Supporting Information

for

Linear Free Energy Relationship and Kinetic Isotope Effects as Measures for the Transition State Variation. A Computational Study

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SI-1. B3LYP/6-31++G** optimized Cartesian coordinates and enthalpies for X-substituted phenylethyl alcohols

X=*p*-OMe Enthalpy (H) = 128.845 kcal/mol (total = -500.551869 hartree)

C ,	-2.351967	-0.031873	-0.667169
C ,	-3.129526	-0.147585	0.643326
C ,	-0.859805	0.070665	-0.446775
H ,	-2.587306	-0.904772	-1.283089
H ,	-2.719137	0.846511	-1.206317
H ,	-2.926265	0.727452	1.274816
H ,	-2.802809	-1.041674	1.190894
C ,	-0.051540	-1.065145	-0.409232
C ,	-0.240650	1.313017	-0.244209
C ,	1.323836	-0.985139	-0.175386
C ,	1.122958	1.414941	-0.010866
C ,	1.916715	0.262694	0.026593
H ,	-0.495685	-2.042238	-0.573119
H ,	-0.837984	2.218971	-0.278193
H ,	1.911763	-1.893159	-0.161244
H ,	1.597489	2.377430	0.139034
O ,	3.248493	0.462771	0.259635
O ,	-4.519959	-0.229443	0.322351
H ,	-5.024878	-0.299204	1.137762
C ,	4.106582	-0.667787	0.306401
H ,	5.103824	-0.277096	0.502778
H ,	4.111137	-1.207578	-0.647061
H ,	3.821956	-1.354003	1.111748

X=*p*-OH Enthalpy (H) = 110.299 kcal/mol (total = -461.272476 hartree)

C ,	1.878052	0.030598	0.684947
C ,	2.695163	-0.015008	-0.605613
C ,	0.388777	0.015546	0.425066
H ,	2.165994	-0.824825	1.303243
H ,	2.159655	0.931719	1.237539
H ,	2.443389	0.848825	-1.235242
H ,	2.450490	-0.925375	-1.168944
C ,	-0.311003	-1.190744	0.292522
C ,	-0.333152	1.202715	0.277081
C ,	-1.674388	-1.218484	0.021484
C ,	-1.700262	1.193680	0.004572
C ,	-2.373856	-0.020513	-0.125077
H ,	0.219552	-2.130311	0.411957
H ,	0.175454	2.155874	0.382459
H ,	-2.209704	-2.155649	-0.073019
H ,	-2.240028	2.130603	-0.100279
O ,	-3.716576	-0.100319	-0.389327
O ,	4.078876	0.003711	-0.248176

H , 4.608607 -0.030128 -1.050113
H , -4.087793 0.785388 -0.457477

X=*p*-Me Enthalpy (H) = 125.223 kcal/mol (total = -425.329225 hartree)
C , 1.912515 0.000841 -0.684515
C , 2.724444 0.000911 0.610456
C , 0.422516 0.000483 -0.428264
H , 2.198577 0.880611 -1.268440
H , 2.199027 -0.878679 -1.268589
H , 2.471322 -0.885771 1.207120
H , 2.474105 0.889658 1.205223
C , -0.287454 1.197194 -0.287279
C , -0.286942 -1.196613 -0.287642
C , -1.654157 1.196825 -0.017114
C , -1.653641 -1.196944 -0.017662
C , -2.363966 -0.000211 0.120550
H , 0.234264 2.143510 -0.394516
H , 0.235201 -2.142662 -0.395159
H , -2.177098 2.142905 0.084572
H , -2.176205 -2.143282 0.083580
C , -3.852313 -0.000691 0.374673
O , 4.109149 -0.001582 0.259333
H , 4.635135 -0.001887 1.064518
H , -4.161191 0.884296 0.936169
H , -4.412149 -0.002473 -0.567226
H , -4.160189 -0.884340 0.938854

X=*m*-Me Enthalpy (H) = 125.204 kcal/mol (total = -425.329310 hartree)
C , 1.744197 , -0.005995 , 0.701174
C , 2.573568 , -0.253581 , -0.558241
C , 0.291318 , 0.272372 , 0.386933
H , 1.834212 , -0.882827 , 1.348989
H , 2.184926 , 0.837642 , 1.240237
H , 2.523299 , 0.624519 , -1.215473
H , 2.166571 , -1.111737 , -1.109147
C , -0.630421 , -0.775484 , 0.286358
C , -0.155857 , 1.576936 , 0.155781
C , -1.972477 , -0.554081 , -0.036885
C , -1.488475 , 1.817562 , -0.171905
C , -2.390084 , 0.760728 , -0.269405
H , -0.293658 , -1.792144 , 0.471442
H , 0.540176 , 2.405995 , 0.235728
C , -2.953493 , -1.700611 , -0.098472
H , -1.825961 , 2.832883 , -0.350033
H , -3.426537 , 0.957590 , -0.524754
O , 3.920913 , -0.505790 , -0.151017
H , 4.460278 , -0.651511 , -0.933869

H , -3.473436 , -1.823424 , 0.858065
H , -3.715475 , -1.532925 , -0.863732
H , -2.451355 , -2.644818 , -0.321349

X=H Enthalpy (H) = 107.023 kcal/mol (total = -386.030817 hartree)
C , 1.384694 , -0.000925 , 0.700823
C , 2.257680 , -0.000797 , -0.553801
C , -0.091124 , -0.000392 , 0.372376
H , 1.642138 , -0.880780 , 1.297494
H , 1.642734 , 0.878585 , 1.297740
H , 2.035174 , 0.886324 , -1.161361
H , 2.037262 , -0.889305 , -1.160104
C , -0.789095 , -1.201443 , 0.200946
C , -0.788286 , 1.201176 , 0.201289
C , -2.141996 , -1.203791 , -0.133999
C , -2.141187 , 1.204523 , -0.133618
C , -2.822850 , 0.000617 , -0.303755
H , -0.269085 , -2.144428 , 0.339293
H , -0.267632 , 2.143770 , 0.339886
H , -2.665167 , -2.145785 , -0.256950
H , -2.663736 , 2.146901 , -0.256263
H , -3.876114 , 0.001014 , -0.560838
O , 3.623554 , 0.001056 , -0.133609
H , 4.188976 , 0.001460 , -0.911583

X=*m*-OH Enthalpy (H) = 110.296 kcal/mol (total = -461.273037 hartree)
C , 1.719687 0.006673 0.702397
C , 2.556256 -0.196868 -0.560671
C , 0.260794 0.252743 0.389727
H , 1.832630 -0.878979 1.334397
H , 2.136055 0.851986 1.257236
H , 2.489227 0.693903 -1.198660
H , 2.167698 -1.050867 -1.131180
C , -0.631032 -0.820525 0.289136
C , -0.216476 1.546704 0.160873
C , -1.970867 -0.606517 -0.035963
C , -1.556839 1.754874 -0.164093
C , -2.440908 0.686571 -0.265900
H , -0.278332 -1.832386 0.474733
H , 0.458431 2.391580 0.245244
O , -2.873615 -1.632245 -0.138720
H , -1.919183 2.762507 -0.335243
H , -3.485106 0.834093 -0.512693
O , 3.905956 -0.430784 -0.153820
H , 4.453544 -0.540031 -0.936827
H , -2.437366 -2.469510 0.050264

X=*p*-Cl Enthalpy (H) = 101.756 kcal/mol (total = -845.662043 hartree)

C ,	-2.330630	0.000289	-0.670030
C ,	-3.107872	-0.001277	0.646794
C ,	-0.834943	0.000230	-0.452838
H ,	-2.631650	-0.878581	-1.247293
H ,	-2.631891	0.880362	-1.245314
H ,	-2.839923	0.885102	1.237523
H ,	-2.841786	-0.890357	1.234306
C ,	-0.124157	-1.198899	-0.334093
C ,	-0.124062	1.199257	-0.333586
C ,	1.249416	-1.209876	-0.101868
C ,	1.249531	1.210099	-0.101438
C ,	1.925114	0.000050	0.013805
H ,	-0.648070	-2.144373	-0.431552
H ,	-0.647927	2.144800	-0.430617
H ,	1.789241	-2.144598	-0.017007
H ,	1.789431	2.144744	-0.016240
Cl ,	3.661615	-0.000129	0.302364
O ,	-4.499039	0.000700	0.328750
H ,	-5.006968	0.000261	1.145535

