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Supplementary Information

The Kinetics of the Reactions of Br Atoms with the Xylenes: An Experimental and Theoretical Study

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Table S1: Calculated unscaled harmonic vibrational wavenumbers and rotational constants of the species involved in *o*-xylene + Br reaction. Imaginary wavenumber is denoted by *i*. Wavenumbers corresponding to the torsional modes are shown in bold.

Species	MP2/aug-cc-pVDZ				G3				G4				B3LYP/cc-pVTZ			
	Wavenumbers			B(GHZ)	Wavenumbers			B(GHZ)	Wavenumbers			B(GHZ)	Wavenumbers			B(GHZ)
***o*-xylene**	**116**	172	**186**	3.1386	**131**	183	**188**	3.1774	**134**	165	**175**	3.1673	**137**	162	**173**	3.1758
	256	299	402	2.1171	280	325	440	2.1518	256	300	409	2.1523	255	302	413	2.1613
	431	491	494	1.2847	489	543	566	1.3037	450	508	521	1.3020	450	512	525	1.3066
	577	593	743		630	789	796		588	732	746		592	734	747	
	745	822	847		842	892	980		766	833	883		759	839	881	
	910	912	997		1057	1081	1101		926	969	1004		950	994	1004	
	1000	1029	1043		1113	1150	1156		1009	1044	1073		1013	1048	1076	
	1064	1132	1165		1182	1235	1236		1076	1140	1185		1077	1147	1187	
	1202	1256	1287		1295	1339	1342		1203	1249	1312		1207	1244	1323	
	1389	1400	1437		1439	1564	1575		1334	1410	1421		1327	1415	1424	
	1461	1465	1484		1609	1626	1640		1464	1476	1492		1471	1480	1493	
	1486	1500	1506		1641	1645	1668		1494	1501	1525		1497	1506	1528	
	1614	1639	3047		1780	1814	3198		1619	1647	3022		1620	1649	3019	
	3048	3122	3125		3202	3247	3249		3023	3069	3071		3020	3059	3061	
	3156	3157	3188		3279	3282	3347		3113	3114	3160		3102	3104	3154	
	3192	3210	3225		3353	3367	3383		3164	3179	3194		3158	3172	3187	
3,4-dimethyl phenyl	145	204	214	3.2665	117	173	177	3.2980	134	166	177	3.1992	137	163	176	3.2083
	299	312	423	2.2631	270	322	437	2.2956	263	301	413	2.2410	261	303	417	2.2510
	512	520	587	1.3597	438	528	530	1.3765	440	507	509	1.3396	439	511	512	1.3447
	603	754	783		606	707	756		577	704	742		581	701	743	
	820	909	987		825	863	891		795	812	864		790	815	860	
	992	1028	1056		983	1066	1082		941	1005	1009		949	1005	1012	
	1104	1105	1126		1109	1137	1159		1043	1072	1075		1046	1074	1077	
	1145	1187	1228		1207	1255	1295		1132	1182	1233		1135	1185	1229	
	1278	1308	1387		1377	1388	1469		1287	1311	1399		1292	1305	1401	
	1405	1465	1468		1564	1574	1594		1411	1422	1476		1415	1425	1480	
	1486	1489	1525		1616	1626	1633		1479	1486	1492		1484	1490	1493	
	1586	1823	1873		1641	1653	1673		1498	1575	1626		1501	1576	1626	
	3054	3058	3130		3197	3202	3246		3024	3024	3071		3020	3021	3061	
	3139	3165	3171		3250	3279	3281		3073	3115	3116		3063	3104	3106	
	3205	3231	3255		3353	3363	3379		3157	3170	3189		3151	3160	3178	
2,3-dimethyl phenyl	140	198	206	3.3910	111	161	173	3.4191	128	158	173	3.3133	131	154	171	3.3229

	280	296	408	2.1592	254	304	419	2.1924	246	284	394	2.1402	244	286	398	2.1496
	512	544	588	1.3415	478	512	527	1.3583	471	497	511	1.3215	472	500	513	1.3265
	616	768	782		608	711	757		589	706	743		592	703	744	
	830	875	988		795	876	921		767	823	890		758	827	894	
	1015	1022	1062		1010	1054	1066		959	986	999		974	990	1000	
	1110	1131	1134		1126	1132	1158		1037	1071	1087		1039	1073	1086	
	1147	1167	1234		1224	1244	1278		1134	1181	1218		1140	1182	1218	
	1255	1306	1386		1351	1383	1536		1266	1315	1405		1268	1307	1410	
	1402	1465	1470		1562	1563	1577		1417	1433	1477		1421	1439	1480	
	1486	1487	1537		1613	1626	1633		1481	1492	1493		1483	1494	1495	
	1592	1815	1891		1640	1648	1688		1493	1557	1645		1496	1559	1644	
	3057	3061	3134		3198	3202	3247		3025	3026	3073		3022	3023	3063	
	3141	3171	3180		3250	3280	3287		3076	3115	3127		3066	3104	3116	
	3215	3233	3256		3350	3366	3382		3162	3178	3190		3156	3170	3182	
PC$_o$	36	47	69	1.3512	13	14	40	1.3891	17	19	65	1.5119	6	15	50	1.5666
	156	175	215	0.6857	109	142	157	0.6399	159	177	257	0.5063	153	172	247	0.4582
	234	288	333	0.6289	186	264	345	0.5945	292	325	351	0.4735	257	280	326	0.4367
	416	438	504		425	439	507		411	421	494		416	421	494	
	509	558	601		529	554	614		504	540	588		507	543	593	
	706	749	776		708	750	763		712	745	746		716	744	747	
	837	857	959		789	887	903		783	855	873		787	862	873	
	985	1011	1037		971	1010	1039		932	967	975		952	978	990	
	1063	1085	1091		1067	1109	1146		1002	1058	1063		1005	1061	1063	
	1154	1164	1207		1211	1246	1271		1147	1178	1198		1152	1180	1198	
	1266	1280	1319		1344	1409	1413		1291	1308	1335		1292	1317	1331	
	1398	1466	1477		1564	1567	1586		1412	1452	1481		1417	1458	1485	
	1500	1510	1540		1632	1634	1644		1486	1496	1508		1493	1501	1512	
	1680	1714	2601		1653	1669	2806		1563	1600	2514		1567	1605	2556	
	3056	3136	3169		3201	3252	3283		3026	3076	3118		3021	3064	3107	
	3210	3214	3218		3343	3352	3357		3166	3168	3172		3159	3160	3167	
	3236	3252	3328		3369	3384	3439		3186	3202	3267		3179	3192	3256	
RC$_o$	75	105	138	1.4214	23	32	38	1.6786	40	60	113	1.6097	39	59	108	1.6157
	176	**201**	211	0.8924	120	175	179	0.6843	**133**	**167**	195	0.7202	136	167	192	0.7106
	268	303	401	0.7400	269	322	434	0.6051	258	301	408	0.6020	256	303	412	0.5961
	463	491	498		463	532	534		446	499	514		447	504	519	
	572	646	743		614	738	760		581	706	743		586	709	746	
	773	820	874		802	883	927		772	829	897		767	834	894	
	911	943	996		1001	1047	1066		938	976	1001		951	1000	1005	
	1003	1036	1058		1086	1116	1142		1008	1039	1070		1011	1044	1073	
	1068	1130	1169		1165	1220	1254		1073	1135	1187		1074	1142	1191	

	1205	1253	1287		1277	1306	1377		1197	1238	1304		1202	1236	1315	
	1390	1400	1430		1421	1564	1574		1343	1409	1421		1338	1414	1425	
	1460	1470	1479		1585	1622	1626		1449	1473	1490		1459	1479	1493	
	1484	1506	1515		1638	1640	1649		1491	1492	1514		1495	1498	1520	
	1609	1649	3048		1685	1720	3198		1595	1608	3029		1601	1612	3025	
	3053	3127	3138		3203	3248	3251		3030	3079	3083		3026	3067	3071	
	3160	3168	3194		3280	3282	3349		3120	3131	3170		3108	3119	3163	
	3204	3216	3232		3354	3368	3383		3191	3199	3213		3183	3191	3204	
2-methyl benzyl	171	215	282	3.2523	156	186	262	3.2897	156	186	258	3.2304	154	182	257	3.2389
	333	416	444	2.2387	345	424	439	2.2705	326	412	421	2.2355	327	416	422	2.2448
	504	516	562	1.3372	506	529	555	1.3546	493	504	540	1.3321	493	508	542	1.3368
	602	704	750		614	706	744		589	706	736		594	713	735	
	774	826	859		763	783	880		746	779	856		747	780	861	
	948	985	1009		903	965	1005		867	924	960		868	947	979	
	1025	1044	1082		1038	1067	1109		977	1003	1058		983	1006	1061	
	1085	1150	1165		1145	1210	1246		1065	1147	1177		1065	1152	1179	
	1205	1269	1281		1270	1343	1409		1198	1290	1308		1197	1291	1316	
	1319	1397	1466		1415	1564	1566		1335	1413	1453		1330	1418	1458	
	1477	1500	1510		1587	1633	1635		1482	1489	1498		1486	1493	1502	
	1539	1675	1709		1644	1653	1669		1510	1566	1604		1513	1570	1606	
	3055	3134	3167		3199	3248	3279		3024	3072	3115		3019	3061	3104	
	3208	3211	3216		3341	3348	3353		3162	3165	3169		3156	3158	3163	
	3235	3250	3325		3366	3381	3436		3182	3197	3263		3176	3190	3252	
TS$_o$	763*i*	44	55	1.9479	1545*i*	45	52	1.9567	306*i*	37	44	1.9011	489*i*	40	45	1.9199
	165	**209**	274	0.5184	149	177	250	0.4993	152	**181**	258	0.4749	148	175	255	0.4753
	330	402	419	0.4760	342	358	432	0.4574	326	408	437	0.4318	327	411	432	0.4316
	481	513	530		454	512	530		482	504	525		460	505	528	
	558	607	728		542	616	723		556	600	726		528	599	724	
	787	825	853		766	787	894		748	779	832		750	770	835	
	879	930	981		902	978	1003		853	863	885		861	878	897	
	1008	1020	1061		1029	1047	1073		940	975	992		964	997	1000	
	1082	1100	1105		1111	1150	1197		1007	1060	1069		1011	1063	1071	
	1146	1158	1176		1227	1252	1280		1148	1183	1209		1153	1182	1188	
	1236	1270	1283		1287	1349	1405		1225	1311	1336		1212	1306	1324	
	1324	1398	1467		1421	1569	1574		1349	1415	1458		1335	1421	1465	
	1481	1497	1524		1604	1630	1635		1485	1494	1500		1489	1501	1505	
	1560	1739	1765		1646	1657	1687		1506	1575	1613		1509	1581	1618	
	3057	3140	3155		3202	3257	3289		3029	3082	3122		3026	3071	3111	
	3172	3217	3222		3306	3357	3362		3142	3171	3177		3133	3164	3170	
	3239	3253	3264		3374	3388	3392		3189	3202	3236		3182	3195	3223	

Table S2: Calculated harmonic vibrational wavenumbers and rotational constants of the species involved in *m*-xylene + Br reaction. Imaginary wavenumber is denoted by *i*. Wavenumbers corresponding to the torsional modes are shown in bold.

