JOC The Journal of Organic Chemistry

J. Org. Chem., 1997, 62(26), 9267-9275, DOI:10.1021/jo971587b

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Supplementary Information

Cartesian coordinates (in Å) for all stationary points

1. trans-2,3-dimethylcyclopropylidene **1b**, C2, B3LYP/TZP

13

C	.000000	.000000	1.304589
C	.000000	.746877	.010631
C	.000000	-.746877	.010631
C	-1.195006	-1.594066	-.389091
C	1.195006	1.594066	-.389091
H	.965488	-1.225314	-.169432
H	-.965488	1.225314	-.169432
H	1.189173	1.786363	-1.465237
H	-1.189173	-1.786363	-1.465237
H	1.184471	2.552291	.136710
H	-1.184471	-2.552291	.136710
H	-2.132584	-1.089988	-.145053
H	2.132584	1.089988	-.145053

2. cis-2,3-dimethylcyclopropylidene **1c**, Cs, B3LYP/TZP

13

C	-.169441	.680411	1.677556
C	-.169441	.680411	-1.677556
C	-.169441	-.527083	.756610
C	-.169441	-.527083	-.756610
C	1.074187	-.829492	.000000
H	-.681730	-1.396342	1.165790
H	-.681730	-1.396342	-1.165790
H	.276132	.421092	-2.641337
H	.405664	1.508493	-1.260698
H	.276132	.421092	2.641337
H	-1.189332	1.035268	1.850256
H	.405664	1.508493	1.260698
H	-1.189332	1.035268	-1.850256

3. **TS1** for ring opening of **1c**, Cs, B3LYP/TZP

13

C	-1.051048	-.720570	.000000
C	.157685	-.503772	.789958
C	.157685	-.503772	-.789958
C	.157685	.630082	1.795687
C	.157685	.630082	-1.795687
H	.788782	-1.343869	1.062431
H	.788782	-1.343869	-1.062431
H	1.157754	1.061632	1.897903
H	1.157754	1.061632	-1.897903
H	-.157823	.260572	2.775964
H	-.157823	.260572	-2.775964
H	-.527795	1.425515	1.501714
H	-.527795	1.425515	-1.501714

4. **TS2** for ring opening of **1b**, C1, B3LYP/TZP

13

C	-.625185	-.117426	-.325064
C	-.130609	1.227030	-.345701
C	.793178	.394693	.383446
C	-2.029188	-.386519	.171759
H	-.205970	-.927547	-.912611
C	1.940430	-.503301	-.039676
H	-2.038358	-1.204526	.898838
H	-2.670204	-.679019	-.666665
H	-2.454651	.500798	.640236
H	2.015777	-1.395070	.587455
H	1.855491	-.813837	-1.082560
H	2.873424	.057843	.067016
H	.932730	.774491	1.399704

5. 1,3-dimethylallene (**2**)

13

C	0.485876	-1.211764	0.411271
C	0.000000	0.000000	0.413308
C	-0.485876	1.211764	0.411271
C	0.000000	-2.343112	-0.459135
H	1.307523	-1.438785	1.090186
H	-1.307523	1.438785	1.090186
C	0.000000	2.343112	-0.459135
H	-0.809189	2.721642	-1.091928
H	0.820157	2.024673	-1.103718
H	0.348145	3.181558	0.152716
H	0.809189	-2.721642	-1.091928
H	-0.820157	-2.024673	-1.103718
H	-0.348145	-3.181558	0.152716

6. Bicyclo[4.1.0]hepta-7-ylidene (**3**), B3LYP/DZP

17

C	-1.143124	-.678665	-.344877
C	-1.079099	.826794	-.260907
C	-1.646267	.025471	.884252
C	.260634	1.535016	.026067
C	.118966	-1.537634	-.240199
C	1.470016	.614754	-.224656
C	1.278572	-.768827	.421423
H	-1.942961	-1.100710	-.961242
H	-1.806438	1.402353	-.836940
H	.276366	1.881002	1.069707
H	.329851	2.428966	-.605943
H	-.107815	-2.454174	.321702
H	.421029	-1.837964	-1.254433
H	1.620219	.487285	-1.306717
H	2.375480	1.093505	.173011
H	2.201023	-1.358340	.338092
H	1.075061	-.643382	1.496135