X=*m*-CHO Enthalpy (H) = 114.002 kcal/mol (total = -499.377517 hartree)

C ,	2.078033	-0.097283	0.693465
C ,	2.863805	-0.399303	-0.583088
C ,	0.652296	0.311892	0.402582
H ,	2.097512	-0.987588	1.328083
H ,	2.598719	0.695854	1.237524
H ,	2.882033	0.489087	-1.228447
H ,	2.373493	-1.209713	-1.138757
C ,	-0.374992	-0.634325	0.354582
C ,	0.324864	1.646817	0.139697
C ,	-1.688441	-0.264544	0.048663
C ,	-0.983990	2.027369	-0.167400
C ,	-1.993984	1.076508	-0.215697
H ,	-0.154554	-1.677876	0.564378
H ,	1.103781	2.401852	0.181926
C ,	-2.743298	-1.303248	0.014229
H ,	-1.208584	3.069858	-0.362855
H ,	-3.017170	1.346423	-0.448309
O ,	4.185308	-0.774164	-0.196413
H ,	4.698182	-0.974278	-0.985049
O ,	-3.909240	-1.101792	-0.243552
H ,	-2.387725	-2.329269	0.249028

X=*m*-Cl Enthalpy (H) = 101.766 kcal/mol (total = -845.662325 hartree)

C ,	2.062309	-0.079055	0.702158
C ,	2.843028	-0.437844	-0.562717

C , 0.654892 0.378787 0.393417
H , 2.044654 -0.955309 1.356000
H , 2.608697 0.706534 1.231536
H , 2.891627 0.433137 -1.229561
H , 2.329830 -1.246391 -1.099880
C , -0.390868 -0.548234 0.325150
C , 0.375377 1.725553 0.137119
C , -1.675400 -0.123880 0.003105
C , -0.916145 2.136441 -0.183744
C , -1.957274 1.213161 -0.254646
H , -0.207190 -1.596677 0.528179
H , 1.173916 2.457533 0.195949
Cl , -2.976440 -1.309188 -0.072840
H , -1.119823 3.183803 -0.375837
H , -2.965169 1.522295 -0.499342
O , 4.151100 -0.844388 -0.160732
H , 4.658631 -1.083206 -0.941962

X=*p*-CHO Enthalpy (H) = 113.995 kcal/mol (total = -499.378116 hartree)
C , -2.265381 0.044032 -0.662905
C , -3.036853 -0.156443 0.643095
C , -0.772782 0.099264 -0.441961
H , -2.519599 -0.776919 -1.339328
H , -2.616221 0.968363 -1.129763
H , -2.819388 0.668932 1.333844
H , -2.719746 -1.091608 1.122975
C , -0.010181 -1.079632 -0.410556
C , -0.122528 1.321192 -0.235044
C , 1.356348 -1.042137 -0.177105
C , 1.248166 1.365543 -0.000798
C , 1.998480 0.185946 0.031399
H , -0.499981 -2.033159 -0.580547
H , -0.694432 2.242821 -0.265474
H , 1.947476 -1.950304 -0.156713
H , 1.743010 2.319599 0.154220
C , 3.454708 0.250281 0.278885
O , -4.425670 -0.196196 0.318138
H , -4.932591 -0.326254 1.125120
O , 4.195603 -0.707180 0.326747
H , 3.852141 1.277263 0.426524

X=*m*-CN Enthalpy (H) = 107.284 kcal/mol (total = -478.297094 hartree)
C , 1.950409 -0.109101 0.700263
C , 2.734585 -0.460068 -0.565173
C , 0.540976 0.340827 0.391637
H , 1.936943 -0.987028 1.351715
H , 2.491667 0.677996 1.232568

H , 2.776899 0.412029 -1.231354
H , 2.228117 -1.272017 -1.103655
C , -0.503068 -0.582966 0.324558
C , 0.255198 1.687112 0.133613
C , -1.803912 -0.171861 0.001681
C , -1.035900 2.102149 -0.187303
C , -2.072798 1.179194 -0.256605
H , -0.315169 -1.630992 0.528852
H , 1.053622 2.419773 0.191319
C , -2.860534 -1.136375 -0.059195
H , -1.235455 3.149959 -0.379184
H , -3.080208 1.490984 -0.502082
O , 4.044019 -0.855451 -0.160664
H , 4.551641 -1.103940 -0.938931
N , -3.712849 -1.915232 -0.109257

X=*p*-CN Enthalpy (H) = 107.297 kcal/mol (total = -478.297433 hartree)
C , 2.192416 0.000376 -0.663018
C , 2.967041 0.000647 0.656684
C , 0.697937 0.000216 -0.446862
H , 2.493599 0.880500 -1.237899
H , 2.493887 -0.879806 -1.237652
H , 2.698474 -0.886480 1.245968
H , 2.700268 0.889282 1.244515
C , -0.010452 1.202367 -0.328157
C , -0.010258 -1.202095 -0.328306
C , -1.380237 1.211423 -0.096381
C , -1.380022 -1.211414 -0.096653
C , -2.075695 -0.000011 0.022303
H , 0.517180 2.145318 -0.425900
H , 0.517523 -2.144950 -0.426151
H , -1.917060 2.148290 -0.011120
H , -1.916754 -2.148348 -0.011600
C , -3.486897 -0.000265 0.257732
O , 4.356302 -0.000965 0.336859
H , 4.866342 -0.001296 1.152463
N , -4.626695 -0.000322 0.449778

X=*m*-NO_2 Enthalpy (H) = 110.076 kcal/mol (total = -590.589638 hartree)
C , 2.295151 -0.090983 0.683947
C , 3.038954 -0.488318 -0.592221
C , 0.907256 0.433140 0.396791
H , 2.244381 -0.964455 1.339333
H , 2.886424 0.667852 1.203777
H , 3.112397 0.376507 -1.265296
H , 2.483999 -1.277865 -1.115981
C , -0.181265 -0.438834 0.322447

C ,	0.683473	1.797000	0.168951
C ,	-1.443118	0.063269	0.023385
C ,	-0.588802	2.283603	-0.127988
C ,	-1.672778	1.415602	-0.204577
H ,	-0.063820	-1.500049	0.499393
H ,	1.517326	2.488487	0.232581
N ,	-2.585267	-0.877034	-0.047644
H ,	-0.737833	3.343702	-0.295458
H ,	-2.671536	1.762380	-0.429293
O ,	4.333782	-0.944496	-0.206563
H ,	4.810718	-1.235675	-0.989426
O ,	-3.688809	-0.412375	-0.304410
O ,	-2.359775	-2.064195	0.152157

X=*p*-NO_2 Enthalpy (H) = 110.118 kcal/mol (total = -590.589993 hartree)

C ,	2.610610	0.000576	-0.660972
C ,	3.367750	0.000747	0.668962
C ,	1.113994	0.000376	-0.464001
H ,	2.919104	0.880751	-1.231538
H ,	2.919403	-0.879719	-1.231191
H ,	3.092883	-0.886383	1.254748
H ,	3.095285	0.889671	1.253154
C ,	0.405570	1.204399	-0.355060
C ,	0.405981	-1.203860	-0.354728
C ,	-0.967642	1.215491	-0.141006
C ,	-0.967226	-1.215370	-0.140720
C ,	-1.635623	-0.000033	-0.035405
H ,	0.935030	2.146598	-0.446444
H ,	0.935784	-2.145897	-0.445829
H ,	-1.522553	2.139936	-0.059791
H ,	-1.521821	-2.139986	-0.059313
N ,	-3.095635	-0.000241	0.189639
O ,	4.760879	-0.001367	0.364205
H ,	5.261931	-0.001109	1.185284
O ,	-3.658347	1.084481	0.278180
O ,	-3.658292	-1.085131	0.276494

