

## Supporting Information

### Thermodynamic stabilities of propylenebenzenium ions in the gas phase. Substituent effect of unsymmetrical phenonium ions

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**Table S1.** Cartesian coordinates of B3LYP/6-311+G\*\* and B3LYP/6-31+G\* of optimized  $\alpha$ -methylphenonium ions

B3LYP/6-311+G**			
<i>p</i> -NMe <sub>2</sub>			
H	-2.18949715	-1.0060651411	-0.4941579913
C	-1.1934897092	-0.65355601	-0.2543695107
C	1.3924910992	0.2480577285	0.3767244155
C	-0.053293876	-1.3460187159	-0.804317241
C	-1.0593053391	0.4251977644	0.5589094977
C	0.2428292353	0.9318089745	0.9093603297
C	1.2431659401	-0.8334569484	-0.4297649891
H	-1.9462358045	0.9055254214	0.9446433399
H	2.1270631696	-1.3339761419	-0.8116985963
H	2.3870905326	0.590158568	0.6211576923
N	0.3784569286	1.9984044488	1.7011567036
C	1.7107245416	2.5243347663	2.045391336
H	2.2874933094	1.7874321519	2.6090307705
H	1.5890709622	3.4094164886	2.6627069939
H	2.260824223	2.8066344319	1.1454808473
C	-0.7989098445	2.6857257108	2.2592855365
H	-1.3963778476	2.002450435	2.8662378111
H	-1.4194688311	3.1042176456	1.4636516093
H	-0.461046669	3.4993981491	2.8941702582
C	-0.1770710862	-2.8855189947	-1.112202168
H	0.6991714675	-3.4656706709	-0.8514649317
H	-1.1198920704	-3.3208135135	-0.8022912022
C	-0.1580617466	-2.0054166336	-2.2719197175
H	0.7947146546	-1.9090820435	-2.781898469
C	-1.3614275918	-1.7504392598	-3.1455039004
H	-1.3514996343	-0.7397257075	-3.5579976554
H	-2.3046540122	-1.910362706	-2.6214521431
H	-1.3318645371	-2.4526788019	-3.983776791
<i>p</i> -MeO			
C	-1.0110724673	0.2277368061	-0.6209013732
C	-1.0296654409	0.2118891229	0.8157772033
C	0.1275593706	0.1880930823	1.5340241861
C	1.3820260243	0.1764253733	0.863112575
C	1.4360984868	0.1944835569	-0.5553130744

**Table S1. Continued**

C	0.2675146225	0.2250248265	-1.2667531099
H	-1.9787109237	0.2247133511	1.337649147
H	0.1283643766	0.1802729291	2.6165642524
O	2.4371640633	0.1482947885	1.6450979903
H	2.3852299954	0.1885698375	-1.0723958455
H	0.3064135508	0.246996548	-2.3509075769
C	-2.2047516894	-0.5821699923	-1.4373452626
C	-2.2369329794	0.8617521679	-1.3970925343
C	-3.1526783816	-1.4726817799	-0.6797627026
H	-1.7690579273	-1.0315010752	-2.3231988473
H	-2.9455388689	1.3517579397	-0.7395977466
H	-1.947764505	1.4389962885	-2.2663378087
H	-3.9640101989	-1.7474734114	-1.3615924009
H	-3.6034451655	-0.9786289213	0.1812241645
H	-2.6687426626	-2.3949839743	-0.354386615
C	3.7808108613	0.1355076359	1.104885442
H	4.4307628723	0.1149285108	1.9745953117
H	3.9615082929	1.0407545929	0.5233364253
H	3.9352095515	-0.759527184	0.5003229631
<b>3-Cl-4-MeO</b>			
C	-1.0627444321	-1.2131388887	0.1210798903
C	0.3520172856	-1.3185725219	0.1530636047
C	1.1458926749	-0.1269798175	0.2054140458
C	0.5357491942	1.0942729723	0.2219086005
C	-0.8933896573	1.2163823641	0.1781460935
C	-1.6651860008	0.0154189385	0.1324175913
H	-1.6664197328	-2.1093464975	0.0890510186
O	1.00763705	-2.4498227059	0.1360917392
C	0.3256503838	-3.7271832396	0.0809392181
H	1.1468082771	1.988546254	0.267946771
Cl	2.8708550384	-0.2630914522	0.2485141607
H	-2.7464437751	0.0732832743	0.1100321993
C	-1.546964313	2.5256930461	0.7890943244
H	1.1225664037	-4.4646950768	0.0738469097
C	-1.4559951587	2.5452172101	-0.651373977
C	-2.633349129	2.4082899168	-1.5778877004
H	-0.2997360801	-3.8575254286	0.9652150751
H	-0.2620779156	-3.7993880722	-0.8352302578

**Table S1. Continued**

H	-0.8559254389	3.1053386034	1.3883537501
H	-2.510383671	2.3444181135	1.2510516161
H	-0.5992953503	3.0576872601	-1.0755058751
H	-2.36890206	1.8768512524	-2.4934044735
H	-3.4892322838	1.9212037271	-1.1098765129
H	-2.9466755116	3.4183630434	-1.8617650135
<hr/>			
<i>p</i> -Me			
C	-0.7151250371	0.3048354847	0.34150173
C	-0.1271787998	-0.9697961205	0.5803996621
C	1.2212468799	-1.1590076354	0.390558329
C	2.0476501862	-0.1036856945	-0.054664565
C	1.4707737798	1.160593082	-0.2946790362
C	0.1242669443	1.3667265676	-0.1012505863
H	-0.7424940503	-1.7916246638	0.9263661328
H	1.6605786642	-2.1296639536	0.5883925048
C	3.5065403336	-0.3326087384	-0.2917029059
H	2.0984522649	1.9780596143	-0.6289395426
H	-0.3058985699	2.3464913461	-0.2805614423
C	-2.2826033052	0.3294800565	-0.382145326
C	-2.1095168724	0.6576612516	1.0050345186
C	-2.8635814496	-0.951472784	-0.8990516226
H	-2.283629686	1.1559497057	-1.0843159639
H	-2.4087778948	-0.068162167	1.7525629371
H	-2.1666806411	1.6906671595	1.3261411878
H	-3.912889602	-0.7461843345	-1.1423856512
H	-2.8476300092	-1.7567996639	-0.1651444907
H	-2.3760994607	-1.2799056776	-1.8180435183
H	3.6560557998	-0.6962062127	-1.3163320619
H	3.9094507752	-1.0913432676	0.3810347319
H	4.0832087138	0.5870656829	-0.1859697419
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H (unsubstituted)			
C	0.1951411884	-0.276818273	0.367271645
C	-0.2817721778	1.050566824	0.5224186672
C	-1.5952821677	1.3498486036	0.2190810793
C	-2.4459990932	0.3435726247	-0.2580623136
C	-1.9912620785	-0.9687797875	-0.4288161986
C	-0.680826818	-1.2818264618	-0.1206134144
H	0.3789258561	1.8244575862	0.8938049721

**Table S1. Continued**

H	-1.9675628328	2.3580741854	0.3506223711
H	-3.4743181084	0.5868281403	-0.5006934119
H	-2.6622393036	-1.7347260396	-0.79676721
H	-0.3192626126	-2.2974837824	-0.2402209333
C	1.8424441572	-0.4423844098	-0.3188964618
C	1.5494102646	-0.7070899949	1.0585979956
C	2.5205287272	0.7779583746	-0.8450409749
H	1.7803190159	-1.2793328165	-1.0061638049
H	1.8776422637	0.011419356	1.801642498
H	1.5194419812	-1.7331435054	1.4065058571
H	3.5595831949	0.4836531277	-1.0453490436
H	2.5417344527	1.6027777435	-0.1339474933
H	2.0964236453	1.1097173445	-1.7938866785
<i>m</i> -Cl			
H	-1.5612146089	-2.0912054707	0.2495379105
C	0.577113234	-2.1414355208	0.0721770377
C	-0.6455307747	-1.5111653701	0.2291338433
C	0.5003602029	0.6540039954	0.351648264
C	1.7119530443	0.0047582041	0.1996119474
Cl	3.189033667	0.9151272789	0.1842552332
H	0.6262695843	-3.2175134516	-0.0372688725
C	-0.6951996156	-0.1046804439	0.381938598
C	-2.031412965	0.5744544194	0.8663347222
C	-2.0950237785	0.605831271	-0.5660214008
C	-1.8324042855	1.7916803082	-1.4244564314
C	1.7536431584	-1.3908243975	0.0573948823
H	0.477088042	1.7301236676	0.466309652
H	-1.8509570271	1.5083145878	1.3880844756
H	-2.6665175271	-0.1216773802	1.4027735483
H	-2.5508531735	-0.2462171459	-1.0592750078
H	-1.2829403699	1.5347718077	-2.3315007203
H	-2.8217924972	2.1476691965	-1.7463042366
H	-1.339729627	2.6094693204	-0.9005677426
H	2.7116770085	-1.8815824682	-0.0666062774
<i>m</i> -F			
H	-1.5314871443	-2.078637724	0.2533238897
C	0.6062799557	-2.1268464205	0.0696122986
C	-0.6175277368	-1.4962273684	0.2311245325

**Table S1. Continued**

C	0.5184075605	0.6737297197	0.3578807262
C	1.716484622	0.0120185563	0.2017297759
F	2.8506608064	0.7141590535	0.1901027815
H	0.6541379022	-3.2025804162	-0.0421687472
C	-0.6730688337	-0.0907255733	0.3898073947
C	-2.014054957	0.5809034241	0.8653828323
C	-2.0867076036	0.6109724829	-0.567073247
C	-1.8292777803	1.7939097287	-1.4282231093
C	1.7816319935	-1.3756794549	0.0540024096
H	0.5144466973	1.7499426805	0.4762648257
H	-1.8408930539	1.5178065456	1.3843700791
H	-2.6457440224	-0.1167290314	1.4040700835
H	-2.5355637077	-0.2465511404	-1.0574836316
H	-1.2860073041	1.5360187321	-2.3387899883
H	-2.8219754862	2.1461076155	-1.7456194068
H	-1.3361503123	2.6143557324	-0.9089849992
H	2.7499700962	-1.846044734	-0.0721290746
<hr/> <i>m</i> -CF <sub>3</sub> <hr/>			
H	-1.5310538195	-0.6834482267	0.3237064341
C	0.6014263688	-0.7252884155	0.157005397
C	-0.6213342874	-0.0954846773	0.288449078
C	0.5171302635	2.0719074193	0.3436990882
C	1.735049182	1.427206322	0.2221933746
C	0.6926472972	-2.2361290795	0.0459585035
H	2.654250892	1.9988898731	0.2020310559
C	-0.6777872666	1.3156783894	0.3948693528
C	-2.0233419131	1.9962176211	0.8512954559
C	-2.0860209234	1.9871006947	-0.5810616353
C	-1.8338011857	3.1481688638	-1.4739756778
F	1.4150250334	-2.7438563673	1.0587942586
F	1.2934389402	-2.5893043791	-1.1045911412
F	-0.5243304536	-2.8055701498	0.0728955522
C	1.7793150962	0.0337658465	0.1253698957
H	0.4813139548	3.1520421688	0.419588124
H	-1.8534364044	2.9460701271	1.3473768859
H	-2.6536738125	1.3095513434	1.405695029
H	-2.5277565127	1.1139905532	-1.0504794046
H	-1.2830237552	2.86891422	-2.3735692184