Species	MP2/aug-cc-pVDZ				G3				G4				B3LYP			
	Wavenumbers			B(GHZ)	Wavenumbers			B(GHZ)	Wavenumbers			B(GHZ)	Wavenumbers			B(GHZ)
***m*-xylene**	**30**	**34**	201	3.5365	**27**	**31**	215	3.5772	**24**	**36**	200	3.5844	**16**	**42**	196	3.5947
	213	270	397	1.7323	244	291	431	1.7641	222	270	398	1.7598	221	275	405	1.7678
	427	505	506	1.1801	485	557	577	1.1992	444	519	530	1.1979	445	525	529	1.2026
	531	620	724		578	770	786		543	716	734	1.4519	547	715	739	
	758	865	882		873	984	998		795	897	902		788	901	911	
	924	926	991		1012	1078	1093		920	961	998		922	990	1001	
	1002	1027	1038		1106	1109	1172		1013	1034	1061		1021	1036	1065	
	1047	1108	1173		1174	1211	1246		1063	1123	1183		1066	1125	1181	
	1189	1278	1302		1288	1330	1378		1198	1273	1324		1199	1274	1321	
	1392	1397	1438		1466	1565	1567		1344	1410	1413		1351	1415	1417	
	1460	1475	1476		1588	1632	1632		1450	1486	1487		1453	1489	1491	
	1491	1500	1501		1635	1650	1668		1488	1507	1525		1492	1508	1530	
	1624	1644	3055		1792	1816	3202		1629	1649	3026		1631	1650	3022	
	3055	3137	3137		3202	3253	3253		3029	3082	3084		3022	3073	3073	
	3157	3157	3180		3279	3280	3341		3112	3112	3152		3100	3101	3145	
	3187	3195	3217		3345	3357	3376		3160	3168	3187		3154	3163	3181	
3,5-dimethyl phenyl	28	29	230	3.9454	3	30	199	3.9820	15	33	201	3.8766	30	44	199	3.8930
	244	282	420	1.7698	224	287	430	1.7975	213	272	405	1.7473	213	275	409	1.7545
	526	550	563	1.2409	480	513	536	1.2579	467	503	519	1.2227	470	507	517	1.2278
	607	737	770		561	682	747		542	680	720		544	674	724	
	912	980	997		865	893	926		839	863	892		835	859	895	
	1002	1014	1015		971	1042	1071		929	994	1004		929	998	1009	
	1038	1109	1110		1110	1141	1151		1026	1059	1061		1027	1062	1063	
	1146	1166	1222		1152	1259	1329		1098	1179	1256		1100	1177	1256	
	1292	1297	1392		1362	1404	1517		1283	1309	1409		1287	1303	1413	
	1393	1475	1478		1528	1565	1567		1411	1434	1471		1415	1437	1472	
	1479	1484	1553		1617	1633	1635		1484	1485	1495		1487	1489	1496	
	1594	1824	1891		1639	1646	1700		1498	1553	1643		1500	1555	1642	
	3071	3071	3160		3198	3199	3253		3029	3030	3086		3023	3026	3074	
	3160	3175	3175		3254	3277	3278		3086	3114	3115		3076	3103	3103	
	3212	3234	3235		3340	3362	3365		3161	3171	3172		3154	3160	3162	

2,4-dimethyl phenyl	78	93	223	3.6978	17	43	195		30	63	194	3.6532	36	64	193	3.6695
	268	273	408	1.8094	235	281	422	3.7508	233	266	398	1.7876	233	270	404	1.7941
	495	536	558	1.2338	436	538	540	1.8321	429	517	533	1.2184	429	520	534	1.2231
	606	746	760		559	705	751	1.2500	538	692	724		541	690	727	
	918	944	995		828	928	948		801	893	904		795	886	907	
	1003	1011	1022		982	1029	1074		939	995	998		948	999	1002	
	1070	1110	1124		1110	1149	1152		1033	1057	1065		1034	1061	1067	
	1140	1215	1221		1199	1244	1315		1144	1177	1246		1143	1176	1247	
	1295	1323	1397		1376	1390	1496		1292	1327	1405		1294	1321	1408	
	1400	1475	1477		1548	1565	1570		1411	1415	1452		1415	1420	1457	
	1479	1486	1540		1630	1632	1634		1483	1487	1497		1485	1490	1499	
	1572	1829	1877		1642	1660	1680		1502	1597	1629		1505	1598	1629	
	3066	3073	3151		3199	3204	3249		3029	3036	3083		3026	3032	3072	
	3163	3169	3175		3257	3277	3279		3092	3114	3117		3081	3103	3106	
	3184	3214	3245		3338	3354	3376		3144	3162	3183		3137	3155	3174	
2,6-dimethyl phenyl	58	64	216	3.7434	28	33	196	3.7887	18	30	191	3.6888	27	39	189	3.7007
	260	266	398	1.7682	219	273	412	1.7942	219	258	387	1.7501	217	261	391	1.7578
	524	540	562	1.2194	473	522	536	1.2363	470	506	518	1.2046	475	509	517	1.2095
	587	764	767		561	713	758		544	697	736		546	696	740	
	885	937	975		809	943	963		789	893	911		780	893	913	
	1018	1024	1050		1012	1027	1061		963	973	1005		979	980	1008	
	1086	1117	1120		1132	1147	1150		1051	1055	1058		1051	1057	1062	
	1147	1169	1237		1161	1246	1344		1111	1185	1253		1111	1186	1253	
	1295	1317	1397		1346	1396	1487		1275	1326	1410		1273	1320	1414	
	1400	1474	1477		1564	1568	1586		1411	1412	1478		1415	1416	1483	
	1478	1487	1552		1630	1630	1638		1482	1483	1496		1485	1485	1498	
	1574	1811	1888		1642	1659	1672		1501	1579	1640		1504	1579	1640	
	3073	3074	3164		3204	3205	3257		3036	3037	3093		3032	3033	3082	
	3164	3175	3175		3258	3279	3279		3093	3117	3118		3082	3106	3106	
	3204	3212	3243		3346	3355	3375		3156	3161	3189		3150	3155	3183	
PC_m	31	46	73	1.2452	12	16	39	1.2651	22	24	53	1.2767	20	23	43	1.2783
	95	221	230	0.7089	50	118	129	0.6712	66	202	210	0.5987	68	199	209	0.5720
	253	285	302	0.5960	202	214	299	0.5678	281	303	366	0.5111	280	282	292	0.4925
	413	448	513		429	436	537		407	424	510		412	426	511	
	520	557	576		538	548	568		514	545	546		518	544	549	
	710	754	758		683	736	767		692	734	742		693	740	746	
	846	963	964		810	900	914		800	875	891		798	882	903	
	984	989	995		973	1008	1035		932	968	980		934	982	992	
	1037	1069	1091		1049	1112	1152		989	1038	1062		995	1040	1066	
	1157	1174	1215		1166	1248	1269		1120	1184	1198		1121	1185	1198	

	1246	1285	1331		1362	1406	1450		1289	1327	1344		1290	1328	1349	
	1399	1472	1476		1514	1568	1598		1414	1434	1484		1419	1440	1488	
	1493	1511	1543		1631	1632	1639		1493	1495	1504		1497	1498	1509	
	1686	1721	2531		1650	1683	2807		1574	1600	2493		1577	1604	2523	
	3064	3149	3171		3201	3253	3281		3034	3089	3119		3029	3077	3107	
	3201	3206	3218		3331	3350	3354		3158	3163	3170		3149	3158	3163	
	3230	3244	3322		3360	3377	3425		3180	3194	3257		3173	3187	3245	
RC$_m$	79	**85**	108	1.3420	16	**20**	26	1.3391	65	**75**	84	1.3294	62	**66**	74	1.3335
	126	141	225	0.9053	**30**	37	217	0.8813	**84**	112	221	0.8768	**80**	107	220	0.8663
	262	270	397	0.7222	243	291	431	0.7073	228	275	399	0.6591	225	277	403	0.6541
	451	503	530		486	556	577		437	511	527		440	515	529	
	535	681	731		578	771	785		534	697	733		538	701	737	
	772	888	907		874	983	1000		796	904	908		791	905	910	
	930	967	988		1013	1079	1093		909	977	983		915	986	1002	
	1004	1036	1042		1108	1109	1172		1017	1041	1056		1022	1042	1061	
	1078	1111	1178		1174	1211	1246		1062	1116	1180		1065	1119	1180	
	1185	1279	1303		1288	1331	1376		1191	1269	1329		1193	1271	1329	
	1393	1396	1428		1466	1566	1568		1345	1406	1407		1351	1411	1413	
	1464	1472	1474		1585	1631	1633		1425	1479	1480		1432	1483	1483	
	1488	1498	1515		1635	1649	1668		1488	1497	1530		1491	1501	1535	
	1620	1661	3053		1790	1812	3203		1581	1624	3033		1589	1627	3028	
	3057	3135	3144		3203	3256	3257		3034	3092	3093		3029	3079	3080	
	3161	3171	3191		3282	3282	3342		3124	3125	3173		3111	3112	3166	
	3197	3206	3222		3348	3359	3378		3185	3189	3197		3177	3180	3189	
3-methyl benzyl	97	216	228	3.6854	51	201	212	3.7365	60	198	209	3.6744	57	197	208	3.6878
	285	413	453	1.8451	299	427	436	1.8694	282	407	423	1.8387	285	412	424	1.8457
	521	522	558	1.2391	538	538	547	1.2557	509	514	543	1.2348	510	519	541	1.2394
	579	711	755		569	681	730		546	689	724		550	690	731	
	758	841	951		768	804	894		743	797	869		747	794	876	
	962	980	982		908	973	1001		887	933	958		898	935	983	
	994	1035	1061		1035	1048	1111		981	990	1039		984	995	1041	
	1088	1154	1171		1151	1166	1248		1062	1119	1183		1065	1120	1184	
	1216	1244	1282		1269	1362	1408		1198	1288	1327		1197	1289	1328	
	1331	1397	1473		1450	1515	1567		1343	1414	1437		1348	1418	1442	
	1477	1494	1510		1598	1631	1632		1485	1493	1495		1488	1497	1498	
	1540	1682	1718		1640	1650	1683		1504	1576	1605		1509	1578	1607	
	3064	3149	3169		3199	3249	3278		3030	3083	3115		3026	3072	3103	
	3200	3206	3214		3329	3345	3349		3156	3162	3164		3147	3157	3158	
	3226	3241	3318		3356	3374	3422		3175	3190	3253		3169	3183	3242	
TS$_m$	871*i*	33	45	1.9814	1562*i*	39	44	2.0156	326*i*	34	46	2.0084	505*i*	33	39	2.0286