SI-2.B3LYP/6-311+G** optimized Cartesian coordinates and enthalpies for X-substituted protonated phenylethyl alcohols

X=*p*-OMe Enthalpy (H) = 136.360 kcal/mol (total = -500.855541 hartree)

C ,	2.288329	-0.000782	0.768705
C ,	2.872796	-0.146543	-0.602185
C ,	0.793301	0.088806	0.492872
H ,	2.516973	-0.863771	1.398784
H ,	2.645456	0.904787	1.265342
H ,	2.762984	0.712106	-1.258563
H ,	2.653334	-1.078182	-1.115952
C ,	0.003520	-1.063256	0.447687
C ,	0.184860	1.333076	0.255597
C ,	-1.362382	-0.990477	0.191474
C ,	-1.170145	1.420159	-0.000696
C ,	-1.960005	0.257364	-0.036671
H ,	0.445690	-2.036111	0.640054
H ,	0.772045	2.245332	0.297711
H ,	-1.948714	-1.898741	0.182245
H ,	-1.650489	2.376269	-0.166658
O ,	-3.266783	0.447944	-0.289791
O ,	4.532821	-0.246559	-0.582530
H ,	4.876582	-1.020788	-0.104767
H ,	4.972678	0.551855	-0.243393
C ,	-4.150960	-0.677159	-0.330289
H ,	-5.134335	-0.265931	-0.544426
H ,	-4.172213	-1.192922	0.633794
H ,	-3.864179	-1.372095	-1.124564

X=*p*-OH Enthalpy (H) = 117.942 kcal/mol (total = -461.573796 hartree)

C ,	1.810325	0.023855	0.774630
C ,	2.459352	-0.001120	-0.577973
C ,	0.319966	0.012960	0.462795
H ,	2.086197	-0.852594	1.366874
H ,	2.081989	0.924043	1.331969
H ,	2.315271	0.887957	-1.185816
H ,	2.307221	-0.908349	-1.156414
C ,	-0.366734	-1.200743	0.310064
C ,	-0.384499	1.210707	0.299030
C ,	-1.720080	-1.220580	0.016134
C ,	-1.742363	1.202653	0.004746
C ,	-2.416475	-0.015340	-0.140025
H ,	0.154034	-2.143521	0.446434
H ,	0.118763	2.164248	0.424739
H ,	-2.259283	-2.153866	-0.086099
H ,	-2.278896	2.139481	-0.102313
O ,	-3.734916	-0.103544	-0.423199

O , 4.098712 -0.007571 -0.490180
H , 4.469361 -0.797917 -0.060472
H , 4.476664 0.785897 -0.072834
H , -4.138643 0.769183 -0.495449

X=*p*-Me Enthalpy (H) = 132.929 kcal/mol (total = -425.630907 hartree)
C , -1.847152 0.000342 0.760564
C , -2.504604 0.000031 -0.589820
C , -0.353030 0.000215 0.460686
H , -2.121568 0.889292 1.334964
H , -2.121658 -0.888258 1.335469
H , -2.352850 -0.897334 -1.183927
H , -2.353224 0.897344 -1.184101
C , 0.340069 1.205300 0.305663
C , 0.339925 -1.205022 0.305982
C , 1.700531 1.200707 0.017349
C , 1.700354 -1.200693 0.017647
C , 2.406456 -0.000057 -0.130439
H , -0.174392 2.153396 0.430684
H , -0.174674 -2.153013 0.431257
H , 2.223635 2.144770 -0.087711
H , 2.223339 -2.144850 -0.087169
C , 3.887265 -0.000276 -0.406362
O , -4.125687 -0.000272 -0.488555
H , -4.495472 0.791994 -0.060925
H , -4.495258 -0.793339 -0.062231
H , 4.189212 0.885490 -0.968083
H , 4.450959 -0.001524 0.532576
H , 4.188560 -0.885065 -0.969987

X=*m*-Me Enthalpy (H) = 132.949 kcal/mol (total = -425.630311 hartree)
C , 1.678902 , -0.023274 , 0.771884
C , 2.376660 , -0.181663 , -0.549621
C , 0.223819 , 0.264132 , 0.416631
H , 1.752399 , -0.936597 , 1.368277
H , 2.103026 , 0.805977 , 1.344732
H , 2.427401 , 0.714660 , -1.162343
H , 2.071847 , -1.043275 , -1.138118
C , -0.691197 , -0.789596 , 0.306959
C , -0.192014 , 1.574301 , 0.168939
C , -2.025568 , -0.557523 , -0.034701
C , -1.519765 , 1.818544 , -0.175733
C , -2.422082 , 0.764840 , -0.278103
H , -0.369793 , -1.806603 , 0.514096
H , 0.502224 , 2.403067 , 0.266090
C , -3.019153 , -1.687939 , -0.124448
H , -1.851136 , 2.834054 , -0.357141

H , -3.453630 , 0.970103 , -0.543485
O , 3.952809 , -0.497351 , -0.374991
H , 4.139252 , -1.335300 , 0.084114
H , 4.453833 , 0.218720 , 0.053934
H , -3.792659 , -1.587177 , 0.642424
H , -3.523658 , -1.691251 , -1.094250
H , -2.539188 , -2.658506 , 0.010755

X=H Enthalpy (H) = 114.797 kcal/mol (total = -386.329871 hartree)
C , -1.318148 , 0.000016 , 0.765293
C , -2.054103 , 0.000053 , -0.546263
C , 0.161071 , 0.000013 , 0.395161
H , -1.562628 , 0.888448 , 1.353985
H , -1.562652 , -0.888530 , 1.353794
H , -1.932189 , -0.896420 , -1.148845
H , -1.932620 , 0.896626 , -1.148782
C , 0.840417 , 1.209270 , 0.211478
C , 0.840378 , -1.209256 , 0.211327
C , 2.187132 , 1.207632 , -0.142449
C , 2.187081 , -1.207636 , -0.142605
C , 2.860177 , -0.000012 , -0.321805
H , 0.328453 , 2.153956 , 0.366943
H , 0.328361 , -2.153935 , 0.366662
H , 2.711326 , 2.147148 , -0.269656
H , 2.711244 , -2.147152 , -0.269921
H , 3.909070 , -0.000033 , -0.593093
O , -3.653190 , -0.000328 , -0.348416
H , -3.998921 , 0.794529 , 0.094938
H , -3.997950 , -0.792496 , 0.100484

X=*m*-OH Enthalpy (H) = 118.027 kcal/mol (total = -461.570765 hartree)
C , 1.650012 -0.079970 0.771141
C , 2.368429 -0.111993 -0.549837
C , 0.192953 0.204783 0.422761
H , 1.739540 -1.037203 1.291390
H , 2.047166 0.708180 1.416751
H , 2.400239 0.832675 -1.086149
H , 2.092929 -0.929462 -1.211331
C , -0.711751 -0.855040 0.290955
C , -0.224636 1.517674 0.197737
C , -2.041476 -0.595426 -0.050420
C , -1.554409 1.764533 -0.148354
C , -2.459539 0.721240 -0.275327
H , -0.393967 -1.876788 0.479934
H , 0.465510 2.346208 0.316198
O , -2.977953 -1.567268 -0.178549
H , -1.887380 2.782429 -0.311467

H , -3.495071 0.901407 -0.535739
O , 3.946558 -0.397888 -0.379303
H , 4.155401 -1.263357 0.014544
H , 4.426731 0.297794 0.103755
H , -2.617445 -2.435444 0.032985