**Table S1. Continued**

H	-2.8276170751	3.48228727	-1.8065426575
H	-1.3516949074	3.9879153623	-0.9754985653
H	2.7357939721	-0.4664925323	0.0209872938
<hr/>			
3,5-(CF <sub>3</sub> ) <sub>2</sub>			
H	-2.3567972977	-1.3127773355	0.2743280927
C	-0.223569656	-1.3302914511	0.0974664303
C	-1.4541921384	-0.7135769622	0.2458999078
C	-0.3404048291	1.4615433673	0.3311216696
C	0.8812206125	0.8293802031	0.1891179146
C	-0.1186286243	-2.8411756272	-0.0271032978
C	2.1737063745	1.6281079488	0.163810059
C	-1.5226137613	0.6909599228	0.379185734
C	-2.8806885408	1.3625957808	0.7947426562
C	-2.9559676141	1.3840646573	-0.6385973703
C	-2.6930345526	2.5520912371	-1.5097198503
F	2.9308151063	1.3356876885	1.2330492403
F	2.883964571	1.3373074113	-0.9387329192
F	1.9302152661	2.9498520019	0.1700421846
F	0.5150937371	-3.3592130752	1.0372120259
F	0.5768845348	-3.1754939986	-1.1263233292
F	-1.3339932945	-3.4085160158	-0.1094699027
C	0.9446290989	-0.5638528207	0.0686214438
H	-0.379220779	2.539594055	0.4221889457
H	-2.7287735152	2.3088905144	1.3044365843
H	-3.5199164231	0.6695005058	1.3319451714
H	-3.3716046629	0.506353749	-1.1247885267
H	-2.1434618922	2.2855770624	-2.414395881
H	-3.6888546167	2.8850239598	-1.843756599
H	-2.2178285907	3.3877576012	-0.9983288492
H	1.9062882961	-1.0501228339	-0.0566430415
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B3LYP/6-31+G*			
<hr/>			
<i>p</i> -NMe <sub>2</sub>			
H	-2.1937903819	-1.0104863519	-0.4913079298
C	-1.1952000491	-0.6559707387	-0.2540879301
C	1.3953203496	0.250351918	0.3776284371
C	-0.0531245807	-1.3492076601	-0.808793432
C	-1.0607478276	0.4259241569	0.5620989613
C	0.2435338988	0.934565937	0.9120397022

**Table S1. Continued**

C	1.245731616	-0.8337808646	-0.4325473584
H	-1.950368023	0.903871467	0.9513979475
H	2.1324972822	-1.332972708	-0.8166617075
H	2.3925188666	0.5937587421	0.6204959
N	0.3793781237	2.0039910154	1.7057176082
C	1.7132373713	2.5216696787	2.0574073316
H	2.2910947543	1.7701459619	2.6051861125
H	1.5951484124	3.3955729542	2.695349361
H	2.2625530079	2.8221083405	1.1594564844
C	-0.800057855	2.6960342708	2.2542944289
H	-1.3909527399	2.0207174332	2.881390618
H	-1.4284170721	3.0916364302	1.4497829931
H	-0.4652638222	3.5294942813	2.8690723879
C	-0.1755304908	-2.8898173885	-1.114817762
H	0.7033970933	-3.4727990586	-0.8553313417
H	-1.1197153447	-3.3294849221	-0.803592774
C	-0.1586875633	-2.0076531965	-2.2760623969
H	0.7946735631	-1.9119367236	-2.7918161358
C	-1.3664034337	-1.7552764653	-3.149978662
H	-1.3639583966	-0.739288781	-3.5573575707
H	-2.3111385943	-1.9243759737	-2.6254674446
H	-1.332354084	-2.4549360855	-3.9937080762
<hr/> <i>p</i> -MeO <hr/>			
C	-1.0143195196	0.2218436861	-0.6234528007
C	-1.0307003774	0.2072154718	0.817454349
C	0.1302644258	0.1850627017	1.5376305786
C	1.3864690737	0.1752283064	0.864044891
C	1.4410875682	0.1937031598	-0.5573918111
C	0.2687578166	0.2223977909	-1.2702067495
H	-1.9814094508	0.2190915517	1.3414239328
H	0.1307049743	0.1776149797	2.6226313006
O	2.4449333337	0.1490075153	1.6480291993
H	2.3923338376	0.1896378308	-1.0758111793
H	0.3081137032	0.2445001644	-2.3568545523
C	-2.2066950559	-0.5826806973	-1.4385984145
C	-2.2381329673	0.8642150928	-1.3976627187
C	-3.1611799126	-1.4726515564	-0.6812192854
H	-1.77630429	-1.0342069259	-2.3297156915



**Table S1. Continued**

H	-2.9488437734	1.3566826527	-0.7389180021
H	-1.9491998209	1.4442089987	-2.2692850646
H	-3.9705214298	-1.7515215385	-1.3677521209
H	-3.6184593585	-0.9738590251	0.1772860948
H	-2.6771464544	-2.3948832173	-0.346112905
C	3.7882841097	0.139209319	1.1079601298
H	4.4385857068	0.1199256197	1.9805987496
H	3.9660331664	1.0471073349	0.5250491385
H	3.9436355525	-0.7576181964	0.5018776945
<b>3-Cl-4-MeO</b>			
C	-1.0652827848	-1.2164330151	0.1197603699
C	0.3524126211	-1.3209716615	0.1522321367
C	1.1490530961	-0.1284553243	0.2056458391
C	0.536665666	1.096405882	0.2215556665
C	-0.8960325383	1.2208143666	0.1755800374
C	-1.6693268467	0.0156340938	0.1308731929
H	-1.6704001776	-2.1145955225	0.0881420095
O	1.0100606974	-2.4560563107	0.1361919758
C	0.3280215561	-3.7328968254	0.0815449068
H	1.1497828051	1.9922452468	0.2683098089
Cl	2.8743368895	-0.2635707962	0.2512015108
H	-2.7531010987	0.0729673722	0.1088305636
C	-1.548240656	2.5289557677	0.7908122522
H	1.1275446521	-4.4713580273	0.0755604476
C	-1.456618722	2.5487767068	-0.6526070556
C	-2.6379686923	2.4140878459	-1.5800143106
H	-0.299446962	-3.8616621845	0.9676166239
H	-0.2605003053	-3.8046928	-0.8370912617
H	-0.8565643574	3.1115215584	1.3925297208
H	-2.5149348232	2.3496734318	1.2544351264
H	-0.600006522	3.0662454476	-1.0786861189
H	-2.376622105	1.875469129	-2.4957075046
H	-3.497997131	1.930898744	-1.1087752169
H	-2.9480628713	3.4269346054	-1.8674239002
<b><i>p</i>-Me</b>			
C	-0.7218268404	0.3031469316	0.3283977346
C	-0.1297549744	-0.973752078	0.5726947085
C	1.223407369	-1.1623734659	0.3882922555

**Table S1. Continued**

C	2.052844679	-0.1040887323	-0.0545920307
C	1.4745504545	1.1630944004	-0.2974149663
C	0.1234707246	1.368588679	-0.1100085676
H	-0.7466890604	-1.7982605684	0.9172333776
H	1.6636832533	-2.1349613882	0.5884388815
C	3.515766503	-0.3316244299	-0.2869575264
H	2.1047330301	1.9828748244	-0.6297152518
H	-0.3070463552	2.3505081723	-0.2921688641
C	-2.282353453	0.3298736663	-0.3823759242
C	-2.1098127199	0.660726439	1.007423035
C	-2.8735155351	-0.9538052177	-0.8948197742
H	-2.2942881383	1.1578637362	-1.0872324895
H	-2.4079352214	-0.0658175899	1.759277175
H	-2.1649278372	1.6967233036	1.3300318126
H	-3.9243379396	-0.7453208023	-1.1386768009
H	-2.8606437465	-1.757912124	-0.1551460875
H	-2.3848993341	-1.2919182449	-1.8131106361
H	3.6750383086	-0.6721267722	-1.3209039932
H	3.9151867812	-1.1068846483	0.373490828
H	4.0954690157	0.5865149465	-0.1553516167
<hr/>			
H (unsubstitued)			
<hr/>			
C	0.2042866025	-0.2752973345	0.3508843046
C	-0.2778118767	1.0549039244	0.5125578037
C	-1.5969985915	1.3534681014	0.2175591182
C	-2.4521718412	0.3429464072	-0.2541417723
C	-1.996206294	-0.9730386475	-0.4273861
C	-0.6799548661	-1.2846685674	-0.1276841986
H	0.3858344361	1.8316303042	0.8800722847
H	-1.9704381249	2.3637094674	0.3517187017
H	-3.4849093727	0.5854239838	-0.4897323333
H	-2.670771342	-1.7419651396	-0.7902052444
H	-0.3173864346	-2.3024844572	-0.2494267794
C	1.8359138119	-0.4431397578	-0.3183646313
C	1.5497384529	-0.7099943052	1.0630743677
C	2.5245906911	0.7793624114	-0.8427963212
H	1.7874582909	-1.2841922492	-1.0061089174
H	1.8758098051	0.0112098088	1.8089311607
H	1.5159546682	-1.7381106281	1.4140449543

