723203	4.824855
39	6	0	2.999190	1.662630	6.415624
40	8	0	3.874016	1.069556	5.776861
41	8	0	3.366290	2.323050	7.559816
42	6	0	2.468415	3.261569	8.252375
43	6	0	1.682751	0.348256	2.959979
44	6	0	-0.460274	0.152554	6.111715
45	1	0	-0.441206	0.705693	-0.982291
46	1	0	0.162521	-0.945592	-0.781021
47	1	0	-0.491223	-0.632861	1.494028
48	1	0	-0.400158	1.139469	1.355407
49	1	0	2.580254	-1.111996	0.394291
50	1	0	1.804335	1.646777	-0.640090
51	1	0	2.146621	0.199231	-1.610892
52	1	0	-4.264277	1.983688	5.965264
53	1	0	-3.243501	1.768361	4.511604
54	1	0	-4.367175	3.152636	4.608455
55	1	0	-4.371504	5.284367	2.268019
56	1	0	-3.982783	3.767386	1.380967
57	1	0	-2.918796	5.183770	1.213933
58	1	0	5.198559	-1.646016	-0.423504
59	1	0	6.173605	-1.821107	-2.682836
60	1	0	6.202938	0.160136	-4.194102

61	1	0	5.212576	2.309824	-3.416564
62	1	0	4.195849	2.465038	-1.163109
63	1	0	3.250161	-1.807642	2.259062
64	1	0	4.673239	-3.109696	3.766301
65	1	0	7.034364	-2.432276	4.177160
66	1	0	7.952534	-0.429681	3.010505
67	1	0	6.535772	0.860239	1.465152
68	1	0	6.782679	4.495999	1.021445
69	1	0	5.810546	4.079261	-0.401585
70	1	0	6.860582	2.862978	0.340138
71	1	0	6.506350	2.500341	3.434660
72	1	0	4.891734	2.385397	4.145826
73	1	0	5.655155	3.967470	3.962514
74	1	0	2.888037	4.637372	0.849819
75	1	0	4.000618	5.626567	1.820493
76	1	0	2.827459	4.575841	2.632132
77	1	0	0.915597	2.058044	6.809060
78	1	0	0.721504	2.847890	2.862298
79	1	0	-0.351621	0.288193	3.580441
80	1	0	3.122480	3.810719	8.927826
81	1	0	1.712844	2.719697	8.828217
82	1	0	1.993095	3.944609	7.546568
83	1	0	2.716630	0.408544	3.279161
84	1	0	-0.925710	-0.767794	5.739990
85	1	0	-1.153290	0.977840	5.937408
86	1	0	-0.326496	0.049726	7.194576
87	6	0	1.763595	-0.888629	5.731799
88	1	0	1.225100	-1.775298	5.377459
89	1	0	2.747449	-0.857754	5.265513
90	1	0	1.910746	-0.995171	6.814194

Structure **osrrs-TS2**

Imaginary Frequency: -179

E(RB3LYP) = -2383.635267 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.002434	-0.137915	0.017316
2	6	0	0.003235	-0.051587	1.572254
3	7	0	1.444648	0.048823	1.931598
4	6	0	2.193875	-0.717031	0.878489
5	6	0	1.488502	-0.231565	-0.401776

