Proton Transfer Reactions of nitroalkanes: The Role of *Aci*-Nitro Species

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Supporting Information

Table S1. Optimized structures for the proton-transfer reactions of small carbon acids with CN^- at B3LYP/6-31+G* S2

Table S2. Optimized structures for the proton-transfer reactions of small carbon acids with CN^- at MP2/6-31+G* S7

Table S3. Optimized structures for the proton-transfer reactions of X-substituted $PHCH_2NO_2$ at B3LYP/6-31+G* S10

Table S1. Optimized structures for the proton-transfer reactions of small carbon acids with CN^- at B3LYP/6-31+G*

acid, name of compound, enthalpy

HCN, −93.408790

C	0.000000	0.000000	−0.502193
N	0.000000	0.000000	0.655294
H	0.000000	0.000000	−1.573899

CH_3NO_2, −244.970415

C	−1.328723	−0.034945	−0.001312
N	0.171988	−0.000086	−0.004806
O	0.698164	1.110025	0.001243
O	0.769226	−1.072974	0.001294
H	−1.647057	−1.064078	−0.153101
H	−1.672002	0.629831	−0.794415
H	−1.651642	0.348112	0.968738

$C_2H_5NO_2$, −284.258058

C	1.830297	0.086603	−0.321457
C	0.693190	−0.536303	0.479615
N	−0.646991	0.023211	0.052061
O	−1.512840	−0.775534	−0.298245
O	−0.782821	1.243843	0.091201
H	2.779719	−0.335578	0.025105
H	1.858299	1.170318	−0.183747
H	1.728106	−0.133604	−1.389233
H	0.771827	−0.296720	1.544150

$CH_2(NO_2)_2$, −449.452962

C	−0.000579	−0.883366	0.000232
N	1.232878	−0.023131	0.122667
O	2.194368	−0.364773	−0.554592
H	0.084409	−1.481343	−0.905177
O	1.183565	0.898396	0.924009
H	−0.086746	−1.480881	0.905815
N	−1.232864	−0.021320	−0.122567
O	−1.179876	0.904804	−0.918270
O	−2.197343	−0.366731	0.548511

CH_3COCH_3, −193.076985

C	1.293541	−0.613856	−0.000113
C	0.000000	0.182491	−0.000099
O	0.000001	1.401569	0.000023
C	−1.293541	−0.613854	0.000120
H	1.342885	−1.260641	0.885583
H	2.151218	0.062382	−0.007053
H	1.336951	−1.272360	−0.877369
H	−2.151220	0.062387	0.006517
H	−1.337100	−1.271761	0.877825
H	−1.342736	−1.261242	−0.885135

CH_3COCH_2Cl, −652.671357

C	0.257164	−0.779703	−0.079291
Cl	1.858690	0.011731	0.035718
C	−0.927320	0.188829	−0.024420
O	−0.801638	1.393278	−0.030498
C	−2.282813	−0.494465	0.049133
H	0.175509	−1.508477	0.733546
H	−2.336062	−1.376297	−0.600140
H	−3.065531	0.217336	−0.222620
H	−2.460352	−0.834807	1.078233
H	0.219624	−1.331373	−1.024788

$CH_3COCHCl_2$, −1112.265835

C	0.250702	0.087056	0.465069
Cl	1.732374	−0.824448	0.103941
Cl	0.288625	1.750056	−0.257275
C	−1.034181	−0.640915	−0.013185
O	−0.975164	−1.690721	−0.608632
C	−2.342380	0.040077	0.335023
H	−2.289162	0.589856	1.280355
H	−3.130749	−0.715010	0.378319
H	−2.593270	0.763242	−0.449977
H	0.212671	0.235051	1.545590

$CH_3COCH_2COCH_3$, −345.680323

C	0.000096	−0.001089	0.996340
C	−1.213275	−0.294418	0.099180
C	1.213066	0.294150	0.099336
O	1.438634	1.428896	−0.280952
C	2.061451	−0.891193	−0.300576
O	−1.440134	−1.428677	−0.281738
C	−2.060224	0.892179	−0.300058
H	0.182911	−0.882271	1.617663
H	2.795221	−0.594964	−1.053334
H	2.582844	−1.284327	0.582560
H	1.426329	−1.700939	−0.680727
H	−2.580830	1.285735	0.583347
H	−2.794546	0.597176	−1.052754
H	−1.424089	1.701206	−0.680048
H	−0.182524	0.878864	1.619482

CH_3CHO, −153.779250

C	1.171214	−0.148597	−0.000015
C	−0.231994	0.399344	0.000007
H	−0.310112	1.509493	−0.000022
H	1.711302	0.222825	0.881655
O	−1.239008	−0.277356	−0.000004
H	1.163865	−1.241545	−0.000445
H	1.711690	0.223593	−0.881111

$CH_2(CHO)_2$, −267.083333

C	−0.011926	0.847550	0.099966
C	−1.048900	−0.241851	0.298652
H	−0.791996	−1.028378	1.033379
H	−0.293480	1.485008	−0.748637
O	−2.111159	−0.258706	−0.285206
H	−0.008894	1.502048	0.988613
C	1.403268	0.336488	−0.089847
H	2.168015	1.125310	−0.254276
O	1.720122	−0.833433	−0.073757

CH_3CN, −132.711657

C	−1.182287	0.000001	−0.000004
C	0.280549	−0.000007	0.000000

N	1.441563	0.000002	−0.000001
H	−1.560151	0.979203	−0.311390
H	−1.560162	−0.219908	1.003712
H	−1.560203	−0.759270	−0.692294