**Table S1. Continued**

H	3.5646767739	0.4833831329	-1.0448792269
H	2.548466113	1.6036812286	-0.1266488212
H	2.096988653	1.1204611559	-1.7899812032
<hr/>			
<i>m</i> -Cl			
<hr/>			
H	-1.5661242407	-2.0966398375	0.2444123898
C	0.5777140614	-2.1465618622	0.0739795235
C	-0.6485587532	-1.5146632592	0.2241096554
C	0.4989660941	0.6574613934	0.3409893805
C	1.7150091586	0.0073000618	0.1964682377
Cl	3.1911141829	0.9180135135	0.1847087297
H	0.6282720936	-3.2256908052	-0.0303892008
C	-0.7020487093	-0.1021385609	0.3667476592
C	-2.0343200263	0.5739628084	0.8723040253
C	-2.0892765535	0.600841479	-0.5631670925
C	-1.8322259666	1.7945567369	-1.4232758694
C	1.7572223949	-1.3928560723	0.0597116803
H	0.4743917141	1.7365467145	0.4515681642
H	-1.8508980442	1.509696025	1.3959788258
H	-2.6688576207	-0.1245095817	1.4124958001
H	-2.5571234425	-0.2468413918	-1.0585217831
H	-1.2713454372	1.5424241752	-2.327974933
H	-2.8226099771	2.1486626459	-1.7495700047
H	-1.3436459476	2.6156679116	-0.8945681064
H	2.7179067107	-1.8853296864	-0.0588076565
<hr/>			
<i>m</i> -F			
<hr/>			
H	-1.5362008565	-2.0844764042	0.2479618332
C	0.6070992014	-2.1323183361	0.0718042043
C	-0.6205333646	-1.4998449253	0.2264599432
C	0.5159915436	0.6779965913	0.3473086534
C	1.7170675356	0.0137268168	0.1981122322
F	2.8551582531	0.7188033041	0.1878792554
H	0.6563281949	-3.2111146799	-0.0348926302
C	-0.6805680063	-0.088217507	0.3748776651
C	-2.0184817222	0.5802371473	0.8713354889
C	-2.0808187587	0.6057168843	-0.5641216288
C	-1.8282399718	1.7967135886	-1.4266717214
C	1.7855179999	-1.3780760281	0.0568484694
H	0.5110628561	1.7570592401	0.4606048644

**Table S1. Continued**

H	-1.8422299322	1.518830911	1.3925000776
H	-2.649458747	-0.1202344108	1.4132417561
H	-2.5411819677	-0.2475403233	-1.0570599183
H	-1.2752430553	1.5432962294	-2.335902843
H	-2.8217127964	2.1493224848	-1.7465845013
H	-1.3367685553	2.6191320518	-0.9027717292
H	2.756773841	-1.8491102267	-0.0637300457
<i>m</i> -CF <sub>3</sub>			
H	-1.5397752666	-0.684048582	0.3140140917
C	0.5989118327	-0.7277945942	0.1571451252
C	-0.62716199	-0.096126361	0.2809479526
C	0.513543668	2.0778271672	0.3362191771
C	1.7351476473	1.4315877103	0.221820741
C	0.6943401745	-2.2392927617	0.0492099166
H	2.6567753559	2.0043269443	0.2048694091
C	-0.6868483723	1.320354575	0.3798171425
C	-2.030066351	1.9976914682	0.8553416901
C	-2.0807070544	1.9855837862	-0.5799972399
C	-1.8313690325	3.1552153612	-1.4732055208
F	1.4464634664	-2.7415823241	1.0486450405
F	1.272295436	-2.5948430343	-1.1172457453
F	-0.521658993	-2.8178928697	0.1065142779
C	1.7795805852	0.0340838283	0.1287520573
H	0.4771426661	3.1605771379	0.4098899571
H	-1.8586036352	2.9489227299	1.354863243
H	-2.6605309098	1.3076546015	1.4112898668
H	-2.5332698428	1.1170947895	-1.0536620811
H	-1.2680768859	2.8812080093	-2.3699917487
H	-2.8251371519	3.4890058199	-1.8113261781
H	-1.3530966165	3.9972709365	-0.9684262498
H	2.7384464565	-0.4679294115	0.0309512828
<i>3,5</i> -(CF <sub>3</sub> ) <sub>2</sub>			
H	-2.3666858555	-1.3137292865	0.2662334818
C	-0.2271590146	-1.333321966	0.1012634076
C	-1.4613039421	-0.7145392004	0.239059335
C	-0.3453954585	1.4676221612	0.3224058579
C	0.880191363	0.8338662578	0.1920583259
C	-0.1173532165	-2.8444384145	-0.0224159636

**Table S1. Continued**

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C	2.1751870428	1.6295460888	0.1689740273
C	-1.5327453604	0.695560075	0.3633732142
C	-2.8889778928	1.3645595171	0.795693033
C	-2.9494072527	1.3777016876	-0.6405880576
C	-2.6876559857	2.5514300219	-1.5161724908
F	2.9589810434	1.2887854873	1.2096089295
F	2.8610605981	1.3797112921	-0.9643230255
F	1.9394792301	2.9550113099	0.2342525005
F	0.5773677661	-3.3551519438	1.0121007699
F	0.5268246845	-3.1785854793	-1.1582598176
F	-1.333428455	-3.4249138404	-0.0415734626
C	0.9435105683	-0.563610659	0.0783981817
H	-0.3868708432	2.5480583666	0.4102169238
H	-2.7359823112	2.3140260748	1.3055231242
H	-3.528510976	0.669707425	1.3362071413
H	-3.3744263754	0.5024578002	-1.1284617126
H	-2.1222621523	2.2870828088	-2.4149122248
H	-3.682064964	2.8831598273	-1.8597005536
H	-2.2175212685	3.3908894554	-1.000021164
H	1.908415837	-1.0516173207	-0.0336312875

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**Table S2.** Cartesian coordinates of B3LYP/6-311+G\*\* and B3LYP/6-31+G\* of optimized phenonium ions

B3LYP/6-311+G**			
<i>p</i> -NMe <sub>2</sub>			
H	-2.3273043737	-1.2635441054	-0.932791132
C	-1.3385350005	-0.9021402821	-0.6700153175
C	1.2402429911	0.0054227467	-0.0113709869
C	-0.18626219	-1.5907914077	-1.2085885115
C	-1.219396615	0.1730854838	0.14696073
C	0.0794970539	0.67923428	0.5160495365
C	1.1077301771	-1.0688916569	-0.8274847622
H	-2.1114896005	0.6517414444	0.522414649
H	1.9968908423	-1.5583091945	-1.2111411577
H	2.2293923612	0.3558397457	0.2430003603
N	0.2032997111	1.7364460329	1.3192807149
C	1.5305409615	2.2546004557	1.6970257283
H	2.1048641878	1.4968848403	2.2340485783
H	1.3984512905	3.1113378749	2.3509248973
H	2.0869829914	2.5774409066	0.8146858126
C	-0.9824998413	2.4259470231	1.8589236238
H	-1.58074612	1.7481266534	2.4713224728
H	-1.5981900646	2.8288949607	1.0521159306
H	-0.6533819248	3.2511087283	2.4832799817
C	-0.308717379	-3.140117789	-1.4702940444
H	0.5846749325	-3.7060452472	-1.2401009923
H	-1.2336394017	-3.5821064441	-1.1230510511
C	-0.3232034651	-2.2572581419	-2.6301836225
H	0.5595552335	-2.1754256348	-3.2510326444
H	-1.2587566577	-2.0514813732	-3.1339784936
<i>p</i> -MeO			
C	-1.2422559045	0.6950854658	-0.5807358488
C	-1.257239173	-0.7465167423	-0.5877276927
C	-0.2101602939	-1.4629927252	-0.0982253119
C	0.9252911432	-0.7860193733	0.4325805987
C	0.9742327058	0.6359149651	0.4554469565
C	-0.0819650138	1.3466874709	-0.0383182541
H	-2.1227696218	-1.2601626271	-0.9923464023
H	-0.2054567727	-2.5454169631	-0.0960175404
O	1.8805252495	-1.5641179319	0.8791417876

**Table S2. Continued**

H	1.8347874876	1.1513553264	0.8577401651
H	-0.0506511562	2.4311367232	-0.0236871026
C	-2.0275119502	1.4480823897	-1.7465397106
C	-2.6403324007	1.4481066219	-0.4357177681
H	-2.3972748786	0.7820077031	-2.5152240942
H	-1.5261731419	2.3366283926	-2.1074833122
H	-3.4672897946	0.7820576034	-0.2264893301
H	-2.5957886251	2.3366767956	0.1803945437
C	3.1012380963	-1.0279872087	1.4498057345
H	3.6861684	-1.9009346453	1.7232638134
H	2.8722031505	-0.436267697	2.3370001653
H	3.6350982333	-0.4362856527	0.7051006479
<b>3-Cl-4-MeO</b>			
H	-2.5752251711	-1.5629904513	-0.0362607266
C	-0.4519391457	-1.5832961437	-0.025111793
C	-1.6698401499	-0.9658958594	-0.0228137912
C	-0.5612100675	1.2322904669	0.0147423731
C	0.6585943534	0.624396857	0.0125893726
O	1.9425075999	-1.3152927264	-0.0083750275
H	-0.391344427	-2.662363905	-0.0402858778
C	-1.7779078623	0.4635746072	-0.0028741839
C	-3.0550643392	1.0942574708	0.7219140979
C	-3.0470402198	1.1149019492	-0.7237509496
H	-2.8159744078	2.0322439618	-1.2494066852
Cl	2.1197340459	1.5493871975	0.0337595606
C	2.1758736652	-2.747386138	-0.0277306712
H	3.2567969234	-2.8491254329	-0.0234247151
H	1.7500898599	-3.2074314422	0.8647649725
H	1.7597096978	-3.1815119893	-0.93757901
C	0.7399467744	-0.8094425067	-0.007559489
H	-0.6151394588	2.3149164808	0.0300173243
H	-2.8301093188	1.9962282143	1.2760538672
H	-3.6577569978	0.3659448926	1.2486474106
H	-3.6436344914	0.4019657832	-1.277752544
<b><i>p</i>-Me</b>			
C	-2.1289371979	1.5198676274	-1.8330730814
H	-2.2276961258	1.0592189875	-2.8169084698

H	-3.1112530827	1.4585661843	-1.3460536366
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**Table S2. Continued**

