

Supplementary Information

Table S1. Optimized geometries and computed vibrational frequencies of the reactants, various intermediates, transition states and products of the reaction of meta-tolyl radical with 1,3-butadiene.

Species	Optimized Cartesian Coordinates, Å	Computed Vibrational Frequencies, cm ⁻¹		
meta-tolyl	C,0,-3.7627529663,-0.4005702977,0.8842169466	27.9810	208.3799	348.7248
	C,0,-3.6910741583,0.9526853905,0.539295308	417.4490	483.2838	518.7533
	C,0,-2.5517943162,1.4985211598,-0.0530933974	629.3056	671.6545	756.0077
	C,0,-1.4373671302,0.6936461164,-0.3189053619	789.2978	854.4398	888.9952
	C,0,-1.5521358824,-0.6294825055,0.0362610849	974.4978	998.0693	1000.5238
	C,0,-2.6456641933,-1.217728536,0.6183151199	1058.0257	1060.3308	1098.6321
	C,0,-4.9967486811,-0.984922817,1.5298486938	1177.5261	1208.6276	1299.0866
	H,0,-4.5443266586,1.592865661,0.7369986673	1307.4149	1414.3321	1436.2255
	H,0,-2.5271685306,2.5527481794,-0.3093139107	1486.4770	1487.7948	1495.6030
	H,0,-0.544434452,1.101425418,-0.7789004575	1562.4246	1637.5835	3025.4573
	H,0,-2.6645773868,-2.2732056111,0.8716746113	3075.4889	3104.4748	3154.2212
	H,0,-5.3858953712,-1.8272668403,0.9502924855	3154.5000	3169.5318	3180.0302
	H,0,-5.790325611,-0.2400703086,1.6142722769			
	H,0,-4.7777516619,-1.3563570089,2.5358209331			
[0]	C,0,-3.7490320601,-0.4080883095,0.8797954913	7.6082	10.0321	12.9535
	C,0,-3.7253415221,0.9510773736,0.548085834	22.5501	35.6024	38.6895
	C,0,-2.6190671151,1.5356530514,-0.0676086208	46.4215	175.3901	207.1676
	C,0,-1.4890832547,0.7668254337,-0.374985562	299.9053	345.2608	419.0260
	C,0,-1.5586238402,-0.5624135234,-0.0326361033	482.5147	518.7044	519.5623
	C,0,-2.6184720621,-1.1896838097,0.5717876062	543.4435	629.4991	670.3367
	C,0,-4.9405666444,-1.0271006536,1.5710368003	760.0411	783.6862	789.1383
	H,0,-4.5916635828,1.563995595,0.774067988	852.8014	893.9634	900.9538
	H,0,-2.6325295406,2.592216201,-0.3150810141	935.1368	943.5016	977.3082
	H,0,-0.6207972253,1.2018660864,-0.8560417465	994.8294	1001.8505	1002.4399
	H,0,-2.6020408419,-2.2490029876,0.8084481712	1005.1428	1057.0066	1058.6730
	H,0,-5.1491330631,-2.0277869833,1.1844931408	1059.3438	1098.5850	1178.3138
	H,0,-5.8371334696,-0.4182799719,1.4373370391	1208.3212	1226.1732	1299.5238

	H,0,-4.763039865,-1.1231254684,2.6475866219 C,0,2.16312824,-0.714957467,-1.2813834571 C,0,2.7753528131,0.09880561,-0.4142319782 C,0,4.0573260985,0.7451454225,-0.6572261184 C,0,4.6693535787,1.5580376778,0.2100355172 H,0,2.6025623094,-0.946253734,-2.2470094062 H,0,1.207943576,-1.1726052466,-1.0522483441 H,0,2.3034372142,0.3054339025,0.5443257281 H,0,4.5284782323,0.5360672208,-1.615778404 H,0,5.6248506765,2.0160609045,-0.0156247673 H,0,4.2303733484,1.789313676,1.1756005837	1305.6751 1412.3611 1474.1153 1493.0936 1651.4340 3077.8209 3128.9650 3154.8832 3182.9627	1314.2810 1415.9750 1485.4224 1561.9551 1704.4282 3104.2380 3134.0328 3155.2825 3217.0935	1320.1278 1436.1145 1489.3631 1636.6262 3023.5817 3122.2017 3135.8720 3170.7013 3219.2564
[1]	C,0,-3.4759157154,0.7393343245,0.5698280267 C,0,-3.4062463631,-0.6405402134,0.7212019991 C,0,-2.1737558469,-1.2726626719,0.9291703633 C,0,-1.0238009169,-0.4837725224,0.9745994322 C,0,-1.0759233385,0.9073724938,0.8283372531 C,0,-2.3162374126,1.5120010249,0.623728206 C,0,0.2024641273,1.732060191,0.8839683532 C,0,1.1550222961,1.426163268,-0.2340398379 C,0,2.4759243498,1.04429537,-0.0599726778 C,0,3.3698471778,0.765902577,-1.0772289645 C,0,-2.098306746,-2.7691285559,1.1195955992 H,0,-4.4358271745,1.2175125184,0.4072349782 H,0,-4.3130501203,-1.2354728818,0.6760100514 H,0,-0.05951121,-0.9614676449,1.1220714399 H,0,-2.376985316,2.5891433868,0.5059758375 H,0,0.7041858122,1.5716551407,1.8448746581 H,0,-0.0736874259,2.7945745702,0.8537132349 H,0,0.7649097142,1.513242375,-1.2457708044 H,0,2.836944018,0.959881159,0.9646384007 H,0,4.3907576368,0.4744797259,-0.8668730161 H,0,3.0734145785,0.8312625224,-2.118302027 H,0,-1.0808683934,-3.1384319486,0.9755635123	19.4601 112.0716 229.0188 389.9473 531.4457 605.3985 763.8232 888.4512 934.7802 996.7725 1062.0924 1172.0409 1206.5053 1290.1686 1368.7348 1475.4229 1501.1034 1627.8516 3021.0534 3101.7137 3139.2503 3159.1037	27.1852 194.2991 291.2523 440.4150 542.7172 716.7989 791.9327 900.2740 964.8597 1013.9048 1106.8057 1188.7613 1260.3036 1334.1698 1414.6875 1490.2686 1517.4712 1648.1219 3039.6176 3111.0643 3150.4389 3177.6471	46.1466 213.2132 306.5124 482.0156 562.2707 731.6438 804.4512 908.9967 983.0364 1020.7713 1117.4826 1196.2416 1279.4475 1345.1578 1457.0600 1495.2657 1523.4897 2992.1082 3073.3269 3133.9032 3151.2380 3233.0063