7. Cyclohepta-1,2-diene (**4**), C2

a) B3LYP/DZP

13

C	.000000	.000000	1.429306
C	.000000	1.271239	1.038684
C	.000000	-1.271239	1.038684
C	.605874	1.492836	-.267394
C	-.605874	-1.492836	-.267394
H	1.177339	2.400127	-.469262
H	-1.177339	-2.400127	-.469262
H	-.474987	2.082183	1.589241
H	.474987	-2.082183	1.589241
C	.382141	.615994	-1.293994
C	-.382141	-.615994	-1.293994
H	.766017	.907335	-2.271674
H	-.766017	-.907335	-2.271674

b) MP2/DZP

13

C	.000000	.000000	1.433413
C	.000000	1.286519	1.031363
C	.000000	-1.286519	1.031363
C	.642877	1.487669	-.260286
C	-.642877	-1.487669	-.260286
H	1.249824	2.374716	-.462577
H	-1.249824	-2.374716	-.462577
H	-.474481	2.100138	1.581208
H	.474481	-2.100138	1.581208
C	.406342	.599362	-1.295624
C	-.406342	-.599362	-1.295624
H	.807830	.882888	-2.271590
H	-.807830	-.882888	-2.271590

c) CCSD/DZP

13

C	.000000	1.278203	1.040393
C	.000000	.000000	1.432038
C	.000000	-1.278203	1.040393
C	.640294	1.491132	-.270913
C	-.640294	-1.491132	-.270913
H	1.245167	2.379209	-.462596
H	-1.245167	-2.379209	-.462596
H	-.507845	2.082627	1.570298
H	.507845	-2.082627	1.570298
C	.411237	.610109	-1.292491
C	-.411237	-.610109	-1.292491
H	.832912	.868055	-2.265749
H	-.832912	-.868055	-2.265749

8. Tricyclo[4.1.0.02,7]heptane (**5**), B3LYP/DZP

17

C	.087712	-.618100	1.137294
C	.835919	-1.267549	.000000
C	-.671263	-1.273933	.000000
C	.087712	-.618100	-1.137294
C	.087712	.906433	1.276094
C	.087712	.906433	-1.276094
C	-.468213	1.565867	.000000
H	.098994	-1.176450	2.076987
H	1.510092	-2.117125	.000000
H	.098994	-1.176450	-2.076987
H	-.524573	1.204288	2.139433
H	1.113666	1.248301	1.477364
H	1.113666	1.248301	-1.477364
H	-.524573	1.204288	-2.139433
H	-.269390	2.646315	.000000
H	-1.559331	1.438818	.000000
H	-1.341294	-2.126580	.000000

9. Tricyclo[4.1.0.03,7]heptane (**6**), B3LYP/DZP

17

C	-1.276881	.565653	-.340603
C	.032616	1.258581	.033841
C	-.630352	.331764	1.026036
C	1.353581	.669893	-.476953
C	-1.021008	-.893766	-.741042
C	1.383339	-.764158	.129710
C	-.083385	-1.032375	.507919
H	-2.168910	1.144809	-.575093
H	-.047192	2.331856	.201141
H	2.206965	1.270590	-.138080
H	1.388520	.647534	-1.574197
H	-1.929568	-1.497349	-.631500
H	-.574497	-1.091276	-1.726437
H	1.777332	-1.510726	-.572829
H	2.012525	-.784978	1.030237
H	-.243697	-1.919499	1.128374
H	-.968929	.595487	2.024926

10. **TS4** for ring opening **3** -> **4**, B3LYP/DZP

17

C	-.386572	-1.286307	-.729945
C	-1.374129	-.906722	.144291
C	.672599	-1.334647	.198489
C	-1.567861	.599598	.174773
C	1.736864	-.300602	-.088459
C	-.314822	1.376822	-.349388
C	1.070562	1.069645	.297797
H	-1.891049	-1.520311	.900040
H	.511318	-1.479551	1.287955
H	-2.449574	.882944	-.422639
H	-1.792867	.887003	1.213821
H	1.977915	-.303257	-1.158574
H	2.653609	-.435951	.505623
H	-.237840	1.223240	-1.431949
H	-.522525	2.444493	-.187107
H	.976018	1.112180	1.393528
H	1.755157	1.882487	.013954

11. **TS5** for CH insertion **3** -> **5**, B3LYP/DZP

17

C	.744268	1.072947	-.119185
C	1.351441	-.216853	-.563538
C	1.508818	.183269	.896428
C	.459084	-1.263250	.043250
C	-.753907	1.351671	-.191858
C	-1.045716	-1.176059	-.226916
C	-1.596937	.161841	.296936
H	1.374292	1.951800	-.292393
H	2.135489	-.417318	-1.289037
H	.906962	-2.261479	.036306
H	-.991506	2.240778	.408956
H	-1.016381	1.591690	-1.234030
H	-1.218148	-1.270739	-1.308816
H	-1.561847	-2.012619	.263262
H	-2.646801	.286603	.001878
H	-1.573657	.136037	1.395540
H	.589295	-.926156	1.207636