C	-1.1210437583	0.812857846	-0.9875981814
H	-1.8914099137	2.5783259045	-1.9475640303
C	-0.8786228001	-0.5681123375	-1.1695020444
C	-0.416803495	1.5119933518	0.019467514
H	-1.4140942143	-1.1035704344	-1.944385379
C	0.0265291353	-1.2308312407	-0.379103564
C	0.4915692823	0.8637697445	0.8181543234
H	-0.5981924416	2.571377235	0.1561791568
H	1.0286136248	1.4075534815	1.5881581179
C	0.7431464786	-0.5330703179	0.6430135121
C	1.1779546804	-1.3773022643	1.9511156961
H	0.207589344	-2.2904456084	-0.5255885541
H	2.5703728479	-1.8296592567	0.3225723379
C	2.2211243312	-1.0720393462	1.0118705946
H	2.9169750346	-0.2685094443	1.2149121726
H	0.7374321021	-2.3655330272	1.971950221
H	1.0840493392	-0.8043136967	2.8643297772
H (unsubstituted)			
C	-0.4654641608	0.3206812674	-0.2758793972
C	-0.4735788236	-1.1056842478	-0.2807406119
C	0.5495402818	-1.8022574887	0.3256958006
C	1.5925629825	-1.0972165655	0.9439790765
C	1.623804741	0.3049005553	0.9625479472
C	0.6069598405	1.0137806422	0.359831088
H	-1.2886776513	-1.6336384712	-0.7639141425
H	0.5504102266	-2.884902045	0.3261735419
H	2.3951805034	-1.6501876601	1.4197159063
H	2.4411741235	0.8238107816	1.4470679584
H	0.6140042322	2.0984515807	0.3640457362
C	-1.1857180906	1.0681435112	-1.5340641345
C	-1.9149421058	1.0681160114	-0.303892552
H	-1.4439599743	0.372646524	-2.3219791397
H	-0.6401147292	1.9493800252	-1.8454387357
H	-2.7301172193	0.3726090953	-0.1523166266
H	-1.9262728249	1.9493409886	0.3242234772
<i>m</i> -Cl			



H	-2.1136735083	-2.0419784326	0.0374566654
C	0.0322346279	-2.0546395621	0.0184246291

**Table S2. Continued**

C	-1.2071537635	-1.4473345444	0.0239324416
C	-0.1053616447	0.7583060167	-0.0060697161
C	1.1243926828	0.1309785505	-0.0113073662
Cl	2.5843751921	1.063715707	-0.0328655394
H	0.1152354852	-3.1341148666	0.0275546079
C	-1.2939930251	-0.0270927533	0.0117125889
C	-2.6029946804	0.6412580131	0.7319484522
C	-2.6159060301	0.6282888768	-0.6964589998
H	-2.3683620239	1.5225389905	-1.2536555955
C	1.192232875	-1.2725904394	0.0009221049
H	-0.1670100931	1.8403969342	-0.0154206085
H	-2.3454446997	1.5453821827	1.2682819588
H	-3.1690880287	-0.0925740722	1.2908506508
H	-3.1920060009	-0.1154099505	-1.2315922629
H	2.1652643532	-1.7504527529	-0.0033860535
<i>m</i> -F			
H	-1.736584135	-1.8799660167	0.0322336735
C	0.4087121221	-1.8914513739	0.0136443469
C	-0.8316559159	-1.2831765558	0.0188246295
C	0.2585155536	0.9284016095	-0.0111611678
C	1.4744375012	0.2871032271	-0.0158264973
F	2.5964075781	1.0046218914	-0.032255614
H	0.4903805728	-2.9708055335	0.0229319466
C	-0.9263221732	0.1370124943	0.0064704251
C	-2.2405814125	0.7957383544	0.7272819905
C	-2.2536243079	0.7828607344	-0.7008648558
H	-2.011696573	1.6785140228	-1.2582413289
C	1.5671939261	-1.1084024501	-0.0037069992
H	0.2152655006	2.0113870708	-0.0208358315
H	-1.9882043356	1.7010564379	1.2640161402
H	-2.8020784711	0.0587256621	1.2864784696
H	-2.8255427884	0.0362120873	-1.2362216807
H	2.5507402649	-1.5652369932	-0.0080320937
<i>m</i> -CF <sub>3</sub>			
H	-1.7131013181	-0.4189025778	0.0071739054

C	0.4256221862	-0.4253961769	-0.000909259
C	-0.8104139899	0.1810967824	0.0027762339
C	0.2926731428	2.3819492139	-0.0050123424

**Table S2. Continued**

C	1.524363522	1.7588649765	-0.0086584926
C	0.5583021403	-1.9383874702	0.0011418552
H	2.435649674	2.3430309266	-0.0130743671
C	-0.8988591667	1.6028734975	0.0007815891
C	-2.2137392487	2.2598833444	0.7185542739
C	-2.2190360938	2.2574915909	-0.7096068337
H	-1.9722886069	3.1566074389	-1.2593333396
F	1.2372168127	-2.3482031315	1.0857215653
F	1.2300957619	-2.3517889222	-1.0865020987
F	-0.6442414281	-2.5346529436	0.0060749849
C	1.5903164723	0.361837921	-0.0066186836
H	0.2242871072	3.4644464603	-0.0065272189
H	-1.9630090643	3.1608660907	1.2634024834
H	-2.7801021276	1.5198390576	1.2693094506
H	-2.789383804	1.5155718298	-1.2536840621
H	2.5595989729	-0.1255815728	-0.0095121932
<hr/>			
biscf3phenonium			
H	2.1713597206	1.764049296	0.0002775606
C	1.2201786836	-0.1529209702	-0.0007083776
C	1.2298783506	1.2264946684	-0.00104584
C	-1.2299194849	1.2264535065	0.0007455669
C	-1.2201734088	-0.1529618553	0.0007472745
C	2.5170194917	-0.9480433378	-0.0232401828
C	-2.5169874947	-0.9481222326	0.0234747566
C	-0.000032559	1.939008459	-0.0002377572
C	0.0008593595	3.4203961669	-0.7133775795
C	-0.0009743467	3.420571467	0.7125378569
H	-0.9190489352	3.5932660494	1.2598362331
F	-3.577938568	-0.1471499743	-0.1583253976
F	-2.513716951	-1.8776367615	-0.9432703525
F	-2.6571775038	-1.5738978847	1.203109911
F	2.6572298291	-1.5741056882	-1.2027207726
F	2.513780761	-1.8773191209	0.9437345518
F	3.5779437594	-0.1469905509	0.1583614356

C	0.0000142336	-0.8424399154	0.0001041962
H	-2.1714189432	1.7639761126	-0.0007100362
H	-0.9158024324	3.5925466226	-1.2632425607
H	0.918928139	3.5929871048	-1.2607183946

**Table S2. Continued**

H	0.9156816608	3.5928879298	1.2623604804
H	0.0000324858	-1.9279549001	0.0002376226

B3LYP/6-31+G\*

<i>p</i> -NMe <sub>2</sub>			
H	-2.3323459591	-1.2651452795	-0.933954926
C	-1.3408732656	-0.9036804294	-0.6711601336
C	1.242616714	0.0070776004	-0.0101225337
C	-0.1867294682	-1.5947856865	-1.2116341509
C	-1.2213700539	0.1750327512	0.1484757902
C	0.0798136062	0.6820762774	0.5182375474
C	1.1096700269	-1.070711249	-0.8289023886
H	-2.116021819	0.6541929224	0.5243329085
H	2.0014824386	-1.5605418569	-1.2129233627
H	2.2343911846	0.3576446141	0.2443436116
N	0.2039247708	1.7419012192	1.3234966507
C	1.5325123037	2.2585677151	1.7000345174
H	2.1071790924	1.4975317405	2.2373942611
H	1.4029914676	3.1175808239	2.3556027642
H	2.0892086631	2.5808499248	0.8143709285
C	-0.9835102219	2.4301618406	1.8621268553
H	-1.582509066	1.7491184789	2.4749437604
H	-1.5999501027	2.832642336	1.0520754259
H	-0.6563615238	3.2578815504	2.4884762873
C	-0.3092152901	-3.1452914902	-1.4728401844
H	0.5861961571	-3.7145657391	-1.2426856754
H	-1.2365575252	-3.5903566848	-1.1253366589
C	-0.3237423215	-2.2610940002	-2.634486971
H	0.560974501	-2.1801562471	-3.2586115768
H	-1.2617742091	-2.0559312322	-3.1412524467
<i>p</i> -MeO			
C	-1.2457710024	0.6972258938	-0.5823689222
C	-1.259480102	-0.7481577605	-0.5887689045
C	-0.2089958887	-1.46706272	-0.0976784519

C	0.9280233997	-0.7877508144	0.4338613014
C	0.9778423945	0.6369027604	0.457139577
C	-0.0816922876	1.3496287014	-0.0381815344
H	-2.1265965402	-1.2638117577	-0.9941281975
H	-0.2050787062	-2.551990789	-0.0958412766

**Table S2. Continued**

O	1.8864793348	-1.568163111	0.881921025
H	1.8404987748	1.1534101361	0.8604128263
H	-0.0495759661	2.4365317667	-0.0231727068
C	-2.030309907	1.4497306522	-1.7493314781
C	-2.6442715272	1.4497561428	-0.4360825228
H	-2.4027479429	0.7834576537	-2.5212959914
H	-1.5296703411	2.341799922	-2.1126851262
H	-3.4754676399	0.7835136111	-0.226812842
H	-2.6020346806	2.3418535514	0.181033854
C	3.1066487041	-1.0302520784	1.4523290915
H	3.6924667143	-1.9056274526	1.7262058481
H	2.8747797652	-0.4369659097	2.3407431411
H	3.6396291835	-0.4369905074	0.7046633347

**3-Cl-4-MeO**

H	-2.579596943	-1.5666995043	-0.0362336904
C	-0.4510581314	-1.5871915065	-0.0251044811
C	-1.6725241609	-0.9676364828	-0.0227711735
C	-0.5609444733	1.2350026814	0.0148465995
C	0.6628435067	0.6251963777	0.0126660735
O	1.9488686973	-1.3190722346	-0.0084028179
H	-0.3904184834	-2.6687473626	-0.0403188798
C	-1.7816708941	0.4657200277	-0.0027814613
C	-3.0585830644	1.096927807	0.7231495196
C	-3.0504858534	1.1175632987	-0.7250330929
H	-2.8207185049	2.0381353718	-1.2524475385
Cl	2.1242783795	1.5506747944	0.0338182636
C	2.1813498137	-2.7509651034	-0.0278133743
H	3.2649444142	-2.8516043305	-0.0235534717
H	1.7537720445	-3.2106085638	0.8669656077
H	1.7632933728	-3.1845853867	-0.9399131738
C	0.7427528938	-0.8111495704	-0.0075258108
H	-0.6143326192	2.3201365253	0.0301674915

H	-2.8350378292	2.0021314414	1.2790750769
H	-3.664983467	0.3680666878	1.2517401402
H	-3.6506818355	0.4040763188	-1.2809662919
<hr/>			
<i>p</i> -Me			
C	-2.133768987	1.5233497586	-1.8359136357
H	-2.197457854	1.0905175049	-2.838873338