	86	202	237	0.4405	53	186	219	0.4289	**47**	196	215	0.4082	48	191	214	0.4090
	281	408	415	0.4069	296	357	428	0.3976	279	403	432	0.3788	282	407	434	0.3794
	456	497	529		442	523	542		492	508	521	0.3932	455	503	523	
	566	583	733		548	572	695		543	584	698		544	570	695	
	761	842	888		767	813	916		744	798	827		747	791	838	
	936	974	983		932	972	1004		864	889	914		880	901	923	
	1014	1018	1032		1022	1042	1058		938	970	993		942	995	999	
	1036	1089	1108		1107	1154	1171		1001	1040	1065		1009	1042	1069	
	1140	1169	1184		1215	1252	1266		1123	1183	1192		1125	1169	1194	
	1231	1252	1291		1303	1367	1405		1242	1324	1345		1218	1308	1336	
	1337	1400	1473		1455	1533	1569		1349	1416	1444		1353	1421	1449	
	1478	1481	1534		1608	1622	1631		1484	1487	1495		1487	1491	1499	
	1567	1740	1772		1643	1668	1698		1513	1584	1614		1519	1590	1618	
	3068	3149	3155		3203	3256	3283		3034	3089	3121		3030	3077	3108	
	3174	3210	3216		3295	3353	3357		3131	3170	3171		3123	3163	3165	
	3229	3246	3260		3364	3381	3383		3182	3198	3227		3175	3190	3214	
												HBr	2620			250.2888
																250.2888

Table S3: Calculated harmonic vibrational wavenumbers and rotational constants of the species involved in *p*-xylene + Br reaction. Imaginary wavenumber is denoted by *i*. Wavenumbers corresponding to the torsional modes are shown in bold.

	MP2/aug-cc-pVDZ				G3				G4				B3LYP/cc-pVTZ			
Species	**Wavenumbers**			**B(GHZ)**	**Wavenumbers**			**B(GHZ)**	**Wavenumbers**			**B(GHZ)**	**Wavenumbers**			**B(GHZ)**
***p*-xylene**	**40**	**48**	138	5.2991	27	35	151	5.3876	**25**	**48**	137	5.4100999	26	45	138	5.4361
	283	307	378	1.4129	304	337	413	1.4344	285	311	383	1.430163	287	311	388	1.4346
	400	452	478	1.1314	458	493	544	1.1490	416	462	502	1.1472284	420	465	500	1.1511
	621	638	728		706	774	780		655	725	729		661	726	731	
	785	832	832		893	902	952		815	836	862		817	839	855	
	893	932	986		1064	1068	1094		942	956	989		961	979	990	
	1014	1021	1036		1112	1127	1172		1024	1036	1061		1025	1046	1065	
	1048	1124	1191		1175	1195	1302		1064	1142	1209		1068	1144	1211	
	1237	1241	1309		1311	1333	1338		1230	1239	1332		1223	1241	1325	
	1395	1396	1406		1466	1567	1567		1336	1412	1413		1348	1417	1417	
	1474	1476	1479		1570	1632	1632		1436	1486	1487		1441	1488	1489	
	1482	1498	1526		1637	1646	1695		1489	1501	1549		1492	1505	1553	
	1609	1653	3055		1775	1828	3200		1615	1658	3026		1617	1660	3023	
	3055	3137	3137		3201	3251	3251		3026	3082	3083		3023	3068	3069	
	3158	3158	3180		3278	3278	3338		3111	3111	3154		3100	3100	3147	
	3186	3198	3204		3346	3359	3367		3156	3172	3175		3151	3164	3169	
4-methyl benzyl	59	146	299	5.4274	19	135	303	5.5070	34	133	293	5.4060264	33	131	296	5.4269
	330	393	425	1.5115	313	395	417	1.5313	303	386	392	1.5077041	300	391	397	1.5132
	473	521	529	1.1911	483	505	543	1.2072	464	501	512	1.1876214	467	497	514	1.1920
	658	706	751		676	697	733		646	697	733		652	707	737	
	759	873	896		782	842	845		750	830	837		752	832	834	
	923	978	1014		857	980	990		844	940	959		846	967	969	
	1032	1033	1073		1035	1074	1093		968	1013	1013		977	1015	1021	
	1080	1148	1168		1145	1209	1256		1054	1147	1185		1058	1151	1184	
	1245	1273	1278		1284	1358	1400		1238	1296	1322		1237	1296	1315	
	1336	1398	1475		1440	1531	1567		1332	1412	1446		1343	1416	1452	
	1476	1495	1512		1613	1622	1634		1485	1488	1494		1488	1491	1497	
	1545	1674	1716		1637	1645	1677		1513	1556	1610		1518	1559	1611	
	3059	3139	3166		3194	3249	3274		3019	3078	3110		3013	3067	3098	
	3200	3205	3209		3329	3344	3345		3156	3159	3160		3147	3153	3154	
	3227	3229	3318		3363	3366	3422		3178	3181	3253		3172	3175	3242	
2,5-dimethyl phenyl	75	93	156	5.8894	18	42	137	5.9641	28	52	134	5.7776134	34	54	133	5.8066

	285	350	391	1.4388	295	307	403	1.4590	277	302	378	1.4252907	279	300	383	1.4303
	471	490	590	1.1735	425	475	522	1.1896	420	454	519	1.159672	422	456	517	1.1641
	680	744	767		678	701	766		649	691	730		655	689	730	
	864	920	977		840	853	890		826	829	867		822	831	861	
	1001	1030	1048		994	1050	1080		945	980	1013		958	982	1018	
	1066	1111	1124		1107	1148	1152		1024	1057	1062		1027	1060	1065	
	1140	1212	1234		1219	1263	1297		1157	1209	1231		1160	1210	1228	
	1299	1311	1395		1370	1382	1502		1280	1316	1410		1282	1309	1414	
	1401	1470	1476		1558	1567	1574		1410	1412	1479		1415	1416	1480	
	1478	1486	1527		1626	1630	1633		1482	1485	1497		1485	1488	1499	
	1606	1818	1894		1642	1648	1691		1503	1565	1645		1506	1566	1644	
	3068	3071	3154		3198	3204	3252		3029	3035	3083		3024	3031	3073	
	3160	3172	3172		3257	3277	3278		3091	3113	3116		3080	3102	3104	
	3198	3224	3228		3344	3356	3364		3151	3163	3176		3145	3153	3169	
TS$_p$	800*i*	36	43	2.4788	1554*i*	19	43	2.5021	296*i*	25	36	2.5228284	485*i*	37	38	2.5534
	59	135	298	0.3919	53	129	285	0.3839	**50**	125	293	0.3652446	50	125	296	0.3655
	331	389	423	0.3853	310	372	407	0.3775	309	383	401	0.3609453	306	389	405	0.3616
	438	488	490		416	490	518		455	507	511	0.363088587	439	502	505	
	547	663	747		523	679	716		562	645	723		512	652	725	
	756	848	893		779	844	857		757	813	837		755	813	835	
	928	935	958		866	986	1010		838	853	872		844	864	894	
	999	1033	1048		1011	1045	1088		952	970	982		977	985	989	
	1064	1090	1112		1097	1150	1200		1019	1021	1055		1024	1032	1060	
	1137	1152	1209		1224	1267	1268		1149	1188	1235		1154	1173	1208	
	1247	1274	1293		1303	1363	1398		1239	1330	1339		1238	1315	1327	
	1342	1398	1476		1450	1538	1568		1351	1411	1448		1349	1417	1455	
	1476	1478	1530		1619	1625	1634		1486	1486	1487		1485	1491	1494	
	1577	1740	1770		1647	1651	1696		1528	1565	1617		1534	1571	1622	
	3066	3149	3151		3199	3257	3282		3025	3086	3119		3024	3069	3108	
	3176	3212	3217		3295	3354	3355		3132	3169	3169		3123	3161	3164	
	3231	3234	3259		3371	3374	3381		3186	3189	3227		3179	3182	3214	
RC$_p$	59	**76**	**126**	1.5890	7	19	23	1.5556	**47**	58	**63**	1.4184472	43	55	60	1.4139
	135	143	197	0.7743	32	36	152	0.7670	78	120	156	0.7673933	69	115	152	0.7603
	286	317	381	0.6275	304	337	413	0.6169	285	313	381	0.5637961	287	312	387	0.5586
	400	452	525		459	493	545		407	455	500		411	458	499	
	630	674	727		706	774	780		645	694	729		651	699	730	
	805	830	856		893	904	954		822	830	875		824	833	870	
	922	954	986		1065	1069	1097		947	966	985		953	986	989	
	1015	1020	1037		1112	1127	1173		1023	1034	1058		1026	1042	1062	
	1067	1126	1193		1176	1195	1302		1065	1137	1201		1069	1141	1203	