6	6	0	1.022136	4.402666	3.393277
7	6	0	0.598460	5.147358	4.565678
8	8	0	-0.309928	4.753297	5.345969
9	8	0	1.240466	6.335314	4.809759
10	6	0	0.783552	7.090004	5.981131
11	6	0	2.066745	4.783960	2.452765
12	8	0	2.504125	4.004330	1.566954
13	8	0	2.555871	6.062980	2.561541
14	6	0	3.590781	6.453566	1.601748
15	6	0	3.754124	-0.669766	0.889825
16	6	0	4.223473	-1.539566	-0.310481
17	6	0	4.407537	-2.925749	-0.171963
18	6	0	4.778213	-3.711855	-1.269188
19	6	0	4.973428	-3.125126	-2.523685
20	6	0	4.785670	-1.746443	-2.673753
21	6	0	4.408641	-0.962792	-1.577770
22	6	0	4.357645	-1.239463	2.201016
23	6	0	3.605764	-1.945877	3.155685
24	6	0	4.209326	-2.468840	4.307684
25	6	0	5.578603	-2.298999	4.527680
26	6	0	6.342670	-1.611133	3.577525
27	6	0	5.737731	-1.095775	2.428458
28	8	0	4.108574	0.709220	0.703822
29	14	0	5.396624	1.864257	0.429403
30	6	0	6.997996	1.117748	-0.321634
31	6	0	5.797109	2.690332	2.098078
32	6	0	4.651379	3.108526	-0.797513
33	6	0	0.129790	0.805354	4.652325
34	6	0	-0.960562	1.883989	4.891832
35	6	0	-0.955199	2.794344	3.667319
36	6	0	0.397600	3.167136	3.106382
37	6	0	1.378991	1.438886	4.003405
38	8	0	-1.985015	3.116910	3.051394
39	6	0	-2.329221	1.248412	5.134251
40	8	0	-2.553935	0.058935	4.884180
41	8	0	-3.328257	1.992917	5.697375
42	6	0	-3.294923	3.460223	5.825154
43	6	0	1.991412	0.823011	2.890854
44	1	0	-0.487240	0.737974	-0.422098
45	1	0	-0.561087	-1.020604	-0.309394
46	1	0	-0.443169	-0.946785	2.020855
47	1	0	-0.541324	0.814912	1.938869
48	1	0	1.923064	-1.773808	1.031287
49	1	0	1.888196	0.751523	-0.665093

50	1	0	1.637314	-0.910582	-1.242791
51	1	0	1.398893	7.987883	5.981530
52	1	0	0.933468	6.509357	6.894413
53	1	0	-0.275828	7.338661	5.886232
54	1	0	3.797908	7.496446	1.835743
55	1	0	3.226441	6.345827	0.577484
56	1	0	4.486289	5.840585	1.729768
57	1	0	4.275677	-3.394616	0.796758
58	1	0	4.919699	-4.780180	-1.139162
59	1	0	5.266726	-3.733489	-3.373176
60	1	0	4.927785	-1.279932	-3.643643
61	1	0	4.245962	0.099782	-1.707417
62	1	0	2.540672	-2.089988	3.024249
63	1	0	3.603243	-3.007680	5.029135
64	1	0	6.045207	-2.701399	5.420810
65	1	0	7.410267	-1.483005	3.725939
66	1	0	6.350697	-0.594370	1.691099
67	1	0	7.588841	0.543116	0.398291
68	1	0	7.619970	1.955004	-0.664071
69	1	0	6.789745	0.476075	-1.182093
70	1	0	6.580037	3.447278	1.966234
71	1	0	6.146173	1.962445	2.837630
72	1	0	4.898459	3.183043	2.480373
73	1	0	4.382130	2.629870	-1.745454
74	1	0	5.374017	3.905097	-1.014630
75	1	0	3.757679	3.553950	-0.351440
76	1	0	-0.319303	0.076408	3.977020
77	1	0	-0.680892	2.511698	5.744782
78	1	0	0.540900	2.846003	2.079376
79	1	0	-4.010805	3.680314	6.616160
80	1	0	-3.614622	3.898128	4.879360
81	1	0	-2.304802	3.837547	6.083974
82	1	0	3.048057	1.005902	2.734300
83	6	0	0.496211	0.009240	5.937106
84	6	0	1.412995	0.769506	6.908661
85	1	0	1.012763	-0.908938	5.620860
86	1	0	-0.429553	-0.310140	6.428294
87	6	0	2.356803	2.102087	4.979065
88	6	0	2.700737	1.211773	6.193281
89	1	0	1.647717	0.129870	7.769469
90	1	0	0.896572	1.654167	7.310745
91	1	0	3.270886	2.387263	4.444676
92	1	0	1.925573	3.036627	5.357530
93	1	0	3.260040	0.324792	5.862193