**Table S2. Continued**

H	-3.1290849937	1.4187385059	-1.3772268924
C	-1.1230627604	0.8164061039	-0.9893076561
H	-1.9245543882	2.5937047239	-1.9156118869
C	-0.8839391397	-0.5690617763	-1.1683709953
C	-0.4129056595	1.5171178681	0.016755601
H	-1.4240942884	-1.1065873121	-1.9422593714
C	0.0229170652	-1.2344915296	-0.3759393954
C	0.4975433482	0.8665116503	0.8179472676
H	-0.5914675788	2.5797597187	0.1521091329
H	1.0382018835	1.4125850508	1.5872325705
C	0.7466871146	-0.5355183246	0.6465760573
C	1.1792838735	-1.3766226243	1.9552206563
H	0.2002546632	-2.2974427583	-0.5207809806
H	2.5733467999	-1.8392355291	0.3228649385
C	2.2237845108	-1.0757198037	1.0106428038
H	2.9269019752	-0.2738061522	1.2124814704
H	0.7375867105	-2.3677686172	1.9823551043
H	1.091130876	-0.8022930695	2.8720450319
<hr/>			
H (unsubstituted)			
C	-0.4684976423	0.3227624905	-0.277655832
C	-0.4748732627	-1.1081950956	-0.2814952567
C	0.5507601794	-1.8067027117	0.3264164959
C	1.5965200168	-1.0999405743	0.9463174527
C	1.6277439285	0.3057919388	0.9648802593
C	0.6082288427	1.0163004239	0.3605955796
H	-1.291551382	-1.6378104374	-0.7655979551
H	0.5510738268	-2.891908582	0.3265561009
H	2.4008085461	-1.6540593454	1.4230335058
H	2.4467804706	0.8265044008	1.4503797597
H	0.615766644	2.1033759574	0.3651075923
C	-1.1847670142	1.0682062323	-1.5358687507

C	-1.9160733882	1.0681822587	-0.3022010278
H	-1.4470926029	0.3739925236	-2.3279454863
H	-0.641692391	1.9537678905	-1.850484566
H	-2.736869717	0.3739674834	-0.1522235845
H	-1.9314733547	1.9537403339	0.3252411115
<hr/>			
<i>m</i> -Cl			
H	-1.7700987767	-1.898434476	0.0330096487

**Table S2. Continued**

C	0.3808977194	-1.9105387356	0.0140295884
C	-0.8618278016	-1.3018412186	0.0194821232
C	0.2421698335	0.9091699129	-0.0105937941
C	1.4759308071	0.2812396958	-0.015791595
Cl	2.9349501546	1.2144481949	-0.0373050507
H	0.4643278202	-2.9925556213	0.0232088027
C	-0.9510086347	0.1227760202	0.007207502
C	-2.2567712281	0.7905441016	0.7293572745
C	-2.2697476795	0.7775587822	-0.7026829612
H	-2.0251266203	1.675440501	-1.2615351005
C	1.5439876513	-1.1261620117	-0.0034854541
H	0.1804468927	1.9937715918	-0.0200017653
H	-2.0020268002	1.6982892305	1.2673584942
H	-2.828408881	0.0573804075	1.2897323775
H	-2.8515029061	0.0345500291	-1.2391754426
H	2.5189711777	-1.6053846284	-0.0077411298
<hr/>			
<i>m</i> -F			
H	-1.7409323982	-1.8848900973	0.0322000676
C	0.4096037861	-1.8962946031	0.0137068654
C	-0.8342924293	-1.2861381966	0.0187977962
C	0.2580686014	0.9313480284	-0.0112670931
C	1.476582831	0.2874480912	-0.0158303369
F	2.6022793317	1.0078902335	-0.0322755841
H	0.4913951168	-2.97826851	0.023064448
C	-0.9308577183	0.1384521687	0.0063575349
C	-2.2430576362	0.7964191777	0.7291687329
C	-2.2561861181	0.7835436958	-0.7026586856
H	-2.0164844662	1.6827904367	-1.261525888
C	1.5714592072	-1.1114530906	-0.0036485828
H	0.2150839265	2.0166596066	-0.0210120299

H	-1.9927373802	1.7052857012	1.2674234892
H	-2.8090617758	0.0594326868	1.2901800209
H	-2.8327788493	0.0369663602	-1.2397110416
H	2.5570786992	-1.5689399133	-0.0078961952
<hr/>			
<i>m</i> -CF <sub>3</sub>			
H	-1.7184442833	-0.419942143	0.007225819
C	0.4259035071	-0.4289801413	-0.0009030976
C	-0.8130117737	0.179947896	0.0028082353

**Table S2. Continued**

C	0.2938054019	2.3857803912	-0.0050050382
C	1.5285452776	1.7604028586	-0.0086761714
C	0.5602582966	-1.9421186071	0.0011350904
H	2.4424476963	2.3453118179	-0.0131098455
C	-0.902446561	1.6058455806	0.0008183242
C	-2.2152709567	2.2617361339	0.72031218
C	-2.2205684844	2.2593308993	-0.7113752672
H	-1.9766382277	3.1621167799	-1.2627368523
F	1.2428363655	-2.3529970182	1.0887349726
F	1.2356511107	-2.3565864032	-1.0895795141
F	-0.6445846556	-2.5440195376	0.0061073648
C	1.5937505907	0.3595304559	-0.0066342629
H	0.2261440278	3.4708015939	-0.0065199223
H	-1.9673731303	3.1664083076	1.2667934779
H	-2.7861215132	1.5215377064	1.2726034565
H	-2.7953888039	1.5172369941	-1.2569621021
H	2.5644570598	-0.1298972293	-0.0095393965
<hr/>			
3,5-(CF <sub>3</sub> ) <sub>2</sub>			
H	2.1755897194	1.7695413015	0.0016888564
C	1.223707311	-0.1531499576	0.0000791111
C	1.2329724823	1.2296430152	0.0004067939
C	-1.2330137331	1.2296016357	-0.0007085136
C	-1.2237022086	-0.1531910341	-0.0000403858
C	2.518751512	-0.9520643386	-0.0122055478
C	-2.5187195707	-0.9521460022	0.0124391479
C	-0.0000326221	1.9454263231	-0.0002382158
C	0.0012092991	3.4233300161	-0.7151539011
C	-0.0013240865	3.4235065577	0.7143155645
H	-0.9216302307	3.6006979408	1.2626583943

F	-3.590898301	-0.1440175465	-0.0815072961
F	-2.5459622778	-1.8184539287	-1.0174236989
F	-2.6189709049	-1.6595138541	1.1540707808
F	2.6190186159	-1.6597171804	-1.1536596798
F	2.5460314119	-1.8181108577	1.0178760136
F	3.5909029457	-0.1438753535	0.0815283917
C	0.0000140976	-0.8436731003	0.0001046768
H	-2.175649106	1.7694678863	-0.0021197807
H	-0.917132353	3.6001864305	-1.2669056608

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**Table S2. Continued**

H	0.921509348	3.6004178109	-1.2635404256
H	0.9170118864	3.600528854	1.2660235361
H	0.0000324422	-1.9313404268	0.0002420975

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**Table S3.** Cartesian coordinates of B3LYP/6-311+G\*\* and B3LYP/6-31+G\* of optimized  $\alpha$ -cumyl cations

B3LYP/6-311+G**			
<i>p</i> -NMe <sub>2</sub>			
H	-2.1925201108	-0.615537054	-0.9116300728
C	-1.229281034	-0.3347719983	-0.5095960752
C	1.2430815169	0.4195760947	0.5642478244
C	-0.0721625267	-1.1424719038	-0.8013536193
C	-1.1680398305	0.7751312078	0.2740704247
C	0.0760399475	1.208526917	0.8479290145
C	1.1641221943	-0.6943376505	-0.2120984357
H	-2.0727659322	1.3342474153	0.4619058177
H	2.0748040902	-1.2471192071	-0.3948371311
H	2.2012227376	0.7078060743	0.9708336703
C	-0.1436391063	-2.2783117448	-1.5982682724
C	-1.4053854538	-2.7455767137	-2.2518991731
H	-1.7904051354	-3.6122200167	-1.6984676692
H	-1.1880053099	-3.1065180057	-3.2610596897
H	-2.1957503018	-2.0025247311	-2.3124129996
C	1.0339128055	-3.1543785179	-1.887573454
H	1.877047867	-3.0303380499	-1.2135805533
H	1.3799607579	-2.9553178882	-2.9104464045
H	0.7274409861	-4.2039782281	-1.87327868
N	0.1449483655	2.3017399831	1.614907933
C	1.4237712285	2.7401403048	2.1979649033
H	1.8327257458	1.9738081294	2.8601575296
H	1.2530163582	3.640442681	2.7807312271
H	2.150344034	2.9693486521	1.4152501213
C	-1.055687951	3.103892853	1.902241326
H	-0.7755414499	3.9391944888	2.5371484807
H	-1.8053402887	2.5082220703	2.4278696483
H	-1.487914004	3.5013248382	0.981244109
<i>p</i> -MeO			
C	-0.9865872577	-0.9613308245	-0.0590215255
C	0.4524296647	-0.9727707314	-0.0156146042
C	1.1040667813	0.3047978541	0.0398826596
C	0.4039565913	1.4811569592	0.0451328029
C	-1.0140661875	1.4498736024	0.0093477239
C	-1.6942421143	0.2030860421	-0.039377015

**Table S3. Continued**

H	-1.5334151813	-1.8929718966	-0.0947162571
C	1.17893895	-2.1673015488	-0.024742967
H	2.1832475979	0.3581342411	0.0664816065
H	0.9336456551	2.4228524783	0.0793705746
O	-1.7834703479	2.5146992581	0.0177244047
H	-2.7765085487	0.2131140437	-0.0633516041
C	-1.2278905612	3.8510023826	0.0617245421
H	-0.6535924214	3.9899177268	0.9789087127
C	0.5309126187	-3.5088552844	-0.1188478381
H	-2.0896800636	4.5117175836	0.0571937515
C	2.6662561376	-2.2259545536	0.0670739464
H	-0.6119444304	4.031791158	-0.8204635324
H	1.1708517622	-4.199662759	-0.6726665229
H	0.4465707726	-3.9224134609	0.8962118238
H	-0.4595691262	-3.5081763946	-0.5657162181
H	3.1486443699	-1.3172348512	0.4143740911
H	2.9627648297	-3.0549295422	0.7163975935
H	3.0640998299	-2.4719557773	-0.9271656076
<b>3-Cl-4-MeO</b>			
C	-0.3937734195	-0.9972388336	-0.03779902
C	1.0419039636	-0.9898781085	-0.0183925065
C	1.6862467538	0.2871833163	0.0315263379
C	0.9687273781	1.453235069	0.0595718294
C	-0.4475419515	1.4251996406	0.0399455325
C	-1.1185054221	0.1593535233	-0.0098256966
H	-0.9336033275	-1.9330045281	-0.0751204736
C	1.7632846104	-2.1897461263	-0.0474424242
H	2.7645439518	0.3526165175	0.0478358298
H	1.4859685674	2.4016974742	0.0969709506
O	-1.2106238651	2.4871026169	0.0641567371
Cl	-2.8484110592	0.127636802	-0.033584633
C	-0.6551120977	3.8241902317	0.1146410378
H	-0.0726179356	3.9540043516	1.0278034345
C	1.0726899951	-3.5179840698	-0.1005594697
H	-1.5192341389	4.4816157861	0.1244866167
C	3.2470449217	-2.2633783545	-0.028478641
H	-0.0489108637	4.0121290166	-0.7726112717
H	1.7887808856	-4.3374001316	-0.1230661041