	H,0,-2.7511762906,-3.2932706823,0.416551319 H,0,-2.4136364405,-3.0538805264,2.1292876631			
[2]	C,0,1.0537455714,0.6242179801,-0.2385212292 C,0,2.3479928618,1.0894532505,-0.0056307199 C,0,3.3836719334,0.1515741464,0.0981234699 C,0,3.1219807592,-1.2068502214,-0.0324018114 C,0,1.8218451207,-1.6533440548,-0.2695240006 C,0,0.7728486479,-0.7407032129,-0.376583243 C,0,-0.6543117311,-1.2049028329,-0.6226532568 C,0,-1.5492800133,-0.9713764551,0.5606904656 C,0,-2.7813377613,-0.3275265859,0.5481507734 C,0,-3.4314387958,0.2276965465,-0.537744123 C,0,2.6346442611,2.5671500791,0.1199625375 H,0,0.2390329721,1.3387657041,-0.3121459976 H,0,4.398084135,0.4911488106,0.2827088328 H,0,3.9317598949,-1.9237754008,0.0502305079 H,0,1.6243742295,-2.7154578077,-0.3728883686 H,0,-0.6364787006,-2.2775868786,-0.8566200237 H,0,-1.0531705218,-0.7060267064,-1.5100297894 H,0,-1.1829184237,-1.3493956242,1.5105237508 H,0,-3.2888597079,-0.2576913374,1.5081730414 H,0,-4.3963354357,0.7037499432,-0.4195686034 H,0,-3.0130419364,0.2119601194,-1.5366695103 H,0,3.2119329196,2.9313515212,-0.73635808 H,0,3.2189446227,2.7833256989,1.0190411389 H,0,1.7122910982,3.1490793182,0.1701172387	20.7484 106.7900 249.3769 398.9623 534.4228 611.4613 758.1451 886.0326 937.0716 1003.0696 1036.5818 1169.0951 1214.8324 1305.7195 1414.8814 1473.3988 1501.7860 1627.9109 3022.8518 3103.0659 3151.6812 3159.9646	25.7544 210.7282 273.1206 449.8865 539.9902 706.4763 786.8820 901.0086 982.4237 1012.9441 1062.2309 1176.4987 1241.0228 1334.3755 1433.2497 1479.7450 1523.3177 1648.3230 3066.0802 3124.4517 3152.9823 3178.6798	32.0102 217.8758 343.6751 508.9448 573.1340 717.9477 798.5599 908.6834 995.2012 1024.3070 1116.1515 1195.5434 1261.1657 1346.0478 1457.2784 1489.3259 1524.5986 2999.9163 3072.5902 3146.8043 3157.9595 3235.6742
[3]	C,0,0.3084566377,0.75937275,0.2131410304 C,0,0.3582384919,-0.6827791721,0.65033918 C,0,1.4652794013,-1.4355397787,-0.150665638 C,0,2.7421181077,-0.6405431438,-0.2252500979 C,0,2.8066528925,0.6699097091,0.0052146251 C,0,1.6016381729,1.5178846834,0.337583084 C,0,-0.8405131385,1.3154685792,-0.2747118749	28.9540 198.6320 378.4206 437.9614 576.4056 679.5276 840.6692	68.9284 234.3656 390.1854 479.9562 624.9784 733.3394 886.0825	127.1210 258.6741 398.4800 501.5657 669.0794 768.3785 918.0506

	C,0,-2.0639742848,0.6054281443,-0.3671389745 C,0,-2.0812354919,-0.7505875161,0.0732322668 C,0,-0.9726638549,-1.3693910125,0.5575282823 C,0,-3.3099443841,1.2486206465,-0.9079309902 H,0,0.7036896547,-0.7088479285,1.7010145306 H,0,1.0948976571,-1.6513539243,-1.1609231181 H,0,1.6531576219,-2.4080506656,0.3193933563 H,0,3.6484385218,-1.1829685365,-0.4819086123 H,0,3.7642601296,1.1810180696,-0.0472439012 H,0,1.7170926903,1.9033809235,1.3650042342 H,0,1.5819184265,2.4061124774,-0.3044829254 H,0,-0.8210221846,2.3522256559,-0.6039076373 H,0,-3.0163824072,-1.3018290269,0.0178925482 H,0,-1.0239405552,-2.4034794849,0.8853420045 H,0,-4.1204516215,1.2426103546,-0.1689750222 H,0,-3.6869194901,0.7192383572,-1.7915752701 H,0,-3.1314159931,2.2869098391,-1.1956650803	923.2356 981.9737 1006.9584 1056.5092 1186.8201 1245.6144 1310.8742 1407.0783 1449.7235 1481.1217 1619.0380 2940.2625 3029.0739 3093.8973 3135.7379	952.3631 985.3699 1032.0838 1139.4848 1200.6696 1282.3899 1326.7578 1411.7716 1465.8276 1486.9649 1716.4397 2998.5723 3034.6979 3129.0140 3152.8536	962.3080 1003.9718 1034.9459 1181.6082 1204.4760 1288.8709 1354.0061 1419.6726 1480.1409 1528.3945 2888.7535 3004.7797 3035.0278 3129.3971 3158.2445
[4]	C,0,-0.0554481204,1.083118625,-0.1567901287 C,0,-0.0158028819,-0.3655336252,0.2659005734 C,0,1.101718181,-1.1004648735,-0.5433333126 C,0,2.3750159521,-0.2987167988,-0.606985962 C,0,2.4408777137,1.005350694,-0.3447925132 C,0,1.2333939082,1.8399334866,0.0095000973 C,0,-1.1872577162,1.6399389224,-0.677468501 C,0,-2.3899567111,0.9054632966,-0.7926820483 C,0,-2.4406149301,-0.4341342148,-0.3408179947 C,0,-1.3501659268,-1.0722006618,0.1810500272 C,0,-1.4251621232,-2.477899399,0.7035707687 H,0,0.3280201672,-0.4036552193,1.3170566735 H,0,0.7346418685,-1.3075219936,-1.5571126192 H,0,1.3055565393,-2.0746782312,-0.0865570327 H,0,3.2803219046,-0.8352431952,-0.8793298819 H,0,3.3978103321,1.5185207029,-0.386879615	73.4932 222.3810 387.3355 450.8793 543.6700 707.7795 827.2580 918.9194 979.0853 1015.6276 1072.6166 1184.4062 1225.0072 1316.7451 1396.4940 1434.2908	118.3929 230.1652 399.2004 485.3816 610.1782 721.9937 895.6603 950.9998 994.1936 1032.3037 1132.2650 1198.2412 1285.9480 1338.2820 1409.8954 1463.4123	160.4540 255.1507 427.1012 510.0076 667.9790 765.6118 903.1838 952.0566 1002.5719 1051.6813 1156.2543 1203.9141 1299.2960 1349.6952 1415.5980 1475.8445