X=*p*-Cl Enthalpy (H) = 109.471 kcal/mol (total = -845.956825 hartree)
C , -2.264802 0.002489 0.739165
C , -2.900571 -0.000120 -0.624795
C , -0.762617 0.001574 0.484529
H , -2.553419 0.891940 1.305913
H , -2.554263 -0.884003 1.310086
H , -2.732763 -0.896971 -1.215835
H , -2.734863 0.895743 -1.217878
C , -0.066020 1.207773 0.352698
C , -0.067083 -1.205550 0.355375
C , 1.302402 1.212821 0.105677
C , 1.301312 -1.212371 0.108392
C , 1.978660 -0.000201 -0.017872
H , -0.582480 2.155886 0.464514
H , -0.584346 -2.152973 0.469396
H , 1.842936 2.146295 0.017317
H , 1.841038 -2.146512 0.022164
Cl , 3.693026 -0.001332 -0.324658
O , -4.509069 -0.001489 -0.548786
H , -4.889285 0.787196 -0.122789
H , -4.889127 -0.800525 -0.142436

X=*m*-CHO Enthalpy (H) = 121.729 kcal/mol (total = -499.668492 hartree)
C , 2.022637 -0.037141 0.747303
C , 2.679293 -0.349867 -0.571989
C , 0.583510 0.345615 0.419006
H , 2.041150 -0.906982 1.409782
H , 2.529071 0.792198 1.248868
H , 2.777963 0.492127 -1.252787
H , 2.290649 -1.223690 -1.089258
C , -0.415823 -0.630146 0.375232
C , 0.253677 1.675777 0.136588
C , -1.729117 -0.281121 0.056808
C , -1.058585 2.026839 -0.180895
C , -2.048336 1.052367 -0.224408
H , -0.185729 -1.666868 0.608471
H , 1.015463 2.447911 0.183902
C , -2.786687 -1.333250 0.024445
H , -1.303584 3.062073 -0.385314
H , -3.074800 1.302532 -0.465568
O , 4.213206 -0.769003 -0.399449

H , 4.351954 -1.589703 0.106215
H , 4.784366 -0.066948 -0.039679
O , -3.936800 -1.118810 -0.263656
H , -2.441162 -2.354579 0.287670

X=*m*-Cl Enthalpy (H) = 109.537 kcal/mol (total = -845.956638 hartree)
C , 2.002905 -0.027048 0.759901
C , 2.660855 -0.354455 -0.554824
C , 0.583866 0.411223 0.414552
H , 1.980571 -0.901737 1.415723
H , 2.532925 0.780138 1.272928
H , 2.805007 0.489396 -1.224920
H , 2.240380 -1.205308 -1.085279
C , -0.435468 -0.542571 0.341758
C , 0.305350 1.753503 0.140695
C , -1.725258 -0.142569 0.002584
C , -0.990613 2.137246 -0.195595
C , -2.011975 1.193683 -0.268889
H , -0.244088 -1.585653 0.566445
H , 1.086888 2.502765 0.210297
Cl , -2.995671 -1.336631 -0.075400
H , -1.211153 3.178797 -0.395458
H , -3.021115 1.488491 -0.526199
O , 4.173351 -0.843287 -0.367119
H , 4.266225 -1.678279 0.125473
H , 4.765970 -0.173654 0.018651

X=*p*-CHO Enthalpy (H) = 121.725 kcal/mol (total = -499.669125 hartree)
C , 2.201357 0.060237 0.719585
C , 2.847968 -0.140845 -0.626352
C , 0.699351 0.113649 0.464788
H , 2.439788 -0.767329 1.393719
H , 2.540253 0.992768 1.178954
H , 2.739466 0.687514 -1.322264
H , 2.624500 -1.087523 -1.112204
C , -0.048397 -1.072220 0.434971
C , 0.065515 1.339238 0.240638
C , -1.413265 -1.031387 0.189332
C , -1.304823 1.378314 -0.003217
C , -2.047649 0.196403 -0.032969
H , 0.432608 -2.026471 0.626743
H , 0.630899 2.264871 0.277604
H , -2.007854 -1.937196 0.172974
H , -1.798880 2.330787 -0.164463
C , -3.517119 0.240663 -0.295522
O , 4.439032 -0.231932 -0.520741
H , 4.765237 -0.998599 -0.016199

H , 4.867203 0.578267 -0.190725
O , -4.212998 -0.742569 -0.347704
H , -3.939117 1.254609 -0.444095

X=*m*-CN Enthalpy (H) = 115.075 kcal/mol (total = -478.585295 hartree)
C , 1.892042 -0.035579 0.747990
C , 2.558449 -0.386530 -0.558736
C , 0.468684 0.389178 0.404074
H , 1.875644 -0.897568 1.420677
H , 2.418822 0.782841 1.246484
H , 2.700947 0.445201 -1.244499
H , 2.139595 -1.246474 -1.076079
C , -0.544076 -0.567337 0.338149
C , 0.173430 1.729508 0.130462
C , -1.849457 -0.185714 0.002298
C , -1.125055 2.108804 -0.200834
C , -2.138411 1.158474 -0.269063
H , -0.342380 -1.608901 0.562999
H , 0.950252 2.484583 0.194768
C , -2.879094 -1.178416 -0.057921
H , -1.349358 3.149481 -0.399789
H , -3.149977 1.448403 -0.523758
O , 4.061864 -0.865750 -0.353726
H , 4.157339 -1.700652 0.139102
H , 4.653909 -0.192823 0.027790
N , -3.698396 -1.990345 -0.105201

X=*p*-CN Enthalpy (H) = 115.056 kcal/mol (total = -478.584754 hartree)
C , 2.128775 0.000213 0.719203
C , 2.782615 -0.000475 -0.639547
C , 0.625210 0.000171 0.470048
H , 2.415664 -0.887111 1.290377
H , 2.415755 0.888039 1.289539
H , 2.616384 0.894357 -1.234535
H , 2.616742 -0.896085 -1.233462
C , -0.068198 -1.208404 0.344442
C , -0.068245 1.208691 0.344182
C , -1.436145 -1.213482 0.102340
C , -1.436198 1.213660 0.102117
C , -2.126579 0.000079 -0.022903
H , 0.451637 -2.154313 0.456280
H , 0.451563 2.154640 0.455779
H , -1.973812 -2.149204 0.016630
H , -1.973906 2.149345 0.016265
C , -3.535766 0.000006 -0.273399
O , 4.372830 -0.000139 -0.540824
H , 4.752950 -0.794931 -0.125232

H , 4.752770 0.795988 -0.127633
N , -4.671600 -0.000338 -0.479473

X=*m*-NO_2 Enthalpy (H) = 117.837 kcal/mol (total = -590.876991 hartree)
C , 2.245092 0.031567 0.725739
C , 2.855495 -0.417865 -0.578789
C , 0.836237 0.516144 0.402566
H , 2.202934 -0.795802 1.439661
H , 2.829458 0.842093 1.169446
H , 3.033474 0.372421 -1.304320
H , 2.369261 -1.269972 -1.048060
C , -0.212463 -0.401885 0.336928
C , 0.585289 1.870576 0.150802
C , -1.485449 0.055831 0.024882
C , -0.702058 2.305808 -0.155017
C , -1.754455 1.395679 -0.221819
H , -0.073736 -1.457153 0.538285
H , 1.391098 2.594695 0.212599
N , -2.594522 -0.934517 -0.040362
H , -0.888531 3.357097 -0.335631
H , -2.764292 1.706397 -0.453790
O , 4.326701 -0.984415 -0.384733
H , 4.379523 -1.807500 0.134000
H , 4.969335 -0.338798 -0.039409
O , -3.709996 -0.507392 -0.279624
O , -2.303331 -2.107817 0.146607

X=*p*-NO_2 Enthalpy (H) = 117.880 kcal/mol (total = -590.875389 hartree)
C , -2.548709 0.001041 0.715218
C , -3.191061 -0.000768 -0.649920
C , -1.041579 0.000696 0.486481
H , -2.841990 0.889264 1.281667
H , -2.842129 -0.885531 1.284183
H , -3.018454 -0.896469 -1.241956
H , -3.018252 0.893358 -1.244265
C , -0.348578 1.210804 0.370654
C , -0.349131 -1.209759 0.370912
C , 1.024258 1.217068 0.147382
C , 1.023725 -1.216701 0.147799
C , 1.684322 0.000012 0.037221
H , -0.870705 2.156064 0.475128
H , -0.871668 -2.154773 0.475625
H , 1.582909 2.139552 0.065101
H , 1.581992 -2.139455 0.065934
N , 3.154719 -0.000354 -0.202492
O , -4.776740 -0.000411 -0.563250
H , -5.161398 0.794653 -0.152102