	1237	1241	1310		1311	1332	1339		1218	1240	1336		1216	1244	1333	
	1395	1397	1408		1466	1565	1567		1340	1407	1414		1349	1413	1418	
	1472	1473	1476		1570	1632	1632		1419	1479	1484		1427	1483	1487	
	1488	1501	1523		1636	1646	1694		1486	1497	1533		1490	1500	1541	
	1594	1682	3057		1772	1825	3202		1579	1630	3033		1584	1634	3027	
	3057	3139	3144		3202	3253	3254		3033	3089	3091		3028	3077	3077	
	3163	3172	3189		3279	3280	3341		3120	3123	3166		3107	3110	3158	
	3199	3208	3215		3348	3361	3368		3184	3186	3204		3177	3178	3195	
PC$_p$	27	46	58	1.1942	13	17	23	1.2072	18	21	33	1.2341088	15	22	33	1.2336
	78	148	172	0.7538	36	119	121	0.7117	67	135	293	0.5806185	53	132	257	0.5568
	255	299	333	0.5546	137	305	313	0.5324	301	317	324	0.4479453	294	300	303	0.4345
	393	419	473		397	417	483		387	393	464		392	397	467	
	510	529	657		507	541	676		503	513	645		499	514	651	
	706	749	756		699	738	782		704	739	750		711	743	752	
	875	905	937		847	852	857		835	842	847		837	840	845	
	979	1016	1033		985	997	1035		950	963	968		969	971	984	
	1046	1078	1091		1074	1093	1146		1012	1014	1055		1015	1020	1058	
	1149	1168	1246		1209	1256	1284		1146	1185	1237		1150	1185	1237	
	1272	1277	1336		1358	1397	1440		1297	1322	1333		1297	1315	1344	
	1399	1473	1476		1530	1568	1612		1412	1444	1485		1416	1451	1488	
	1494	1512	1547		1622	1633	1636		1487	1495	1512		1490	1499	1518	
	1679	1720	2583		1645	1677	2807		1553	1606	2509		1557	1609	2546	
	3059	3140	3168		3196	3252	3278		3023	3082	3113		3017	3070	3101	
	3202	3206	3213		3331	3348	3349		3158	3162	3164		3150	3155	3157	
	3227	3232	3322		3366	3369	3425		3180	3184	3257		3173	3177	3245	

Table S4 Optimized geometries in cartesian coordinates (**Å**) of various species involved in the reaction of *o*-xylene + Br.

Species		MP2/aug-cc-pVDZ			B3LYP/cc-pVTZ		
***o*-xylene**	C	-0.632046294	-0.534212122	-0.206662932	-0.618665521	-0.513546829	-0.203515161
	C	-0.988467689	0.476226111	-1.116979503	-0.969481005	0.482964779	-1.10237351
	C	-0.32856555	1.718033533	-1.067886554	-0.317412393	1.709396957	-1.053491723
	C	0.685982058	1.972318652	-0.122410999	0.685293413	1.965243443	-0.119786786
	C	1.045836326	0.95213564	0.796680086	1.040985811	0.954835943	0.791422108
	C	0.379417222	-0.289074897	0.740340813	0.379645484	-0.270667883	0.732451344
	H	-1.772928984	0.300721877	-1.85913365	-1.744618174	0.310461968	-1.837244134
	H	-0.60463824	2.506832815	-1.776219554	-0.591503856	2.487461761	-1.755492681
	C	1.383132933	3.313904464	-0.086156703	1.371258379	3.305975835	-0.095738344
	H	1.251139748	3.806618404	0.892053079	1.249626897	3.804618208	0.868985022
	H	2.468317754	3.20503631	-0.252304373	2.44654577	3.212600019	-0.266622839
	H	0.983893238	3.983334782	-0.86271815	0.968583621	3.964679359	-0.863724
	H	-1.135997926	-1.504957184	-0.232375046	-1.116369259	-1.473939978	-0.227548078
	H	0.658790876	-1.074937688	1.450641781	0.653467835	-1.048741614	1.434593639
	C	2.130326084	1.195608065	1.82224943	2.11859027	1.183239354	1.818769506
	H	1.873679384	2.041595396	2.482189762	1.877050303	2.020853977	2.477622496
	H	3.090896895	1.440047152	1.337856512	3.077876896	1.41887464	1.351448934
	H	2.281286486	0.305294059	2.450842289	2.25917985	0.30021543	2.440250495
3,4-dimethyl phenyl	C	-0.447384782	-0.694165794	0.58611558	-0.453188193	-0.701509481	0.584834476
	C	-0.724796796	0.330615567	-0.260867808	-0.728861924	0.330081817	-0.269250648
	C	-0.094540277	1.54413535	-0.265542941	-0.09840365	1.545777822	-0.276318739
	C	0.906581091	1.755144202	0.661963418	0.917968897	1.769010839	0.663676104
	C	1.238607685	0.742313057	1.559289487	1.247805334	0.744175967	1.570246432
	C	0.561822486	-0.456214345	1.507346537	0.561800384	-0.468753627	1.518337497
	H	-0.36599816	2.3293488	-0.975827893	-0.364274094	2.324370242	-0.98058861
	C	1.637683536	3.07954183	0.701952914	1.636490005	3.092365536	0.689143529
	H	1.519527021	3.563161014	1.685463648	1.527656697	3.589682486	1.655924645
	H	2.717804048	2.936419449	0.534622614	2.70849854	2.970573662	0.516520941
	H	1.254226881	3.762420776	-0.069203813	1.249347744	3.762726662	-0.076480582
	H	-0.976616328	-1.648226262	0.554655593	-0.977731822	-1.64708115	0.555323019
	H	0.828751461	-1.24758129	2.216277977	0.821706108	-1.25268262	2.220203115
	C	2.334288314	0.960449842	2.58134032	2.334798483	0.947255347	2.59460902
	H	2.09928106	1.809919512	3.243906511	2.115082049	1.789597937	3.254821103
	H	3.297531375	1.183187119	2.093108891	3.298091651	1.15922341	2.124432782
	H	2.466563816	0.065592596	3.206419696	2.456546222	0.06124657	3.215586646
2,3-dimethyl phenyl	C	-0.422671775	-0.67388737	0.596741602	-0.428974726	-0.686702876	0.597737114
	C	-0.771677569	0.317414618	-0.292652393	-0.775845725	0.321427009	-0.303264446
	C	-0.067025364	1.484154221	-0.185087885	-0.068101347	1.489406851	-0.195012311
	C	0.931194565	1.767925114	0.696773653	0.937023795	1.780080404	0.693023826
	C	1.259681066	0.742816762	1.582953857	1.272421257	0.74539095	1.596602888
	C	0.582411829	-0.456498924	1.521088272	0.58122759	-0.46466516	1.527781221
	C	1.64126905	3.103645388	0.719905128	1.636591327	3.114349001	0.70380542
	H	1.522355799	3.594420611	1.699681974	1.525411006	3.615147176	1.668284809
	H	2.721506846	2.9770114	0.540981315	2.708281745	3.004334854	0.522875975
	H	1.234965364	3.767935703	-0.054548597	1.229434291	3.767356932	-0.065033962
	H	-0.942402941	-1.63635492	0.571709534	-0.945586537	-1.637862725	0.571918248
	H	0.849053727	-1.252966742	2.221435223	0.841852793	-1.25354506	2.222064031
	C	2.356769717	0.959054426	2.603120871	2.360195347	0.947387314	2.618889909
	H	2.116451316	1.807211876	3.264929871	2.136431086	1.785586745	3.282879345

	H	3.313935674	1.190671496	2.107841246	3.320007785	1.168106902	2.145860914
	H	2.494851493	0.062409258	3.223791021	2.487177478	0.057742858	3.23380032
	H	-1.560353227	0.176948355	-1.03401487	-1.557231594	0.178370095	-1.03756348
PC*o*	C	0.013292325	0.257061965	-1.635687179	0.161992715	0.210821846	-1.662772553
	C	-0.426617619	1.278249059	-0.794125093	-0.227396518	1.137255158	-0.691929054
	C	0.448837539	2.307271698	-0.445594214	0.62823051	2.190995393	-0.359902725
	C	1.745630929	2.349998324	-0.907356584	1.864471014	2.35176513	-0.964113679
	C	2.204311425	1.316906388	-1.775253229	2.276308037	1.406897809	-1.962026103
	C	1.30232062	0.278708108	-2.117160702	1.385166643	0.343504318	-2.28186672
	H	-1.445255006	1.269870221	-0.400409018	-1.190642887	1.050399604	-0.207781789
	H	0.101323224	3.097431688	0.226477798	0.316865221	2.90580114	0.3917383
	C	2.676070648	3.460107352	-0.483107297	2.754310423	3.498963209	-0.576136872
	H	3.54411829	3.053211278	0.061851419	3.709951145	3.148993857	-0.178719013
	H	3.05748777	4.015278697	-1.355675613	2.980556883	4.13888706	-1.432250735
	H	2.155677271	4.16813155	0.177423506	2.281194323	4.115139699	0.186474866
	H	1.629358749	-0.163782368	0.22826655	0.925777329	-0.206238401	1.134853742
	H	1.655469504	-0.523260944	-2.7721384	1.691279723	-0.372497804	-3.033761694
	Br	2.244431589	-0.54671308	1.463032832	1.309542872	-0.982250151	2.275478769
	H	-0.659039341	-0.560533124	-1.906838752	-0.494644456	-0.607020898	-1.92754105
	C	3.5298002	1.290276503	-2.278617562	3.508506222	1.499619711	-2.61730635
	H	4.258149849	2.060304957	-2.030722601	4.215575933	2.286085618	-2.407453358
	H	3.847764105	0.477128948	-2.932267791	3.786086939	0.768524922	-3.362885912
RC*o*	C	-0.132684763	-0.235660258	-0.322916587	-0.181209902	-0.219792968	-0.359302192
	C	-0.727132756	0.985051081	-0.757271045	-0.744530856	0.978883667	-0.813683146
	C	0.047334806	2.155416426	-0.759495676	0.02751685	2.142056082	-0.776917456
	C	1.398164742	2.15126147	-0.34351099	1.33807822	2.149621541	-0.299282634
	C	1.989424754	0.961382413	0.095513914	1.898763724	0.976298369	0.158181756
	C	1.22346338	-0.225644821	0.110593161	1.138698796	-0.205286098	0.135337982
	H	-0.409986284	3.093889558	-1.090582392	-0.410497721	3.067938237	-1.128754707
	C	-0.892984949	-1.536342201	-0.418163286	-0.952860724	-1.506790121	-0.389176963
	H	-0.329811076	-2.352620869	0.057005046	-0.359903164	-2.330620582	0.001772982
	H	-1.066836037	-1.798534821	-1.476062079	-1.26439769	-1.759278095	-1.405719526
	H	-1.873133081	-1.462743803	0.077831863	-1.860551747	-1.435307139	0.213567802
	H	1.686163611	-1.17114533	0.411326759	1.609222458	-1.142971175	0.393652886
	Br	-0.245881311	-0.014334107	2.449738303	0.522748146	-0.235391497	2.84300184
	H	1.975380339	3.080344612	-0.359468987	1.902588865	3.071596049	-0.285560449
	H	3.029437376	0.944485686	0.432324442	2.909989964	0.952161838	0.538164514
	C	-2.177888332	1.010980063	-1.172974509	-2.157699196	1.025311958	-1.328985366
	H	-2.8260212	0.744343025	-0.320360232	-2.870551656	0.719634058	-0.559817962
	H	-2.379974425	0.288137159	-1.980693265	-2.300160221	0.352340101	-2.177379334
	H	-2.466047114	2.012583195	-1.524789238	-2.424256465	2.030444256	-1.651054828
2-methyl benzyl	C	-0.368749552	-0.715015758	0.572270435	-0.367940206	-0.714975723	0.573016043
	C	-0.722319522	0.300204326	-0.315405102	-0.721839811	0.300869824	-0.315960292
	C	-0.111146297	1.527545447	-0.223929662	-0.110679488	1.531971846	-0.226153097
	C	0.878011727	1.793467956	0.756557897	0.882985689	1.805823501	0.756068517
	C	1.231737998	0.746683786	1.659653202	1.236630792	0.752354396	1.663077495
	C	0.603579696	-0.472943235	1.545417372	0.602900032	-0.473599088	1.545959173
	C	1.483291656	3.072132622	0.816615401	1.476814648	3.071245302	0.809118398
	H	2.246329918	3.31778033	1.553376045	2.233432571	3.324348192	1.534670398
	H	1.188102953	3.848812658	0.109781484	1.184610213	3.840648816	0.108888124
	H	-0.846974024	-1.695151174	0.510270242	-0.841447599	-1.685372559	0.511329082
	H	0.875647819	-1.274860885	2.238497134	0.871123592	-1.267676982	2.232122306
	C	2.279425986	0.97625472	2.723378516	2.277602694	0.969571333	2.725444728
	H	1.984342674	1.795057072	3.40018133	1.999045075	1.781435258	3.401610168
	H	3.247988979	1.249830112	2.273248631	3.245105921	1.235047502	2.292370672