	H,0,1.3381159245,2.1867132451,1.0516703885 H,0,1.2166836558,2.7507761442,-0.5997651084 H,0,-1.1678796731,2.6764342057,-1.0031906751 H,0,-3.2749258821,1.3714916322,-1.208068607 H,0,-3.3840441867,-0.970019638,-0.3996402614 H,0,-2.4516701097,-2.8503533438,0.6955314448 H,0,-1.0501765684,-2.5366993048,1.7336036374 H,0,-0.8156503173,-3.1719484555,0.1123306503	1483.0879 1618.7271 2941.5963 3031.3448 3094.2912 3144.0855	1490.6940 1718.0770 2996.2288 3032.0984 3129.5936 3153.5689	1546.1199 2887.5436 3003.5442 3044.1021 3142.0310 3188.9182
[5]	C,0,-1.7550097623,-0.3188801729,0.018667533 C,0,-1.7621493394,-1.709189475,-0.0715654011 C,0,-0.6061297991,-2.434913553,0.1973158017 C,0,0.5756924728,-1.7807086991,0.5627433501 C,0,0.5644218283,-0.3864616101,0.644962206 C,0,-0.5888198974,0.3587900617,0.3784877017 C,0,0.0998891799,2.3925198225,1.697292299 C,0,-0.5672388648,1.8821337911,0.4548127665 C,0,0.0026808111,2.5548045026,-0.7837576892 C,0,0.4176071954,1.9640347977,-1.8987788465 C,0,1.825537733,-2.5650295783,0.8859847902 H,0,-2.6587667298,0.2429093902,-0.1946461598 H,0,-2.6724370767,-2.2274022198,-0.3531184817 H,0,-0.6191768991,-3.5178539238,0.1240143971 H,0,1.4741506649,0.1373034509,0.9217296247 H,0,0.7018841245,3.2925423864,1.6790853067 H,0,-0.1165760741,1.9334544652,2.6539691984 H,0,-1.6263779878,2.1994238527,0.5040826645 H,0,0.048170398,3.6407233484,-0.712412267 H,0,0.7990850899,2.5486120812,-2.7285151334 H,0,0.3916593879,0.8877757616,-2.0246285863 H,0,2.7227401125,-1.9557269649,0.7573803195 H,0,1.9197334609,-3.4464754025,0.2467868547 H,0,1.8123989715,-2.9154151129,1.9239717513	37.7251 104.2713 212.8610 349.5782 461.2184 575.7835 722.4926 846.8105 921.8541 1014.6792 1035.6598 1102.9613 1194.1644 1290.8586 1348.0040 1453.0158 1499.7002 1646.7419 3021.3126 3114.9353 3152.4725 3179.1631	52.9901 112.8485 249.4820 433.4917 493.6603 620.9886 758.2614 905.7193 951.9153 1017.4041 1062.1212 1120.9995 1233.5131 1325.7850 1414.0221 1460.0123 1521.5859 1703.4740 3075.0949 3136.9607 3158.0488 3219.5761	95.9373 173.2895 321.2044 440.6295 533.7312 691.8155 803.6448 921.3697 984.2082 1032.4935 1078.3308 1178.8729 1260.0041 1342.8822 1442.9123 1492.3799 1627.6249 2890.2875 3102.8143 3139.7590 3160.5612 3245.4419
TS [0]-[1]	C,0,-3.480559801,0.274312042,1.0501307261	112.6512i	20.2574	28.3714