$CH_2(CN)_2$, −224.936850

C	0.000002	0.837944	0.000019
C	−1.225191	0.024231	0.000006
H	0.000053	1.488831	0.883782
N	−2.206882	−0.592591	−0.000002
H	−0.000053	1.489013	−0.883609
C	1.225190	0.024229	−0.000104
N	2.206882	−0.592591	0.000045

$CH_3CO_2CH_3$, −268.292539

C	0.671955	1.348129	−0.000008
C	0.604466	−0.166967	−0.000123
O	1.582413	−0.877912	−0.000125
O	−0.625433	−0.753017	0.000317
C	−1.826042	0.028199	−0.000157
H	0.175966	1.770373	−0.881403
H	1.721909	1.642555	−0.004390
H	0.184156	1.768995	0.886675
H	−2.641626	−0.696338	0.004255
H	−1.901012	0.649329	−0.899430
H	−1.897510	0.656347	0.894483

$CH_3CO_2C_2H_5$, −307.581421

C	−1.114213	1.354660	0.030601
C	−1.046555	−0.162083	−0.018024
O	−1.990767	−0.849534	−0.334444
H	−2.088692	1.657139	−0.354481
H	−1.013992	1.718076	1.060363
H	−0.327872	1.825337	−0.568776
O	0.112560	−0.777310	0.337811
C	1.329961	−0.059245	0.627039
H	1.106812	0.914382	1.074084
H	1.828791	−0.668755	1.385654
C	2.202698	0.074405	−0.614062
H	1.723152	0.690379	−1.383256
H	2.407570	−0.911240	−1.044323
H	3.158536	0.543016	−0.349523

$CH_2(CO_2C_2H_5)_2$, −574.702579

C	0.140642	0.618221	0.955543
C	1.159554	1.214949	−0.026234
O	0.935195	2.258671	−0.596512
H	−0.410785	1.452754	1.388633
H	0.626618	0.054012	1.757346
O	2.318978	0.568271	−0.252484
C	2.660981	−0.692604	0.380119
H	1.838680	−1.399246	0.243889
H	2.824113	−0.515460	1.450994
C	3.933192	−1.190578	−0.282006
H	4.241164	−2.136075	0.179627
H	4.745255	−0.465272	−0.166883
H	3.769675	−1.363111	−1.350528
C	−0.822914	−0.321788	0.240858
O	−0.487097	−1.338363	−0.336226
O	−2.088911	0.110179	0.333152
C	−3.102430	−0.696369	−0.329754
H	−3.084347	−1.698792	0.109221
H	−2.832128	−0.782247	−1.386396
C	−4.436880	−0.003985	−0.130883
H	−4.427253	1.000119	−0.567444
H	−4.682651	0.081602	0.932968
H	−5.226537	−0.585419	−0.620732

CH_3CO_2H, −229.019378,

C	−1.376719	−0.056384	0.000000
H	−1.866526	0.918178	−0.000201
C	0.128372	0.139293	−0.000018
O	0.683889	1.208873	0.000004
H	−1.695336	−0.617404	−0.887303
H	−1.695323	−0.617017	0.887553
O	0.871975	−1.007382	0.000005
H	0.300351	−1.793139	−0.000008

$CH_2(CO_2H)_2$, −417.581324

C	−0.021921	−0.820259	0.202052
C	−1.381418	−0.128928	−0.007861
O	−2.382483	−0.794777	−0.125933
H	0.016264	−1.704202	−0.440435
H	−0.014063	−1.203428	1.232583
O	−1.409817	1.210562	−0.013117
H	−0.493047	1.570345	0.044729
C	1.227788	0.008309	0.019985
O	1.274209	1.229044	0.021484
O	2.324195	−0.752276	−0.121636
H	3.095324	−0.157858	−0.208319

CH_3CONH_2, −209.147974

C	1.376483	−0.300224	−0.000005
C	−0.076790	0.150017	−0.000134
O	−0.410796	1.328554	0.000182
N	−1.000540	−0.862402	−0.001337
H	1.600816	−0.898541	0.891434
H	2.018073	0.582108	−0.008224
H	1.597468	−0.913332	−0.882124
H	−1.982890	−0.622571	0.003520
H	−0.741482	−1.838041	0.004134

$CH_2(CONH_2)_2$, −377.820547

C	−0.078379	−0.720973	0.604395
C	1.259499	−0.280842	0.023056
O	1.826102	−0.895849	−0.867434
H	−0.191550	−1.790545	0.421431
H	−0.108936	−0.562646	1.690850
N	1.755209	0.915386	0.508143
H	2.700505	1.152250	0.228094
H	1.462006	1.257150	1.414718
C	−1.334235	−0.040981	0.025138
O	−2.420914	−0.598435	0.089425
N	−1.175196	1.209985	−0.493661
H	−0.264638	1.629310	−0.625829
H	−1.980297	1.647929	−0.922101

anion, name of compound, enthalpy

CN, −92.857284

C 0.000000 0.000000 -0.637274
N 0.000000 0.000000 0.546235

CH_2NO_2, -244.409555
C -1.037025 -0.580416 -0.519609
N 0.034131 0.019174 0.017281
O 0.908664 -0.671385 0.666128
O 0.199430 1.291533 -0.111025
H -1.744988 0.035567 -1.055450
H -1.136533 -1.648465 -0.388684