**Table S3. Continued**

H	0.4228873663	-3.6563459918	0.7697289312
H	0.4369113161	-3.594942652	-0.9883909121
H	3.7710617169	-1.3138681653	0.0127523377
H	3.5568127754	-2.8785770077	0.8259733173
H	3.5820067374	-2.8169337395	-0.9150263154
<i>p</i> -Me			
C	-1.093886137	-0.5493540992	-0.043197963
C	0.3371079815	-0.5585713659	0.0024977348
C	0.9951069193	0.7120733082	0.0533524243
C	0.278911525	1.8841507794	0.0492082847
C	-1.1322980725	1.8741740103	0.0104310673
C	-1.7980622921	0.6300109427	-0.0294341047
H	-1.6429135769	-1.4798847063	-0.0733147716
C	1.0646565498	-1.7632828639	-0.0011690293
H	2.0741794346	0.7647242664	0.0850109522
H	0.80133666	2.8329505549	0.0827954393
C	-1.9030766268	3.1532222314	-0.0141390799
H	-2.8812554064	0.609148278	-0.0511873852
H	-1.3712013018	3.9561895522	0.4984674942
H	-2.8958931419	3.0371778558	0.4227225606
C	0.4184365781	-3.1006339448	-0.1007727918
H	-2.0418492401	3.4710371863	-1.0560670789
C	2.5494473957	-1.8143126031	0.0931123394
H	1.0458192818	-3.7790346039	-0.6846070278
H	0.3777244054	-3.5308204685	0.9109304431
H	-0.5877371103	-3.0994669089	-0.5096346157
H	3.0180638071	-0.9256231989	0.5056552426
H	2.8598806446	-2.6887437121	0.6707628626
H	2.9457826173	-1.9725124644	-0.9208674055
H (unsubstituted)			
C	-1.341595563	-0.1495705329	0.0432748667
C	0.0875458378	-0.1435068112	0.000259059
C	0.7485824149	1.1234486047	-0.0461990158
C	0.0260255083	2.297633599	-0.059155078
C	-1.3733448584	2.2546654369	-0.0062004616
C	-2.0535565209	1.0310995592	0.0499293078
H	-1.8820294412	-1.0844571784	0.0862350337
C	0.8232082445	-1.3513927499	0.0036695266

**Table S3. Continued**

H	1.8272951028	1.174742069	-0.0868249763
H	0.5377130014	3.250694656	-0.1053804542
H	-1.9374756297	3.1807254463	-0.0087105417
H	-3.1352579697	1.0137698784	0.0936167248
C	0.177288767	-2.6897684593	-0.0116550601
C	2.3085756133	-1.3920352231	0.0232442893
H	0.7891587009	-3.399094039	-0.5744761909
H	0.1675741567	-3.0646824384	1.0235430162
H	-0.8412844589	-2.7086402596	-0.3880946343
H	2.7926378547	-0.4923679851	0.391636226
H	2.655702453	-2.2556676161	0.5960802284
H	2.6487300598	-1.5670996213	-1.0091785951
<i>m</i> -Cl			
C	-0.9499134503	-0.247277549	-0.0207077103
C	0.4774372554	-0.2561926866	-0.0024311424
C	1.1615982174	0.995857704	0.0233567372
C	0.4537662498	2.1810567644	0.0195386094
C	-0.9437284291	2.1661325378	0.0115079308
C	-1.6402383143	0.9477574296	-0.0026933233
H	-1.5121907433	-1.1694254663	-0.0324010581
C	1.1914555929	-1.480434068	-0.0110874661
H	2.2412143347	1.0321208592	0.0304351642
H	0.9767951893	3.1290279971	0.0278706843
H	-1.5003802772	3.0960380428	0.0165553443
Cl	-3.3750609478	0.953847478	-0.0058731011
C	0.5195827351	-2.8017179871	-0.1062269215
C	2.6715417373	-1.5512358236	0.0769760855
H	1.1601103325	-3.5203957203	-0.6223270091
H	0.4054879433	-3.1876781959	0.9191952438
H	-0.4625900027	-2.7879449308	-0.570724794
H	3.1581453422	-0.6697198036	0.4832382365
H	2.9726358159	-2.43319436	0.6487760194
H	3.0546404637	-1.7193234971	-0.9417640221
<i>m</i> -F			
C	-0.9706915694	-0.257983481	-0.0221396922
C	0.4562066428	-0.2582188321	-0.0036862442
C	1.1332272981	0.9980331265	0.0233194421
C	0.4227531478	2.1835252741	0.0221730395

**Table S3. Continued**

C	-0.9741855867	2.1652646408	0.0147695248
C	-1.6447214105	0.9395547749	-0.0020535375
H	-1.5479935895	-1.171319645	-0.0352234787
C	1.1779510333	-1.4786611799	-0.013449862
H	2.2125185806	1.0383605339	0.0294492908
H	0.9451293708	3.1316425145	0.0318379883
H	-1.5516145268	3.0828410018	0.0217005949
F	-2.9784099867	0.9390171319	-0.00500418
C	0.5093782999	-2.8012824409	-0.1082992639
C	2.657483951	-1.5429222552	0.0757033657
H	1.1551360339	-3.5232530653	-0.6127373935
H	0.3827027852	-3.1802841433	0.9184098785
H	-0.4680607364	-2.7891865834	-0.5832513924
H	3.1421223074	-0.6541223883	0.4678514894
H	2.9598591663	-2.4154438216	0.6616029622
H	3.0415178339	-1.728262438	-0.9397590245
<hr/>			
<i>m</i> -CF <sub>3</sub>			
C	-0.0179638278	-0.4942265891	0.025868438
C	1.4092303333	-0.4679319533	0.0251208422
C	2.0559944653	0.803643765	0.0160564684
C	1.3199989836	1.972041797	0.0196739307
C	-0.0758735119	1.9156462092	0.0101248763
C	-0.7400796135	0.6787708195	0.0074265939
H	-0.5532381128	-1.4322942616	0.0271735049
C	2.1568589764	-1.6731207292	0.0326505877
H	3.1348878604	0.8685402879	0.0228693598
H	1.8206051281	2.9318778698	0.0257873267
H	-0.6528592134	2.8340070095	0.0073564544
C	-2.2573769906	0.6612713367	-0.0293796488
F	-2.7415320547	-0.5794655205	0.1465130106
F	-2.7039392875	1.1188895936	-1.2130030702
C	1.5224027637	-3.0119852413	0.1186324387
F	-2.7641083919	1.4502036259	0.933246133
C	3.6387365403	-1.6984889336	-0.0462559581
H	1.461817708	-3.4132646943	-0.9056936844
H	2.1685019163	-3.703984458	0.6645377039
H	0.5243450189	-3.0275642546	0.5471085275
H	4.0964925408	-0.8118936531	-0.4753322386

**Table S3. Continued**

H	4.0204293455	-1.820336319	0.9799383962
H	3.9744823283	-2.5857155204	-0.5889978684
<hr/>			
3,5-(CF <sub>3</sub> ) <sub>2</sub>			
C	-0.5807630188	-1.4037332689	0.0442815223
C	0.8428873751	-1.4010157636	0.0007238887
C	1.5123067604	-0.1445926596	-0.0435085711
C	0.7937283029	1.0331756457	-0.0556100124
C	-0.604813545	1.0053977516	-0.000599831
C	-1.2846167702	-0.2171013833	0.0550918437
H	-1.131528809	-2.3321017744	0.0841354368
C	1.5760207867	-2.6197595732	0.0013858816
H	2.5905332768	-0.0929745163	-0.0828958485
C	1.496893729	2.3780043316	-0.1419798736
H	-1.1641824776	1.9351877839	-0.0011363117
C	-2.8021972768	-0.2081932061	0.1407371839
F	-3.306231626	-1.4463081946	0.0116108491
F	-3.3243623546	0.5637769204	-0.825097073
C	0.918074762	-3.9474031392	-0.0401575876
F	-3.2003016609	0.2848146991	1.3256570693
C	3.0571149314	-2.6608012987	0.0438416195
F	2.8268199959	2.2433186723	-0.0123430543
F	1.0592306862	3.20166573	0.8231456216
F	1.2482250017	2.9598678288	-1.3273810145
H	1.5433047649	-4.6659848234	-0.5758138488
H	0.868293522	-4.3188329001	0.9966830081
H	-0.0879880318	-3.9562930276	-0.4503608473
H	3.5365678773	-1.7751510232	0.4515214455
H	3.3982908941	-3.5483472312	0.5824903265
H	3.4090558268	-2.7945215419	-0.9923634962
<hr/>			
B3LYP/6-31+G*			
<hr/>			
<i>p</i> -NMe <sub>2</sub>			
H	-2.1976135219	-0.6152602876	-0.9101740275
C	-1.2314528402	-0.3347271509	-0.5088400547
C	1.2454799434	0.4236641311	0.5662041365
C	-0.0723214654	-1.1441104353	-0.8024632501
C	-1.1699864352	0.778620437	0.2773304059
C	0.0763572934	1.2136211998	0.8514564397

C	1.1662515999	-0.6938155118	-0.2124665462
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**Table S3. Continued**