	H	2.423488598	0.067110325	3.324769611	2.414877162	0.069577226	3.322696029
	H	-1.481803181	0.121422305	-1.080515917	-1.473620555	0.122900952	-1.073467872
	H	-0.383597058	2.328830323	-0.917123628	-0.38224236	2.322991134	-0.913746881
TS_o	C	-0.803125725	-0.476378981	-0.075511095	-0.818809828	-0.490005094	-0.062924942
	C	-1.181313347	0.512336123	-0.97273915	-1.159412559	0.501652798	-0.98174312
	C	-0.572719937	1.742447473	-0.908304263	-0.536213447	1.729647446	-0.916350991
	C	0.407117995	2.017803033	0.054980241	0.438780281	2.011862294	0.070127289
	C	0.800542368	1.003536097	0.953756849	0.792721017	0.986961436	0.996731401
	C	0.180973709	-0.223234562	0.872898598	0.147533194	-0.237960358	0.908757198
	H	-1.950049727	0.313606163	-1.722683823	-1.905513417	0.309536488	-1.740526589
	H	-0.85637216	2.532438318	-1.609911194	-0.791176887	2.505572486	-1.626554869
	C	1.037098492	3.321233939	0.081262347	1.062368996	3.292169487	0.088287416
	H	1.505545027	3.674930232	1.004371608	1.601588064	3.621089603	0.965844735
	H	2.291531229	3.058813846	-0.614402233	2.343211734	3.138522726	-0.772332556
	H	0.622179443	4.100053975	-0.567298181	0.632360145	4.080341549	-0.51701055
	H	-1.274929876	-1.461387889	-0.115465358	-1.299424286	-1.458102721	-0.10450395
	H	0.47689927	-1.017042425	1.564544182	0.407535286	-1.018853208	1.611968923
	C	1.894276145	1.2558523	1.96442073	1.847261235	1.216098802	2.043185463
	H	1.607738314	2.056605759	2.665908264	1.577612491	2.034176814	2.71526888
	H	2.822568387	1.565858519	1.457379615	2.807482491	1.474139466	1.591948591
	H	2.099359095	0.346311544	2.546362232	1.990446752	0.322861617	2.6482871
	Br	3.707704456	2.812742588	-1.263841019	3.676671898	3.11681442	-1.602731079

Table S5 Optimized geometries in cartesian coordinates (**Å**) of various species involved in the reaction of *m*-xylene + Br.

Species		MP2/aug-cc-pVDZ			B3LYP/cc-pVTZ		
***m*-xylene**	C	-0.59379	-0.54352	-0.22015	-0.54092	-0.55226	-0.25777
	C	-0.85092	0.41735	-1.21464	-0.81600	0.41086	-1.22139
	C	-0.20084	1.66411	-1.17778	-0.21547	1.66036	-1.15550
	C	0.71356	1.96444	-0.14649	0.67427	1.96409	-0.12386
	C	0.95720	0.98714	0.84086	0.93432	0.98645	0.83433
	C	0.31601	-0.26899	0.82233	0.33780	-0.27454	0.78765
	H	-1.55866	0.19432	-2.01919	-1.50243	0.18501	-2.02719
	H	-0.40488	2.40887	-1.95499	-0.43640	2.40548	-1.90984
	H	1.66636	1.21062	1.64705	1.62213	1.21242	1.64182
	C	1.41265	3.30675	-0.10797	1.35701	3.30626	-0.06489
	H	2.08878	3.37651	0.75759	1.68372	3.54342	0.94738
	H	2.00907	3.46698	-1.02111	2.24149	3.32593	-0.70713
	H	0.68248	4.12968	-0.03826	0.69500	4.10413	-0.40290
	H	-1.10297	-1.51303	-0.25374	-1.01329	-1.52491	-0.31725
	C	0.59189	-1.30406	1.89216	0.61953	-1.29652	1.85871
	H	-0.33163	-1.56739	2.43344	0.00225	-1.11927	2.74337
	H	1.32239	-0.93054	2.62568	1.66117	-1.26104	2.17973
	H	0.99460	-2.23018	1.45018	0.40713	-2.30679	1.50968
3,5-dimethyl phenyl	C	-0.46062	-0.28085	-0.37741	-0.53710	-0.25339	-0.33156
	C	-0.69610	0.68694	-1.30619	-0.78585	0.72295	-1.25914
	C	-0.13299	1.92608	-1.35275	-0.18789	1.95077	-1.32487
	C	0.77134	2.22684	-0.34956	0.77866	2.24135	-0.34745
	C	1.04674	1.27912	0.61917	1.06227	1.27386	0.61584
	C	0.44574	0.03362	0.61972	0.42857	0.02930	0.64552
	H	-0.37536	2.64971	-2.13485	-0.44005	2.67887	-2.08586
	H	1.76278	1.52241	1.41021	1.80267	1.49784	1.37475
	C	1.44876	3.58284	-0.31964	1.49077	3.56968	-0.35555
	H	2.13450	3.66254	0.53580	2.10300	3.69669	0.53634
	H	2.02416	3.74613	-1.24379	2.14582	3.65872	-1.22521
	H	0.69967	4.38570	-0.24165	0.78229	4.39854	-0.39991
	H	-0.95502	-1.25482	-0.40925	-1.05625	-1.20360	-0.33650
	C	0.77113	-0.98166	1.69763	0.78876	-0.99889	1.68692
	H	-0.13825	-1.25849	2.25278	-0.07149	-1.61273	1.95419
	H	1.50480	-0.57902	2.41036	1.16609	-0.52875	2.59493
	H	1.18626	-1.89798	1.25061	1.56730	-1.67212	1.31877
2,4-dimethyl phenyl	C	-0.49614	-0.16162	-0.32842	-0.51359	-0.15982	-0.31150
	C	-0.88701	0.73960	-1.26169	-0.91662	0.74812	-1.24909
	C	-0.24110	1.97176	-1.25692	-0.25847	1.98421	-1.25668
	C	0.74535	2.24312	-0.33986	0.75585	2.25261	-0.34083
	C	1.08955	1.26493	0.58626	1.10899	1.26666	0.58613
	C	0.47962	0.03107	0.62150	0.47782	0.01831	0.62833
	H	-0.52510	2.73002	-1.99346	-0.54271	2.73568	-1.98336
	C	1.45569	3.58211	-0.32554	1.46093	3.58584	-0.33323
	H	1.31573	4.08926	0.64201	1.21633	4.15801	0.56472
	H	2.53784	3.45296	-0.48429	2.54520	3.46276	-0.35094
	H	1.06881	4.24019	-1.11711	1.17881	4.18844	-1.19570
	C	0.85620	-1.03153	1.63042	0.86345	-1.04345	1.62419
	H	-0.01339	-1.30545	2.24657	0.00251	-1.35713	2.21628
	H	1.65542	-0.66946	2.29311	1.63192	-0.68092	2.30580

