Electronic Supplementary Material (ESI) for RSC Advances.

Kinetic investigations of chlorine atom initiated photo oxidation reactions of 2,3-dimethyl-1,3-butadiene in gas phase: An experimental and theoretical study

S. Vijayakumar and B. Rajakumar*

Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, India.

*Address for correspondence: rajakumar@iitm.ac.in

Table S.1: Optimized geometries of the reactant, pre-reactive complexes, transition states, product complexes and products for the reaction of 2,3-dimethyl-1,3-butadiene + Cl at MP2/6-31 G (d,p) level of theory.

Table S.1.1: Optimized parameters of 2,3-dimethyl-1,3-butadiene.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-0.70429	0.222046	0.000007
2	6	0	0.704289	-0.22205	0.000013
3	6	0	-1.03003	1.529752	-0.00032
4	1	0	-2.06532	1.841823	-0.00033
5	1	0	-0.28724	2.313119	-0.00059
6	6	0	1.030025	-1.52975	-0.00032
7	1	0	2.065314	-1.84182	-0.00037
8	1	0	0.287238	-2.31312	-0.00061
9	6	0	-1.78764	-0.82465	0.000288
10	1	0	-2.77014	-0.35698	0.00058
11	1	0	-1.71439	-1.46585	0.879191
12	1	0	-1.71493	-1.46581	-0.8787
13	1	0	2.770139	0.356979	0.000542
14	6	0	1.787643	0.82465	0.000289
15	1	0	1.714912	1.465829	-0.87868
16	1	0	1.714414	1.465833	0.879207

Table S.1.2: Optimized parameters of pre-reactive complex RC1a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.150511	0.603651	0.513621
2	6	0	1.254378	-0.19398	-0.05058
3	6	0	-0.62489	0.115499	1.528788
4	1	0	-1.40543	0.722741	1.963836
5	1	0	-0.48779	-0.87517	1.933458
6	6	0	2.113694	0.348913	-0.93707
7	1	0	2.929251	-0.23451	-1.34136
8	1	0	2.028998	1.368738	-1.28059
9	6	0	-0.0487	2.019147	0.046954
10	1	0	-0.94619	2.443679	0.490224
11	1	0	-0.14999	2.06042	-1.03558
12	1	0	0.805075	2.634864	0.332262
13	1	0	2.239721	-2.09356	-0.13357
14	6	0	1.414595	-1.62236	0.396273
15	1	0	1.622493	-1.68123	1.465542
16	1	0	0.507544	-2.19223	0.197977
17	17	0	-1.9236	-0.57523	-0.68119

Table S.1.3: Optimized parameters of transition state TS1a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.215759	0.597182	0.465418
2	6	0	1.315749	-0.26955	-0.03158
3	6	0	-0.70242	0.118539	1.331789
4	1	0	-1.44924	0.77283	1.755077
5	1	0	-0.65014	-0.88209	1.729331
6	6	0	2.303473	0.251133	-0.71679
7	1	0	3.116443	-0.36569	-1.07234
8	1	0	2.359734	1.300736	-0.96045
9	6	0	0.141013	2.021966	0.012237
10	1	0	-0.75611	2.497333	0.397123
11	1	0	0.121831	2.068941	-1.07446
12	1	0	1.012834	2.574871	0.362997
13	1	0	2.082656	-2.25739	-0.19356
14	6	0	1.255245	-1.73843	0.284075
15	1	0	1.319844	-1.9148	1.35802
16	1	0	0.317616	-2.16037	-0.07389
17	17	0	-2.03814	-0.44232	-0.60581

Table S.1.4: Optimized parameters of transition state TS2a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-0.03307	0.539296	0.418076
2	6	0	1.231166	-0.11942	-0.05416
3	6	0	-0.59939	0.116924	1.591282
4	1	0	-1.41562	0.667652	2.03208
5	1	0	-0.29992	-0.79939	2.071514
6	6	0	2.150144	0.60029	-0.63452
7	1	0	3.088183	0.15628	-0.93804
8	1	0	2.032128	1.653323	-0.83945
9	6	0	-0.37467	1.905626	-0.1051
10	1	0	-1.38369	2.177568	0.188752
11	1	0	-0.30278	1.932287	-1.18759
12	1	0	0.324326	2.62986	0.316049
13	1	0	2.325902	-1.94144	-0.24606
14	6	0	1.408431	-1.58601	0.217161
15	1	0	1.47412	-1.78983	1.286227
16	1	0	0.562313	-2.14121	-0.18153
17	17	0	-1.7118	-0.66385	-0.65285

Table S.1.5: Optimized parameters of transition state TS1.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-0.46484	0.21545	-5.9E-05
2	6	0	-1.95273	-0.0831	0.000042
3	6	0	0.378686	-0.75935	0.000027
4	1	0	1.880916	-0.4257	0.000098
5	1	0	0.340808	-1.83655	0.00014
6	6	0	-2.82231	0.882494	0.000297
7	1	0	-3.88233	0.66918	0.000374
8	1	0	-2.54567	1.925478	0.000438
9	6	0	-0.03148	1.657597	-0.00027
10	1	0	1.050613	1.736491	-0.00036
11	1	0	-0.42361	2.163004	0.881101
12	1	0	-0.42376	2.16278	-0.88169
13	1	0	-3.44077	-1.62058	-0.00019
14	6	0	-2.35737	-1.52922	-0.00016
15	1	0	-1.9656	-2.03933	-0.88034
16	1	0	-1.96564	-2.03957	0.879904
17	17	0	3.227953	-0.17638	0.000071

Table S.1.6: Optimized parameters of transition state TS2.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.910766	0.767251	-0.1596
2	6	0	0.945789	-0.72625	-0.04287
3	6	0	0.751188	1.335564	-1.32924
4	1	0	0.737589	2.412547	-1.43023
5	1	0	0.619439	0.752596	-2.22963
6	6	0	-0.13696	-1.42334	-0.00111
7	1	0	-0.38542	-2.47119	0.08424
8	1	0	-1.47035	-0.67468	-0.00457
9	6	0	1.073228	1.520566	1.130532
10	1	0	1.098344	2.593214	0.948518
11	1	0	1.992034	1.234838	1.644276
12	1	0	0.240432	1.295959	1.797126
13	1	0	2.249321	-2.44208	0.147546
14	6	0	2.313502	-1.36197	0.036029
15	1	0	2.868813	-1.12489	-0.87105
16	1	0	2.866166	-0.95369	0.882086
17	17	0	-2.70361	-0.07609	0.072305