12. **TS6** for CH insertion **3** -> **6**, B3LYP/DZP

17

C	1.317677	-.427387	-.334948
C	.115934	-1.281122	-.003179
C	.851456	-.606178	1.133984
C	-1.284221	-.829342	-.409322
C	.967538	1.016998	-.642008
C	-1.471275	.630643	.078899
C	-.114398	1.196958	.433491
H	2.244206	-.885519	-.681051
H	.296164	-2.358126	-.028123
H	-2.045256	-1.477648	.043047
H	-1.403559	-.906447	-1.499108
H	1.823668	1.674170	-.442484
H	.609222	1.231775	-1.663315
H	-1.932982	1.250138	-.705985
H	-2.132916	.672290	.953135
H	-.123827	2.147721	.979155
H	.369015	.448226	1.503234

13. Bicyclo[3.1.0]hexa-6-ylidene, boat conformer (**7**), B3LYP/DZP

14

C	.225542	-.881255	.767073
C	.225542	-.881255	-.767073
C	-.930206	-1.433433	.000000
C	.225542	.587904	1.221944
C	.225542	.587904	-1.221944
C	-.277679	1.380300	.000000
H	.722736	-1.597179	1.427145
H	.722736	-1.597179	-1.427145
H	-.407161	.733172	2.107016
H	-.407161	.733172	-2.107016
H	1.251494	.876263	1.489182
H	1.251494	.876263	-1.489182
H	-1.375588	1.396869	.000000
H	.075760	2.417635	.000000

14. Bicyclo[3.1.0]hexa-6-ylidene, chair conformer (**7**), B3LYP/DZP

14

C	-.836141	-.751695	-.356942
C	-.836142	.751693	-.356943
C	-1.608598	.000000	.692085
C	.556537	-1.230264	.129498
C	.556535	1.230265	.129498
H	-1.405974	-1.391488	-1.031766
H	-1.405976	1.391486	-1.031768
H	.521794	-1.535496	1.184571
H	.521792	1.535496	1.184572
C	1.470295	.000000	-.062775
H	2.316048	.000001	.637695
H	1.871407	.000000	-1.083738
H	.882994	2.098924	-.453049
H	.882997	-2.098922	-.453049

15. Cyclohexa-1,2-diene (**8**), C1

a) B3LYP/DZP

14

C	-.006879	-1.410389	-.086572
C	-.057928	1.323007	-.155029
C	1.177937	-.895017	.230125
C	-1.200994	-.853584	-.277702
C	1.326667	.579004	-.170903
C	-1.264745	.502757	.423672
H	1.914085	-1.362560	.883593
H	-1.922513	-1.143008	-1.041188
H	2.011666	1.036480	.557039
H	1.797306	.699429	-1.155329
H	-2.204883	1.031809	.219620
H	-1.166275	.395467	1.509557
H	-.320888	1.616778	-1.178470
H	.047165	2.250944	.423633

b) MP2/DZP

14

C	-.018260	-1.410847	-.104370
C	-.058818	1.307927	-.178904
C	1.173190	-.896411	.227358
C	-1.215801	-.831787	-.277554
C	1.323099	.578134	-.162286
C	-1.238419	.503762	.453799
H	1.903772	-1.375471	.879471
H	-1.936394	-1.082546	-1.055735
H	1.974292	1.029189	.599896
H	1.826332	.710740	-1.129229
H	-2.182003	1.045473	.304481
H	-1.076537	.370801	1.530098
H	-.342633	1.525075	-1.216652
H	.043223	2.272064	.339420

c) CCSD/DZP

14

C	-.049247	1.316555	-.170765
C	-.023303	-1.419237	-.098464
C	1.166212	-.901473	.228384
C	-1.214239	-.833711	-.274413
C	1.328977	.571871	-.161988
C	-1.243742	.515451	.438641
H	1.901194	-1.387180	.868535
H	-1.947265	-1.107702	-1.031091
H	1.992289	1.023330	.588761
H	1.823863	.694906	-1.134113
H	-2.181907	1.058026	.263983
H	-1.112966	.393254	1.520251
H	-.320682	1.557174	-1.206973
H	.057525	2.271455	.362280

16. **TS7** for ring opening **7** -> **8**, B3LYP/DZP

14

C	-.205807	.856677	.835383
C	-.205807	.856677	-.835383
C	.699304	1.627627	.000000
C	-.205807	-.631139	1.194865
C	-.205807	-.631139	-1.194865
C	.393709	-1.374975	.000000
H	-.757297	1.481272	1.548931
H	-.757297	1.481272	-1.548931
H	.365297	-.770540	2.123158
H	.365297	-.770540	-2.123158
H	-1.235622	-.964927	1.388369
H	-1.235622	-.964927	-1.388369
H	1.486234	-1.270426	.000000
H	.150289	-2.443559	.000000