	C,0,-3.2302378344,-1.0652792642,0.7550670755	47.1181	51.3920	83.9528
	C,0,-1.9623878328,-1.5011803214,0.3537462229	132.9289	206.2379	225.4020
	C,0,-0.9298325287,-0.5501283541,0.2570233712	299.7012	348.3882	420.5306
	C,0,-1.2221653115,0.7582557968,0.5572049055	484.2672	516.4956	521.0693
	C,0,-2.4564853523,1.2240770474,0.9514701636	573.4339	610.8562	680.6114
	C,0,-1.7065526182,-2.9487159064,0.0062579057	758.6346	778.7183	783.8093
	H,0,-4.4737061999,0.5830295496,1.3611574342	873.2897	889.6216	901.8355
	H,0,-4.0356115473,-1.7876234499,0.840059805	903.7006	923.8085	973.4102
	H,0,0.0687994641,-0.851510103,-0.0451223135	981.7306	992.2451	1002.0519
	H,0,-2.6402365024,2.2681093239,1.1814225011	1005.7331	1047.5119	1054.5412
	H,0,-1.7493633268,-3.105104783,-1.0771184059	1059.8952	1101.4418	1179.4182
	H,0,-2.4503811077,-3.6049485517,0.4633503619	1209.5669	1227.5543	1301.9905
	H,0,-0.7176343997,-3.2700507601,0.342515292	1303.8312	1309.0637	1318.2411
	C,0,0.7949915422,2.4369889735,0.4184346532	1406.5391	1413.1352	1436.6032
	C,0,1.7755493621,1.8299717378,-0.28026623	1472.0420	1486.1652	1489.9390
	C,0,2.8082882985,1.0060138822,0.3149308341	1493.8852	1563.6879	1613.3154
	C,0,3.7766116156,0.3853709221,-0.3741719464	1636.0219	1661.5218	3022.1521
	H,0,0.7668835152,2.3950728359,1.5013357622	3076.3008	3102.4528	3124.1814
	H,0,0.077133522,3.0860578772,-0.0654645288	3134.0492	3136.9740	3144.8222
	H,0,1.7985935464,1.9343260246,-1.3628896709	3149.6712	3151.1015	3162.9600
	H,0,2.7765666591,0.8998628735,1.3976884303	3174.0918	3220.5493	3234.2601
	H,0,4.5294370088,-0.2171481436,0.119372752			
	H,0,3.8434618285,0.467522751,-1.4544891009			
TS r-[5]	C,0,-1.329327362,-0.2098025039,1.3889512575	297.5035i	22.4788	26.8420
	C,0,-1.2579907312,-1.6012784262,1.5090986088	75.6606	90.2098	136.5097
	C,0,-0.4013780782,-2.3364111742,0.6906997923	187.0428	207.9739	233.6475
	C,0,0.4053027322,-1.7107488521,-0.2656391763	303.2553	355.5626	423.7476
	C,0,0.3378615608,-0.3107145463,-0.3821081292	484.7870	504.0837	520.8148
	C,0,-0.5223162098,0.3801319238,0.4396134231	529.7132	595.0767	687.1076
	C,0,1.3136923401,-2.5118804937,-1.1684934009	710.3257	767.4358	779.4350
	H,0,-1.9873063854,0.3733127435,2.0237001958	841.9158	877.7425	885.0639
	H,0,-1.8697718042,-2.111274769,2.2467258633	897.0363	930.6370	954.3884
	H,0,-0.3558357004,-3.4152660235,0.7990749797	975.7376	996.3138	1000.4046

	H,0,0.9654499878,0.2087212484,-1.1006164066 H,0,1.5413080567,-3.4893746886,-0.7376975998 H,0,2.2580952628,-1.9912041914,-1.3460021368 H,0,0.8469958394,-2.6823636994,-2.1448661231 C,0,-1.3595712214,3.0932772305,1.2721646209 C,0,-0.738596531,2.6800086303,0.1279573801 C,0,0.666015365,2.9927316768,-0.1504634102 C,0,1.2108041002,3.0118855011,-1.3695993902 H,0,-0.7921110504,3.4831193662,2.1101450555 H,0,-2.4299801456,2.9936085867,1.4017757619 H,0,-1.3512417813,2.420591672,-0.7306795557 H,0,1.2774266687,3.245978935,0.7129808035 H,0,2.2499475778,3.2779799298,-1.5224351832 H,0,0.6296395095,2.7730599241,-2.2549142304	1003.9327 1060.7310 1210.4835 1303.9635 1391.7522 1468.1236 1493.8593 1635.9664 3074.9775 3134.3854 3146.7752 3174.6413	1037.6564 1104.3540 1216.7879 1313.8436 1411.5423 1488.0084 1552.2436 1685.4582 3101.3359 3138.1753 3149.3417 3217.2278	1058.9170 1180.4364 1273.2771 1317.7587 1436.8030 1490.3053 1573.1679 3021.0997 3127.5622 3146.2062 3164.5399 3228.9784
TS [1]-[5]	C,0,-1.0476945859,-0.155724153,0.8924058165 C,0,-0.8155245942,-1.1778844828,1.7757057102 C,0,0.5137176362,-1.4668993648,2.1824753425 C,0,1.5817273406,-0.6661300441,1.7300473031 C,0,1.3754600589,0.3670816022,0.8578276626 C,0,0.0386661966,0.6489744441,0.3129201335 C,0,-0.2707464745,2.0593546811,-0.1843454403 C,0,0.0582270793,1.0459902034,-1.2366218207 C,0,-0.8698213293,0.6032653088,-2.3052037628 C,0,-2.017258345,-0.0713670205,-2.24183326 C,0,-1.9558923631,-1.9866122515,2.3481583847 H,0,-2.068001879,0.1064992946,0.6404608583 H,0,0.7005097589,-2.2827547921,2.8713556937 H,0,2.5855685147,-0.8667020378,2.0902551551 H,0,2.2040375694,0.9849823747,0.527322323 H,0,0.4498748449,2.8398584596,0.035591793 H,0,-1.3084191075,2.3656478856,-0.1101994336 H,0,1.0828312438,1.1087384392,-1.5910401405 H,0,-0.5217662695,0.8936058926,-3.2966968044	131.4939i 122.2127 262.5611 399.7569 510.6581 654.0001 727.1113 828.4802 941.9312 982.8415 1043.7806 1093.3605 1178.4045 1316.9161 1373.9256 1449.8041 1485.1616 1600.4807 3069.9403	67.7378 184.1197 320.8437 432.8792 535.4207 667.1028 786.8534 875.5232 958.6495 1007.4278 1059.1550 1102.8075 1188.0062 1336.5275 1412.1569 1459.5631 1497.4011 1699.0143 3097.8573	101.1211 229.1007 366.1260 486.1609 621.0758 700.2727 811.5705 927.3417 961.6819 1023.9020 1071.2223 1133.9611 1240.6226 1345.7335 1415.6524 1477.3308 1558.7667 3021.3881 3101.1076