H ,	-5.162070	-0.797405	-0.156503
O ,	3.702173	1.086332	-0.293771
O ,	3.701974	-1.087312	-0.291709

SI-3. B3LYP/6-311+G** optimized Cartesian coordinates, enthalpies and imaginary frequencies for X-substituted protonated phenylethyl alcohols

X = *p*-OMe Enthalpy (H) = 135.386 kcal/mol (total = -500.856966 hartree), -181.2 cm-1

C ,	2.287021	0.020594	0.824069
C ,	2.785398	-0.149623	-0.563482
C ,	0.794909	0.101904	0.516198
H ,	2.515831	-0.832752	1.464123
H ,	2.644478	0.938195	1.293639
H ,	2.694606	0.701654	-1.229973
H ,	2.582370	-1.097756	-1.050005
C ,	0.008971	-1.056142	0.470901
C ,	0.185910	1.343357	0.252744
C ,	-1.352980	-0.989832	0.204020
C ,	-1.165569	1.422892	-0.014355
C ,	-1.952269	0.255725	-0.042000
H ,	0.454151	-2.024801	0.675943
H ,	0.771897	2.256400	0.287458
H ,	-1.937478	-1.899252	0.198763
H ,	-1.648175	2.374858	-0.196472
O ,	-3.254363	0.439402	-0.306428
O ,	4.553454	-0.269035	-0.649479
H ,	4.928696	-1.025239	-0.170196
H ,	5.024203	0.532293	-0.368913
C ,	-4.139595	-0.687081	-0.344703
H ,	-5.120296	-0.276467	-0.571086
H ,	-4.168630	-1.192886	0.624108
H ,	-3.845162	-1.387945	-1.130483

X=*p*-OH Enthalpy (H) = 116.749 kcal/mol (total = -461.575172 hartree) -213.9 cm-1

C ,	1.803030	0.009645	0.866307
C ,	2.321202	0.007559	-0.518939
C ,	0.320305	0.004079	0.499289
H ,	2.077235	-0.881479	1.431426
H ,	2.073677	0.904592	1.427032
H ,	2.210799	0.916068	-1.100443
H ,	2.203981	-0.900578	-1.099812
C ,	-0.366373	-1.210542	0.319167
C ,	-0.375869	1.209212	0.318256
C ,	-1.711937	-1.223145	0.004120
C ,	-1.725666	1.206545	0.003271
C ,	-2.401418	-0.011676	-0.156290
H ,	0.151759	-2.154035	0.457477
H ,	0.131500	2.158781	0.454252
H ,	-2.254138	-2.152755	-0.113917
H ,	-2.258332	2.144577	-0.111085
O ,	-3.710556	-0.094341	-0.460198

O , 4.143542 0.001128 -0.589936
H , 4.563255 -0.793553 -0.224627
H , 4.570549 0.775394 -0.190885
H , -4.113820 0.778619 -0.539432

X=*p*-Me Enthalpy (H) = 131.393 kcal/mol (total = -425.631864 hartree) -225.7 cm-1
C , 1.837386 -0.000047 0.892069
C , 2.305722 -0.000045 -0.501255
C , 0.352830 -0.000013 0.509894
H , 2.107264 -0.895898 1.449776
H , 2.107303 0.895777 1.449800
H , 2.209537 0.911553 -1.079051
H , 2.209460 -0.911634 -1.079055
C , -0.333890 -1.210890 0.324565
C , -0.333833 1.210884 0.324578
C , -1.684554 -1.204574 0.009355
C , -1.684511 1.204628 0.009364
C , -2.386482 0.000038 -0.151414
H , 0.181877 -2.156610 0.457070
H , 0.181970 2.156583 0.457086
H , -2.206937 -2.146957 -0.110494
H , -2.206852 2.147033 -0.110477
C , -3.858215 0.000011 -0.459890
O , 4.197764 0.000041 -0.631542
H , 4.642039 -0.782469 -0.271793
H , 4.641894 0.782494 -0.271489
H , -4.148702 -0.885598 -1.027515
H , -4.438316 -0.001737 0.469572
H , -4.149372 0.887194 -1.024681

X=*m*-Me Enthalpy (H) = 131.298 kcal/mol (total = -425.630657 hartree) -226.7 cm-1
C , 1.662931 , 0.020308 , 0.927169
C , 2.147088 , -0.146727 , -0.445150
C , 0.220982 , 0.282632 , 0.463145
H , 1.729649 , -0.877934 , 1.538484
H , 2.079717 , 0.880172 , 1.448641
H , 2.268641 , 0.730090 , -1.069289
H , 1.903951 , -1.057327 , -0.978926
C , -0.681093 , -0.788296 , 0.336374
C , -0.190031 , 1.588131 , 0.156099
C , -2.004279 , -0.571345 , -0.042725
C , -1.507530 , 1.813216 , -0.225436
C , -2.398704 , 0.747182 , -0.323532
H , -0.353385 , -1.796696 , 0.570513
H , 0.501113 , 2.419240 , 0.247547
C , -2.991431 , -1.705859 , -0.139835
H , -1.842335 , 2.820153 , -0.443075

H , -3.423586 , 0.939251 , -0.622842
O , 4.047659 , -0.538043 , -0.515707
H , 4.332112 , -1.361633 , -0.092938
H , 4.642042 , 0.164965 , -0.214840
H , -3.789384 , -1.589328 , 0.599033
H , -3.463357 , -1.730577 , -1.125515
H , -2.514050 , -2.671485 , 0.032214

X=H Enthalpy (H) = 113.016 kcal/mol (total = -386.329643 hartree) -224.7 cm-1
C , 1.292504 , 0.000000 , 0.939932
C , 1.798710 , -0.000023 , -0.431521
C , -0.165143 , 0.000003 , 0.447388
H , 1.524424 , -0.898205 , 1.508914
H , 1.524434 , 0.898217 , 1.508891
H , 1.757864 , 0.914348 , -1.010230
H , 1.757871 , -0.914421 , -1.010192
C , -0.831757 , -1.216701 , 0.219684
C , -0.831748 , 1.216709 , 0.219664
C , -2.161261 , -1.212304 , -0.180998
C , -2.161251 , 1.212313 , -0.181019
C , -2.824698 , -0.000005 , -0.381665
H , -0.319862 , -2.158403 , 0.388118
H , -0.319847 , 2.158410 , 0.388081
H , -2.682361 , -2.149500 , -0.333179
H , -2.682346 , 2.149510 , -0.333217
H , -3.862068 , -0.000007 , -0.694683
O , 3.770488 , 0.000028 , -0.502370
H , 4.222985 , -0.780607 , -0.151449
H , 4.222856 , 0.780485 , -0.150884

X=*m*-OH Enthalpy (H) = 116.276 kcal/mol (total = -461.570615 hartree) -217.7 cm-1
C , 1.630699 -0.033586 0.941036
C , 2.117661 -0.079547 -0.437735
C , 0.187612 0.223435 0.476054
H , 1.715984 -0.974753 1.480804
H , 2.019166 0.794438 1.530645
H , 2.242752 0.844877 -0.987058
H , 1.906732 -0.951671 -1.043937
C , -0.700473 -0.856279 0.322587
C , -0.226974 1.532201 0.190111
C , -2.016943 -0.613604 -0.062656
C , -1.545457 1.758914 -0.199604
C , -2.434302 0.701102 -0.327744
H , -0.375478 -1.868417 0.543940
H , 0.458408 2.364139 0.305583
O , -2.948383 -1.582908 -0.201675
H , -1.882653 2.768255 -0.400669