Table S.1.7: Optimized parameters of transition state TS3.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-0.4694	-0.18187	-0.10895
2	6	0	-1.89314	0.197076	0.025122
3	6	0	-0.0736	-1.46867	-0.18974
4	1	0	0.969277	-1.73056	-0.28284
5	1	0	-0.78401	-2.2801	-0.1509
6	6	0	-2.28234	1.487766	0.026676
7	1	0	-3.32668	1.749644	0.122968
8	1	0	-1.58609	2.307803	-0.07343
9	6	0	0.517657	0.933578	-0.17179
10	1	0	1.811725	0.402392	-0.02012
11	1	0	0.52561	1.620983	0.669033
12	1	0	0.646618	1.428931	-1.13046
13	1	0	-3.90797	-0.48828	0.264903
14	6	0	-2.90953	-0.90603	0.153647
15	1	0	-2.90597	-1.54894	-0.72695
16	1	0	-2.70096	-1.53342	1.020373
17	17	0	3.171791	-0.01762	0.111623

Table S.1.8: Optimized parameters of transition state TS4.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-0.61834	0.797934	-0.08762
2	6	0	-1.39382	-0.47943	-0.11118
3	6	0	-0.83689	1.762839	-0.96672
4	1	0	-0.26656	2.68192	-0.94898
5	1	0	-1.59566	1.66586	-1.72961
6	6	0	-1.06373	-1.44228	-0.94017
7	1	0	-1.60664	-2.37833	-0.9563
8	1	0	-0.23226	-1.34037	-1.62293
9	6	0	0.416768	0.929661	0.93597
10	1	0	0.819339	1.928674	1.078454
11	1	0	1.417482	0.283291	0.48233
12	1	0	0.247387	0.395046	1.866509
13	1	0	-3.01654	-1.54138	0.813624
14	6	0	-2.5275	-0.57073	0.872969
15	1	0	-2.1719	-0.42624	1.894432
16	1	0	-3.26496	0.208421	0.676388
17	17	0	2.694786	-0.43911	0.013326

Table S.1.9: Optimized parameters of product complex PC1.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-0.65579	0.677732	0.221382
2	6	0	-1.4141	-0.59779	0.006443
3	6	0	-0.11998	0.957324	1.397724
4	1	0	0.421289	1.880179	1.563583
5	1	0	-0.21984	0.280393	2.234433
6	6	0	-0.75683	-1.70258	-0.09377
7	1	0	-0.98434	-2.74221	-0.26511
8	1	0	1.714995	-0.0668	0.285607
9	6	0	-0.55159	1.592651	-0.96727
10	1	0	0.005111	2.494875	-0.7205
11	1	0	-1.54092	1.883745	-1.3216
12	1	0	-0.04955	1.080089	-1.78823
13	1	0	-3.37433	-1.46338	-0.22658
14	6	0	-2.91705	-0.48596	-0.08794
15	1	0	-3.31084	-0.0364	0.824031
16	1	0	-3.20552	0.151752	-0.92393
17	17	0	2.884468	-0.35944	-0.1483

Table S.1.10: Optimized parameters of product complex PC3.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.659063	-0.10745	0.142377
2	6	0	2.099056	0.164371	-0.03953
3	6	0	0.173038	-1.36486	0.227324
4	1	0	-0.88333	-1.54991	0.358095
5	1	0	0.814333	-2.23112	0.162349
6	6	0	2.567036	1.427782	-0.08759
7	1	0	3.62174	1.625272	-0.21943
8	1	0	1.916076	2.285095	0.006527
9	6	0	-0.26676	1.046862	0.237768
10	1	0	-2.40512	0.344938	-0.02401
11	1	0	-0.44359	1.666642	-0.63067
12	1	0	-0.50348	1.477458	1.200959
13	1	0	4.059183	-0.65939	-0.3077
14	6	0	3.03702	-1.00574	-0.16927
15	1	0	3.007682	-1.63392	0.721551
16	1	0	2.76922	-1.63154	-1.02102
17	17	0	-3.62138	-0.03879	-0.1243

Table S.1.11: Optimized parameters of product P1a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.286833	0.535461	0.349669
2	6	0	1.372119	-0.2836	-0.00348
3	6	0	-0.97613	-0.05014	0.861706
4	1	0	-1.46766	0.61718	1.565408
5	1	0	-0.83914	-1.01888	1.329648
6	6	0	2.521839	0.240096	-0.52024
7	1	0	3.35176	-0.3967	-0.78614
8	1	0	2.64817	1.297906	-0.68674
9	6	0	0.301075	2.01533	0.100991
10	1	0	-0.59242	2.48473	0.507785
11	1	0	0.334904	2.238896	-0.96728
12	1	0	1.168883	2.489327	0.561329
13	1	0	2.159041	-2.27195	-0.21265
14	6	0	1.275561	-1.78095	0.188706
15	1	0	1.199754	-2.04562	1.243752
16	1	0	0.403088	-2.18807	-0.32127
17	17	0	-2.17966	-0.30965	-0.47635

Table S.1.12: Optimized parameters of product P2a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-0.33058	0.313595	0.300247
2	6	0	1.118901	0.062953	-0.06242
3	6	0	-0.61237	-0.03404	1.711062
4	1	0	-1.46306	0.413492	2.20199
5	1	0	-0.16608	-0.90336	2.164226
6	6	0	1.887097	1.020257	-0.60677
7	1	0	2.922479	0.817399	-0.84369
8	1	0	1.524981	2.011482	-0.82929
9	6	0	-0.8324	1.712645	-0.02337
10	1	0	-1.88898	1.785859	0.22463
11	1	0	-0.70935	1.937786	-1.07956
12	1	0	-0.2824	2.443069	0.569063
13	1	0	2.670448	-1.40314	-0.21581
14	6	0	1.687067	-1.29856	0.23835
15	1	0	1.799562	-1.45763	1.311155
16	1	0	1.042872	-2.08599	-0.14903
17	17	0	-1.3504	-0.83647	-0.74684

Table S.1.13: Optimized parameters of product P1.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.714325	0.361393	-1.4E-05
2	6	0	-0.65058	-0.28505	-7E-06
3	6	0	0.8459	1.64866	-6.8E-05
4	1	0	0.198542	2.508505	-0.00011
5	6	0	-0.78812	-1.58102	-5.9E-05
6	1	0	-1.76977	-2.03439	-5.5E-05
7	1	0	0.051213	-2.2596	-0.00011
8	6	0	1.923712	-0.53824	0.000058
9	1	0	2.834759	0.053903	0.000104
10	1	0	1.922447	-1.18032	-0.88059
11	1	0	1.922346	-1.18031	0.880713
12	1	0	-2.76427	0.06956	0.000093
13	6	0	-1.83684	0.637347	0.00006
14	1	0	-1.82279	1.282032	0.879054
15	1	0	-1.82287	1.282052	-0.87892