	H,0,-2.5671372176,-0.2938617002,-3.1491480509 H,0,-2.4392477482,-0.4410270752,-1.317922232 H,0,-1.8534346604,-3.0448138514,2.0869343061 H,0,-2.921142992,-1.640411542,1.9733874944 H,0,-1.9747706773,-1.9241652706,3.4407399685	3107.2958 3151.5637 3181.3898	3128.7635 3166.5295 3198.0092	3151.2333 3176.0394 3239.6746
TS [1]-[2]	C,0,1.4883562933,1.4479038866,-0.5758824147 C,0,2.8668232554,1.4915135574,-0.3690858452 C,0,3.5770995543,0.320953899,-0.1295746918 C,0,2.9206696339,-0.9156217335,-0.0936870133 C,0,1.5405711001,-0.9386255221,-0.2997001151 C,0,0.8093280655,0.2297476548,-0.5432497708 C,0,-0.6908971754,0.1619384176,-0.738968695 C,0,-1.4567584248,-0.0753480835,0.5316945356 C,0,-2.9040713436,-0.3416548651,0.5088702402 C,0,-3.46953362,-1.5470850607,0.5569531916 C,0,3.6947945359,-2.1908745703,0.142287955 H,0,0.939240133,2.3649555762,-0.76369434 H,0,3.3865917812,2.4431834832,-0.3951970788 H,0,4.649928273,0.3634611501,0.0306114671 H,0,1.016608454,-1.8898218962,-0.2701944019 H,0,-0.9411653643,-0.6295550263,-1.4585010085 H,0,-1.0355698844,1.0952662501,-1.2150427019 H,0,-0.9875725406,0.2010999073,1.4719199413 H,0,-3.5627068333,0.5306551644,0.4380310207 H,0,-4.5472038563,-1.6674317661,0.5300043266 H,0,-2.8734345107,-2.4510476332,0.6303556174 H,0,3.0276745862,-3.0282490459,0.3565752438 H,0,4.3863378339,-2.0866626602,0.9829994333 H,0,4.2911010536,-2.4585350835,-0.7365258955	230.8338i 37.6565 228.9621 314.1941 488.9371 606.1180 754.2599 897.6951 952.4881 1006.6523 1061.7718 1117.5727 1195.4629 1314.7449 1371.2257 1458.3756 1501.2558 1649.2087 2999.2596 3073.1644 3143.9129 3160.2931	19.1360 99.5215 258.0788 393.8158 521.5226 666.3305 797.3680 910.8463 975.8547 1013.4758 1064.3177 1169.0133 1257.8215 1328.7670 1414.8663 1467.7320 1524.2298 1681.8230 3022.2198 3101.6551 3149.2310 3178.6883	33.2853 212.1409 268.6576 449.0604 539.6527 718.2690 881.6379 938.4416 983.1735 1021.2763 1112.0419 1178.0180 1276.2341 1344.3378 1447.0007 1489.6897 1629.1443 2939.6865 3035.8082 3126.4888 3151.8840 3210.2449
TS [1]-p1 ^a	C,0,-3.1969124015,0.4896673667,0.631315954 C,0,-3.3979035948,-0.7958346202,0.1234770849 C,0,-2.3868429827,-1.4421191963,-0.5881148658 C,0,-1.1646866889,-0.820713927,-0.8005074575	496.1532i 98.3041 209.7491 310.5687	30.9955 111.0916 233.3802 312.8185	40.7997 160.7385 253.8887 349.7694

	C,0,-0.929473982,0.469489484,-0.2976667876 C,0,-1.963168368,1.1040012808,0.4054999168 C,0,0.3458900773,1.1788600712,-0.471932815 C,0,1.5294237591,0.6386324987,-0.8656024498 C,0,2.7678767824,1.3776303184,-0.9208119564 C,0,3.9428917686,0.859554313,-1.3095121964 C,0,-4.2735680541,1.1934260336,1.4227553494 H,0,-4.3506803928,-1.2914982436,0.2779928471 H,0,-2.5606541959,-2.4358463526,-0.986210666 H,0,-0.3989967647,-1.3316384716,-1.3718612976 H,0,-1.7956522352,2.1075618308,0.7862818445 H,0,0.3613794287,2.1989380865,-0.095894801 H,0,1.5731159656,-0.4033134708,-1.1712640491 H,0,2.7232359588,2.4234014961,-0.6234189238 H,0,4.8470433814,1.4553550884,-1.3309623691 H,0,4.0303779764,-0.17758298,-1.6171275759 H,0,-4.0928675462,1.1022948622,2.4992854535 H,0,-5.2588942207,0.7695167291,1.2179319124 H,0,-4.3083920934,2.2601633563,1.1877318511 H,0,-0.1612485776,2.1934954466,-2.2596470026	387.5109 530.3502 656.8763 796.5145 915.8993 968.0007 1013.6389 1062.6472 1191.7623 1292.3036 1342.1984 1435.3153 1498.9725 1629.3762 3023.1894 3128.4815 3148.5781 3173.4010	447.9928 562.1476 711.0726 876.6268 925.1260 973.5352 1021.6850 1120.4345 1198.7355 1308.9433 1349.9780 1463.5967 1526.1801 1642.6998 3076.9260 3134.3647 3150.8911 3188.6003	521.8890 639.6428 773.1205 897.9111 931.2023 984.2053 1038.9299 1184.9721 1262.5766 1320.5548 1415.8985 1491.9423 1614.4816 1659.3481 3103.6501 3136.8071 3158.6048 3223.8989
TS [2]-[3]	C,0,-0.2252812409,0.6752226116,0.8626154645 C,0,-0.374528891,-0.7526815086,0.9323518333 C,0,2.0072109115,0.5803324921,2.0571383206 C,0,0.7281925839,1.3512750396,1.8200695214 C,0,-0.8366506844,1.3646862207,-0.1658024486 C,0,-1.6688409852,0.7305985067,-1.1111914887 C,0,-1.8891160755,-0.6486437137,-0.9773430284 C,0,-1.299686881,-1.3712502679,0.0450560621 C,0,1.5978627447,-1.1726403225,0.3345152598 C,0,2.3608948872,-0.544881308,1.4128599503 C,0,-2.2976690993,1.5218034888,-2.2294641334 H,0,-0.1737131719,-1.2420693083,1.8791662521 H,0,2.6424615354,0.9509899988,2.8566049389	587.8918i 141.7417 256.9820 405.1842 519.7091 662.6045 790.8651 875.9628 943.2346 986.3562 1038.3035 1097.8238 1206.2528	38.8859 202.4439 347.3909 432.3036 560.6761 703.7709 810.1468 898.5149 958.8421 1011.2347 1052.6189 1164.8418 1233.2794	75.1086 219.6500 394.9778 512.8354 652.5328 714.6637 865.6990 934.4101 971.4969 1021.0062 1088.3237 1186.9439 1256.5390