H , -3.462333 0.864907 -0.627132
O , 4.058811 -0.437312 -0.531183
H , 4.372315 -1.279433 -0.171035
H , 4.649911 0.256343 -0.204480
H , -2.599176 -2.452740 0.023913

X=*p*-Cl Enthalpy (H) = 107.724 kcal/mol (total = -845.956724 hartree) -231.0 cm-1
C , 2.254702 0.000006 0.902287
C , 2.648301 -0.000016 -0.508896
C , 0.761121 0.000010 0.549141
H , 2.539407 -0.897104 1.449080
H , 2.539413 0.897132 1.449054
H , 2.553118 0.913846 -1.082296
H , 2.553110 -0.913904 -1.082258
C , 0.070679 -1.213718 0.384018
C , 0.070691 1.213735 0.383955
C , -1.287410 -1.217298 0.108071
C , -1.287398 1.217313 0.108006
C , -1.961404 -0.000001 -0.029581
H , 0.589664 -2.158791 0.504176
H , 0.589686 2.158809 0.504060
H , -1.827385 -2.149398 0.004085
H , -1.827364 2.149413 0.003969
Cl , -3.659265 -0.000008 -0.375450
O , 4.592563 0.000067 -0.737766
H , 5.070793 -0.781482 -0.424391
H , 5.070864 0.780897 -0.422713

X=*m*-CHO Enthalpy (H) = 119.750 kcal/mol (total = -499.666846 hartree) -224.3 cm-1
C , 2.007419 0.008586 0.948697
C , 2.390201 -0.262294 -0.430671
C , 0.581562 0.362374 0.480992
H , 2.012726 -0.857653 1.606410
H , 2.505066 0.860923 1.405753
H , 2.586792 0.561353 -1.105024
H , 2.085947 -1.188988 -0.900305
C , -0.411715 -0.630581 0.423619
C , 0.264577 1.684619 0.119355
C , -1.710773 -0.294893 0.058519
C , -1.036028 2.015989 -0.245025
C , -2.019962 1.031597 -0.277106
H , -0.178447 -1.656659 0.694687
H , 1.028251 2.454564 0.154574
C , -2.775624 -1.345744 0.023901
H , -1.280679 3.039743 -0.500078
H , -3.039528 1.268011 -0.560047
O , 4.331763 -0.835584 -0.587260

H , 4.599434 -1.678777 -0.195509
H , 5.023072 -0.190361 -0.382591
O , -3.910821 -1.123083 -0.307519
H , -2.448114 -2.360736 0.326665

X=*m*-Cl Enthalpy (H) = 107.558 kcal/mol (total = -845.955086 hartree) -220.8 cm-1
C , 1.981691 0.007822 0.961207
C , 2.378691 -0.253874 -0.415883
C , 0.578915 0.421943 0.473536
H , 1.942374 -0.868824 1.603682
H , 2.501255 0.834037 1.441110
H , 2.622958 0.572299 -1.071106
H , 2.046848 -1.159611 -0.907109
C , -0.436786 -0.545762 0.382330
C , 0.317734 1.758446 0.125596
C , -1.712205 -0.156988 -0.005321
C , -0.965217 2.127467 -0.258064
C , -1.982469 1.176362 -0.325793
H , -0.245065 -1.580217 0.641926
H , 1.102656 2.503880 0.187516
Cl , -2.982747 -1.342389 -0.091861
H , -1.181773 3.159631 -0.504192
H , -2.982857 1.462281 -0.625653
O , 4.300746 -0.905363 -0.544660
H , 4.519407 -1.773023 -0.176772
H , 5.012807 -0.299434 -0.296132

X=*p*-CHO Enthalpy (H) = 119.670 kcal/mol (total = -499.667043 hartree) -218.6 cm-1
C , 2.187991 0.055339 0.933039
C , 2.532419 -0.092610 -0.472160
C , 0.696407 0.104886 0.541356
H , 2.410313 -0.806786 1.557485
H , 2.515742 0.983978 1.394233
H , 2.525974 0.771558 -1.123864
H , 2.410651 -1.051130 -0.960036
C , -0.054303 -1.086761 0.480917
C , 0.082586 1.338495 0.260509
C , -1.408017 -1.035362 0.198323
C , -1.276278 1.381040 -0.020334
C , -2.023387 0.198942 -0.052434
H , 0.420928 -2.039732 0.688357
H , 0.659224 2.256523 0.296321
H , -2.010965 -1.935214 0.169167
H , -1.760553 2.332417 -0.212692
C , -3.490092 0.246010 -0.359558
O , 4.564676 -0.247910 -0.753163
H , 5.026103 -1.032072 -0.424975

H , 5.127351 0.515734 -0.564082
O , -4.177427 -0.741031 -0.414605
H , -3.906726 1.256388 -0.535719

X=*m*-CN Enthalpy (H) = 112.892 kcal/mol (total = -478.581916 hartree) -215.1 cm-1
C , 1.867651 0.009398 0.981365
C , 2.231969 -0.274775 -0.394049
C , 0.463788 0.402716 0.467713
H , 1.829911 -0.851697 1.643649
H , 2.380238 0.852773 1.437047
H , 2.486915 0.531760 -1.068914
H , 1.925403 -1.203214 -0.857889
C , -0.544164 -0.571051 0.383186
C , 0.187442 1.735702 0.108194
C , -1.832278 -0.202195 -0.008110
C , -1.096631 2.096051 -0.277307
C , -2.105381 1.136477 -0.336906
H , -0.341366 -1.602503 0.647866
H , 0.967934 2.486811 0.162029
C , -2.865378 -1.190809 -0.073724
H , -1.317665 3.125314 -0.530647
H , -3.107450 1.414940 -0.639411
O , 4.219108 -0.933214 -0.550579
H , 4.465896 -1.824842 -0.269865
H , 4.954209 -0.348245 -0.322596
N , -3.691284 -1.994924 -0.128400

X=*p*-CN Enthalpy (H) = 112.898 kcal/mol (total = -478.582032 hartree) -217.0 cm-1
C , 2.114944 0.000206 0.939200
C , 2.450500 0.000044 -0.474844
C , 0.622518 0.000124 0.547400
H , 2.389913 -0.900659 1.482340
H , 2.389841 0.901213 1.482144
H , 2.393764 0.917373 -1.046268
H , 2.393857 -0.917425 -1.046052
C , -0.062721 -1.217639 0.377979
C , -0.062778 1.217810 0.377650
C , -1.418904 -1.219452 0.098455
C , -1.418959 1.219484 0.098126
C , -2.102728 -0.000024 -0.042526
H , 0.460126 -2.160150 0.498044
H , 0.460028 2.160379 0.497452
H , -1.956475 -2.152829 -0.009019
H , -1.956574 2.152808 -0.009599
C , -3.501926 -0.000098 -0.334586
O , 4.507709 -0.000087 -0.782103
H , 5.032118 -0.779297 -0.552099

H , 5.032834 0.777653 -0.548785
N , -4.631540 -0.000159 -0.573208

X=*m*-NO_2 Enthalpy (H) = 115.606 kcal/mol (total = -590.873001 hartree) -214.8 cm-1
C , 2.217898 0.030131 0.973227
C , 2.534191 -0.265734 -0.410116
C , 0.830774 0.503608 0.479091
H , 2.140945 -0.830129 1.632927
H , 2.783877 0.842575 1.421562
H , 2.827123 0.526414 -1.086521
H , 2.172708 -1.176281 -0.869892
C , -0.224956 -0.418500 0.386615
C , 0.613752 1.856559 0.148359
C , -1.475272 0.045245 0.019603
C , -0.654088 2.290527 -0.213303
C , -1.713036 1.383010 -0.280205
H , -0.097848 -1.468632 0.620250
H , 1.431213 2.566940 0.206731
N , -2.599427 -0.932229 -0.060427
H , -0.825452 3.334632 -0.442780
H , -2.710818 1.694865 -0.561400
O , 4.492158 -1.038625 -0.611742
H , 4.686281 -1.963957 -0.410427
H , 5.267644 -0.521805 -0.355454
O , -3.691614 -0.491971 -0.367403
O , -2.332452 -2.097916 0.185190