Table S.1.14: Optimized parameters of product P3.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.752571	-0.16962	0.00195
2	6	0	-0.67327	0.214519	-0.0036
3	6	0	1.141482	-1.46341	-0.00589
4	1	0	2.19007	-1.72465	0.003946
5	1	0	0.433028	-2.27862	-0.01918
6	6	0	-1.04149	1.511084	-0.02038
7	1	0	-2.08516	1.793881	-0.02429
8	1	0	-0.31332	2.309167	-0.03329
9	6	0	1.779835	0.897617	0.0178
10	1	0	1.986962	1.448919	0.922032
11	1	0	2.238319	1.239308	-0.89703
12	1	0	-2.71239	-0.44873	0.013411
13	6	0	-1.71142	-0.87567	0.010891
14	1	0	-1.61758	-1.51964	-0.86419
15	1	0	-1.60615	-1.50679	0.893903

Table S.1.15: Optimized parameters of product HCl.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	1	0	0.000000	0.000000	-1.198748
2	17	0	0.000000	0.000000	0.070515

Table S.2: Vibrational frequencies for the reactant, pre-reactive complexes, transition states, product complexes and products for the reaction of 2,3-dimethyl-1,3-butadiene + Cl at MP2/6-31 G (d,p) level of theory.

Table S.2.1: Normal mode frequencies of R1, RC1a, TS1a, TS2a, TS1 and TS2 (cm^{-1}).

R1	RC1a	TS1a	TS2a	TS1	TS2
73.6	71.5	-383.4	-421.9	-342.5	-414.5
225.9	98.1	57.9	67.7	30.6	32.3
237.2	157.1	105.7	171.8	58.1	70.3
304.2	220.7	174.2	214.6	89.9	85.4
323.5	227.0	210.1	264.9	245.8	200.0
406.3	267.2	251.4	298.2	257.5	204.5
473.4	307.2	317.2	304.2	290.3	237.2
493.5	407.1	334.8	316.8	372.0	246.6
529.1	434.5	415.5	402.3	399.4	317.2
685.8	471.7	479.4	464.9	466.3	438.8
752.7	505.8	497.1	472.7	485.3	529.2
800.6	618.4	564.9	560.0	523.2	571.4
899.1	681.5	757.6	659.6	587.4	625.1
901.0	764.4	784.7	733.3	744.2	747.0
952.7	801.4	891.6	856.8	807.7	762.6
1009.0	917.0	965.1	946.1	829.8	823.6
1037.3	949.3	992.7	970.8	900.3	855.3
1070.1	1008.2	1020.7	1014.5	963.6	987.2
1091.3	1029.2	1050.4	1046.7	1006.5	1009.1
1094.2	1038.7	1084.3	1083.2	1044.9	1049.5
1235.4	1073.8	1088.4	1088.5	1088.9	1051.2
1409.0	1093.5	1100.0	1110.1	1109.9	1058.1
1456.1	1218.8	1132.9	1143.2	1112.2	1105.6
1460.5	1238.5	1254.6	1250.5	1137.9	1130.0
1478.5	1413.4	1407.0	1403.3	1202.8	1185.5
1500.0	1454.5	1453.0	1450.4	1348.3	1286.8
1537.3	1462.2	1457.2	1462.1	1362.4	1373.9
1537.4	1468.3	1497.1	1481.0	1457.5	1444.6
1555.9	1505.0	1518.5	1524.4	1461.5	1457.0
1569.2	1532.5	1528.8	1532.3	1520.3	1515.7
1690.1	1537.9	1535.8	1536.8	1534.6	1527.5
1729.8	1551.9	1549.6	1551.0	1540.8	1536.9
3122.8	1569.3	1568.7	1566.7	1553.5	1540.7
3123.0	1646.5	1717.2	1609.3	1564.2	1551.4

3206.6	1896.8	1890.0	2491.4	1868.4	2037.0
3206.9	3124.8	3132.0	3134.6	2082.6	2759.8
3229.6	3131.8	3137.4	3138.1	3128.2	3124.1
3230.2	3212.2	3222.8	3223.3	3141.7	3129.0
3246.0	3223.0	3229.8	3239.4	3213.7	3211.1
3246.7	3235.5	3247.0	3252.8	3229.5	3223.2
3345.3	3245.0	3262.0	3275.8	3242.1	3235.9
3346.1	3248.9	3266.0	3279.2	3265.2	3242.7
	3264.1	3274.2	3283.0	3270.1	3299.9
	3349.3	3361.8	3355.3	3344.4	3321.7
	3364.6	3380.1	3397.2	3356.2	3344.1

Table S.2.2: Normal mode frequencies of TS3, TS4, PC1, PC3, P1a and P2a (cm^{-1}).

TS3	TS4	PC1	PC3	P1a	P2a
-1117.7	-1445.4	29.8	21.9	52.6	74.0
34.3	42.6	40.2	47.5	63.7	165.6
70.8	55.1	65.2	73.5	120.5	215.8
106.9	97.8	104.8	82.8	172.3	261.2
232.4	204.2	188.8	229.9	207.8	316.0
247.7	229.4	197.8	265.6	298.2	343.4
308.8	252.7	227.7	294.9	378.7	352.6
362.8	339.4	251.4	318.9	405.9	378.1
412.6	417.4	318.2	359.1	464.4	401.4
472.6	459.4	350.2	377.7	506.6	452.7
489.4	477.1	398.9	396.6	548.2	476.7
522.0	592.4	434.3	455.6	641.5	519.7
550.1	625.7	564.3	494.0	718.3	644.7
683.1	764.3	612.8	518.6	759.7	703.0
771.5	779.5	750.6	653.6	858.3	744.1
794.1	837.0	812.6	683.4	932.6	919.0
899.0	974.5	859.3	775.3	960.6	944.2
917.1	993.1	926.2	791.0	1010.8	951.4
941.9	1024.5	984.7	899.0	1043.9	1000.5
955.0	1047.1	1017.5	905.7	1052.6	1032.6
963.2	1058.9	1049.9	965.5	1097.6	1054.4
1009.3	1065.0	1059.4	1012.4	1170.0	1099.9
1052.8	1080.6	1107.1	1051.4	1261.7	1196.3
1084.1	1126.9	1119.2	1064.0	1304.7	1233.9
1093.6	1203.5	1189.3	1093.9	1338.5	1321.3
1170.2	1242.4	1363.1	1222.4	1357.6	1394.7
1258.0	1293.9	1446.6	1413.9	1448.0	1453.7
1405.6	1384.3	1456.7	1457.8	1459.2	1459.0
1457.4	1456.3	1512.0	1466.6	1498.9	1511.8
1475.7	1498.8	1528.1	1502.0	1537.7	1524.3
1503.5	1520.1	1537.9	1523.2	1543.9	1543.5
1513.9	1526.6	1546.3	1536.8	1546.9	1551.8
1536.1	1535.8	1551.6	1561.0	1552.5	1554.3
1561.7	1552.5	1961.1	1648.7	1567.0	1564.1
1667.2	1750.5	2484.1	1810.1	1614.2	2037.5
1764.1	2788.1	2966.2	2961.5	3114.8	3131.4
3124.9	3120.0	3123.7	3123.5	3128.7	3137.1
3186.1	3185.4	3126.0	3208.0	3183.7	3217.3