$C_2H_4NO_2$, -283.698576
C -1.888908 -0.015371 -0.000269
C -0.562687 -0.703992 0.000202
N 0.572191 0.000233 0.001424
O 1.721288 -0.594353 -0.000666
O 0.517897 1.292767 -0.000322
H -2.694224 -0.765657 -0.001522
H -2.031767 0.637436 -0.878448
H -2.033075 0.635943 0.878814
H -0.450182 -1.780487 -0.000504

$CH(NO_2)_2$, -448.952881
C 0.000001 -0.654655 0.000117
N 1.232522 -0.034932 -0.000161
O 2.230703 -0.822274 0.000034
O 1.374601 1.206399 0.000027
N -1.232521 -0.034935 0.000033
O -2.230704 -0.822271 -0.000049
O -1.374602 1.206396 0.000010
H 0.000006 -1.729003 0.000021

CH_2COCH_3, -192.491901
C 1.295425 -0.482957 0.000030
C -0.134025 0.110692 -0.000197
O -0.195536 1.387383 0.000053
C -1.191978 -0.790676 0.000011
H 1.313091 -1.582558 -0.000014
H 1.841013 -0.119817 0.883276
H 1.841284 -0.119730 -0.883007
H -2.220825 -0.432497 0.000172
H -1.026810 -1.866810 0.000083

$CH_3COCHCl$, -652.109542
C 0.229610 -0.678453 0.000018
Cl 1.897473 -0.024550 -0.000002
C -0.878880 0.148418 -0.000023
O -0.935667 1.417132 0.000002
C -2.225998 -0.609264 0.000006
H -2.121151 -1.703634 -0.000052
H -2.805981 -0.310184 -0.884417
H -2.805904 -0.310179 0.884480
H 0.212929 -1.759919 -0.000008

CH_3COCCl_2, -1111.715129
C 0.192563 0.001516 0.001231
Cl 1.540441 -1.139890 0.000176
Cl 0.732734 1.706346 -0.000448
C -1.125894 -0.435033 -0.000114
O -1.482719 -1.654167 -0.000952
C -2.250808 0.611934 0.000550
H -1.915999 1.653380 0.001641
H -2.880811 0.439001 0.883498
H -2.880565 0.440694 -0.882900

$CH_3COCHCOCH_3$, -345.145422
C -0.028375 -0.724370 0.000047
C 1.335180 -0.294860 -0.000048
C -1.192232 0.083103 0.000030
O -1.261084 1.343098 -0.000060
C -2.542339 -0.664200 0.000010
O 2.301755 -1.100017 -0.000040
C 1.653272 1.202364 0.000009
H -0.160097 -1.805060 0.000108
H -3.121358 -0.360531 0.882897
H -3.121347 -0.360207 -0.882758
H -2.440082 -1.756647 -0.000200
H 1.210119 1.699562 -0.870822
H 2.742176 1.327183 -0.001044
H 1.212190 1.698837 0.872331

CH_2CHO, -153.200341
C -1.186474 -0.169873 -0.000014
C 0.098052 0.356417 -0.000241
O 1.228026 -0.231523 0.000086
H -1.361931 -1.246430 0.000089
H -2.049523 0.496071 0.000356
H 0.117781 1.483275 0.000400

$CH(CHO)_2$, -266.563005
C 0.000000 0.933276 0.000002
C 1.288862 0.332812 -0.000044
H 2.110306 1.104407 0.000136
H 0.000000 2.025701 0.000028
O 1.634648 -0.864245 0.000013
C -1.288861 0.332812 -0.000045
O -1.634648 -0.864245 0.000014
H -2.110305 1.104408 0.000136

CH_2CN, -132.121603
C 1.203359 0.000208 -0.044653
C -0.182696 -0.001015 -0.000480
N -1.373594 0.000388 0.006908
H 1.746980 -0.928618 0.111331
H 1.744200 0.930740 0.111114

$CH(CN)_2$, -224.414204
C 0.000000 0.714737 -0.000193
C -1.229926 0.050806 -0.000308
H 0.000021 1.801081 0.001078
N -2.285050 -0.478508 0.000215
C 1.229916 0.050785 -0.000031
N 2.285055 -0.478499 0.000087

$CH_3CO_2CH_3$, -267.710341
C -0.630013 1.362237 0.000015
C -0.659308 -0.028645 0.000647
O -1.634442 -0.809996 -0.000225
O 0.606489 -0.735464 -0.000097
C 1.805435 -0.003640 -0.000043
H 0.276272 1.956362 -0.000402
H -1.579743 1.887996 -0.000643

H 2.625654 −0.735173 −0.000273
H 1.902421 0.637186 0.892400
H 1.902341 0.637592 −0.892217

$CH_2CO_2C_2H_5$, −307.004767
C −2.167374 −0.586296 0.340437
C −1.042560 0.130046 −0.023085
O −0.834203 1.366910 −0.094593
H −3.072731 −0.051693 0.609766
H −2.165634 −1.671524 0.342909
O 0.063676 −0.751137 −0.385503
C 1.305602 −0.121122 −0.609685
H 1.841961 −0.746997 −1.340464
H 1.146318 0.875077 −1.040809
C 2.135893 0.003646 0.673009
H 2.296188 −0.981629 1.130819
H 1.609850 0.639170 1.393629
H 3.118897 0.453765 0.460851