X=*p*-NO_2 Enthalpy (H) = 115.550 kcal/mol (total = -590.871150 hartree) -206.8 cm-1
C , -2.535944 -0.000029 0.960163
C , -2.821526 0.000046 -0.458814
C , -1.036909 -0.000015 0.571970
H , -2.813292 0.902782 1.497647
H , -2.813279 -0.902897 1.497561
H , -2.773945 -0.918560 -1.028510
H , -2.773944 0.918744 -1.028366
C , -0.352384 1.220311 0.412260
C , -0.352406 -1.220331 0.412100
C , 1.010236 1.222554 0.153353
C , 1.010215 -1.222565 0.153195
C , 1.662467 -0.000004 0.029779
H , -0.878721 2.161811 0.523085
H , -0.878760 -2.161836 0.522797
H , 1.569696 2.142437 0.048669
H , 1.569659 -2.142445 0.048395
N , 3.131964 0.000003 -0.253442
O , -4.925948 -0.000101 -0.831275
H , -5.475533 0.777793 -0.668135

H ,	-5.475972	-0.776955	-0.664691
O ,	3.670330	1.087887	-0.358033
O ,	3.670350	-1.087874	-0.357991

SI-4. B3LYP/6-31+1+G** optimized Cartesian coordinates and enthalpies for X-substituted phenonium ions

X = *p*-OMe Enthalpy (H) = 118.166 kcal/mol (total = -424.437065 hartree)

C ,	-2.946996	-0.216956	-0.723554
C ,	-2.946996	-0.216956	0.723448
C ,	-1.535638	-0.046450	0.000066
H ,	-3.050631	-1.149504	-1.262840
H ,	-3.261848	0.666845	-1.263112
H ,	-3.261931	0.666825	1.262996
H ,	-3.050796	-1.149499	1.262717
C ,	-0.653178	-1.180470	0.000037
C ,	-0.938476	1.265678	0.000025
C ,	0.704276	-1.032332	0.000035
C ,	0.412243	1.423201	-0.000081
C ,	1.259676	0.277918	-0.000042
H ,	-1.082446	-2.176974	-0.000005
H ,	-1.585105	2.136667	0.000104
H ,	1.345355	-1.902568	0.000011
H ,	0.876815	2.400971	-0.000105
O ,	2.544250	0.534238	-0.000107
C ,	3.536663	-0.523401	0.000157
H ,	4.491880	-0.007090	-0.002511
H ,	3.436122	-1.132271	-0.899245
H ,	3.439133	-1.128698	0.902300

X=*p*-OH Enthalpy (H) = 99.673 kcal/mol (total = -385.151649 hartree)

C ,	2.513476	-0.009481	0.722362
C ,	2.513476	-0.009481	-0.722018
C ,	1.085531	-0.001898	-0.000074
H ,	2.716685	-0.924672	1.263066
H ,	2.722183	0.904464	1.263133
H ,	2.722097	0.904468	-1.262821
H ,	2.717344	-0.924610	-1.262585
C ,	0.339601	-1.229700	-0.000101
C ,	0.348566	1.233864	-0.000090
C ,	-1.025680	-1.226735	-0.000065
C ,	-1.014759	1.243161	-0.000063
C ,	-1.717105	0.011801	-0.000040
H ,	0.876094	-2.172521	-0.000140
H ,	0.894215	2.171374	-0.000114
H ,	-1.582714	-2.157253	-0.000042
H ,	-1.583944	2.163997	-0.000048
O ,	-3.034079	0.092360	0.000008
H ,	-3.467954	-0.773327	0.000009

X=*p*-Me Enthalpy (H) = 114.195 kcal/mol (total = -349.203104 hartree)

C , -2.562721 -0.000087 0.724630
C , -2.568590 -0.000063 -0.711971
C , -1.118158 -0.000022 0.000569
H , -2.753094 0.915641 1.268951
H , -2.753750 -0.915778 1.268785
H , -2.763561 -0.915800 -1.254621
H , -2.764401 0.915591 -1.254457
C , -0.386106 1.228523 -0.002951
C , -0.385962 -1.228509 -0.002987
C , 0.986135 1.220125 -0.010443
C , 0.986236 -1.219903 -0.010396
C , 1.700721 0.000186 -0.013020
H , -0.927031 2.168967 -0.002084
H , -0.926782 -2.169014 -0.002148
H , 1.532706 2.155600 -0.017339
H , 1.532925 -2.155321 -0.017241
C , 3.193980 -0.000011 0.008381
H , 3.606837 0.893315 -0.461953
H , 3.536662 -0.005471 1.051716
H , 3.606281 -0.889160 -0.470478

X=*m*-Me Enthalpy (H) = 114.237 kcal/mol (total = -349.198068 hartree)
C , 2.307815 , -0.678599 , 0.715719
C , 2.307468 , -0.678420 , -0.715598
C , 0.976111 , -0.072457 , -0.000160
H , 2.093914 , -1.588446 , 1.260994
H , 2.856230 , 0.077771 , 1.261640
H , 2.855268 , 0.078277 , -1.261692
H , 2.095199 , -1.588845 , -1.260556
C , -0.190358 , -0.895418 , -0.000108
C , 0.837645 , 1.344831 , -0.000112
C , -1.458562 , -0.342393 , 0.000194
C , -0.423635 , 1.900750 , 0.000029
C , -1.547686 , 1.065933 , 0.000166
H , -0.070165 , -1.974123 , -0.000297
H , 1.721721 , 1.972868 , -0.000245
C , -2.704220 , -1.188942 , -0.000064
H , -0.549137 , 2.976209 , 0.000000
H , -2.532784 , 1.522528 , 0.000210
H , -3.315340 , -0.978367 , 0.881487
H , -3.315977 , -0.976764 , -0.880799
H , -2.466386 , -2.252815 , -0.001135

X=H Enthalpy (H) = 96.034 kcal/mol (total = -309.895161 hartree)
C , -2.094493 , -0.000016 , -0.714911
C , -2.094164 , -0.000005 , 0.715207
C , -0.628213 , 0.000000 , -0.000275

H , -2.276141 , -0.916503 , -1.261030
H , -2.276681 , 0.916445 , -1.260898
H , -2.275608 , 0.916472 , 1.261403
H , -2.276157 , -0.916455 , 1.261272
C , 0.090822 , -1.231831 , -0.000103
C , 0.090787 , 1.231837 , -0.000126
C , 1.469099 , -1.224666 , 0.000018
C , 1.469072 , 1.224670 , 0.000003
C , 2.152684 , 0.000009 , 0.000052
H , -0.454931 , -2.169222 , -0.000104
H , -0.454981 , 2.169219 , -0.000139
H , 2.021875 , -2.155548 , 0.000085
H , 2.021824 , 2.155569 , 0.000077
H , 3.237239 , 0.000031 , 0.000144

X=*m*-OH Enthalpy (H) = 99.227 kcal/mol (total = -385.136484 hartree)
C , 2.316794 -0.575863 0.714542
C , 2.317302 -0.576047 -0.713555
C , 0.944581 -0.038438 -0.000821
H , 2.148598 -1.494440 1.261171
H , 2.816676 0.212979 1.261196
H , 2.818477 0.212266 -1.259806
H , 2.149716 -1.494825 -1.260056
C , -0.160037 -0.931832 -0.000540
C , 0.729815 1.368191 -0.000424
C , -1.454777 -0.432004 -0.000064
C , -0.563348 1.849896 0.000061
C , -1.644143 0.962281 0.000233
H , -0.007968 -2.005168 -0.000766
H , 1.575341 2.045943 -0.000556
O , -2.460484 -1.325707 0.000108
H , -0.750409 2.916267 0.000320
H , -2.654506 1.360599 0.000638
H , -3.329171 -0.905072 0.000396