	H,0,0.2410567074,1.4972467387,2.7955605422	1308.8829	1325.5850	1347.0321
	H,0,0.9569062806,2.361599278,1.4574156663	1405.9328	1414.7753	1453.1211
	H,0,-0.6688238565,2.4354761551,-0.2517195595	1470.6691	1476.0079	1484.3643
	H,0,-2.5564169435,-1.1485725671,-1.6728932207	1486.7214	1506.4870	1551.7494
	H,0,-1.5139313386,-2.4285128025,0.1566789547	1615.3096	1650.3164	2979.7910
	H,0,1.6980497876,-2.2511428386,0.2305935012	3011.1139	3013.3886	3059.7638
	H,0,1.5125525071,-0.6609223552,-0.6173628066	3094.5335	3096.8814	3105.4576
	H,0,3.2409206256,-1.0774452783,1.7726478482	3137.4791	3146.8954	3150.4831
	H,0,-1.5615127309,1.7793915291,-3.0000550132	3152.7647	3175.3315	3184.2083
	H,0,-2.7212666336,2.4624810711,-1.8646143483			
	H,0,-3.0970040389,0.9582541405,-2.715599068			
TS [2]-[4]	C,0,-0.5544316552,0.9495528627,0.3905234418	583.4476i	78.2265	98.5316
	C,0,-0.6860357271,-0.4792456678,0.4181556239	138.9843	162.6762	232.1857
	C,0,1.699643982,0.8428003602,1.5432479436	244.0218	368.5037	395.8232
	C,0,0.4072145377,1.604915418,1.3538905244	402.7389	453.0102	514.2647
	C,0,-1.1856775252,1.6617126288,-0.6135410737	525.7696	543.5708	651.9720
	C,0,-2.0103409835,1.01682488,-1.5450348709	663.1256	699.6522	730.4451
	C,0,-2.2192397142,-0.3644241525,-1.4579596741	761.6157	794.1838	870.8068
	C,0,-1.6128011065,-1.1194076095,-0.4648531433	894.8883	909.0026	939.5709
	C,0,1.2849022239,-0.85303915,-0.2349912793	945.4538	955.6023	965.7976
	C,0,2.0566616044,-0.2540476594,0.8536043929	985.3254	1018.0198	1019.3236
	C,0,-1.8638446982,-2.5973545717,-0.3262806868	1029.8455	1057.8343	1091.0647
	H,0,-0.4559118741,-0.9887457276,1.3490587894	1099.8057	1166.2533	1177.6876
	H,0,2.3434342107,1.1931190075,2.3450394746	1203.8957	1234.0476	1246.4905
	H,0,-0.063635099,1.7140907588,2.3420816719	1314.2982	1327.2730	1347.5967
	H,0,0.6182727938,2.628870026,1.020027085	1404.6367	1413.9014	1414.6371
	H,0,-1.0378029657,2.7352382345,-0.6802095039	1466.0025	1476.2085	1482.8947
	H,0,-2.5026141474,1.5909227962,-2.3215623115	1493.3453	1524.3317	1566.1256
	H,0,-2.8871506904,-0.8493951081,-2.1632543675	1607.5026	1650.6315	2979.7599
	H,0,1.4064041333,-1.9240287643,-0.3830700781	3009.3430	3013.5925	3052.4845
	H,0,1.1728466342,-0.3045975854,-1.1633272239	3095.3228	3099.1303	3106.0392
	H,0,2.9492315765,-0.7874273307,1.1795301838	3135.2541	3150.3436	3150.8108
	H,0,-0.9566304148,-3.1776254202,-0.5318843832	3155.7388	3182.9081	3185.0552