3210.3	3203.5	3211.1	3231.2	3192.9	3236.2
3232.6	3231.9	3215.8	3235.7	3214.5	3237.8
3244.3	3245.7	3234.1	3242.0	3226.9	3251.5
3262.6	3285.3	3237.6	3252.7	3236.4	3257.6
3284.6	3304.4	3260.4	3340.2	3264.0	3264.9
3340.9	3344.7	3340.3	3347.1	3265.5	3353.5
3364.4	3353.3	3347.7	3352.3	3370.0	3389.6

Table S.2.3: Normal mode frequencies of products P1, P2, P3 and P4 (cm^{-1}).

P1	P2	P3	P4
47.6	63.8	81.8	43.5
245.1	197.3	216.3	215.8
258.9	200.6	229.9	238.0
297.8	225.5	279.2	248.1
360.2	249.4	321.8	342.6
395.3	317.2	343.3	460.9
457.1	433.1	416.2	574.0
487.4	564.1	474.6	590.4
579.8	612.4	510.6	598.6
760.7	754.0	528.1	642.8
811.1	811.7	683.4	775.5
905.9	853.9	771.9	785.5
906.5	932.3	792.1	807.1
989.8	985.8	896.5	822.4
1039.4	1032.1	899.3	995.2
1081.6	1051.2	966.4	1002.1
1084.0	1058.1	1012.4	1028.5
1104.5	1108.3	1050.4	1074.6
1132.5	1126.0	1059.9	1090.2
1200.7	1189.9	1093.7	1122.1
1360.3	1364.6	1224.1	1269.1
1450.4	1445.8	1416.0	1278.2
1458.8	1456.0	1456.3	1448.5
1518.2	1514.4	1463.6	1472.5
1534.6	1529.1	1497.5	1519.5
1538.7	1538.9	1524.1	1527.4
1552.9	1546.5	1537.0	1536.4
1563.2	1553.9	1560.8	1552.1
1783.9	1962.9	1646.7	1602.6
2016.6	2728.6	1808.5	2707.8
3127.5	3121.5	3122.1	3119.0
3130.2	3124.0	3205.9	3204.3
3212.5	3207.5	3229.1	3229.2
3216.6	3212.8	3240.3	3248.0
3240.0	3231.0	3246.9	3254.9
3248.3	3234.0	3259.0	3284.4
3260.3	3286.6	3340.2	3337.3
3351.4	3338.5	3346.8	3365.5
3361.1	3341.2	3372.8	3367.1

Table S.3: Optimized geometries of the reactant, pre-reactive complexes, transition states, product complexes and products for the reaction of 2-methyl-1,3-butadiene (isoprene) + Cl at MP2/6-311+G(2df,2p) level of theory.

Table S.3.1: Optimized parameters of 2-methyl-1,3-butadiene (isoprene).

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.825737	-0.69049	-1.3E-05
2	6	0	-0.514547	-0.09589	0.00001
3	6	0	1.982993	-0.00049	0.000013
4	1	0	2.933875	-0.51472	-2.3E-05
5	1	0	2.009052	1.080565	0.000059
6	6	0	-1.600946	-0.89774	0.000015
7	1	0	-2.603954	-0.492	-2.3E-05
8	1	0	-1.501951	-1.97594	0.000023
9	1	0	-1.689201	1.699961	-4.8E-05
10	6	0	-0.641686	1.403053	-1.1E-05
11	1	0	-0.161347	1.83377	0.880233
12	1	0	-0.161297	1.833763	-0.88023
13	1	0	0.865519	-1.77606	-8.3E-05

Table S.3.2: Optimized parameters of pre-reactive complex Rc1a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.150626	0.368883	-0.93318
2	6	0	1.256415	-0.08114	-0.09215
3	6	0	-0.63697	1.454385	-0.67676
4	1	0	-1.40566	1.752853	-1.37424
5	1	0	-0.50987	2.05369	0.213224
6	6	0	2.04712	-1.07738	-0.54386
7	1	0	2.890212	-1.43448	0.032368
8	1	0	1.855266	-1.55853	-1.49444
9	1	0	2.343184	0.150505	1.73931
10	6	0	1.495659	0.600716	1.225693
11	1	0	1.706365	1.662222	1.083192
12	1	0	0.616918	0.515301	1.866155
13	1	0	-0.0101	-0.17732	-1.85747
14	17	0	-1.96256	-0.621	0.34785

Table S.3.3: Optimized parameters of transition state Ts1a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	1.30807	-0.76912	0.334694
2	6	0	0.435884	0.417121	0.385891
3	6	0	2.437292	-0.8259	-0.32835
4	1	0	3.046255	-1.7178	-0.30952
5	1	0	2.806502	0.000807	-0.91855
6	6	0	-0.56875	0.446098	1.290709
7	1	0	-1.16917	1.332934	1.428645
8	1	0	-0.70355	-0.36049	1.997004
9	1	0	-0.05968	2.337637	-0.40561
10	6	0	0.69806	1.568837	-0.52919
11	1	0	1.678867	1.996509	-0.31447
12	1	0	0.692327	1.233055	-1.56538
13	1	0	0.970191	-1.62369	0.908848
14	17	0	-1.94853	-0.4836	-0.4555

Table S.3.4: Optimized parameters of transition state Ts2a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	1.196981	-0.69811	0.385451
2	6	0	0.241376	0.439404	0.277317
3	6	0	2.358411	-0.7253	-0.2054
4	1	0	3.036836	-1.5522	-0.0508
5	1	0	2.693851	0.061512	-0.86668
6	6	0	-0.45877	0.777751	1.403718
7	1	0	-1.05692	1.675735	1.436592
8	1	0	-0.47207	0.127099	2.264715
9	1	0	-0.43816	2.107011	-0.87377
10	6	0	0.404913	1.422131	-0.84335
11	1	0	1.319956	1.994082	-0.67494
12	1	0	0.48072	0.910485	-1.79898
13	1	0	0.885105	-1.50767	1.034268
14	17	0	-1.7004	-0.65361	-0.38687