	H	1.20791	-1.94130	1.12104	1.24810	-1.93185	1.12024
	H	-1.67208	0.51837	-1.98856	-1.70485	0.53573	-1.95973
	H	1.87724	1.48060	1.31911	1.90087	1.47141	1.29953
2,6-dimethyl phenyl	C	-0.59881	-0.17703	-0.23806	-0.61464	-0.18595	-0.23534
	C	-0.96190	0.79972	-1.14107	-0.98224	0.80296	-1.14064
	C	-0.27528	1.99412	-1.19844	-0.28793	2.00562	-1.20482
	C	0.79377	2.24125	-0.35199	0.80149	2.24911	-0.35515
	C	1.08940	1.22503	0.51147	1.09859	1.22206	0.50793
	C	0.46241	0.01751	0.63165	0.46772	0.00801	0.63578
	H	-0.57232	2.76284	-1.91957	-0.58432	2.76739	-1.91635
	C	1.57068	3.54000	-0.38630	1.57619	3.54073	-0.39015
	H	1.51896	4.04906	0.58782	1.48030	4.08100	0.55332
	H	2.63090	3.35218	-0.61299	2.63958	3.35738	-0.54972
	H	1.16268	4.21273	-1.15452	1.21841	4.18900	-1.18906
	H	-1.15119	-1.12187	-0.20123	-1.16438	-1.11906	-0.19633
	C	0.88945	-1.03161	1.63588	0.89643	-1.03767	1.63194
	H	0.24855	-1.92185	1.55901	0.28474	-1.93460	1.54379
	H	0.82049	-0.63828	2.66119	0.80822	-0.66548	2.65399
	H	1.93244	-1.33511	1.46036	1.93932	-1.32011	1.48090
	H	-1.80213	0.62551	-1.81798	-1.81937	0.63382	-1.80487
PC$_m$	C	-0.09471	0.12900	-1.39102	-0.18490	0.16969	-1.47306
	C	-0.46094	1.24329	-0.66723	-0.56533	1.29800	-0.77494
	C	0.42117	2.30333	-0.49658	0.33688	2.33752	-0.55424
	C	1.70691	2.25306	-1.05706	1.65367	2.25594	-1.03654
	C	2.07257	1.14248	-1.78198	2.03540	1.12045	-1.73062
	C	1.18801	0.04824	-1.97341	1.13538	0.04418	-1.98013
	H	-1.45507	1.29149	-0.21497	-1.57487	1.37788	-0.39347
	H	0.12087	3.17642	0.08903	0.02252	3.21604	-0.00566
	H	3.07505	1.08736	-2.21940	3.04451	1.04682	-2.11832
	C	2.67322	3.39440	-0.83053	2.61867	3.38796	-0.79880
	H	2.91492	3.48364	0.24099	2.74831	3.57748	0.26848
	H	3.61020	3.23666	-1.38364	3.59827	3.17292	-1.22304
	H	2.23123	4.34883	-1.15653	2.25318	4.31346	-1.24820
	H	2.20182	0.44529	0.37849	2.65903	0.26917	0.54530
	Br	2.53369	-0.14943	1.64318	3.21277	-0.23372	1.76819
	C	1.59158	-1.09371	-2.71329	1.53892	-1.08909	-2.69507
	H	0.91314	-1.93629	-2.84982	0.85366	-1.90314	-2.88136
	H	2.58780	-1.15066	-3.15283	2.54541	-1.18018	-3.07699
	H	-0.79088	-0.70478	-1.51355	-0.89090	-0.63278	-1.64167
RC$_m$	C	-0.13798	-0.23350	-0.32693	-0.17979	-0.20392	-0.39540
	C	-0.73362	0.99019	-0.72715	-0.74267	1.00317	-0.78053
	C	0.01805	2.16904	-0.74406	0.00632	2.17690	-0.73938
	C	1.37935	2.15799	-0.35770	1.33483	2.16665	-0.32151
	C	2.00249	0.96889	0.04631	1.93852	0.98204	0.07200
	C	1.23586	-0.22444	0.04322	1.16107	-0.19958	0.05443
	H	-1.78889	1.00371	-1.01760	-1.77023	1.03232	-1.11790
	H	-0.44948	3.10915	-1.05239	-0.44997	3.11061	-1.04127
	C	-0.90562	-1.52996	-0.43034	-0.95076	-1.49030	-0.44843
	H	-0.41442	-2.32735	0.14591	-1.05227	-1.91698	0.55090
	H	-0.96841	-1.84688	-1.48513	-0.43664	-2.23006	-1.06591
	H	-1.93028	-1.40808	-0.04711	-1.94735	-1.33862	-0.85943
	H	1.71461	-1.17325	0.31208	1.64916	-1.14569	0.24502
	Br	-0.10387	-0.06663	2.44888	0.63368	-0.29513	2.73292
	H	1.95140	3.09150	-0.36432	1.90135	3.08824	-0.30666
	C	3.43621	0.93589	0.51875	3.37626	0.92809	0.49808

	H	3.93906	1.89641	0.33077	3.83566	1.91464	0.47079
	H	4.00440	0.14039	0.01002	3.95208	0.26775	-0.15454
	H	3.47166	0.73346	1.60276	3.46128	0.53640	1.51277
3-methyl benzyl	C	-0.72718	-0.42121	-0.10488	-0.73087	-0.42058	-0.10306
	C	-1.00434	0.58228	-1.02817	-1.00786	0.58481	-1.02853
	C	-0.23685	1.72489	-1.07620	-0.23666	1.72801	-1.07719
	C	0.84667	1.89357	-0.18457	0.85443	1.90211	-0.18497
	C	1.10677	0.85442	0.74661	1.10940	0.85704	0.74630
	C	0.34130	-0.28487	0.79431	0.33872	-0.28886	0.79728
	H	-1.84057	0.46090	-1.72215	-1.83670	0.46581	-1.71436
	H	-0.45764	2.51123	-1.80303	-0.45625	2.50579	-1.79702
	H	1.94392	0.97474	1.44215	1.93839	0.97354	1.43414
	C	1.64945	3.06197	-0.21704	1.64757	3.05510	-0.21936
	H	2.48411	3.18595	0.47376	2.47749	3.18340	0.46047
	H	1.44605	3.85799	-0.93419	1.44981	3.84684	-0.92744
	H	-1.34470	-1.32356	-0.07752	-1.34520	-1.31178	-0.07702
	C	0.63063	-1.38512	1.79313	0.63049	-1.38313	1.79124
	H	-0.23862	-1.55345	2.44847	-0.23332	-1.57549	2.43086
	H	1.49451	-1.12986	2.42382	1.47181	-1.12454	2.43291
	H	0.84812	-2.33271	1.27529	0.87038	-2.32088	1.28551
TS*m*	C	-0.96910	-0.31088	-0.17329	-0.97782	-0.33649	-0.18044
	C	-1.33850	0.78316	-0.93697	-1.34889	0.76808	-0.94299
	C	-0.48439	1.85622	-1.07067	-0.49465	1.84625	-1.07166
	C	0.76182	1.83507	-0.44043	0.76649	1.83401	-0.43722
	C	1.11469	0.71894	0.33448	1.11407	0.70234	0.33655
	C	0.26838	-0.35382	0.47372	0.26378	-0.38111	0.47109
	H	-2.31232	0.79438	-1.43298	-2.31211	0.78078	-1.43514
	H	-0.77326	2.72512	-1.66796	-0.78394	2.70771	-1.65877
	H	2.08828	0.71116	0.83538	2.07556	0.69185	0.83510
	C	1.66177	2.96887	-0.54509	1.65117	2.94670	-0.54368
	H	1.28431	3.77152	0.58578	1.29024	3.87872	0.63592
	H	2.71204	2.82381	-0.27063	2.68494	2.82528	-0.24489
	H	1.46946	3.71019	-1.32791	1.46416	3.69238	-1.30629
	H	-1.65572	-1.15690	-0.07266	-1.65788	-1.17380	-0.08600
	C	0.64968	-1.55820	1.30707	0.64878	-1.58229	1.29364
	H	0.64709	-2.47220	0.69281	0.66387	-2.48816	0.68434
	H	-0.06924	-1.70226	2.12868	-0.06572	-1.74943	2.10189
	H	1.65156	-1.43568	1.74234	1.63514	-1.46040	1.73843
	Br	0.94958	4.71598	1.81143	1.03891	4.92205	1.78322

Table S6 Optimized geometries in cartesian coordinates (**Å**) of various species involved in the reaction of *p*-xylene + Br.

		MP2/aug-cc-pVDZ			B3LYP/cc-pVTZ		
Species		**X**	**Y**	**Z**	**X**	**Y**	**Z**
***p*-xylene**	C	-0.29482	-0.29679	-0.04485	-0.28308	-0.28769	-0.04802
	C	-0.66830	0.80823	-0.83402	-0.66777	0.81661	-0.80266
	C	0.05756	2.01487	-0.78434	0.04840	2.00906	-0.75258
	C	1.17914	2.15344	0.05603	1.17511	2.13980	0.05376
	C	1.55397	1.04498	0.84780	1.56319	1.03019	0.80913
	C	0.83033	-0.15797	0.79827	0.85002	-0.15756	0.75913
	H	-1.53696	0.72724	-1.49653	-1.53937	0.74743	-1.44217
	H	-0.25451	2.85912	-1.40875	-0.27650	2.84906	-1.35443
	H	2.42300	1.12571	1.51072	2.43921	1.09779	1.44344
	H	1.14279	-1.00245	1.42310	1.17909	-1.00049	1.35530
	C	1.96622	3.44451	0.11754	1.95082	3.42974	0.12005
	H	1.96339	3.86017	1.13859	1.88094	3.88400	1.11126
	H	3.01707	3.28027	-0.17234	3.01102	3.26805	-0.08432
	C	-1.06689	-1.59757	-0.09003	-1.06104	-1.57739	-0.08633
	H	-1.47211	-1.85069	0.90346	-1.57530	-1.75814	0.86075
	H	-0.41834	-2.43062	-0.40738	-0.40617	-2.43238	-0.26394
	H	-1.90908	-1.53306	-0.79560	-1.81430	-1.56305	-0.87333
	H	1.53971	4.20013	-0.55952	1.57789	4.15449	-0.60290
4-methyl benzyl	C	-0.19647	-0.34856	0.05500	-0.20586	-0.35575	0.05788
	C	1.20893	-0.25585	-0.06322	1.21119	-0.26232	-0.00503
	C	1.85005	0.96170	0.00518	1.85189	0.95667	0.05267
	C	1.14058	2.14787	0.19321	1.13608	2.15569	0.17709
	C	-0.25464	2.06674	0.31171	-0.26296	2.07781	0.23569
	C	-0.90805	0.86403	0.24596	-0.91978	0.86784	0.17943
	H	1.78924	-1.17117	-0.21130	1.78981	-1.17204	-0.10389
	H	2.93947	1.00152	-0.08979	2.93343	0.99123	-0.00092
	H	-0.83119	2.98556	0.45980	-0.83893	2.99110	0.32526
	H	-1.99720	0.82666	0.34116	-2.00114	0.83813	0.22392
	C	1.84133	3.48477	0.26863	1.84438	3.47823	0.27462
	H	1.48542	4.16060	-0.52607	1.25206	4.28154	-0.16464
	H	1.64571	3.97724	1.23515	2.03250	3.74958	1.31783
	C	-0.86750	-1.59550	-0.01375	-0.86490	-1.58850	-0.00133
	H	-0.31047	-2.52139	-0.16081	-0.31294	-2.51251	-0.09543
	H	-1.95258	-1.65148	0.07915	-1.94267	-1.64803	0.04554
	H	2.92932	3.36821	0.15746	2.80978	3.45230	-0.23122
2,5-dimethyl phenyl	C	-0.32918	-0.25235	0.01248	-0.34170	-0.26123	0.02445
	C	-0.74298	0.86776	-0.66759	-0.73817	0.86258	-0.69709
	C	0.02556	2.02336	-0.69177	0.03053	2.02356	-0.72793
	C	1.23501	2.10950	-0.04066	1.24199	2.11834	-0.03296
	C	1.59085	0.95764	0.61920	1.57894	0.97802	0.66212
	C	0.89072	-0.20055	0.68317	0.87087	-0.18748	0.73305
	H	-1.69718	0.85084	-1.20159	-1.67005	0.83461	-1.24786
	H	-0.33922	2.89601	-1.24562	-0.31484	2.87738	-1.30004
	H	1.26179	-1.06700	1.23812	1.21929	-1.03364	1.31345
	C	2.09083	3.35677	-0.05184	2.09277	3.36037	-0.04999
	H	2.24956	3.73133	0.97078	2.26118	3.73651	0.96027
	H	3.07825	3.14961	-0.49152	3.07292	3.15955	-0.48611
	C	-1.16349	-1.51671	0.04265	-1.16407	-1.52330	0.04072
	H	-1.43321	-1.78072	1.07715	-1.26530	-1.91908	1.05237