$CH(CO_2C_2H_5)_2$, −574.167166
C 0.000000 −1.766838 −0.000041
C −1.298075 −1.197724 0.000009
O −2.368505 −1.835829 −0.000056
O −1.358776 0.200030 0.000036
C −2.665405 0.757414 0.000043
C −2.514564 2.273939 −0.000012
C 1.298075 −1.197723 −0.000035
O 2.368506 −1.835829 −0.000037
O 1.358776 0.200030 0.000114
C 2.665405 0.757414 0.000147
C 2.514563 2.273939 −0.000159
H 0.000001 −2.851178 −0.000097
H −3.225634 0.417164 0.881703
H −3.225673 0.417100 −0.881567
H −1.962889 2.609935 −0.886007
H −1.962840 2.609993 0.885931
H −3.502222 2.756523 0.000001
H 3.225754 0.416951 −0.881349
H 3.225553 0.417314 0.881922
H 1.962716 2.610129 0.885656
H 1.963010 2.609799 −0.886281
H 3.502221 2.756524 −0.000084

CH_2CO_2H, −228.443083
C −1.402793 −0.176456 0.000036
C −0.053045 0.118817 −0.000429
O 0.560068 1.225080 0.000105
H −2.125594 0.632880 0.000478
H −1.752650 −1.203962 0.000143
O 0.806164 −1.033586 0.000079
H 1.683420 −0.615037 0.000266

$CH(CO_2H)_2$, −417.039243
C −0.024841 −0.584206 −0.000378
C −1.280497 0.091835 0.000163
O −1.553258 1.286237 0.000173
H −0.011230 −1.671123 −0.000384
O −2.401047 −0.789604 0.000103
H −2.064936 −1.700134 −0.000153
C 1.242665 0.040140 −0.000848
O 1.584324 1.228784 0.000033
O 2.290556 −0.919578 0.000441
H 3.087613 −0.362076 0.000916

CH_2CONH_2, −208.549869
C −1.343493 −0.436672 0.024388
C −0.070372 0.127830 −0.013046
O 0.258973 1.353038 0.008103
N 1.055717 −0.806110 −0.108445
H −1.495318 −1.510028 −0.080368
H −2.217043 0.208787 0.019303
H 1.867457 −0.350557 0.302575
H 0.866289 −1.676684 0.384724

CH(CONH2)2, −377.278476
C −0.008089 −0.743195 −0.064350
C −1.188211 0.026975 −0.017126
O −1.297321 1.286506 0.057030
N −2.424744 −0.699521 −0.083666
C 1.330525 −0.224603 −0.017568
O 2.361317 −0.937146 0.075964
N 1.475186 1.165051 −0.111875
H −0.084243 −1.826647 −0.106318
H −3.168520 −0.153898 0.341070
H −2.373791 −1.633798 0.311493
H 0.619201 1.694425 0.061922
H 2.336948 1.511279 0.290934

TS
name of compound, enthalpy
CH_3NO_2, −337.842003
C −0.311110 −0.000034 1.028913
H 1.035074 −0.000045 0.373224
H −0.328744 0.925333 1.601914
H −0.328772 −0.925429 1.601868
C 2.279093 −0.000030 −0.069367
N 3.415666 0.000030 −0.344636
N −1.292385 0.000003 0.026817
O −1.690518 1.097570 −0.444317
O −1.690535 −1.097532 −0.444377

$C_2H_5NO_2$, −377.129397
C −0.305305 0.450937 −0.626908
H 1.036408 −0.047910 −0.228634
H −0.314681 0.272025 −1.701444
C −0.288396 1.887979 −0.161320
C 2.293916 −0.331167 0.071367
N 3.437375 −0.514858 0.233150
H 0.011639 1.961880 0.890668
H −1.263668 2.392195 −0.258114
H 0.444618 2.444993 −0.760437
N −1.225618 −0.398374 0.001672
O −1.655332 −0.102809 1.149272
O −1.544407 −1.481823 −0.559851

CH_3COCH_3, −285.929816
C 0.261611 −0.541102 1.007091
H −1.115810 −0.238915 0.325141
H 0.157906 0.108798 1.880663
H 0.140871 −1.607608 1.216185
C −2.321314 −0.014304 −0.092791

N	-3.436879	0.218259	-0.354856
C	1.264404	-0.202461	0.053473
O	1.773065	-0.981735	-0.788383
C	1.678733	1.279630	-0.034054
H	1.196077	1.911626	0.721524
H	1.425416	1.664553	-1.030924
H	2.768567	1.357042	0.076150

CH_3COCH_2Cl, -745.542426

C	-0.255747	0.223183	-0.550425
H	1.141467	-0.025219	-0.126459
H	-0.165499	0.149086	-1.635421
Cl	-0.559684	1.949305	-0.106289
C	2.440405	-0.206002	0.150233
N	3.574325	-0.461830	0.285045
C	-1.099393	-0.762706	0.075771
O	-1.813194	-0.617168	1.078707
C	-0.950921	-2.171026	-0.524893
H	-0.304149	-2.203625	-1.409110
H	-0.532438	-2.838159	0.238800
H	-1.945532	-2.550803	-0.789978

$CH_3COCHCl_2$, -1205.147872

C	0.200484	-0.218655	0.037649
H	-1.194406	0.030269	-0.217154
Cl	0.534090	-1.858028	-0.611558
Cl	0.264295	-0.232410	1.860410
C	-2.524338	0.241844	-0.379939
N	-3.655082	0.500175	-0.534235
C	0.999573	0.851465	-0.578421
O	1.539757	0.739650	-1.680766
C	0.980199	2.204783	0.129826
H	-0.010503	2.437568	0.535749
H	1.280729	2.971460	-0.589865
H	1.683642	2.203091	0.971857