Table S.3.5: Optimized parameters of transition state Ts3a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-0.0208	0.763652	-0.44109
2	6	0	1.199756	-0.02006	-0.10681
3	6	0	-0.65214	1.573039	0.451229
4	1	0	-1.43202	2.243602	0.127814
5	1	0	-0.43585	1.526148	1.506831
6	6	0	2.084049	-0.17853	-1.05492
7	1	0	3.02115	-0.68792	-0.87362
8	1	0	1.917568	0.19396	-2.05736
9	1	0	2.288859	-1.09365	1.382808
10	6	0	1.360796	-0.53288	1.293164
11	1	0	1.385959	0.285177	2.01415
12	1	0	0.522442	-1.18097	1.547122
13	1	0	-0.21372	0.906389	-1.49649
14	17	0	-1.81673	-0.69553	-0.17652

Table S.3.6: Optimized parameters of transition state Ts4a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.201097	0.776653	0.61984
2	6	0	1.329133	0.087055	-0.02244
3	6	0	-0.72614	0.185416	1.396407
4	1	0	-1.47754	0.77545	1.897824
5	1	0	-0.67256	-0.86269	1.649039
6	6	0	2.218376	0.820078	-0.6561
7	1	0	3.079119	0.376601	-1.13709
8	1	0	2.120719	1.895286	-0.72443
9	1	0	2.272165	-1.78103	-0.4623
10	6	0	1.407816	-1.40824	0.082753
11	1	0	1.4958	-1.72222	1.123805
12	1	0	0.505488	-1.85652	-0.33296
13	1	0	0.126984	1.843132	0.443492
14	17	0	-2.00188	-0.08434	-0.64589

Table S.3.7: Optimized parameters of transition state Ts1.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-1.01279	1.027324	0.454787
2	6	0	-1.1768	-0.40024	0.054363
3	6	0	-0.6331	1.968021	-0.36981
4	1	0	-0.53351	2.992942	-0.04013
5	1	0	-0.40124	1.752141	-1.40435
6	6	0	-0.16471	-1.16068	-0.19857
7	1	0	-0.02673	-2.19485	-0.48162
8	1	0	1.234941	-0.59017	-0.06367
9	1	0	-2.63666	-1.96354	-0.27482
10	6	0	-2.5984	-0.90808	-0.01223
11	1	0	-3.0796	-0.76526	0.956412
12	1	0	-3.15302	-0.32921	-0.75111
13	1	0	-1.24398	1.254487	1.490736
14	17	0	2.550269	-0.19498	0.058668

Table S.3.8: Optimized parameters of transition state Ts2.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	2.146947	-0.68192	0.00002
2	6	0	0.812529	-0.09868	-5.8E-05
3	6	0	3.308811	0.01645	0.00007
4	1	0	4.253041	-0.49671	0.000138
5	1	0	3.338471	1.090471	0.000032
6	6	0	-0.24774	-0.94122	-0.00011
7	1	0	-1.52954	-0.44279	-2.3E-05
8	1	0	-0.30477	-2.01255	-3.7E-05
9	1	0	-0.40044	1.681809	-0.00036
10	6	0	0.643536	1.402312	-4.4E-05
11	1	0	1.111286	1.837171	0.877406
12	1	0	1.111851	1.837256	-0.87715
13	1	0	2.197901	-1.75829	0.000026
14	17	0	-2.92719	0.004821	0.000042

Table S.3.9: Optimized parameters of transition state Ts3.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-0.23094	0.789378	0.12643
2	6	0	-1.28999	-0.16698	-0.08838
3	6	0	-0.06467	2.030064	0.438635
4	1	0	0.916791	2.480039	0.503199
5	1	0	-0.9238	2.659067	0.652163
6	6	0	-1.94812	-0.15303	-1.24058
7	1	0	-2.746	-0.85786	-1.43432
8	1	0	-1.70755	0.559397	-2.01616
9	1	0	-2.33469	-1.84327	0.747713
10	6	0	-1.52362	-1.16679	1.011711
11	1	0	-0.61912	-1.75133	1.183351
12	1	0	-1.76989	-0.65568	1.942388
13	1	0	0.979353	0.125774	-0.02786
14	17	0	2.267587	-0.51247	-0.17867

Table S.3.10: Optimized parameters of transition state Ts7.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	1.64001	-0.67205	0.49906
2	6	0	1.025212	0.630098	0.121092
3	6	0	1.498806	-1.76622	-0.21003
4	1	0	1.948406	-2.69888	0.102607
5	1	0	0.916305	-1.7736	-1.12204
6	6	0	1.500159	1.37068	-0.86996
7	1	0	1.036204	2.310838	-1.13847
8	1	0	2.368518	1.063099	-1.43471
9	1	0	-0.43511	2.10053	0.762545
10	6	0	-0.14176	1.062055	0.892943
11	1	0	-1.12379	0.419453	0.388465
12	1	0	-0.19033	0.716055	1.922474
13	1	0	2.20644	-0.68543	1.425389
14	17	0	-2.34478	-0.30585	-0.20617

Table S.3.11: Optimized parameters of transition state Ts8.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-1.38104	-0.8166	0.20787
2	6	0	-0.83799	0.545399	-0.05318
3	6	0	-2.60147	-1.18418	-0.09443
4	1	0	-2.95229	-2.1858	0.113112
5	1	0	-3.29643	-0.50207	-0.56727
6	6	0	-1.25029	1.608017	0.620895
7	1	0	-0.82906	2.587321	0.434885
8	1	0	-2.01983	1.529662	1.375539
9	1	0	1.272476	0.183543	-0.46394
10	6	0	0.229926	0.644244	-1.04997
11	1	0	0.162204	-0.04022	-1.89168
12	1	0	0.531339	1.65298	-1.31966
13	1	0	-0.69014	-1.51851	0.665909
14	17	0	2.521585	-0.38166	0.227409

Table S.3.12: Optimized parameters of product complex Pc1.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-1.09286	1.018009	0.498106
2	6	0	-1.44833	-0.38516	0.125939
3	6	0	-0.41082	1.830617	-0.28026
4	1	0	-0.16875	2.836459	0.034593
5	1	0	-0.06859	1.518536	-1.25843
6	6	0	-0.53527	-1.29261	0.2189
7	1	0	-0.44236	-2.35946	0.086947
8	1	0	1.591477	-0.44308	0.100834
9	1	0	-3.04814	-1.69116	-0.50534
10	6	0	-2.87377	-0.63672	-0.29819
11	1	0	-3.55326	-0.31334	0.492246
12	1	0	-3.09878	-0.05113	-1.19027
13	1	0	-1.43374	1.350952	1.473811
14	17	0	2.846378	-0.23839	-0.04832