94	1	0	3.354159	1.766576	6.879531

Structure **orssr-TS2**

Imaginary Frequency: -146

E(RB3LYP) **=** -2383.629132 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.033138	-0.075688	-0.035573
2	6	0	-0.083052	0.083128	1.497454
3	7	0	1.344979	0.094639	1.941317
4	6	0	2.231709	-0.255412	0.768671
5	6	0	1.411230	0.286095	-0.415084
6	6	0	3.044546	-0.065519	6.551923
7	6	0	4.363141	0.465908	6.163527
8	8	0	4.557736	0.964119	5.032767
9	8	0	5.449975	0.410764	7.004097
10	6	0	5.559205	-0.541942	8.115105
11	6	0	2.521523	0.147175	7.880887
12	8	0	3.098966	0.675885	8.854975
13	8	0	1.194735	-0.287685	8.022919
14	6	0	0.638902	-0.205678	9.375303
15	6	0	3.723505	0.222025	0.802785
16	6	0	4.309293	-0.091465	-0.606045
17	6	0	4.753744	-1.387683	-0.920478
18	6	0	5.235518	-1.688775	-2.199100
19	6	0	5.288182	-0.697599	-3.185394
20	6	0	4.846699	0.594879	-2.882648
21	6	0	4.355147	0.892219	-1.606125
22	6	0	4.579279	-0.525993	1.853987
23	6	0	4.132892	-1.676357	2.527043
24	6	0	4.984753	-2.369757	3.399678
25	6	0	6.291288	-1.926778	3.615541
26	6	0	6.747085	-0.787308	2.943665
27	6	0	5.902786	-0.105135	2.067041
28	8	0	3.660490	1.642133	1.022301
29	14	0	4.542390	3.137272	1.260075
30	6	0	3.440281	4.398015	0.342889
31	6	0	6.294535	3.173799	0.482264
32	6	0	4.633142	3.561121	3.107383
33	6	0	-0.310999	0.014542	4.627477
34	6	0	-0.069748	-1.508362	4.940992

35	6	0	1.246399	-1.699222	5.705159
36	6	0	2.306201	-0.656076	5.499174
37	6	0	1.044940	0.712099	4.364102
38	8	0	1.448121	-2.729140	6.361329
39	6	0	-0.072911	-2.416713	3.728663
40	8	0	0.910348	-2.813169	3.089326
41	8	0	-1.358115	-2.773206	3.386771
42	6	0	-1.514900	-3.707426	2.258809
43	6	0	1.748383	0.575694	3.129958
44	6	0	-1.125390	0.611925	5.809704
45	6	0	-1.030414	2.139397	5.896630
46	6	0	0.431997	2.518581	6.170228
47	6	0	1.348906	2.092337	5.009264
48	1	0	-0.774452	0.558371	-0.529946
49	1	0	-0.246232	-1.113931	-0.316689
50	1	0	-0.654621	-0.723272	1.959963
51	1	0	-0.533660	1.035223	1.793865
52	1	0	2.244015	-1.352028	0.707353
53	1	0	1.548184	1.370323	-0.475095
54	1	0	1.713937	-0.157450	-1.364162
55	1	0	6.617075	-0.805361	8.155492
56	1	0	4.954570	-1.432958	7.921812
57	1	0	5.229474	-0.065473	9.035503
58	1	0	-0.376674	-0.589274	9.284730
59	1	0	0.640133	0.827260	9.730430
60	1	0	1.224876	-0.819416	10.063047
61	1	0	4.742707	-2.160394	-0.159765
62	1	0	5.578096	-2.695136	-2.418904
63	1	0	5.670072	-0.928730	-4.174693
64	1	0	4.880417	1.372961	-3.639179
65	1	0	3.995874	1.889237	-1.387051
66	1	0	3.123569	-2.051850	2.403883
67	1	0	4.612169	-3.250979	3.912610
68	1	0	6.946077	-2.459497	4.297404
69	1	0	7.759471	-0.430112	3.101713
70	1	0	6.286255	0.752018	1.528900
71	1	0	3.807069	5.417040	0.515235
72	1	0	2.410530	4.338420	0.710447
73	1	0	3.428293	4.219138	-0.737812
74	1	0	6.337255	2.652849	-0.478523
75	1	0	7.051219	2.744124	1.145586
76	1	0	6.562942	4.224263	0.311265
77	1	0	5.303271	4.418015	3.251878
78	1	0	4.995181	2.721838	3.709111

