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SUPPLEMENTARY MATERIAL FOR:

Epoxidation by Dimethyldioxirane: Effects of Intramolecular and Intermolecular Interactions

Karol Miaskiewicz and Douglas A. Smith

Contribution from The DASGroup, Inc., 1732 Lyter Drive, Johnstown, PA 15905-1801

- Table. Energies (a.u.) of the reactants and transition state structures optimized at the B3LYP/6-31G* level.

	B3LYP/6-31G* energy (a.u.)
Substrates:	
dimethyldioxirane (DMDO)	-268.268944329
2-methyl-2-butene	-196.543583518
3-methyl-2-buten-1-ol	-271.744162330
1-amino-3-methyl-2-butene	-251.882468088
methanol	-115.714406408
Transistion States:	
TS-1 [a]	-464.790816663
TS-2 [a]	-540.002367843
TS-3 [a]	-539.992351153
TS-4 [a]	-464.790816663
TS-5 [a]	580.525640773

[a] see text for numbering of TS structures

- Cartesian coordinates of the B3LYP/6-31G* optimized structures of transition states and some of the reactants:

2-methyl-2-butene

C 0.6303 1.4578 0.0000

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C	0.4494	-0.0407	0.0000
C	-0.7346	-0.6716	0.0002
C	-2.1153	-0.0775	-0.0001
C	1.7413	-0.8241	-0.0001
H	-0.7150	-1.7629	0.0002
H	-2.1153	1.0159	0.0006
H	-2.6832	-0.4089	-0.8805
H	-2.6842	-0.4104	0.8791
H	2.3546	-0.5781	-0.8788
H	1.5648	-1.9043	-0.0024
H	2.3527	-0.5817	0.8810
H	-0.3128	2.0090	0.0008
H	1.2065	1.7790	0.8792
H	1.2055	1.7788	-0.8798

3-methyl-2-buten-1-ol

C	1.3395	1.4085	-0.1241
C	0.9644	-0.0458	0.0270
C	-0.2780	-0.5037	0.2397
C	-1.5474	0.2799	0.3895
C	2.1288	-1.0031	-0.0693
H	-0.4253	-1.5798	0.3315
H	-1.4038	1.3408	0.1385
O	-2.5336	-0.3183	-0.4567
H	-3.3844	0.0979	-0.2499
H	-1.8772	0.2402	1.4432
H	2.6374	-0.9058	-1.0386
H	1.8127	-2.0443	0.0464
H	2.8839	-0.7885	0.7003
H	0.4778	2.0796	-0.1456
H	1.9918	1.7294	0.7003
H	1.9114	1.5625	-1.0493

1-amino-3-methyl-2-butene

C	1.3396	1.4101	0.1336
C	0.9724	-0.0449	-0.0346
C	-0.2625	-0.5073	-0.2842
C	-1.5427	0.2656	-0.4444
C	2.1386	-0.9977	0.0892
H	-0.3983	-1.5849	-0.3805
H	-1.3823	1.3414	-0.2669
H	-1.8886	0.1738	-1.4848
H	2.9119	-0.7775	-0.6605
H	1.8298	-2.0397	-0.0386
H	2.6238	-0.9027	1.0710

H	0.4782	2.0815	0.1062
H	1.8639	1.5682	1.0863
H	2.0341	1.7280	-0.6568
N	-2.5907	-0.3301	0.4030
H	-2.3407	-0.2009	1.3827
H	-3.4685	0.1687	0.2634

TS-1

C	2.4104	-0.5402	1.0951
C	1.6145	-0.4439	-0.1735
C	1.1300	0.7505	-0.6796
C	1.4907	2.1356	-0.2309
C	1.4317	-1.7260	-0.9329
H	0.6402	0.6957	-1.6497
H	1.7607	2.1757	0.8260
H	2.3385	2.5159	-0.8179
H	0.6454	2.8118	-0.3875
H	2.4117	-2.1177	-1.2424
H	0.8220	-1.5928	-1.8308
H	0.9682	-2.4975	-0.3068
H	2.3418	0.3599	1.7071
H	2.0665	-1.3886	1.6976
H	3.4710	-0.7198	0.8641
O	-0.3069	0.3221	0.5603
O	-1.9991	0.4958	1.3590
C	-1.6945	-0.0321	0.1776
C	-1.9002	-1.5425	0.0654
C	-2.1777	0.7511	-1.0444
H	-1.4715	-1.9624	-0.8516
H	-2.9755	-1.7564	0.0624
H	-1.4553	-2.0301	0.9366
H	-1.7322	0.3922	-1.9803
H	-1.9479	1.8115	-0.9103
H	-3.2650	0.6436	-1.1314

TS-2

C	-2.4170	-0.8715	-1.0948
C	-1.6344	-0.7287	0.1787
C	-1.1292	0.4732	0.6389
C	-1.4147	1.8624	0.1163
C	-1.4603	-1.9840	0.9848
H	-0.6426	0.4694	1.6118
H	-1.8546	1.8207	-0.8896