Table S.3.13: Optimized parameters of product complex Pc2.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-1.09286	1.018009	0.498106
2	6	0	-1.44833	-0.38516	0.125939
3	6	0	-0.41082	1.830617	-0.28026
4	1	0	-0.16875	2.836459	0.034593
5	1	0	-0.06859	1.518536	-1.25843
6	6	0	-0.53527	-1.29261	0.2189
7	1	0	-0.44236	-2.35946	0.086947
8	1	0	1.591477	-0.44308	0.100834
9	1	0	-3.04814	-1.69116	-0.50534
10	6	0	-2.87377	-0.63672	-0.29819
11	1	0	-3.55326	-0.31334	0.492246
12	1	0	-3.09878	-0.05113	-1.19027
13	1	0	-1.43374	1.350952	1.473811
14	17	0	2.846378	-0.23839	-0.04832

Table S.3.14: Optimized parameters of product complex Pc3.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-1.09286	1.018009	0.498106
2	6	0	-1.44833	-0.38516	0.125939
3	6	0	-0.41082	1.830617	-0.28026
4	1	0	-0.16875	2.836459	0.034593
5	1	0	-0.06859	1.518536	-1.25843
6	6	0	-0.53527	-1.29261	0.2189
7	1	0	-0.44236	-2.35946	0.086947
8	1	0	1.591477	-0.44308	0.100834
9	1	0	-3.04814	-1.69116	-0.50534
10	6	0	-2.87377	-0.63672	-0.29819
11	1	0	-3.55326	-0.31334	0.492246
12	1	0	-3.09878	-0.05113	-1.19027
13	1	0	-1.43374	1.350952	1.473811
14	17	0	2.846378	-0.23839	-0.04832

Table S.3.15: Optimized parameters of product complex Pc7.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	Coordinates X	(Angstroms) Y	Z
1	6	0	-1.81559	0.730887	0.220243
2	6	0	-1.16872	-0.60743	0.04891
3	6	0	-1.23376	1.871969	-0.06484
4	1	0	-1.74852	2.812309	0.078436
5	1	0	-0.22277	1.915493	-0.44927
6	6	0	-1.18136	-1.20517	-1.19761
7	1	0	-0.74626	-2.18449	-1.34246
8	1	0	-1.61764	-0.71106	-2.0514
9	1	0	-0.20221	-2.22531	1.076712
10	6	0	-0.62364	-1.23192	1.155977
11	1	0	1.381059	-0.26109	0.295756
12	1	0	-0.63853	-0.764	2.128867
13	1	0	-2.83125	0.718058	0.602788
14	17	0	2.515562	0.197061	-0.07738

Table S.3.16: Optimized parameters of product complex Pc8.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	1.326749	-0.84289	-0.13432
2	6	0	0.90672	0.582408	0.041398
3	6	0	2.559487	-1.26437	0.021513
4	1	0	2.817856	-2.3051	-0.119
5	1	0	3.358021	-0.58647	0.295192
6	6	0	0.902341	1.4186	-1.06298
7	1	0	0.580288	2.446879	-0.97314
8	1	0	1.21809	1.067288	-2.03279
9	1	0	-1.56883	0.154085	0.325736
10	6	0	0.495365	1.009884	1.288023
11	1	0	0.515363	0.349905	2.142074
12	1	0	0.183271	2.034044	1.443894
13	1	0	0.544351	-1.54238	-0.41259
14	17	0	-2.63485	-0.41412	-0.0936

Table S.3.17: Optimized parameters of product P1a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	1.506854	-0.76828	0.101786
2	6	0	0.503909	0.161994	0.340734
3	6	0	2.756961	-0.5003	-0.40168
4	1	0	3.473677	-1.29359	-0.54649
5	1	0	3.06456	0.497738	-0.67397
6	6	0	-0.81111	-0.3021	0.852159
7	1	0	-1.17351	0.327197	1.663815
8	1	0	-0.77184	-1.33686	1.182976
9	1	0	-0.03367	2.212977	0.632464
10	6	0	0.648568	1.619036	0.024176
11	1	0	1.663094	1.968677	0.210184
12	1	0	0.409532	1.820524	-1.02333
13	1	0	1.279027	-1.80309	0.338174
14	17	0	-2.0907	-0.21504	-0.42864

Table S.3.18: Optimized parameters of product P2a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	1.138522	-0.51996	0.520473
2	6	0	-0.02809	0.34925	0.124135
3	6	0	2.311355	-0.57786	-0.08308
4	1	0	3.085563	-1.22034	0.296218
5	1	0	2.548508	-0.00448	-0.96039
6	6	0	-0.47322	1.19327	1.266333
7	1	0	-1.12423	2.028383	1.081713
8	1	0	-0.39534	0.817235	2.269836
9	1	0	-0.73519	1.710701	-1.38038
10	6	0	0.169765	1.164197	-1.14729
11	1	0	0.973277	1.878235	-0.99851
12	1	0	0.410403	0.527641	-1.98839
13	1	0	0.963588	-1.1258	1.393946
14	17	0	-1.43745	-0.83912	-0.22338

Table S.3.19: Optimized parameters of product P3a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.317986	0.396804	0.546528
2	6	0	-1.05937	-0.05042	0.117604
3	6	0	0.704127	1.767819	0.131631
4	1	0	1.478213	2.275819	0.676356
5	1	0	0.439926	2.140925	-0.83935
6	6	0	-1.91889	-0.45543	1.039675
7	1	0	-2.91566	-0.76473	0.779045
8	1	0	-1.65813	-0.49434	2.082896
9	1	0	-2.39326	-0.41475	-1.51714
10	6	0	-1.40661	-0.00132	-1.34901
11	1	0	-1.40508	1.018023	-1.72294
12	1	0	-0.69285	-0.56867	-1.93588
13	1	0	0.424801	0.281777	1.612306
14	17	0	1.582267	-0.78934	-0.12082

Table S.3.20: Optimized parameters of product P4a.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-0.30336	-0.83272	0.395771
2	6	0	-1.41085	-0.08108	0.008513
3	6	0	0.966068	-0.25112	0.885038
4	1	0	1.484735	-0.93357	1.55272
5	1	0	0.819697	0.699939	1.388982
6	6	0	-2.53652	-0.70989	-0.46656
7	1	0	-3.4122	-0.15322	-0.76494
8	1	0	-2.57364	-1.78622	-0.55744
9	1	0	-2.28985	1.857339	-0.29295
10	6	0	-1.38383	1.425301	0.126976
11	1	0	-1.31613	1.736895	1.170122
12	1	0	-0.52881	1.842588	-0.40478
13	1	0	-0.33459	-1.90721	0.262715
14	17	0	2.127161	0.078856	-0.4737