H	-2.0777082816	1.337611725	0.46527873
H	2.0798850763	-1.2461227008	-0.3954457205
H	2.2066237753	0.7117256392	0.9723799703
C	-0.1439706399	-2.2827453881	-1.6012745988
C	-1.4071707816	-2.7525121916	-2.2582824494
H	-1.7963375952	-3.6210465023	-1.7054261381
H	-1.187723651	-3.1136754844	-3.2700288447
H	-2.2003078802	-2.0084756976	-2.3230418566
C	1.0347092428	-3.1628514943	-1.8918423066
H	1.879959815	-3.0433695258	-1.2149349779
H	1.3854505957	-2.9644516743	-2.9161106379
H	0.7259023467	-4.2147544618	-1.8778751862
N	0.1454540467	2.3095356287	1.6203387526
C	1.4258420261	2.746668081	2.2017353013
H	1.8354224659	1.9771187335	2.8641602997
H	1.2575950703	3.6490874881	2.7866240627
H	2.1526404218	2.9752746636	1.4153852276
C	-1.0569259644	3.1098518773	1.9071775823
H	-0.778945088	3.9480519817	2.5435028657
H	-1.8070701607	2.5105878222	2.4334958519
H	-1.4900392139	3.5064990985	0.983136769
<i>p</i> -MeO			
C	-0.9864158064	-0.9631202755	-0.0565814231
C	0.4559464591	-0.9735101739	-0.0197890133
C	1.1078598726	0.307768098	0.0328320854
C	0.4045682821	1.4870110737	0.0412700691
C	-1.0163263437	1.4535389056	0.0124300487
C	-1.6975944449	0.204114553	-0.0333271403
H	-1.5341281931	-1.8971377623	-0.0891504423
C	1.1833923458	-2.1709682428	-0.0293942183
H	2.1893279482	0.3636284079	0.0539731607
H	0.9349749178	2.4312399297	0.0728966594
O	-1.7892394384	2.5208206291	0.0246459156
H	-2.78245117	0.2118762817	-0.0519132307
C	-1.2346697299	3.8573039217	0.0662863239
H	-0.6545083424	3.9953704265	0.9828327372

C	0.5318821012	-3.5156855851	-0.1236107754
H	-2.099933892	4.5176752282	0.0662093931

**Table S3. Continued**

C	2.6734804814	-2.2353205573	0.0659204902
H	-0.6217925359	4.0378979421	-0.8211013707
H	1.1900668536	-4.2224047487	-0.6393737785
H	0.3967562752	-3.9118302336	0.8956902121
H	-0.4405442592	-3.5184887622	-0.615912217
H	3.1636091192	-1.3206538586	0.3951089814
H	2.963734	-3.0514812051	0.7391950482
H	3.0760654833	-2.509046983	-0.9218411591
<b>3-Cl-4-MeO</b>			
C	-0.3947492799	-0.9970687027	-0.0376919083
C	1.0439061431	-0.9897263802	-0.0183646217
C	1.6893393482	0.2906585662	0.0316182254
C	0.9691651643	1.4596467392	0.0597289076
C	-0.4500154587	1.4300032913	0.0401051397
C	-1.1228724483	0.1625026973	-0.0096585895
H	-0.9349586406	-1.9354111278	-0.0750013491
C	1.7652051771	-2.1929677969	-0.0475326741
H	2.7698547492	0.3580260482	0.0479360084
H	1.4873663387	2.4104121916	0.0971528088
O	-1.2156246721	2.4951381045	0.0643980733
Cl	-2.8531414742	0.1286845426	-0.0333469744
C	-0.660142564	3.8318721557	0.1148078144
H	-0.0761782904	3.9607199302	1.0300870094
C	1.0715650546	-3.5234932233	-0.1008551318
H	-1.5272480945	4.4895897766	0.1246592801
C	3.2524187502	-2.2717445566	-0.0286232313
H	-0.0525191608	4.0189431937	-0.774659009
H	1.7899058343	-4.3451054723	-0.1230250827
H	0.420345792	-3.6653048924	0.7713586586
H	0.435266296	-3.6039307505	-0.991485096
H	3.7813718975	-1.321623227	0.0127093097
H	3.5634348844	-2.8874443562	0.8283985106
H	3.5888415127	-2.8257101142	-0.9176206535
<b><i>p</i>-Me</b>			
C	-1.0958730417	-0.5508988294	-0.0372239186



C	0.3386571291	-0.559617884	0.0021491125
C	0.9974079054	0.7147051398	0.047017547
C	0.2782416321	1.8896790376	0.0438193133

**Table S3. Continued**

C	-1.1364095834	1.8793603879	0.0114175662
C	-1.8026605927	0.6316526398	-0.0221086148
H	-1.6466596804	-1.4833097086	-0.0619270815
C	1.0677679385	-1.7665139169	-0.0025286307
H	2.0788795411	0.7694701328	0.0722601919
H	0.8021145366	2.8408165955	0.0721624551
C	-1.9090602164	3.1609787518	-0.013491425
H	-2.8884782063	0.6094066234	-0.0389050441
H	-1.3831018769	3.9621863708	0.5143803483
H	-2.9091921311	3.0427220366	0.4131526368
C	0.4214732344	-3.1082381121	-0.1049402063
H	-2.0364097528	3.4907650938	-1.055888859
C	2.5559533748	-1.8211857114	0.0951118151
H	1.0568192558	-3.7904757291	-0.6806759717
H	0.3630365758	-3.5383418456	0.908597446
H	-0.5806593734	-3.1093984288	-0.5314192745
H	3.0290066265	-0.9301236253	0.5049527655
H	2.8621097412	-2.6928738858	0.6847858976
H	2.9595480643	-1.9903726486	-0.9168108615
H (unsubstituted)			
C	-1.3451636562	-0.1485485185	0.0508598258
C	0.0872738734	-0.1427170303	0.0000858978
C	0.7493749457	1.1273937015	-0.0538727544
C	0.0247488798	2.3048490735	-0.0668901112
C	-1.3780562482	2.2621933488	-0.0059264923
C	-2.0593291392	1.0353006602	0.0579992732
H	-1.8867923269	-1.0851511813	0.1013258641
C	0.8240455155	-1.3524339201	0.0033501117
H	1.8301446829	1.179225258	-0.1021809377
H	0.5380808126	3.2596685883	-0.1194582505
H	-1.9435311164	3.1902482647	-0.0082711903
H	-3.1433505905	1.0171047738	0.1082027443
C	0.178563191	-2.695657472	-0.0183609439
C	2.3134439835	-1.3960791101	0.0296325391

H	0.7964096751	-3.4038673476	-0.581538793
H	0.1577578017	-3.0775371181	1.0165541331
H	-0.8383465556	-2.7166178873	-0.4075865514
H	2.7990816192	-0.4980114284	0.4084273655

**Table S3. Continued**

H	2.6562773696	-2.2631629354	0.6052824276
H	2.6648605564	-1.5677033846	-1.0020208871

*m*-Cl

C	-0.9521830256	-0.2469404349	-0.0134818505
C	0.4787093848	-0.2543818479	-0.0039080463
C	1.1630602344	1.0017172463	0.0158878859
C	0.4516211742	2.1892540014	0.0142519002
C	-0.9495701272	2.1728435767	0.015165965
C	-1.6465779523	0.9502270774	0.007387287
H	-1.5143943338	-1.1720376585	-0.0186848337
C	1.1940031147	-1.4802817018	-0.0143998054
H	2.2449673061	1.0403626158	0.0145724575
H	0.9754063792	3.1397963299	0.0173344297
H	-1.5081546607	3.1043887322	0.0222207298
Cl	-3.381529787	0.9530192247	0.0157803918
C	0.5209781107	-2.8056611293	-0.1169251189
C	2.6771695339	-1.5560030674	0.0817390349
H	1.1737251968	-3.5304586687	-0.6142821616
H	0.3726421325	-3.1885241042	0.9076924927
H	-0.4490781962	-2.7931351305	-0.6132455661
H	3.1688246447	-0.6693236328	0.477958091
H	2.9696266227	-2.4292240224	0.6770609701
H	3.0710632929	-1.7483386816	-0.9309107457

*m*-F

C	-0.97248594	-0.2588548772	-0.0139933619
C	0.4581682179	-0.2566343841	-0.0053751235
C	1.1346069471	1.0042892727	0.0157470965
C	0.4202781201	2.1921810146	0.017720323
C	-0.9804444994	2.1722707559	0.020035642
C	-1.6487601193	0.9413238122	0.0093504379
H	-1.5495276655	-1.1750499558	-0.0203996901
C	1.1815010426	-1.4785201491	-0.0173807015
H	2.2161680963	1.0475549346	0.0129273234

H	0.9431736593	3.1430177751	0.022316741
H	-1.5606170037	3.0906491419	0.0298245764
F	-2.9873557392	0.9383205609	0.0163321066
C	0.5107419241	-2.8048915446	-0.1192229351
C	2.6641016806	-1.5479365428	0.0787445506

**Table S3. Continued**

H	1.1701766782	-3.5358114549	-0.5977874958
H	0.3409489225	-3.1767016215	0.9062601976
H	-0.450680516	-2.7935104561	-0.6327904794
H	3.1549697788	-0.6525304067	0.4554012554
H	2.9574931165	-2.4082093491	0.692760386
H	3.0578523439	-1.7636578016	-0.9292573418
<i>m</i> -CF <sub>3</sub>			
C	-0.0187785251	-0.4950214334	0.0251539313
C	1.4119775755	-0.4664213963	0.0299111325
C	2.0583300259	0.8093324885	0.0214891942
C	1.3181387503	1.9796293546	0.0189353163
C	-0.0810480194	1.9204359122	0.0019999325
C	-0.7450756799	0.6793948492	0.0000243648
H	-0.5521102273	-1.4366431857	0.0240331219
C	2.1611974308	-1.6729458265	0.0393876248
H	3.1392832543	0.877049311	0.0347504866
H	1.8184453795	2.9425206415	0.0252666816
H	-0.6611340381	2.839468828	-0.0082171042
C	-2.2628115744	0.6627542946	-0.0381220589
F	-2.7510620098	-0.5864381065	0.0913999949
F	-2.7108824574	1.1679942006	-1.2065722205
C	1.5257641115	-3.0160480813	0.1354712973
F	-2.7714241399	1.4179953886	0.9565289647
C	3.6461330951	-1.7033165712	-0.0507059423
H	1.4208589338	-3.4126214977	-0.8895325892
H	2.1883631139	-3.7156832938	0.6561589446
H	0.5423713503	-3.0318797047	0.6040901576
H	4.1084913206	-0.810181502	-0.4679269016
H	4.0415857738	-1.8534692738	0.9688018645
H	3.9711994609	-2.5812852097	-0.620904069
<i>3,5</i> -(CF <sub>3</sub> ) <sub>2</sub>			
C	-0.5832508582	-1.4054307005	0.0471852456

C	0.843827074	-1.4025081235	0.0006555197
C	1.5150008924	-0.1431389878	-0.0465067456
C	0.7947875194	1.0377603713	-0.0589337048
C	-0.6070369319	1.0090932225	-0.0005463856
C	-1.2891355656	-0.2159108053	0.0584426748
H	-1.1337805629	-2.3360624052	0.0921386244