79	1	0	3.644841	3.836178	3.491174
80	1	0	-0.966472	0.083045	3.755525
81	1	0	-0.881062	-1.866603	5.582549
82	1	0	2.926696	-0.909495	4.643595
83	1	0	-2.585218	-3.893090	2.201203
84	1	0	-0.962969	-4.627686	2.458925
85	1	0	-1.143685	-3.255755	1.335983
86	1	0	2.777999	0.920769	3.150534
87	1	0	-0.749670	0.195190	6.750241
88	1	0	-2.166477	0.280818	5.699008
89	1	0	-1.681532	2.507917	6.699781
90	1	0	-1.381734	2.607054	4.963383
91	1	0	0.744901	2.040932	7.103775
92	1	0	0.538356	3.601075	6.314644
93	1	0	1.250685	2.858438	4.225743
94	1	0	2.398400	2.109610	5.322711

Structure **psrrs-TS2**

Imaginary Frequency: -228

E(RB3LYP) **=** -2422.903384 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.062992	-0.071297	0.213429
2	6	0	0.076523	-0.432790	1.713938
3	7	0	1.498532	-0.137303	2.011044
4	6	0	2.250055	-0.652114	0.813129
5	6	0	1.389203	-0.099358	-0.350140
6	6	0	0.911048	4.247353	4.062769
7	6	0	0.057052	4.747009	5.128424
8	8	0	-1.158695	4.452659	5.257558
9	8	0	0.673326	5.556265	6.052583
10	6	0	-0.187176	6.141760	7.085197
11	6	0	2.181956	4.840964	3.666017
12	8	0	3.007907	4.261543	2.918035
13	8	0	2.417573	6.117937	4.113470
14	6	0	3.691594	6.723504	3.715905
15	6	0	3.791345	-0.424107	0.703493
16	6	0	4.202563	-1.026451	-0.669180
17	6	0	4.451623	-2.403369	-0.802384
18	6	0	4.760395	-2.957421	-2.049776
19	6	0	4.827235	-2.143207	-3.185527

20	6	0	4.573372	-0.772452	-3.064175
21	6	0	4.257126	-0.220909	-1.817514
22	6	0	4.589172	-1.133316	1.827374
23	6	0	3.990644	-1.902143	2.839580
24	6	0	4.767233	-2.539033	3.817705
25	6	0	6.158957	-2.423534	3.802383
26	6	0	6.771259	-1.678008	2.787468
27	6	0	5.994244	-1.051509	1.810513
28	8	0	3.993810	1.005650	0.717862
29	14	0	5.266458	2.229510	0.709377
30	6	0	6.780919	1.800870	-0.391463
31	6	0	5.851327	2.557223	2.491275
32	6	0	4.381696	3.734381	-0.041028
33	6	0	0.198981	0.809662	5.009099
34	6	0	-1.133597	1.571322	4.551288
35	6	0	-0.826127	2.479244	3.354471
36	6	0	0.532619	3.115754	3.315239
37	6	0	1.392234	1.245158	4.114416
38	8	0	-1.611465	2.626627	2.403344
39	6	0	-2.386897	0.746588	4.255641
40	8	0	-2.384378	-0.328396	3.648679
41	8	0	-3.600451	1.230653	4.678041
42	6	0	-3.785218	2.578744	5.235522
43	6	0	1.985583	0.654122	2.984858
44	1	0	-0.509031	0.922065	0.109346
45	1	0	-0.718250	-0.783038	-0.296658
46	1	0	-0.113125	-1.500049	1.881561
47	1	0	-0.599266	0.116977	2.355206
48	1	0	2.115847	-1.744091	0.841395
49	1	0	1.734952	0.907583	-0.597340
50	1	0	1.476649	-0.721582	-1.242588
51	1	0	0.471364	6.800342	7.648546
52	1	0	-0.602095	5.360117	7.726200
53	1	0	-1.006195	6.700990	6.627467
54	1	0	3.685015	7.705893	4.184717
55	1	0	3.752711	6.807326	2.628344
56	1	0	4.530077	6.122843	4.076206
57	1	0	4.418211	-3.045302	0.071383
58	1	0	4.953392	-4.022584	-2.130471
59	1	0	5.072233	-2.571282	-4.152265
60	1	0	4.615220	-0.131642	-3.939505
61	1	0	4.039248	0.836168	-1.733664
62	1	0	2.914842	-2.011480	2.885534
63	1	0	4.276068	-3.123477	4.589230