$CH_3COCH_2COCH_3$, -438.560030

C	-0.211090	0.129533	-0.623346
H	0.833687	-0.642326	-0.208110
H	-0.009466	0.134730	-1.699100
C	-1.419098	-0.659870	-0.320444
C	2.026927	-1.430961	0.150504
N	3.017709	-2.013905	0.382090
C	0.094474	1.407632	0.029137
O	-0.381791	1.819429	1.094789
C	1.183325	2.227340	-0.666297
H	1.361886	3.151688	-0.109418
H	2.111950	1.641155	-0.709623
H	0.900920	2.466589	-1.699775
O	-1.993269	-1.318181	-1.196958
C	-1.897005	-0.739769	1.119547
H	-1.088587	-1.122267	1.757119
H	-2.764142	-1.404728	1.177961
H	-2.134937	0.259082	1.499055

CH_3CHO, -246.637697

C	-0.652910	0.969254	-0.180580
H	0.734936	0.307935	-0.062893
H	-0.691169	1.132922	-1.262333
H	-0.462235	1.869157	0.413436
C	1.982921	-0.097572	-0.020738
N	3.123297	-0.351444	0.038861
C	-1.606544	0.065237	0.361554
O	-2.259501	-0.824586	-0.224918
H	-1.709404	0.125269	1.477691

$CH_2(CHO)_2$, -359.963926

C	0.321033	-0.000011	0.735200
H	-0.886304	-0.000041	0.249439
H	0.039272	-0.000023	1.796637
C	0.910415	-1.290711	0.344648
C	-2.407845	-0.000071	-0.144663
N	-3.572068	0.000006	-0.301082
C	0.910351	1.290723	0.344660
O	1.642402	1.544983	-0.602368
H	0.584306	2.128864	1.010222
O	1.642482	-1.544926	-0.602380
H	0.584405	-2.128876	1.010197

CH_3CN, -225.556932

C	1.643838	-1.143840	-0.000363
H	-0.684477	-0.007513	0.000276
H	1.920059	-1.646099	-0.924827
H	1.903941	-1.647602	0.927983
C	-1.770193	-0.050140	-0.000227
N	-2.929248	-0.109399	-0.000344
C	1.516466	0.234185	-0.000034
N	1.289221	1.403682	0.000388

$CH_2(CN)_2$, -317.833593

C	-0.494095	0.000000	0.538346
H	0.801469	-0.000002	0.195101
H	-0.427044	-0.000001	1.632574
C	-1.113392	-1.214174	0.062315
C	2.268312	0.000000	-0.041712
N	3.436571	-0.000004	-0.145491
N	-1.551079	-2.224501	-0.324059
C	-1.113388	1.214176	0.062315
N	-1.551070	2.224504	-0.324059

$CH_3CO_2CH_3$, -361.154927

C	0.330304	1.133990	-0.758306
H	1.655408	0.302078	-0.226475
H	0.370353	0.885047	-1.819782
H	0.613792	2.156574	-0.506605
C	2.723471	-0.258913	0.078787
N	3.763947	-0.741993	0.296113
C	-0.775192	0.627897	-0.029236
O	-1.222575	0.980863	1.073763
O	-1.354101	-0.502832	-0.656449
C	-2.361014	-1.160085	0.093589
H	-2.689017	-2.005561	-0.521714
H	-3.212462	-0.498306	0.300096
H	-1.977699	-1.527462	1.054173

$CH_3CO_2C_2H_5$, -400.444508

C	-0.897450	1.099739	0.804088
H	-2.173219	0.246153	0.262029
H	-0.889359	0.784084	1.848314
H	-1.243436	2.118909	0.627654

C	-3.230181	-0.355579	-0.054326
N	-4.252283	-0.877048	-0.272355
C	0.214029	0.708424	0.015740
O	0.600784	1.157820	-1.074328
O	0.875746	-0.424242	0.560423
C	1.925168	-0.983295	-0.219834
H	1.929422	-2.055732	0.016900
H	1.704466	-0.851936	-1.284516
C	3.281723	-0.361551	0.114203
H	3.502522	-0.463086	1.184486
H	3.280225	0.702788	-0.142678
H	4.083373	-0.856890	-0.453690

$CH_2(CO_2C_2H_5)_2$, -667.583862

C	-0.041642	0.976476	0.982247
H	-0.415550	1.912687	0.065601
H	0.006526	1.558229	1.902238
C	1.312832	0.592132	0.571015
C	-0.829791	2.948403	-0.895248
N	-1.165108	3.771224	-1.660741
C	-1.194421	0.067816	1.041982
O	-2.079809	0.137090	1.891297
O	-1.283740	-0.824354	0.010077
C	-2.464356	-1.635375	-0.018422
H	-2.520063	-2.234975	0.898787
H	-3.349037	-0.988712	-0.041066
C	-2.382383	-2.513470	-1.257554
H	-3.273849	-3.150887	-1.326452
H	-2.322075	-1.899794	-2.163135
H	-1.496225	-3.157738	-1.223034
O	2.334927	1.117215	1.006393
O	1.369884	-0.352792	-0.419794
C	2.669963	-0.676217	-0.930568
H	2.485520	-1.009358	-1.957506
H	3.289149	0.225443	-0.949404
C	3.342502	-1.777851	-0.116501
H	2.708446	-2.671617	-0.075175
H	3.535152	-1.435938	0.905200
H	4.301436	-2.054668	-0.576359