	H,0,-2.6402514089,-2.937212878,-1.0146038443 H,0,-2.1793086863,-2.8535433473,0.6908683095			
TS [3]-p2 ^b	C,0,0.5743580145,0.5901097533,0.4619933297 C,0,0.6898223937,-0.807179736,0.2580702313 C,0,1.9548557577,-1.5548090662,0.6559869411 C,0,2.8332820136,-0.7948199459,1.6056144698 C,0,2.6366710927,0.4788955938,1.933100855 C,0,1.5135294546,1.3193842727,1.3970757342 C,0,-0.4733800736,1.2830382175,-0.1424266823 C,0,-1.3949472227,0.6619738962,-0.9865743275 C,0,-1.2312284202,-0.7093093768,-1.2437728265 C,0,-0.2014986017,-1.4181186147,-0.6588433958 C,0,-2.5354714115,1.4328358613,-1.6027181605 H,0,2.5246254423,-1.7828736554,-0.2568337607 H,0,1.6918401286,-2.5272324151,1.0864072524 H,0,3.6767616945,-1.3340051024,2.0274173916 H,0,3.3166730949,0.9664558108,2.6261218379 H,0,0.9348194524,1.7275919526,2.2384500539 H,0,1.9269861576,2.1997052547,0.8857638613 H,0,-0.571541257,2.3485397685,0.0493476633 H,0,-1.9141558701,-1.2119998939,-1.9214539246 H,0,-0.0792143526,-2.4740880664,-0.8784371851 H,0,-3.4691103704,1.2580924381,-1.0563780228 H,0,-2.7068419285,1.13061556,-2.6394932897 H,0,-2.344102988,2.5079595845,-1.5898411266 H,0,-0.1890512009,-1.2445960913,1.8065110807	797.5075i 124.3124 313.3764 403.5899 493.4471 603.3435 714.2443 868.4463 946.0965 979.3189 1027.1669 1177.8528 1227.1477 1280.7789 1373.3434 1452.4867 1488.1303 1580.8365 2981.0311 3018.7774 3100.4542 3150.9884	50.4986 184.8760 382.4405 434.1038 538.5089 672.7686 756.9841 892.7446 959.3789 1002.6000 1057.3659 1196.8763 1230.7334 1322.0028 1413.2471 1464.4867 1497.0469 1641.5556 2982.4252 3032.0170 3136.1251 3158.8378	61.3426 252.1405 384.3884 460.8141 569.8024 693.8016 818.2341 919.1853 973.9399 1013.4241 1141.2489 1200.3803 1245.7423 1361.5694 1417.2634 1474.3461 1517.2121 1735.7076 2997.9469 3070.4472 3140.7217 3169.1177
TS [4]-p3 ^c	C,0,-0.0628534496,1.156708318,0.1334420047 C,0,0.0449268523,-0.2421142728,-0.0772352567 C,0,1.2963857429,-0.9890360772,0.3661477964 C,0,2.1653948818,-0.2295192221,1.3247225278 C,0,1.9730742455,1.0453438509,1.646009695 C,0,0.8630703971,1.8836286364,1.0854819945 C,0,-1.0927775798,1.8666264507,-0.4801216283	746.2784i 171.3558 270.1427 431.7787 523.4934 560.2048 737.8470	70.3678 216.7168 384.8264 458.7363 531.6409 669.5048 775.5443	121.7512 266.3293 385.5626 485.8677 541.7909 678.6494 784.9589

	C,0,-1.9887318488,1.2344208097,-1.333219671	846.5601	906.2187	934.3639
	C,0,-1.8524757104,-0.1298128626,-1.5937594469	956.7401	966.7134	976.2483
	C,0,-0.8397149293,-0.874286019,-1.0042234814	979.7202	1010.1134	1017.0297
	C,0,-0.7124525839,-2.3466239944,-1.2954812818	1051.3537	1056.9683	1102.0970
	H,0,1.8862911291,-1.2400857693,-0.5285124466	1187.5732	1192.6431	1198.9055
	H,0,1.0242009788,-1.9532994896,0.8078140501	1229.8252	1237.8618	1239.0549
	H,0,2.9972856932,-0.7758800801,1.7601890431	1267.0462	1316.4274	1368.5281
	H,0,2.6438391377,1.5321880074,2.3483447862	1376.9998	1414.4606	1418.2272
	H,0,0.2688123323,2.2973023591,1.9130658089	1450.3848	1467.9059	1472.7232
	H,0,1.2878559781,2.7607261357,0.5781224118	1487.6823	1493.9808	1509.4560
	H,0,-1.1894612588,2.9307457547,-0.2872439924	1598.8406	1629.1370	1740.8932
	H,0,-2.7832880768,1.8007368313,-1.8060073776	2973.0961	2983.7913	2998.7681
	H,0,-2.5418735805,-0.6183098705,-2.2744987914	3014.0642	3035.2647	3060.2277
	H,0,-0.8391251242,-2.9408841926,-0.3833373992	3105.1692	3136.3750	3151.8195
	H,0,0.2697279658,-2.6002725548,-1.7071350836	3159.1256	3161.1412	3182.5535
	H,0,-1.4690474537,-2.668149267,-2.0129866443			
	H,0,-0.9073057388,-0.7085834822,1.4405603828			
p1 ^a	C,0,-3.1704034635,0.2412844988,-0.0389396174	29.2018	30.7047	100.3515
	C,0,-3.0760334615,-1.1524356723,-0.0638062266	118.4960	165.4159	207.4019
	C,0,-1.831245845,-1.7752346849,-0.1575908135	256.3558	306.1946	314.1537
	C,0,-0.6673687722,-1.023345143,-0.2257330007	384.7974	446.4381	520.3410
	C,0,-0.7260776142,0.3811871023,-0.199637611	531.7682	551.6051	640.5056
	C,0,-1.9904910352,0.9844944199,-0.1045597978	662.3976	711.4617	773.3859
	C,0,0.4587963464,1.2386317002,-0.2624863347	795.3254	876.9893	898.5508
	C,0,1.7473085417,0.8586505066,-0.362658318	917.4206	926.7211	933.2385
	C,0,2.8564774687,1.7895147411,-0.4189917408	967.4200	974.9990	983.8456
	C,0,4.1440682325,1.4337907762,-0.5188184815	1013.8940	1019.0486	1043.5557
	C,0,-4.5135415877,0.928464728,0.0299077955	1062.0961	1119.5751	1185.1404
	H,0,-3.9775809064,-1.7537648619,-0.0073845843	1192.9301	1198.5688	1266.2281
	H,0,-1.7724666743,-2.8581244635,-0.1733391143	1295.5020	1317.5976	1323.9217
	H,0,0.2886504408,-1.5282612915,-0.2942820773	1349.8484	1352.9103	1415.0939
	H,0,-2.0484755721,2.0690228482,-0.0796826431	1437.2889	1463.9618	1491.7410
	H,0,0.2526784117,2.3068451417,-0.2232661085	1498.5236	1526.1946	1621.1815