X=*p*-Cl Enthalpy (H) = 90.723 kcal/mol (total = -769.524291 hartree)
C , 2.942799 0.000005 -0.717653
C , 2.942297 -0.000021 0.718264
C , 1.491956 -0.000006 -0.000359
H , 3.133853 0.915845 -1.261807
H , 3.134442 -0.915785 -1.261685
H , 3.132932 -0.915856 1.262565
H , 3.133579 0.915760 1.262431
C , 0.761903 1.230088 -0.000214
C , 0.761906 -1.230094 -0.000256
C , -0.610202 1.231397 -0.000107
C , -0.610197 -1.231349 -0.000119

C , -1.295695 0.000035 -0.000058
H , 1.302090 2.170754 -0.000227
H , 1.302076 -2.170770 -0.000298
H , -1.169278 2.157989 -0.000059
H , -1.169288 -2.157933 -0.000056
Cl , -3.006412 -0.000019 0.000126

X=*m*-CHO Enthalpy (H) = 102.800 kcal/mol (total = -423.229657 hartree)
C , -2.603600 -0.791745 -0.714750
C , -2.603600 -0.791745 0.714994
C , -1.303898 -0.109679 0.000405
H , -2.338436 -1.687699 -1.261072
H , -3.189913 -0.064888 -1.261955
H , -3.190415 -0.065123 1.261985
H , -2.338525 -1.687660 1.261432
C , -0.091797 -0.860284 0.000098
C , -1.242047 1.314975 0.000164
C , 1.124713 -0.209579 -0.000135
C , -0.019632 1.957811 -0.000149
C , 1.154379 1.199580 -0.000257
H , -0.131724 -1.946100 0.000113
H , -2.163517 1.887502 0.000254
C , 2.416592 -0.978564 -0.000334
H , 0.030149 3.039418 -0.000292
H , 2.125931 1.684170 -0.000463
O , 3.486613 -0.432931 0.000049
H , 2.316886 -2.080801 -0.000601

X=*m*-Cl Enthalpy (H) = 90.585 kcal/mol (total = -769.517455 hartree)
C , 2.509435 -0.955078 0.715008
C , 2.509955 -0.955294 -0.713664
C , 1.287542 -0.134273 -0.001104
H , 2.145957 -1.815402 1.261914
H , 3.168089 -0.293189 1.262177
H , 3.169839 -0.294167 -1.260297
H , 2.147929 -1.816384 -1.260355
C , 0.010128 -0.765438 -0.000827
C , 1.378304 1.285768 -0.000544
C , -1.131912 0.010028 -0.000154
C , 0.224192 2.042581 0.000130
C , -1.024242 1.411116 0.000321
H , -0.063515 -1.846807 -0.001234
H , 2.351810 1.763064 -0.000702
Cl , -2.696871 -0.733191 0.000124
H , 0.276313 3.124008 0.000524
H , -1.930019 2.006667 0.000879

X=*p*-CHO Enthalpy (H) = 102.765 kcal/mol (total = -423.228622 hartree)

C ,	2.902795	-0.170448	0.714359
C ,	2.903039	-0.170181	-0.713495
C ,	1.435818	-0.031021	-0.000359
H ,	2.990255	-1.100439	1.261235
H ,	3.167939	0.724726	1.261949
H ,	3.168605	0.725227	-1.260503
H ,	2.991779	-1.099950	-1.260557
C ,	0.604669	-1.190284	-0.000534
C ,	0.839896	1.262177	-0.000128
C ,	-0.765218	-1.054972	-0.000452
C ,	-0.534373	1.383440	-0.000052
C ,	-1.334772	0.230131	-0.000171
H ,	1.060078	-2.174859	-0.000757
H ,	1.471031	2.144324	-0.000046
H ,	-1.420896	-1.917536	-0.000584
H ,	-0.996871	2.364199	0.000101
C ,	-2.839375	0.362571	-0.000133
O ,	-3.559511	-0.598794	0.000731
H ,	-3.230715	1.396180	-0.000896

X=*m*-CN Enthalpy (H) = 96.035 kcal/mol (total = -402.141239 hartree)

C ,	2.401550	-1.000853	0.713856
C ,	2.401550	-1.000853	-0.712879
C ,	1.183605	-0.163246	-0.000093
H ,	2.026681	-1.855743	1.262123
H ,	3.063614	-0.342723	1.261965
H ,	3.063524	-0.342659	-1.261026
H ,	2.027945	-1.856504	-1.260830
C ,	-0.097564	-0.777866	-0.000113
C ,	1.287393	1.256293	-0.000167
C ,	-1.240091	0.008728	-0.000130
C ,	0.143754	2.030311	-0.000217
C ,	-1.110837	1.414594	-0.000179
H ,	-0.183264	-1.858734	-0.000117
H ,	2.266588	1.722758	-0.000213
C ,	-2.536603	-0.597734	-0.000109
H ,	0.212755	3.110734	-0.000287
H ,	-2.009095	2.021899	-0.000199
N ,	-3.580756	-1.087896	-0.000176

X=*p*-CN Enthalpy (H) = 96.022 kcal/mol (total = -402.142527 hartree)

C ,	-2.845695	-0.000060	0.714577
C ,	-2.845695	-0.000060	-0.713976
C ,	-1.373083	-0.000017	-0.000217
H ,	-3.022425	0.916938	1.261977
H ,	-3.023282	-0.916963	1.261862

H , -3.023135 -0.917027 -1.261203
H , -3.024016 0.916795 -1.261110
C , -0.653885 1.230100 -0.000233
C , -0.653835 -1.230081 -0.000325
C , 0.722420 1.230058 -0.000259
C , 0.722478 -1.229905 -0.000323
C , 1.413999 0.000096 -0.000256
H , -1.195656 2.169633 -0.000245
H , -1.195542 -2.169652 -0.000409
H , 1.277857 2.159085 -0.000263
H , 1.277955 -2.158910 -0.000366
C , 2.840222 0.000086 -0.000099
N , 3.995240 -0.000171 0.000918

X=*m*-NO_2 Enthalpy (H) = 98.760 kcal/mol (total = -514.431615 hartree)
C , 2.707730 -1.000413 0.713617
C , 2.707730 -1.000413 -0.712975
C , 1.515063 -0.126764 0.000600
H , 2.307868 -1.844348 1.261399
H , 3.388994 -0.361996 1.261663
H , 3.388737 -0.361751 -1.261050
H , 2.307978 -1.844352 -1.260825
C , 0.216005 -0.703761 0.000270
C , 1.657718 1.291220 0.000177
C , -0.872511 0.134687 -0.000281
C , 0.540158 2.102533 -0.000429
C , -0.735404 1.525128 -0.000555
H , 0.066392 -1.777653 0.000385
H , 2.650694 1.727735 0.000398
N , -2.243493 -0.464765 -0.000445
H , 0.643554 3.180124 -0.000749
H , -1.630019 2.137412 -0.000825
O , -3.176588 0.314210 0.000153
O , -2.303247 -1.681100 -0.000131

X=*p*-NO_2 Enthalpy (H) = 98.709 kcal/mol (total = -514.428936 hartree)
C , -3.229653 -0.044426 -0.710723
C , -3.229560 0.044401 0.711035
C , -1.744800 -0.000003 -0.000106
H , -3.400571 -0.994376 -1.200944
H , -3.400796 0.836786 -1.315812
H , -3.400342 0.994355 1.201294
H , -3.400438 -0.836834 1.316163
C , -1.032413 -1.229059 0.073848
C , -1.032432 1.229065 -0.074029
C , 0.348299 -1.229073 0.068655
C , 0.348280 1.229121 -0.068902

C ,	1.003854	0.000038	-0.000163
H ,	-1.575395	-2.165995	0.131664
H ,	-1.575429	2.165997	-0.131770
H ,	0.924265	-2.144009	0.112787
H ,	0.924232	2.144064	-0.113013
N ,	2.507748	0.000029	-0.000158
O ,	3.047515	-1.079416	-0.150043
O ,	3.047583	1.079345	0.150423