Table S.3.21: Optimized parameters of product P1.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	-0.91464	-0.19382	0.470165
2	6	0	0.48147	0.184102	0.097433
3	6	0	-1.94922	-0.0643	-0.32654
4	1	0	-2.94168	-0.35438	-0.0092
5	1	0	-1.84082	0.340096	-1.32429
6	6	0	0.808595	1.43264	0.04265
7	1	0	1.701726	2.002631	-0.16011
8	1	0	2.433344	-0.60133	-0.39386
9	6	0	1.431131	-0.96055	-0.16528
10	1	0	1.481486	-1.60963	0.71087
11	1	0	1.064825	-1.55869	-1.00065
12	1	0	-1.04293	-0.60718	1.466671

Table S.3.22: Optimized parameters of product P3.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.889581	0.004787	0.001146
2	6	0	-0.44896	0.098592	0.003321
3	6	0	2.171211	-0.08504	-0.00072
4	1	0	2.737417	-0.12698	-0.92521
5	1	0	2.740999	-0.11693	0.921988
6	6	0	-1.07893	1.3426	-0.00072
7	1	0	-2.15607	1.410461	0.000036
8	1	0	-0.50468	2.255826	-0.00678
9	1	0	-2.32594	-0.94406	0.072928
10	6	0	-1.26579	-1.18075	-0.00053
11	1	0	-1.10052	-1.74296	-0.91835
12	1	0	-0.99388	-1.81649	0.840379

Table S.3.23: Optimized parameters of product P7.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	6	0	0.91943	0.000472	0.491884
2	6	0	-0.52035	-4E-06	0.085407
3	6	0	1.922024	0.000029	-0.356
4	1	0	2.94789	0.000241	-0.01314
5	1	0	1.755325	-0.00076	-1.42571
6	6	0	-1.1683	1.209956	-0.07387
7	1	0	-2.21578	1.242084	-0.33968
8	1	0	-0.64913	2.14662	0.056778
9	1	0	-2.21498	-1.24308	-0.33958
10	6	0	-1.16759	-1.21038	-0.07348
11	1	0	-0.64788	-2.14668	0.057606
12	1	0	1.11322	0.001156	1.560052

Table S.3.24: Optimized parameters of product HCl.

Cartesian Coordinates					
Center No.	Atomic No.	Atomic Type	X	Y	Z
1	1	0	0	0	-1.19945
2	17	0	0	0	0.070556

Table S.4: Vibrational frequencies for the reactant, pre-reactive complexes, transition states, product complexes and products for the reaction of 2-methyl-1,3-butadiene (isoprene) + Cl at MP2/6-311+G(2df,2p) level of theory.

Table S.4.1: Normal mode frequencies of R1, RC1a, TS1a, TS2a, TS3a and TS4a (cm^{-1}).

R1	RC1a	TS1a	TS2a	TS3a	TS4a
118.1998	72.7682	-416.668	-432.79	-428.234	-430.292
192.2848	95.4566	77.1067	94.7921	72.172	66.6562
282.8175	185.9042	106.8776	174.4058	155.1716	99.8693
355.6109	212.6992	170.7216	245.8207	217.6938	211.7294
424.3829	281.469	192.7841	282.0222	273.6442	243.0605
536.0054	393.3914	295.0563	302.4389	292.9764	289.454
623.0178	410.9867	369.7237	327.3211	423.9761	432.2009
758.1741	456.1066	429.717	416.388	471.1782	445.8101
810.2956	558.755	538.8862	501.0641	538.0351	542.1321
873.6426	660.0093	710.7653	651.0555	636.518	715.8911
888.0237	768.5991	816.7764	775.4366	807.8242	822.9266
988.24	821.7019	859.8117	799.9394	850.4354	847.0332
1008.655	907.0997	985.4149	963.5099	977.9936	981.198
1029.438	986.2765	1002.865	989.6229	1005.158	1010.085
1078.281	990.0119	1044.909	1039.838	1041.153	1043.654
1108.512	1029.042	1069.607	1075.711	1066.148	1067.936
1343.955	1078.831	1102.615	1118.448	1100.65	1082.569
1363.67	1101.441	1124.459	1121.112	1126.755	1113.893
1445.414	1191.058	1139.472	1171.671	1138.292	1128.87
1468.082	1361.536	1365.69	1361.504	1328.157	1356.63
1499.164	1387.895	1391.498	1379.763	1367.683	1376.97
1515.473	1442.495	1450.043	1442.402	1454.133	1450.956
1547.846	1468.923	1490.289	1483.41	1490.529	1485.525
1671.081	1497.997	1499.165	1509.727	1516.752	1511.089
1720.97	1514.075	1508.309	1520.143	1522.961	1514.091
3111.231	1549.847	1539.751	1541.453	1550.179	1551.4
3193.277	1633.623	1703.902	1607.676	1625.911	1694.68
3220.578	1789.423	1842.679	2416.126	2381.221	1849.68
3221.911	3113.692	3124.848	3125.48	3123.579	3121.727
3225.649	3198.806	3214.426	3224.308	3211.875	3210.948
3242.106	3225.5	3251.884	3258.535	3236.782	3237.473
3324.166	3228.075	3255.206	3260.365	3256.152	3246.085
3338.028	3240.556	3257.415	3262.899	3277.142	3268.945

	3257.917	3272.362	3294.641	3285.407	3275.503
	3329.489	3358.283	3350.506	3335.121	3345.311
	3360.005	3364.818	3382.267	3394.806	3377.622

Table S.4.2: Normal mode frequencies of TS1, TS2, TS3, TS7, TS8 and PC1 (cm^{-1}).