64	1	0	6.759387	-2.914437	4.561371
65	1	0	7.852863	-1.594872	2.748573
66	1	0	6.487723	-0.517143	1.008748
67	1	0	7.328888	2.735987	-0.566384
68	1	0	6.488056	1.393841	-1.362775
69	1	0	7.474141	1.098382	0.080554
70	1	0	5.023114	2.963732	3.078084
71	1	0	6.658956	3.300072	2.478218
72	1	0	6.230626	1.648390	2.968350
73	1	0	3.577626	4.055330	0.625556
74	1	0	3.965930	3.499319	-1.026688
75	1	0	5.086765	4.566827	-0.156173
76	1	0	-1.372326	2.275124	5.354125
77	1	0	1.019804	3.024085	2.351526
78	1	0	2.150239	1.785373	4.671669
79	1	0	-4.864067	2.726812	5.223298
80	1	0	-3.287076	3.334347	4.628280
81	1	0	-3.415633	2.625875	6.263707
82	1	0	3.013968	0.943794	2.802120
83	1	0	2.396312	-1.368324	7.633238
84	6	0	1.511445	-0.889937	7.193368
85	6	0	1.689543	0.637461	7.159775
86	6	0	1.252335	-1.428144	5.775874
87	1	0	0.657834	-1.145108	7.839720
88	6	0	0.505604	1.330764	6.460657
89	1	0	2.628667	0.882140	6.643917
90	1	0	1.785862	1.036543	8.178344
91	6	0	0.040884	-0.740082	5.115387
92	1	0	1.069344	-2.510655	5.807959
93	1	0	2.150585	-1.275888	5.161913
94	1	0	0.679621	2.413351	6.427223
95	1	0	-0.400210	1.172781	7.064575
96	1	0	-0.161239	-1.186665	4.143172
97	1	0	-0.849118	-0.948628	5.724202

Structure **prssr-TS2**

Imaginary Frequency: -156

E(RB3LYP) **=** -2422.895543 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.212925	0.938218	0.239940

2	6	0	-0.250971	0.683422	1.752446
3	7	0	1.166446	0.483266	2.139829
4	6	0	2.042726	0.251512	0.939988
5	6	0	1.037791	0.168554	-0.231008
6	6	0	2.015389	-3.119222	4.124002
7	6	0	2.728084	-3.182614	2.856057
8	8	0	2.247890	-2.770510	1.775298
9	8	0	4.030636	-3.685363	2.792012
10	6	0	5.016720	-3.498909	3.867845
11	6	0	2.476017	-3.714082	5.390641
12	8	0	2.452454	-3.112725	6.478246
13	8	0	2.935594	-5.022725	5.394061
14	6	0	2.530132	-5.973137	4.343372
15	6	0	3.206539	1.300501	0.763709
16	6	0	2.642959	2.730654	0.705496
17	6	0	2.184540	3.305343	-0.495506
18	6	0	1.605620	4.579779	-0.509007
19	6	0	1.469898	5.306087	0.679176
20	6	0	1.915294	4.743345	1.880065
21	6	0	2.492646	3.468615	1.892296
22	6	0	4.084515	0.916689	-0.450064
23	6	0	4.262411	-0.431377	-0.823065
24	6	0	5.137283	-0.781004	-1.857302
25	6	0	5.868493	0.201594	-2.533141
26	6	0	5.718799	1.541314	-2.160737
27	6	0	4.837916	1.892333	-1.131501
28	8	0	4.005863	1.145196	1.981843
29	14	0	5.688488	1.424863	2.413060
30	6	0	5.631193	1.186706	4.302461
31	6	0	6.267414	3.196962	1.992980
32	6	0	6.846398	0.130170	1.624585
33	6	0	-0.088701	0.043828	5.500468
34	6	0	-0.216649	-1.345424	6.260273
35	6	0	-0.178094	-2.478849	5.250876
36	6	0	0.847152	-2.343224	4.145361
37	6	0	1.160288	-0.184440	4.626311
38	8	0	-0.887509	-3.493001	5.305996
39	6	0	1.655032	0.147969	3.358390
40	6	0	0.273978	1.167226	6.546200
41	6	0	-0.965296	1.850096	7.154997
42	6	0	-1.785683	2.596636	6.068695
43	6	0	-1.590004	1.953681	4.672144
44	6	0	-1.418800	0.424806	4.792010
45	1	0	-0.111595	2.007309	0.035622