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**Table S3. Continued**

C	1.5778595859	-2.6227446999	0.00132883
H	2.5951145705	-0.0927538364	-0.0910328231
C	1.4953361072	2.3845093471	-0.1432194309
H	-1.167542695	1.9407535001	-0.0010258545
C	-2.807181319	-0.2038331576	0.14207669
F	-3.3145779791	-1.449679596	0.06934592
F	-3.330150717	0.5253741537	-0.8623739708
C	0.9207308584	-3.955261299	-0.0534033566
F	-3.2084168679	0.3464658592	1.3052200491
C	3.0628426509	-2.6668456691	0.0569749165
F	2.8336899565	2.2491587925	-0.0700062118
F	1.0958160651	3.1887982396	0.860608265
F	1.1974816688	2.9960648599	-1.3068352505
H	1.5526641308	-4.6694873318	-0.5929087983
H	0.8589931263	-4.3396108569	0.9802880611
H	-0.0825723595	-3.9642398322	-0.4777287026
H	3.5412675663	-1.7832167912	0.4776699714
H	3.3968699901	-3.5576678352	0.600575163
H	3.431727016	-2.7974923804	-0.9759303689

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**Table S4.** Selected bond distances and bond angles of  $\alpha$ -methylphenonium ions optimized at B3LYP/6-311+G(d,p) and B3LYP/6-31+G(d)

Subst.	Bond lengths / Angstrom											
	C $\alpha$ C $\beta$	C1C $\alpha$	C1C $\beta$	C1C2	C1C6	C2C3	C5C6	C3C4	C4C5	$\angle$ C1C $\beta$ C $\alpha$	$\angle$ C1C $\alpha$ C $\beta$	$\angle$ C $\alpha$ C1C $\beta$
<i>p</i> -NMe <sub>2</sub>	1.456 (1.458)	1.612 (1.612)	1.575 (1.575)	1.444 (1.447)	1.443 (1.447)	1.357 (1.362)	1.358 (1.362)	1.440 (1.442)	1.440 (1.443)	64.0 (64.0)	61.5 (61.5)	54.3 (54.4)
<i>p</i> -OMe	1.445 (1.448)	1.657 (1.653)	1.583 (1.584)	1.432 (1.437)	1.437 (1.441)	1.368 (1.372)	1.362 (1.366)	1.420 (1.423)	1.423 (1.425)	66.2 (65.9)	60.9 (61.0)	52.9 (53.0)
3-Cl-4-OMe	1.443 (1.446)	1.664 (1.662)	1.586 (1.583)	1.435 (1.439)	1.428 (1.433)	1.365 (1.370)	1.368 (1.372)	1.433 (1.435)	1.419 (1.422)	66.5 (66.3)	60.9 (60.9)	52.7 (52.8)
<i>p</i> -Me	1.436 (1.439)	1.727 (1.715)	1.584 (1.586)	1.424 (1.429)	1.424 (1.428)	1.376 (1.379)	1.375 (1.379)	1.410 (1.414)	1.412 (1.416)	69.5 (68.9)	59.3 (59.7)	51.2 (51.5)
H	1.433 (1.436)	1.792 (1.749)	1.580 (1.583)	1.420 (1.425)	1.419 (1.424)	1.382 (1.385)	1.381 (1.384)	1.400 (1.403)	1.400 (1.405)	72.8 (71.7)	57.4 (58.1)	49.8 (50.3)
<i>m</i> -F	1.435 (1.437)	1.846 (1.823)	1.573 (1.576)	1.416 (1.421)	1.415 (1.421)	1.378 (1.381)	1.386 (1.390)	1.397 (1.400)	1.395 (1.400)	75.5 (74.3)	55.6 (56.4)	48.8 (49.4)
<i>m</i> -Cl	1.434 (1.437)	1.834 (1.812)	1.575 (1.577)	1.416 (1.421)	1.416 (1.421)	1.383 (1.387)	1.384 (1.388)	1.403 (1.407)	1.396 (1.407)	74.9 (73.7)	56.0 (56.7)	49.0 (49.6)
<i>m</i> -CF <sub>3</sub>	1.434 (1.436)	1.840 (1.818)	1.575 (1.578)	1.416 (1.421)	1.415 (1.420)	1.382 (1.385)	1.383 (1.387)	1.402 (1.405)	1.397 (1.400)	75.2 (74.0)	55.8 (56.5)	48.9 (49.4)
3,5-(CF <sub>3</sub> ) <sub>2</sub>	1.435 (1.438)	1.890 (1.865)	1.571 (1.573)	1.412 (1.417)	1.412 (1.417)	1.383 (1.386)	1.385 (1.387)	1.400 (1.404)	1.397 (1.400)	77.7 (76.4)	54.4 (55.1)	47.9 (48.5)

Values in parentheses are obtained at B3LYP/6-31+G(d).

**Table S5.** Selected bond distances and bond angles of phenonium ions optimized at B3LYP/6-311+G(d,p) and B3LYP/6-31+G(d)

Subst.	Bond lengths / Angstrom										$\angle\text{C1C}\beta\text{C}\alpha$	$\angle\text{C1C}\alpha\text{C}\beta$	$\angle\text{C}\alpha\text{C1C}\beta$
	C $\alpha$ C $\beta$	C1C $\alpha$	C1C $\beta$	C1C2	C1C6	C2C3	C5C6	C3C4	C4C5				
<i>p</i> -NMe <sub>2</sub>	1.458 (1.460)	1.576 (1.577)	1.576 (1.577)	1.446 (1.450)	1.446 (1.450)	1.356 (1.360)	1.356 (1.360)	1.442 (1.445)	1.442 (1.445)	62.5 (62.4)	62.5 (62.4)	55.0 (55.0)	
<i>p</i> -OMe	1.447 (1.450)	1.595 (1.595)	1.595 (1.594)	1.437 (1.441)	1.442 (1.445)	1.365 (1.370)	1.360 (1.364)	1.423 (1.426)	1.425 (1.427)	63.0 (63.0)	63.0 (63.0)	54.0 (54.0)	
3-Cl-4-OMe	1.446 (1.448)	1.598 (1.600)	1.598 (1.600)	1.439 (1.443)	1.434 (1.438)	1.363 (1.367)	1.365 (1.370)	1.436 (1.439)	1.421 (1.424)	63.0 (63.0)	63.0 (63.0)	53.8 (53.9)	
<i>p</i> -Me	1.436 (1.440)	1.616 (1.614)	1.616 (1.615)	1.430 (1.435)	1.430 (1.434)	1.372 (1.376)	1.372 (1.376)	1.414 (1.417)	1.414 (1.417)	63.6 (63.5)	63.6 (63.5)	52.8 (53.0)	
H	1.430 (1.434)	1.631 (1.628)	1.631 (1.628)	1.426 (1.431)	1.426 (1.431)	1.378 (1.382)	1.378 (1.382)	1.403 (1.406)	1.403 (1.406)	64.0 (63.9)	64.0 (63.9)	52.0 (52.3)	
<i>m</i> -F	1.428 (1.432)	1.637 (1.636)	1.637 (1.636)	1.425 (1.429)	1.423 (1.428)	1.375 (1.378)	1.381 (1.385)	1.400 (1.402)	1.398 (1.402)	64.0 (64.0)	64.2 (64.0)	51.7 (51.9)	
<i>m</i> -Cl	1.428 (1.432)	1.637 (1.635)	1.637 (1.635)	1.425 (1.429)	1.423 (1.427)	1.381 (1.384)	1.380 (1.384)	1.405 (1.409)	1.400 (1.403)	64.0 (64.0)	64.0 (64.0)	51.7 (52.0)	
<i>m</i> -CF <sub>3</sub>	1.428 (1.432)	1.636 (1.634)	1.636 (1.635)	1.425 (1.429)	1.424 (1.428)	1.377 (1.380)	1.380 (1.384)	1.406 (1.409)	1.400 (1.402)	64.0 (64.0)	64.0 (64.0)	51.8 (51.9)	
3,5-(CF <sub>3</sub> ) <sub>2</sub>	1.426 (1.429)	1.644 (1.642)	1.644 (1.642)	1.421 (1.426)	1.421 (1.426)	1.379 (1.383)	1.379 (1.383)	1.402 (1.405)	1.400 (1.405)	64.3 (64.2)	64.3 (64.2)	51.4 (51.6)	

Values in parentheses are obtained at B3LYP/6-31+G(d).

**Table S6.** Selected bond distances of  $\alpha$ -cumyl cations optimized at B3LYP/6-311+G(d,p) and B3LYP/6-31+G(d)

Subst.	Bond lengths / Angstrom						
	C1C7	C1C2	C1C6	C2C3	C5C6	C3C4	C4C5
<i>p</i> -NMe <sub>2</sub>	1.389 (1.393)	1.441 (1.444)	1.441 (1.444)	1.360 (1.364)	1.360 (1.364)	1.437 (1.440)	1.437 (1.440)
<i>p</i> -OMe	1.398 (1.400)	1.440 (1.443)	1.435 (1.439)	1.363 (1.367)	1.369 (1.373)	1.421 (1.424)	1.419 (1.422)
3-Cl-4-OMe	1.400 (1.403)	1.436 (1.439)	1.431 (1.435)	1.365 (1.369)	1.369 (1.373)	1.434 (1.436)	1.417 (1.420)
<i>p</i> -Me	1.407 (1.410)	1.432 (1.435)	1.432 (1.435)	1.374 (1.378)	1.374 (1.378)	1.412 (1.415)	1.412 (1.415)
H	1.414 (1.416)	1.430 (1.433)	1.430 (1.433)	1.379 (1.383)	1.379 (1.383)	1.400 (1.405)	1.400 (1.405)
<i>m</i> -F	1.418 (1.420)	1.427 (1.431)	1.427 (1.431)	1.374 (1.378)	1.382 (1.386)	1.397 (1.400)	1.397 (1.400)
<i>m</i> -Cl	1.417 (1.419)	1.427 (1.431)	1.427 (1.431)	1.380 (1.384)	1.380 (1.384)	1.403 (1.407)	1.398 (1.400)
<i>m</i> -CF <sub>3</sub>	1.418 (1.420)	1.427 (1.431)	1.427 (1.430)	1.378 (1.381)	1.381 (1.385)	1.404 (1.408)	1.397 (1.400)
3,5-(CF <sub>3</sub> ) <sub>2</sub>	1.422 (1.424)	1.424 (1.428)	1.424 (1.428)	1.380 (1.383)	1.380 (1.383)	1.400 (1.403)	1.400 (1.403)

Values in parentheses are obtained at B3LYP/6-31+G(d).