	H	-0.60401	-2.36280	-0.38601	-0.69998	-2.30427	-0.56666
	H	-2.09077	-1.38793	-0.53409	-2.16409	-1.34812	-0.35451
	H	1.60664	4.14906	-0.64141	1.61888	4.15002	-0.63186
TS$_p$	C	-0.00098	-0.02262	-0.00252	-0.02422	-0.02962	-0.01631
	C	0.07168	0.12767	1.37702	0.05579	0.12193	1.37259
	C	1.27684	0.03922	2.03629	1.26476	0.03664	2.03387
	C	2.45918	-0.21291	1.33510	2.46335	-0.21392	1.32978
	C	2.38152	-0.35762	-0.05929	2.37608	-0.35732	-0.07505
	C	1.17927	-0.26802	-0.70792	1.16372	-0.27043	-0.72323
	H	-0.84331	0.32120	1.94386	-0.84830	0.31139	1.93708
	H	1.31596	0.16552	3.12218	1.30286	0.16291	3.10809
	H	3.29766	-0.54526	-0.62693	3.28051	-0.53795	-0.64141
	H	1.13813	-0.38758	-1.79481	1.12490	-0.38784	-1.79915
	C	3.73480	-0.27287	2.01907	3.71581	-0.28104	2.00307
	H	4.58669	-0.71244	1.48941	4.57198	-0.68694	1.47886
	H	4.18024	1.10100	1.98303	4.25814	1.17390	2.02223
	C	-1.31924	0.07741	-0.73408	-1.33878	0.05885	-0.73841
	H	-1.53372	-0.85835	-1.27433	-1.58586	-0.88952	-1.22163
	H	-1.28754	0.89132	-1.47570	-1.30638	0.81694	-1.52366
	H	-2.14675	0.27424	-0.03794	-2.15200	0.31055	-0.05965
	H	3.73314	-0.39602	3.10729	3.72611	-0.38995	3.08039
	Br	4.74642	2.57785	1.98908	4.92155	2.59317	2.12135
RC$_p$	C	-0.13150	-0.23849	-0.33647	-0.18347	-0.20917	-0.42613
	C	-0.72694	0.99910	-0.69270	-0.74114	1.01387	-0.77269
	C	0.01141	2.18529	-0.65776	-0.00032	2.18929	-0.69828
	C	1.37867	2.19348	-0.27346	1.33491	2.19613	-0.27412
	C	1.97870	0.97443	0.07243	1.90186	0.98063	0.07152
	C	1.23789	-0.22881	0.04970	1.15909	-0.20988	0.01373
	H	-1.77980	1.01871	-0.99274	-1.76857	1.05425	-1.11068
	H	-0.47190	3.12986	-0.93127	-0.46942	3.12494	-0.97791
	H	3.03022	0.95233	0.37579	2.93156	0.93745	0.40033
	C	2.14604	3.49428	-0.22348	2.10782	3.48386	-0.18075
	H	1.76096	4.13969	0.58337	1.80386	4.05691	0.69854
	H	3.21573	3.31673	-0.03720	3.17805	3.29936	-0.09895
	C	-0.89090	-1.53393	-0.49466	-0.95835	-1.49062	-0.51443
	H	-0.40113	-2.34857	0.05826	-1.07671	-1.93513	0.47553
	H	-0.94018	-1.81364	-1.56061	-0.43918	-2.22232	-1.13711
	H	-1.92019	-1.43205	-0.11805	-1.94851	-1.32721	-0.93662
	H	2.04540	4.04760	-1.17123	1.93733	4.11480	-1.05405
	H	1.72962	-1.17752	0.28745	1.65942	-1.15262	0.18270
	Br	-0.14966	-0.19937	2.45094	0.69422	-0.42541	2.72769
PC$_p$	C	-0.05374	0.14488	-1.52973	-0.11948	0.19942	-1.50062
	C	-0.44530	1.22718	-0.71124	-0.54595	1.34694	-0.77833
	C	0.40811	2.27924	-0.46401	0.30646	2.40458	-0.54272
	C	1.69168	2.31931	-1.00801	1.63079	2.39731	-1.00215
	C	2.08796	1.25436	-1.82959	2.06537	1.27173	-1.71886
	C	1.24904	0.19746	-2.08594	1.22673	0.20289	-1.96243
	H	-1.44239	1.21711	-0.26199	-1.56415	1.38370	-0.41269
	H	0.07792	3.09720	0.18307	-0.05475	3.26356	0.00951
	H	3.09240	1.26139	-2.26493	3.08137	1.24477	-2.09390
	C	2.64500	3.44987	-0.70244	2.56317	3.54008	-0.71312
	H	3.46846	3.09741	-0.05904	3.14606	3.35259	0.19341
	H	3.09068	3.85176	-1.62615	3.27355	3.69147	-1.52648
	C	-0.91992	-0.95190	-1.77953	-0.97867	-0.87562	-1.74989
	H	-1.91773	-0.98458	-1.34133	-1.99918	-0.86739	-1.39568

	H	-0.60027	-1.78259	-2.40924	-0.64328	-1.74226	-2.30079
	H	2.13183	4.26962	-0.17898	2.01722	4.47097	-0.56077
	H	1.98105	0.04079	0.20919	2.40989	-0.52662	0.21499
	H	1.58646	-0.62643	-2.72161	1.58636	-0.64657	-2.52927
	Br	2.33706	-0.44982	1.50756	3.06680	-1.19929	1.29587

Table S7. G3 standard heat of reaction ($\Delta rxn_{,0\,K}H^0$) for various substitution reactions of toluene + Br reaction system. The $\Delta rxn_{,0\,K}H^0$ of Reaction (R1) appears to be lower than the other substitution reactions of Br atoms. However, the transition state responsible for methyl substitution by Br atom lies at 156.7 kJ/mol higher in energy than the reactants. For toluene + Br system, the reactions (R1-R4) appear kinetically irrelevant. These results are taken from our recent work (Giri et al., *Int. J. Chem. Kinet*., 2021, **53**, 390-402).

Reaction	$\Delta_{rxn,0K}H^0$ (kJ/mol)
$C_6H_5CH_3 + Br \rightarrow C_6H_5Br + CH_3$ (R1)	74
$C_6H_5CH_3 + Br \rightarrow$ 2-bromotoluene + H (R2)	113.2
$C_6H_5CH_3 + Br \rightarrow$ 3-bromotoluene + H (R3)	115.1
$C_6H_5CH_3 + Br \rightarrow$ 4-bromotoluene + H (R4)	116.1

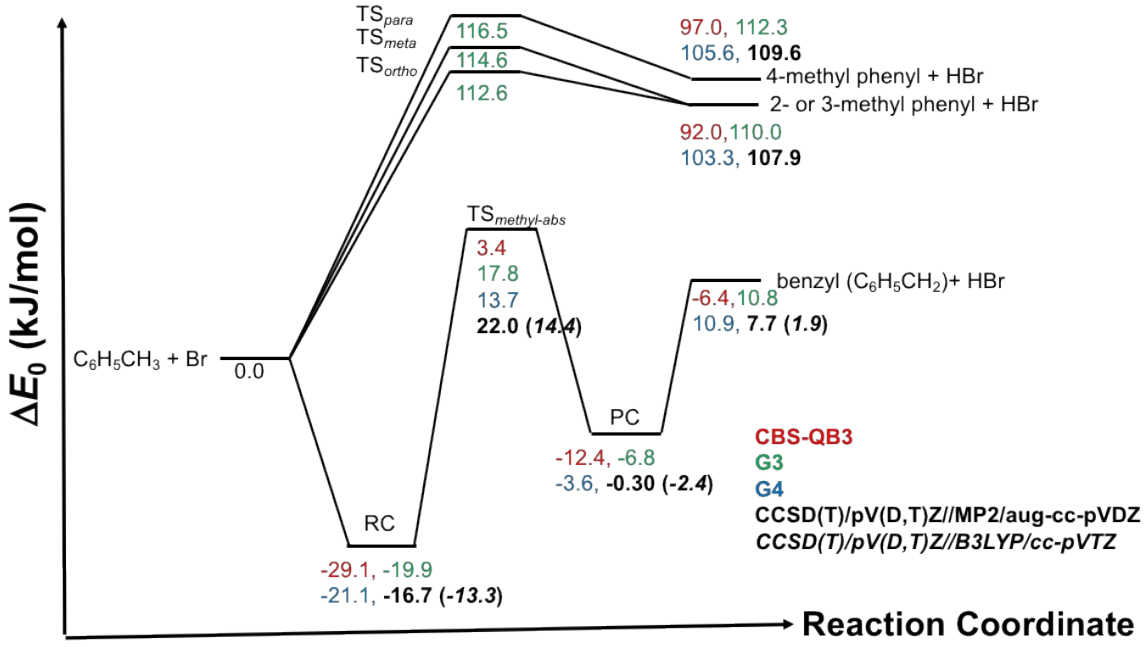

Figure S1: Zero-point energy corrected potential energy surface for the toluene + Br reaction. The relative energies are provided with a color code to identify the various *ab initio* methods employed. These results are taken from our recent work (Giri et al., *Int. J. Chem. Kinet., 2021, **53**, 390-402*).