CH_3CO_2H, -321.883176

C	-0.275476	-0.345219	1.068017
H	1.144472	-0.137777	0.353590
H	-0.210633	0.417035	1.845994
H	-0.183376	-1.373985	1.417885
C	2.328375	0.006856	-0.081752
N	3.448408	0.132599	-0.389854
C	-1.266357	-0.146551	0.073836
O	-1.762464	-0.961119	-0.725728
O	-1.658449	1.198611	-0.073807
H	-2.241261	1.176091	-0.852818

$CH_2(CO_2H)_2$, -510.459063

C	0.214509	0.000002	-0.510043
H	-1.044801	-0.000017	-0.129495
H	0.082913	0.000000	-1.592214
C	0.774320	1.262135	-0.012562
C	-2.543919	-0.000040	0.192935
N	-3.704042	-0.000057	0.371987
O	1.320802	1.509927	1.049201
O	0.546332	2.284432	-0.918102
H	0.849629	3.090846	-0.463207
C	0.774361	-1.262111	-0.012562
O	1.320843	-1.509885	1.049207
O	0.546420	-2.284415	-0.918105
H	0.849743	-3.090818	-0.463209

CH_3CONH_2, -301.990948

C	-0.302331	-0.309188	1.095099
H	1.216017	-0.134230	0.316112
H	-0.204179	-1.315085	1.504103
H	-0.204127	0.496160	1.829393
C	2.350831	-0.001136	-0.095557
N	3.474144	0.133158	-0.380127
C	-1.274528	-0.159995	0.066839
O	-1.747216	-1.061016	-0.667152
N	-1.655709	1.187472	-0.257163
H	-2.523443	1.195091	-0.782987
H	-1.679413	1.823687	0.533340

$CH(CONH_2)_2$ -470.693354

C	0.390187	0.115623	-0.772025
H	-0.936769	-0.546844	-0.602758
H	0.579452	0.154843	-1.843993
C	0.102050	1.438256	-0.220260
C	-2.145723	-1.043464	-0.277009
N	-3.196153	-1.370876	0.121089
C	1.270236	-0.869888	-0.124071
O	1.724400	-1.855643	-0.729936
N	1.584957	-0.699976	1.215389
H	1.131440	0.024855	1.757898
H	1.967859	-1.505944	1.689132
N	-0.351291	1.460298	1.128497
O	0.156345	2.506586	-0.844376
H	-0.731167	2.375292	1.355074
H	-1.019867	0.720970	1.344512

Table S2. Optimized structures for the proton-transfer reactions of small carbon acids with CN^- at MP2/6-31+G*

acid, name of compound, enthalpy

HCN, -93.2813809

C	0.000000	0.000000	-0.512559
N	0.000000	0.000000	0.665547
H	0.000000	0.000000	-1.583473

CH_3NO_2, -244.6736992

C	-0.902662	-0.637767	-0.713275
N	0.110560	0.085801	0.104509
O	0.852598	-0.599413	0.830311
O	0.172056	1.321183	-0.025832
H	-1.741495	0.036169	-0.873718
H	-1.183151	-1.538823	-0.171988
H	-0.426012	-0.891182	-1.661335

$CH_2(NO_2)_2$, −448.9293285

C	0.000625	0.892978	−0.003031
N	−1.205659	0.023296	0.136570
O	−2.190804	0.329096	−0.555948
O	−1.129652	−0.896446	0.965144
N	1.205814	0.020617	−0.135798
O	1.128873	−0.904934	−0.957792
O	2.191102	0.330080	0.554839
H	−0.104912	1.486387	−0.910551
H	0.106920	1.493321	0.899831

CH_3COCH_3, −192.807220

C	−1.415601	0.110879	−0.118569
C	0.096154	0.119080	−0.098625
O	0.746595	0.924542	−0.765860
C	0.770460	−0.909759	0.780392
H	−1.775177	−0.823567	−0.564590
H	−1.781410	0.957656	−0.701239
H	−1.813423	0.156588	0.901000
H	1.850478	−0.872107	0.630411
H	0.394605	−1.913536	0.554475
H	0.539260	−0.706889	1.832441

$CH_3COCHCl_2$, −1111.096778

C	−0.517843	−0.117777	0.110931
Cl	−0.580968	−1.645621	−0.753258
Cl	0.217332	−0.292980	1.727696
C	0.265828	0.960917	−0.661332
O	0.836497	0.706876	−1.711932
C	0.276297	2.333489	−0.033668
H	−0.637738	2.536459	0.531144
H	0.404425	3.073156	−0.826142
H	1.121095	2.409395	0.658224
H	−1.543645	0.222414	0.271198

$CH_3COCH_2COCH_3$, −345.2109648

C	0.917549	−0.252861	−0.371911
C	−0.192620	−1.209964	0.053410
C	0.384802	1.157001	−0.131308
O	0.539077	1.700485	0.962725
C	−0.364204	1.798046	−1.268926
O	−1.054740	−1.558373	−0.753711
C	−0.192745	−1.644569	1.494675
H	1.132592	−0.420009	−1.431172
H	−0.820234	2.731381	−0.934960
H	0.329049	1.999535	−2.093989
H	−1.127037	1.108880	−1.648139
H	0.681685	−2.278085	1.684299
H	−1.105171	−2.200782	1.715389
H	−0.105914	−0.769112	2.147898
H	1.815933	−0.392553	0.236043