H	-2.1495	2.3440	0.7743
H	-2.4412	-2.3702	1.2981
H	-0.8579	-1.8208	1.8828
H	-0.9916	-2.7751	0.3862
H	-2.3184	-0.0081	-1.7540
H	-2.0913	-1.7617	-1.6453
H	-3.4850	-1.0107	-0.8702
O	0.3492	0.1057	-0.5595
O	2.0424	0.4781	-1.2221
C	1.7183	-0.2724	-0.1604
C	1.9638	-1.7690	-0.3288
C	2.1285	0.2828	1.2013
H	1.4829	-2.3589	0.4597
H	3.0412	-1.9663	-0.2866
H	1.5906	-2.0863	-1.3056
H	1.7007	-0.2932	2.0306
H	1.8181	1.3267	1.2885
H	3.2197	0.2325	1.2889
O	-0.2604	2.6775	0.1461
H	0.3994	2.2111	-0.4022

TS-3

C	-1.7976	1.5188	1.1467
C	-1.1441	1.0685	-0.1249
C	-0.9958	-0.2628	-0.4748
C	-1.6998	-1.4300	0.1764
C	-0.6779	2.1589	-1.0439
H	-0.5981	-0.4601	-1.4693
H	-1.7581	-1.2934	1.2566
H	-1.1181	-2.3439	-0.0022
H	-1.5302	2.7897	-1.3352
H	-0.2164	1.7686	-1.9552
H	0.0416	2.8176	-0.5421
H	-1.9926	0.7019	1.8415
H	-1.1726	2.2629	1.6544
H	-2.7559	2.0070	0.9175
O	0.5638	-0.2042	0.6243
O	2.1875	-0.7881	1.3551
C	1.9543	-0.3182	0.1315
C	2.5727	1.0451	-0.1740
C	2.0937	-1.3326	-1.0044
H	2.2026	1.4765	-1.1110
H	3.6597	0.9336	-0.2619
H	2.3625	1.7269	0.6540
H	1.6987	-0.9588	-1.9566

H	1.5812	-2.2586	-0.7299
H	3.1557	-1.5594	-1.1522
O	-3.0476	-1.5637	-0.2793
H	-3.0215	-1.8497	-1.2056

TS-4

C	-2.2778	-1.1352	-1.0950
C	-1.5291	-0.8686	0.1794
C	-1.1750	0.3942	0.6171
C	-1.6227	1.7204	0.0634
C	-1.2365	-2.0744	1.0265
H	-0.7023	0.4728	1.5934
H	-1.9819	1.6009	-0.9703
H	-2.4839	2.0578	0.6599
H	-2.1782	-2.5362	1.3584
H	-0.6519	-1.8259	1.9168
H	-0.6990	-2.8416	0.4555
H	-2.2847	-0.2794	-1.7713
H	-1.8358	-1.9867	-1.6252
H	-3.3211	-1.4056	-0.8733
O	0.3454	0.1225	-0.5645
O	2.0126	0.5983	-1.2369
C	1.7371	-0.1525	-0.1638
C	2.0891	-1.6316	-0.3068
C	2.1082	0.4473	1.1909
H	1.6541	-2.2413	0.4930
H	3.1781	-1.7496	-0.2654
H	1.7379	-1.9921	-1.2770
H	1.7154	-0.1441	2.0271
H	1.7310	1.4699	1.2652
H	3.2005	0.4653	1.2816
N	-0.5494	2.7033	0.2211
H	0.2190	2.4303	-0.3915
H	-0.8744	3.6186	-0.0843

TS-5

C	2.6243	-1.2469	-1.2589
C	2.1940	-0.6995	0.0718
C	1.1118	-1.1778	0.7809
C	0.2881	-2.3953	0.4938
C	3.0914	0.3530	0.6612
H	0.9392	-0.7301	1.7580
H	0.4716	-2.8067	-0.5011
H	0.5227	-3.1753	1.2319
H	-0.7786	-2.1595	0.5731

H	4.0795	-0.0810	0.8733
H	2.6981	0.7616	1.5967
H	3.2584	1.1780	-0.0411
H	1.8647	-1.8750	-1.7253
H	2.8582	-0.4276	-1.9482
H	3.5427	-1.8415	-1.1458
O	0.1658	0.1535	-0.4500
O	-1.2434	1.1724	-1.0317
C	-0.3384	1.4621	-0.0661
C	0.6033	2.6036	-0.4321
C	-0.8784	1.5232	1.3590
H	1.4328	2.6985	0.2765
H	0.0447	3.5465	-0.4247
H	0.9959	2.4404	-1.4390
H	-0.0704	1.5298	2.1001
H	-1.5417	0.6737	1.5383
H	-1.4513	2.4491	1.4867
H	-2.2509	-0.2646	-0.4033
O	-2.7484	-0.9441	0.1025
C	-4.1146	-0.8387	-0.2423
H	-4.6675	-1.5623	0.3660
H	-4.3025	-1.0732	-1.3025
H	-4.5266	0.1625	-0.0381