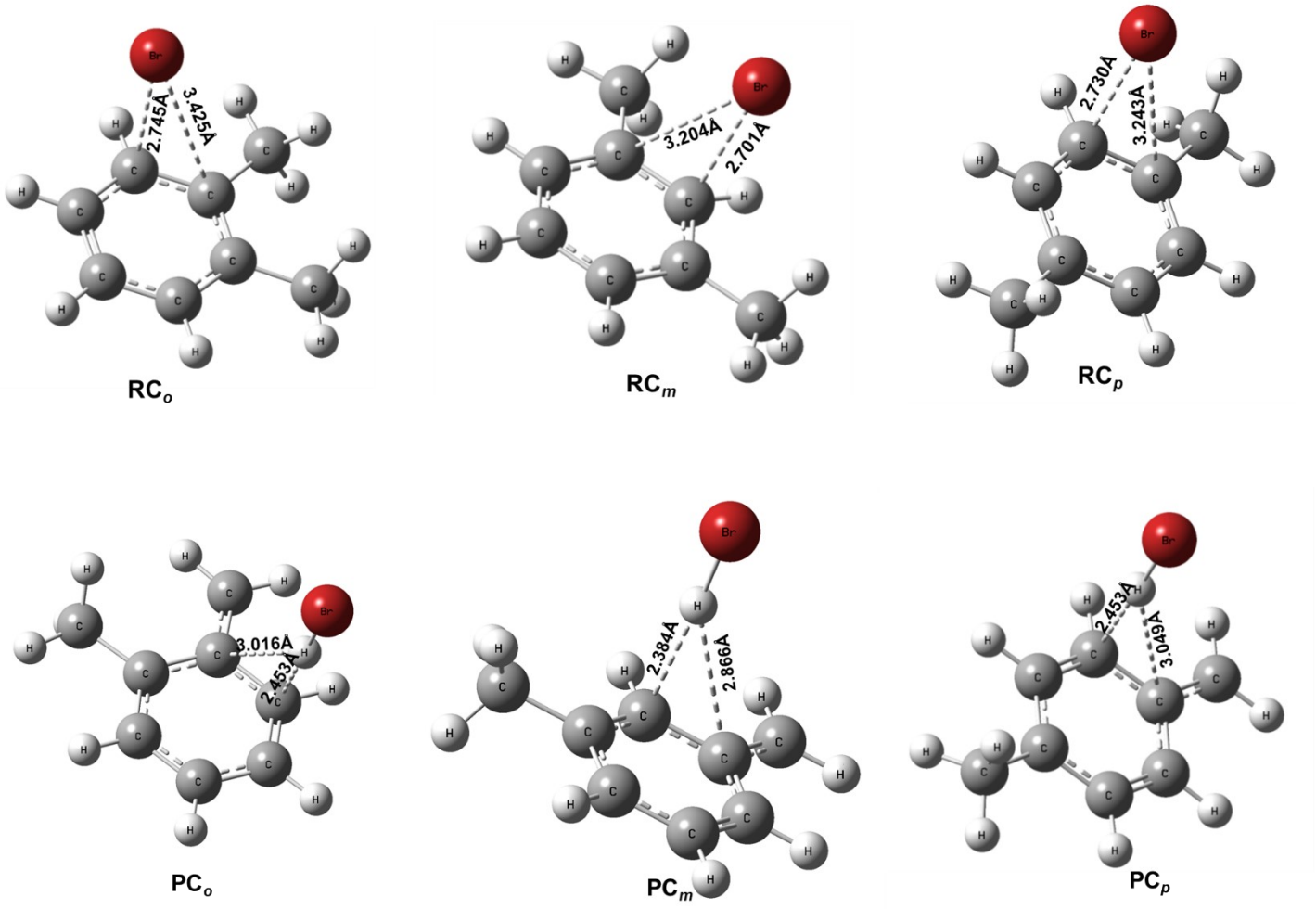

Figure S2: The geometrical parameters for the optimized structures of pre-reactive and post-reactive complexes at B3LYP/6-31G(2df,p) levels of theory.

Table S8: Calculated rate coefficients based on the molecular parameters and energetics from G4 composite method for the hydrogen abstraction reactions of xylenes by Br atoms. For $k_{1b}(T)$ calculations, the barrier heights are lowered by ≤ 1.5 kJ/mol to match with the experimental data (see main text for detail explanation). The units are in cm^3 $molecule^{-1}$, s^{-1} and cm^3 $molecule^{-1}$ s^{-1} for $K_{1a}(T)$, $k_{1b}(T)$ and $k_{ov.}(T)$, respectively.

	***o*-xylene + Br (G4)-parameters**			***m*-xylene + Br (G4)-parameters**			***p*-xylene + Br (G4)-parameters**		
T/K	$K_{1a}(T)$	$k_{1b}(T)$	$k_{ov.}(T)$	$K_{1a}(T)$	$k_{1b}(T)$	$k_{ov.}(T)$	$K_{1a}(T)$	$k_{1b}(T)$	$k_{ov.}(T)$
200	7.57E-19	1.90E+04	1.44E-14	8.87E-18	4.56E+02	4.04E-15	4.99E-19	1.97E+04	9.84E-15
225	1.70E-19	1.48E+05	2.52E-14	1.37E-18	5.90E+03	8.08E-15	1.10E-19	1.75E+05	1.93E-14
250	5.25E-20	7.69E+05	4.04E-14	3.13E-19	4.61E+04	1.44E-14	3.34E-20	1.01E+06	3.38E-14
275	2.03E-20	2.98E+06	6.06E-14	9.49E-20	2.50E+05	2.37E-14	1.28E-20	4.30E+06	5.48E-14
298	9.87E-21	8.54E+06	8.42E-14	3.82E-20	9.27E+05	3.54E-14	6.13E-21	1.32E+07	8.08E-14
300	9.32E-21	9.29E+06	8.65E-14	3.55E-20	1.03E+06	3.66E-14	5.78E-21	1.44E+07	8.34E-14
325	4.86E-21	2.45E+07	1.19E-13	1.56E-20	3.44E+06	5.38E-14	2.99E-21	4.06E+07	1.21E-13
350	2.81E-21	5.65E+07	1.59E-13	7.80E-21	9.75E+06	7.60E-14	1.71E-21	9.91E+07	1.70E-13
375	1.76E-21	1.17E+08	2.06E-13	4.30E-21	2.42E+07	1.04E-13	1.07E-21	2.16E+08	2.30E-13
400	1.17E-21	2.24E+08	2.63E-13	2.57E-21	5.40E+07	1.39E-13	7.07E-22	4.31E+08	3.05E-13
425	8.25E-22	3.98E+08	3.29E-13	1.64E-21	1.10E+08	1.81E-13	4.96E-22	7.96E+08	3.95E-13
450	6.07E-22	6.67E+08	4.05E-13	1.11E-21	2.09E+08	2.32E-13	3.63E-22	1.38E+09	5.02E-13
475	4.63E-22	1.07E+09	4.94E-13	7.85E-22	3.72E+08	2.92E-13	2.76E-22	2.27E+09	6.28E-13
500	3.65E-22	1.63E+09	5.94E-13	5.77E-22	6.28E+08	3.62E-13	2.17E-22	3.58E+09	7.75E-13

Table S9: Calculated rate coefficients based on the molecular parameters and energetics from CCSD(T)/cc-pV(D,T)//MP2/aug-cc-pVDZ level of theory for the hydrogen abstraction reactions of xylenes by Br atoms. The calculated rate coefficients for *o*-xylene + Br are ca. 50% lower than the experimental values (not provided in the table). For $k_{1b}(T)$ calculations, the barrier heights are lowered by ≤ 1.5 kJ/mol to match with the experimental data (see main text for detail explanation). The units are in cm^3 $molecule^{-1}$, s^{-1} and cm^3 $molecule^{-1}$ s^{-1} for $K_{1a}(T)$, $k_{1b}(T)$ and $k_{ov.}(T)$, respectively.

	***m*-xylene + Br (CCSD(T)/cc-pV(D,T)//MP2/aug-cc-pVDZ)-parameters**			***p*-xylene + Br (CCSD(T)/cc-pV(D,T)//MP2/aug-cc-pVDZ)-parameters**		
T/K	$K_{1a}(T)$	$k_{1b}(T)$	$k_{ov.}(T)$	$K_{1a}(T)$	$k_{1b}(T)$	$k_{ov.}(T)$
200	8.68E-19	8.41E+03	7.30E-15	5.71E-19	3.22E+04	1.84E-14
225	1.51E-19	8.13E+04	1.23E-14	1.06E-19	2.71E+05	2.87E-14
250	3.79E-20	5.06E+05	1.92E-14	2.81E-20	1.50E+06	4.22E-14
275	1.24E-20	2.28E+06	2.83E-14	9.61E-21	6.14E+06	5.91E-14
298	5.28E-21	7.37E+06	3.89E-14	4.24E-21	1.84E+07	7.78E-14
300	4.93E-21	8.09E+06	3.99E-14	3.97E-21	2.00E+07	7.96E-14
325	2.29E-21	2.38E+07	5.44E-14	1.90E-21	5.48E+07	1.04E-13
350	1.19E-21	6.04E+07	7.19E-14	1.02E-21	1.31E+08	1.33E-13
375	6.81E-22	1.36E+08	9.28E-14	5.95E-22	2.79E+08	1.66E-13
400	4.20E-22	2.79E+08	1.17E-13	3.74E-22	5.44E+08	2.04E-13
425	2.76E-22	5.29E+08	1.46E-13	2.50E-22	9.85E+08	2.46E-13
450	1.90E-22	9.37E+08	1.78E-13	1.76E-22	1.68E+09	2.94E-13
475	1.37E-22	1.57E+09	2.15E-13	1.29E-22	2.71E+09	3.48E-13
500	1.03E-22	2.51E+09	2.57E-13	9.75E-23	4.18E+09	4.08E-13