46	1	0	-1.126467	0.586037	-0.248421
47	1	0	-0.822430	-0.227405	1.971380
48	1	0	-0.690032	1.512219	2.306044
49	1	0	2.515283	-0.719059	1.100979
50	1	0	1.448184	0.564240	-1.162107
51	1	0	0.792238	-0.885608	-0.401944
52	1	0	5.967650	-3.336888	3.358939
53	1	0	5.066048	-4.385925	4.499271
54	1	0	4.768465	-2.627672	4.480902
55	1	0	2.654775	-6.955412	4.797818
56	1	0	3.172609	-5.871563	3.466869
57	1	0	1.484719	-5.812148	4.069657
58	1	0	2.287465	2.764536	-1.429392
59	1	0	1.266766	5.004040	-1.449135
60	1	0	1.025523	6.296261	0.668157
61	1	0	1.813873	5.295127	2.809657
62	1	0	2.831253	3.032108	2.822726
63	1	0	3.741255	-1.227974	-0.305620
64	1	0	5.250500	-1.826335	-2.126227
65	1	0	6.547065	-0.072982	-3.334434
66	1	0	6.283684	2.316109	-2.669867
67	1	0	4.733841	2.936146	-0.861232
68	1	0	4.948037	1.904892	4.767577
69	1	0	6.626640	1.328488	4.739256
70	1	0	5.289128	0.178150	4.558861
71	1	0	7.239222	3.381004	2.467533
72	1	0	5.556998	3.942271	2.363792
73	1	0	6.384584	3.339724	0.915073
74	1	0	6.954686	0.281028	0.547121
75	1	0	6.463189	-0.882375	1.788645
76	1	0	7.839341	0.201705	2.085828
77	1	0	0.429673	-2.127979	3.165208
78	1	0	2.002487	-0.378969	5.291341
79	1	0	2.726164	0.002266	3.283009
80	1	0	0.880808	1.927892	6.037520
81	1	0	0.906766	0.737465	7.332112
82	1	0	-0.650617	2.547071	7.941393
83	1	0	-1.597041	1.101206	7.646055
84	1	0	-1.487605	3.652502	6.027918
85	1	0	-2.849026	2.581183	6.338896
86	1	0	-0.706783	2.396122	4.191620
87	1	0	-2.446521	2.188269	4.027670
88	1	0	-2.256230	0.031696	5.376435
89	1	0	-1.488922	-0.068480	3.820715

90	1	0	0.713574	-1.477468	6.830251
91	6	0	-1.358315	-1.482356	7.238183
92	8	0	-2.568043	-1.453675	6.982637
93	8	0	-0.882718	-1.649746	8.517684
94	6	0	-1.884881	-1.852458	9.574794
95	1	0	-2.503361	-2.721058	9.340460
96	1	0	-1.302822	-2.014062	10.479579
97	1	0	-2.521012	-0.968989	9.666765