CH_3CHO, −153.5719111

C	1.171368	−0.143472	0.000202
C	−0.226058	0.404198	0.000175
H	−0.313471	1.509294	0.000770
H	1.709962	0.222310	0.882293
O	−1.241038	−0.285442	−0.000449
H	1.149967	−1.234871	0.000092
H	1.709986	0.222446	−0.881824

$CH_2(CHO)_2$, −266.7358006

C	−0.223071	0.617534	−0.616081
C	−0.195227	0.620865	0.893491
H	0.802850	0.627545	1.364730
H	−1.262706	0.598335	−0.966779
O	−1.210673	0.629302	1.580894
H	0.229530	1.545573	−0.998892
C	0.533246	−0.551957	−1.201162
H	0.566628	−0.601675	−2.306333
O	1.082425	−1.415355	−0.524670

$CH_2(CN)_2$, −224.6171531

C	0.343942	0.610163	−0.468187
C	0.337334	0.606213	1.001132
H	1.379477	0.645504	−0.825323
N	0.352401	0.639337	2.181737
H	−0.163491	1.511706	−0.829934
C	−0.320663	−0.576654	−1.023816
N	−0.846819	−1.516426	−1.508729

CH_3CO_2H, −228.7482039

C	−1.380747	0.023690	−0.219000
C	0.097847	0.116500	0.018879
O	0.747990	1.141901	0.151443
O	0.668116	−1.122703	0.074409
H	−1.569909	−0.502608	−1.158487
H	−1.847275	−0.552111	0.584874
H	−1.802424	1.027457	−0.257585
H	1.625781	−0.978740	0.230861

anion, name of compound, enthalpy

CN, −92.7254563

C	0.000000	0.000000	−0.647157
N	0.000000	0.000000	0.554706

CH_2NO_2, −244.106374

C	−1.032925	−0.578150	−0.517627
N	0.045090	0.025238	0.022596
O	0.920254	−0.669643	0.672897
O	0.208151	1.301236	−0.107422
H	−1.736300	0.042979	−1.051473
H	−1.126321	−1.645248	−0.383063

$CH(NO_2)_2$, −448.4128241

C	−0.000006	−0.661948	0.000043
N	1.229410	−0.035032	−0.000004
O	2.236866	−0.820761	0.000033
O	1.360136	1.219302	−0.000076
N	−1.229421	−0.035031	0.000016
O	−2.236878	−0.820759	0.000067
O	−1.360146	1.219303	−0.000054
H	−0.000006	−1.738194	0.000106

CH_2COCH_3, −192.2205483

C	0.979359	−0.596207	−0.759820
C	−0.076130	0.112733	0.104458
O	0.327117	1.186167	0.693122
C	−1.338552	−0.463194	0.164899
H	0.597618	−1.505049	−1.243572
H	1.840036	−0.857370	−0.131603

H 1.336816 0.098390 -1.530138
H -2.123444 -0.002830 0.761935
H -1.574360 -1.377504 -0.375170

CH_3COCCl_2, -1110.539887
C 0.141018 -0.228386 -0.063420
Cl -0.619640 -1.794841 0.080420
Cl 1.465632 0.004843 1.079686
C -0.543494 0.829913 -0.649463
O -1.656747 0.725094 -1.273467
C 0.098380 2.217048 -0.586957
H 1.187448 2.195471 -0.490111
H -0.310248 2.782106 0.261665
H -0.180511 2.740183 -1.506567

$CH_3COCHCOCH_3$, -344.6682683
C 0.632016 -0.044954 -0.375457
C -0.308445 -0.993691 -0.876446
C 0.431705 0.870429 0.683967
O -0.613466 1.027344 1.391264
C 1.612890 1.787252 1.026399
O -0.043160 -1.779330 -1.834219
C -1.691035 -1.077711 -0.245207
H 1.597921 -0.045812 -0.878607
H 1.291185 2.830540 0.925334
H 1.889058 1.630564 2.075842
H 2.489482 1.615457 0.391666
H -1.616154 -1.297865 0.824550
H -2.255891 -1.857860 -0.765799
H -2.206027 -0.113832 -0.309761

CH_2CHO, -152.9888595
C -1.187836 -0.168549 0.000060
C 0.094116 0.362024 0.000042
O 1.231065 -0.236866 -0.000118
H -1.355910 -1.244649 -0.000075
H -2.050870 0.495093 0.000208
H 0.120578 1.483639 0.000193

$CH(CHO)_2$, -359.4789076
C 0.000000 0.953778 0.000000
C 1.280067 0.339316 0.000001
H 2.117099 1.087812 0.000002
H 0.000000 2.045643 0.000000
O 1.600357 -0.875983 -0.000001
C -1.280067 0.339316 -0.000001
O -1.600357 -0.875983 0.000001
H -2.117099 1.087812 -0.000002

$CH(CN)_2$, -224.0848946
C -0.387496 -0.558169 -0.276517
C -0.628670 -0.148747 1.040959
H -0.961636 -1.382464 -0.685945
N -0.857752 0.177451 2.169167
C 0.572928 0.068173 -1.080765
N 1.385802 0.582488 -1.792421

CH_2CO_2H, -228.1586156
C -1.398863 -0.179147 0.000052
C -0.051036 0.117958 0.000000
O 0.570291 1.228349 -0.000027
H -2.120125 0.629918 0.000088
H -1.743934 -1.206789 0.000076
O 0.805418 -1.041746 -0.000031
H 1.683256 -0.612784 -0.000068

