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Supplementary Material

s-trans-1,3-butadiene (1)

RBecke3LYP/6-31G* Energy: -155.9921372 H

1	6	0.000000	0.728726	0.000000
2	6	0.000000	-0.728726	0.000000
3	6	1.107312	1.484259	0.000000
4	6	-1.107312	-1.484259	0.000000
5	1	1.060135	2.569021	0.000000
6	1	-1.060135	-2.569021	0.000000
7	1	2.100101	1.039436	0.000000
8	1	-2.100101	-1.039436	0.000000
9	1	-0.977927	1.211199	0.000000
10	1	0.977927	-1.211199	0.000000

ethylene (2)

RBecke3LYP/6-31G* Energy: -78.5874573 H

1	6	0.000000	0.000000	0.665524
2	6	0.000000	0.000000	-0.665524
3	1	0.000000	0.923558	1.239453
4	1	0.000000	-0.923558	1.239453
5	1	0.000000	0.923558	-1.239453
6	1	0.000000	-0.923558	-1.239453

Concerted T. S. (3)

RBecke3LYP/6-31G* Energy: -234.5438948 H

1	6	0.499253	-0.436584	1.437291
2	6	0.499253	-0.436584	-1.437291
3	6	-0.261329	-1.328804	0.703590
4	6	-0.261329	-1.328804	-0.703590
5	6	-0.261329	1.571834	0.692999
6	6	-0.261329	1.571834	-0.692999
7	1	0.387554	-0.386519	2.517676
8	1	1.459891	-0.095393	1.068674
9	1	0.387554	-0.386519	-2.517676
10	1	1.459891	-0.095393	-1.068674
11	1	-1.040733	-1.893469	1.213289
12	1	-1.040733	-1.893469	-1.213289
13	1	0.525348	2.088050	1.235813
14	1	-1.191624	1.448651	1.235917
15	1	0.525348	2.088050	-1.235813
16	1	-1.191624	1.448651	-1.235917

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cyclohexene (4)

RBecke3LYP/6-31G* Energy: -234.6482863 H

1	6	-0.369136	-0.672890	-1.192312
2	6	0.369136	0.672890	-1.192312
3	6	0.000000	1.503028	0.047936
4	6	0.000000	-1.503028	0.047936
5	6	-0.007775	0.668468	1.306095
6	6	0.007775	-0.668468	1.306095
7	1	-1.452466	-0.487764	-1.192983
8	1	1.452466	0.487764	-1.192983
9	1	-0.145143	-1.237283	-2.105884
10	1	0.145143	1.237283	-2.105884
11	1	0.701013	2.341466	0.163846
12	1	-0.701013	-2.341466	0.163846
13	1	-0.989906	1.967161	-0.089975
14	1	0.989906	-1.967161	-0.089975
15	1	-0.023396	1.204543	2.254680
16	1	0.023396	-1.204543	2.254680

Anti Diradical T. S. (5)

UBecke3LYP/6-31G* Energy: -234.5269466 H

1	6	2.037240	1.126097	.121956
2	6	1.944255	-.184153	-.244515
3	6	.855448	-1.066885	.006655
4	6	-.357890	-.708591	.659192
5	6	-1.459744	.175882	-.573867
6	6	-2.698239	.507269	.012499
7	1	1.252542	1.632008	.677505
8	1	2.914179	1.716665	-.122949
9	1	2.780565	-.607968	-.800787
10	1	.898628	-2.043652	-.472351
11	1	-.286205	.056621	1.430525
12	1	-.984666	-1.540505	.973500
13	1	-1.499448	-.551600	-1.383815
14	1	-.785949	1.004363	-.799689
15	1	-2.793196	1.358029	.682482
16	1	-3.537948	-.181745	-.016486

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Anti Diradical Intermediate (6)

UBecke3LYP/6-31G* Energy: -234.534663 H

1	6	2.144615	1.085981	.047285
2	6	1.969621	-.263456	-.193853
3	6	.823754	-1.019949	.065360
4	6	-.458133	-.486680	.610529
5	6	-1.435905	.013085	-.533851
6	6	-2.726512	.524745	-.013861
7	1	1.364117	1.703571	.481224
8	1	3.081349	1.579351	-.189955
9	1	2.811736	-.798869	-.633434
10	1	.833306	-2.066715	-.233431
11	1	-.281334	.351950	1.293344
12	1	-.978188	-1.262669	1.183855
13	1	-1.599715	-.822651	-1.224991
14	1	-.899580	.792624	-1.089891
15	1	-2.788431	1.512791	.434589
16	1	-3.568819	-.142323	.146328

Gauche-Out Diradical T. S. (7)

UBecke3LYP/6-31G* Energy: -234.5237105 H

1	6	0.003964	0.009132	0.005918
2	6	0.004931	0.009722	1.370295
3	6	1.140468	-0.000002	2.229008
4	6	2.496652	0.021533	1.798191
5	6	3.063109	1.742813	1.283460
6	6	3.483377	2.564410	2.348996
7	1	0.919657	-0.023135	-0.577945
8	1	-0.925386	0.031768	-0.554057
9	1	-0.964418	0.037650	1.868501
10	1	0.946338	0.111201	3.294226
11	1	2.692710	-0.471448	0.845572
12	1	3.236561	-0.250854	2.547697
13	1	2.161109	2.048203	0.751621
14	1	3.859032	1.442942	0.599539
15	1	4.507792	2.536290	2.709708
16	1	2.770472	3.122632	2.949533