TS1	TS2	TS3	TS7	TS8	PC1
-496.724	-451.484	-1100.5	-1438.53	-1445.56	19.2416
66.5172	59.2509	58.4148	57.9013	55.1141	49.0336
79.2712	98.8867	87.1903	77.3132	85.3795	77.4318
120.1505	176.255	173.9595	114.7205	115.0761	123.7826
211.6629	187.2912	180.0431	269.3904	274.503	205.0665
272.5756	265.6696	209.6407	342.1742	339.7594	234.7656
311.8597	341.884	385.7605	406.4917	394.5978	292.1429
376.1489	419.0763	435.1614	442.3419	468.5003	302.8054
533.8019	505.7024	479.1356	479.1866	474.0854	333.4505
610.3545	585.8204	639.2908	617.5812	609.5599	355.2901
715.892	642.1142	689.397	734.4946	738.192	600.8234
768.8328	701.7902	794.736	806.3962	823.1351	745.799
834.9838	772.4902	818.4839	846.2472	846.5361	807.131
848.3093	833.8256	848.4111	961.8377	959.4803	832.1748
1000.539	952.7306	988.7898	1020.945	1016.721	924.3566
1037.447	956.2398	1009.654	1055.648	1061.346	1040.921
1060.395	1027.097	1048.468	1061.613	1065.815	1047.202
1104.146	1052.6	1060.189	1095.774	1093.306	1069.495
1129.086	1138.255	1066.818	1125.503	1128.28	1128.029
1148.239	1141.379	1110.821	1144.508	1156.225	1131.78
1191.363	1210.791	1132.593	1179.602	1179.999	1257.527
1282.744	1330.668	1311.604	1258.162	1259.9	1376.977
1381.142	1378.911	1444.099	1335.628	1330.843	1438.46
1438.206	1520.425	1473.791	1388.182	1386.378	1509.896
1510.538	1546.546	1486.69	1484.32	1482.763	1515.146
1514.745	1553.19	1514.751	1513.011	1513.585	1528.436
1527.362	1611.501	1540.121	1520.351	1521.443	1973.412
2026.576	1627.907	1723.363	1750.484	1754.225	2715.802
2595.883	1663.752	2111.085	2645.676	2563.556	2958.4
3116.748	3192.852	3120.736	3176.118	3178.131	3113.412

3210.757	3249.334	3212.794	3235.205	3235.365	3204.817
3233.426	3301.555	3215.346	3241.798	3242.123	3228.881
3240.982	3318.866	3231.272	3278.665	3281.983	3236.067
3300.046	3329.214	3243.792	3304.534	3290.194	3311.555
3313.882	3398.333	3319.946	3341.72	3339.087	3338.469
3344.969	3413.066	3353.068	3350.261	3349.906	3342.628

Table S.4.3: Normal mode frequencies of PC3, PC7, PC8, P1a, P2a and P3a (cm^{-1}).

PC3	**PC7**	**PC8**	**P1a**	**P2a**	**P3a**
19.2416	33.3031	34.4212	67.3431	109.9785	64.2006
49.0336	48.163	47.5476	94.9378	233.6677	175.6999
77.4318	61.2674	58.2948	143.8405	278.0825	205.6305
123.7826	97.981	93.1532	258.8687	302.1128	217.4781
205.0665	267.1219	259.5612	300.8313	323.9291	294.5604
234.7656	283.3574	277.8052	391.6508	330.5029	306.5227
292.1429	313.3506	322.3451	409.8128	369.8349	443.6873
302.8054	345.2337	344.004	556.2984	422.7037	502.809
333.4505	424.8833	424.0127	603.359	484.6339	578.8887
355.2901	564.6976	556.6242	728.1309	580.0293	618.352
600.8234	600.2163	603.7812	806.398	660.2905	700.4472
745.799	637.7679	638.5272	827.9797	770.6794	811.6341
807.131	763.1278	761.9833	950.8861	838.1274	830.6423
832.1748	808.536	804.4891	1006.529	1009.252	1015.205
924.3566	822.4251	821.7436	1019.303	1059.093	1066.897
1040.921	848.9155	848.9627	1059.453	1084.8	1089.903
1047.202	1000.754	1000.978	1081.63	1131.156	1156.582
1069.495	1084.598	1077.88	1195.475	1137.067	1166.796
1128.029	1087.727	1087.248	1240.98	1182.531	1200.23
1131.78	1117.015	1116.862	1296.334	1328.473	1343.778
1257.527	1148.189	1147.639	1352.188	1392.381	1416.648
1376.977	1262.943	1264.715	1419.452	1447.489	1465.947
1438.46	1371.813	1376.807	1460.883	1544.996	1546.855
1509.896	1445.069	1444.439	1479.399	1575.354	1581.403
1515.146	1519.883	1516.78	1519.253	1587.157	1592.965
1528.436	1523.652	1523.962	1533.455	1618.271	1610.916
1973.412	1593.245	1592.803	1536.394	1625.018	1624.743
2715.802	2631.849	2671.657	1580.021	1852.352	1857.48
2958.4	2978.61	2986.621	3106.997	3201.118	3192.502

3113.412	3237.596	3236.173	3156.082	3274.459	3251.96
3204.817	3238.985	3239.12	3188.965	3295.261	3276.677
3228.881	3248.35	3248.513	3219.033	3305.44	3310.467
3236.067	3302.044	3305.743	3233.072	3323.501	3316.457
3311.555	3337.707	3337.277	3237.711	3342.038	3318.678
3338.469	3356.695	3358.218	3263.6	3409.663	3394.803
3342.628	3367.15	3366.764	3369.79	3416.618	3427.217

Table S.4.4: Normal mode frequencies of P4a, P1, P3 and P8 (cm^{-1}).

P4a	**P1**	**P3**	**P8**
62.18	111.1929	63.3131	62.9768
106.7904	207.8868	278.7799	278.7281
160.199	263.9536	342.3366	342.3345
279.5807	299.1963	422.5878	422.559
336.0683	358.9379	560.4647	560.4689
435.9642	596.2304	588.6801	588.6558
479.2862	752.5775	633.8674	633.8623
541.0764	822.2183	760.9285	760.8725
604.2917	837.1505	790.0108	790.0832
680.7015	921.1204	805.9413	805.9934
786.2199	1045.945	849.2066	849.191
830.8621	1052.32	1001.303	1001.299
834.4717	1073.967	1070.325	1070.235
945.4353	1128.177	1087.619	1087.623
1020.408	1146.309	1115.525	1115.514
1038.688	1257.264	1144.894	1144.81
1085.143	1379.948	1265.211	1265.256
1167.268	1438.839	1370.457	1370.453
1239.403	1507.798	1444.078	1444.056
1278.754	1516.146	1516.265	1516.265
1347.51	1531.13	1524.77	1524.811
1430.759	1957.699	1594.12	1594.148
1463.514	2613.568	2654.425	2654.163
1484.794	3110.928	3235.188	3235.165
1527.624	3200.765	3242.961	3242.954
1530.525	3224.819	3250.111	3250.105
1549.462	3229.705	3300.911	3300.862
1589.019	3293.663	3335.197	3335.186

3121.91	3336.362	3362.572	3362.516
3179.981	3338.863	3364.299	3364.241
3208.368			
3229.728			
3246.636			
3249.415			
3268.115			
3356.777			