	H,0,2.0046556304,-0.1968273938,-0.4065012377 H,0,2.6016943488,2.8468067189,-0.3755226521 H,0,4.9360530375,2.1716420581,-0.5572192295 H,0,4.4421031375,0.3910890925,-0.5649980636 H,0,-4.9084249353,1.1195599424,-0.9739433027 H,0,-4.4438893228,1.89086678,0.5421429387 H,0,-5.2474464059,0.3157634561,0.558403221	1640.5447 3021.5388 3121.4851 3141.2518 3171.4335	1658.7738 3076.1853 3124.0666 3148.1745 3187.4141	1690.5750 3101.9638 3134.3487 3156.1192 3220.5502
p2 ^b	C,0,0.3632744891,0.743466074,-0.0506601623 C,0,0.4300552505,-0.651530367,-0.0986370982 C,0,-0.7669897071,-1.3798300405,-0.113538192 C,0,-2.0005244122,-0.7484278457,-0.0819248018 C,0,-2.0827111966,0.6498631469,-0.0337359887 C,0,-0.8910342283,1.3681702543,-0.0191031255 C,0,1.6119553867,1.6026338275,-0.0316939604 C,0,1.751528013,-1.3921116285,-0.1346627938 C,0,2.9587228266,-0.5004273654,-0.1142835948 C,0,2.8966443577,0.8271601797,-0.0686347222 C,0,-3.4230140749,1.3445256406,0.0006571903 H,0,-0.7232837041,-2.4646148503,-0.1507389531 H,0,-2.9099273874,-1.341372033,-0.0945659929 H,0,-0.9304555002,2.4539304212,0.0181612926 H,0,1.5994567304,2.2431463353,0.8614468242 H,0,1.5851531542,2.3023530831,-0.8789169481 H,0,1.7875926951,-2.0316073682,-1.0279761579 H,0,1.8018984759,-2.0907509546,0.7124679454 H,0,3.9273437807,-0.9922220139,-0.1389771171 H,0,3.8151500804,1.407610924,-0.0564595757 H,0,-3.3081897188,2.4296486891,0.0389145688 H,0,-4.0063623445,1.0390058167,0.8750207194 H,0,-4.0186219662,1.1024290745,-0.8852493561	20.0018 191.8856 383.4851 444.6776 594.5395 719.2579 871.8769 947.0187 980.3951 1028.0595 1178.0506 1226.9907 1282.3227 1375.3777 1450.0778 1487.7135 1616.8974 2983.6050 2994.5968 3099.6635 3142.9109	45.3475 254.3660 405.9173 496.7364 673.0745 751.1757 890.1791 953.6938 1001.9905 1061.0527 1198.3687 1230.6031 1337.3806 1414.7661 1470.5225 1501.3431 1658.6626 2984.9500 3021.1586 3132.0704 3155.0652	122.5567 308.6793 433.2530 543.3012 696.6675 821.5013 921.9519 977.9148 1013.7185 1144.2791 1208.4069 1248.8092 1362.5464 1417.1772 1474.0232 1539.7898 1737.1112 2993.2773 3068.8710 3138.5305 3162.4754
p3 ^c	C,0,-0.0602378223,0.5437637876,-0.0729360487 C,0,0.0019596926,-0.8556105144,-0.0453350022 C,0,-1.1802752016,-1.5978211078,0.0563953999	60.4175 221.6973 386.9623	123.6234 260.3533 430.7137	159.5342 273.4044 471.6554

C,0,-2.4127928167,-0.9673001089,0.1303238455	487.0673	506.1953	519.9558
C,0,-2.474293586,0.4238140477,0.1029115645	553.8290	671.5660	677.1716
C,0,-1.3140050979,1.1898187442,0.0021826005	724.9383	779.9499	783.6826
C,0,1.1977082512,1.3825406894,-0.1824088749	847.5647	903.3454	935.8370
C,0,1.3187826798,-1.6050752319,-0.1224669044	960.6585	964.7774	977.7330
C,0,2.5307447408,-0.7289173295,-0.2297058794	981.4292	1013.2274	1013.9570
C,0,2.4751400269,0.598417093,-0.2561728065	1049.7753	1057.5446	1107.7923
C,0,-1.4131812748,2.6969521467,-0.0251406355	1188.8353	1197.8896	1200.0561
H,0,-1.1237895875,-2.6820515003,0.0771461459	1230.9996	1235.2189	1236.3713
H,0,-3.3228175808,-1.5518210007,0.2089333877	1269.7385	1324.0034	1370.6940
H,0,-3.4362662197,0.9226498445,0.1604832975	1377.8805	1417.2079	1419.8417
H,0,1.2518081805,2.0768474713,0.6684764642	1461.9237	1472.6182	1485.0916
H,0,1.1275220073,2.0372165434,-1.0630183578	1488.8962	1497.3735	1512.0215
H,0,1.2923759346,-2.2949824917,-0.9775762722	1629.4523	1639.5165	1742.4015
H,0,1.4169482242,-2.254713334,0.7585740118	2980.5552	2986.4528	2987.6909
H,0,3.4930588239,-1.2301299505,-0.2873300003	2996.3042	3018.3335	3061.7565
H,0,3.3926545582,1.1751267788,-0.3353309686	3103.6642	3133.5881	3149.3641
H,0,-0.9939746251,3.115409481,-0.9462222274	3156.6646	3158.8354	3179.9413
H,0,-0.8681420395,3.1554464289,0.8067021152			
H,0,-2.4537352679,3.0187275132,0.0422041453			

^ap1 – 1-meta-tolyl-*trans*-1,3-butadiene.

^bp2 – 6-methyl-1,4-dihydronaphthalene.

^cp3 – 5-methyl-1,4-dihydronaphthalene.