TS
name of compound, enthalpy
CH_3NO_2, -337.4069831
C 0.380824 0.729153 -0.755816
H 0.380742 0.729044 0.714919
H 1.423738 0.729213 -1.066764
H -0.215022 1.585085 -1.066791
C 0.419065 0.802463 2.047309
N 0.506659 0.970205 3.222301
N -0.244407 -0.468006 -1.146676
O 0.452484 -1.519449 -1.261286
O -1.505498 -0.496858 -1.261317

$C_2H_5NO_2$, -376.038855
C -0.328213 0.474585 -0.659216
H 0.987763 -0.020424 -0.308445
H -0.427059 0.334345 -1.735031
C -0.302446 1.885086 -0.133846
C 2.247401 -0.323919 0.034089
N 3.405807 -0.528982 0.215594
H 0.101973 1.911881 0.883459
H -1.295651 2.355989 -0.108277
H 0.352105 2.486704 -0.776408
N -1.205787 -0.393345 0.003344
O -1.526426 -0.140986 1.205526
O -1.576039 -1.462354 -0.572279

$CH_2(NO_2)_2$, -541.652553
C 0.526793 0.001667 -0.310279
H 0.526308 0.001457 1.000572
H 1.545684 0.001565 -0.688006
C 0.564123 0.012453 2.486810
N 0.681679 0.049262 3.673498
N -0.122584 -1.230735 -0.736151
O 0.612156 -2.242829 -0.667587
O -1.321861 -1.256478 -1.072038
N -0.144683 1.214227 -0.751543
O -1.333205 1.398173 -0.423938
O 0.559457 2.059262 -1.359369

CH_3COCH_3, -285.5263978
C -0.825831 -0.328580 -0.904917
H -0.824272 -0.329152 0.610182
H -0.829579 -1.404103 -1.096618
H -1.742576 0.190018 -1.193131
C -0.884917 -0.416036 1.931612
N -1.000276 -0.590321 3.103259
C 0.381522 0.365273 -1.205430
O 0.480969 1.600737 -1.448766
C 1.682891 -0.414536 -1.007283
H 1.550857 -1.493424 -1.142432
H 2.041952 -0.239902 0.015387
H 2.439268 -0.038547 -1.702962

$CH_3COCHCl_2$, -1203.845013
C 0.177229 0.091638 -0.259473
H 0.177285 0.091898 1.184420

Cl	1.865358	0.092210	−0.779556
Cl	−0.612738	1.648568	−0.640625
C	0.147914	0.179565	2.524367
N	0.051068	0.201900	3.710494
C	−0.582209	−1.080763	−0.684998
O	−0.049673	−2.151176	−1.033668
C	−2.086905	−1.008720	−0.484527
H	−2.336167	−0.552663	0.479790
H	−2.480006	−2.027123	−0.530524
H	−2.551922	−0.399541	−1.266929

CH_3CHO, −245.886559

C	−0.658432	0.985585	−0.180480
C	−1.591189	0.063005	0.366945
O	−2.224682	−0.847746	−0.227723
H	−0.735155	1.148690	−1.258430
H	−0.512823	1.893563	0.410979
H	−1.687995	0.107277	1.479459
H	0.683418	0.350709	−0.063950
C	1.959081	−0.077234	−0.020781
N	3.113321	−0.363773	0.037089

$CH_2(CHO)_2$, −359.4789076

C	0.581936	−0.000005	−0.582597
H	0.581493	−0.000008	0.743268
H	1.669033	−0.000006	−0.728115
C	−0.010951	−1.279150	−0.972257
C	0.754948	0.000000	2.256740
N	1.059278	0.000018	3.411422
C	−0.010948	1.279142	−0.972252
O	−1.186018	1.520299	−1.275669
H	0.710473	2.128691	−0.931082
O	−1.186022	−1.520303	−1.275674
H	0.710469	−2.128700	−0.931090

CH_3CN, −225.556932

C	1.643269	−1.144090	−0.000555
H	−0.684551	−0.007685	0.001765
H	1.922905	−1.645587	−0.924429
H	1.901947	−1.647386	0.928491
C	−1.770332	−0.049756	0.000555
N	−2.929368	−0.109392	−0.001084
C	1.516687	0.234055	−0.000203
N	1.289648	1.403593	0.000426

$CH_2(CN)_2$, −317.3775708,

C	0.421038	−0.000001	−0.624221
H	0.420843	−0.000001	0.748459
H	1.489708	0.000000	−0.863459
C	−0.215131	1.207944	−1.087406
C	0.531416	0.000003	2.180010
N	0.710852	−0.000001	3.358860
N	−0.723249	2.238966	−1.384937
C	−0.215131	−1.207944	−1.087409
N	−0.723249	−2.238966	−1.384942

CH_3CO_2H, −321.4674035

C	−0.269471	−0.358502	1.097430
H	1.071723	−0.147199	0.406097
H	−0.254958	0.399170	1.881099
H	−0.222644	−1.387781	1.452172
C	2.278398	0.018299	−0.087583
N	3.402205	0.158058	−0.452418
C	−1.250114	−0.155088	0.090671
O	−1.732875	−0.969139	−0.723910
O	−1.615664	1.196944	−0.064575
H	−2.174126	1.178710	−0.867669

Table S3. Optimized structures for the proton-transfer reactions of X-substituted PHCH2NO2 at B3LYP/6-31+G*

enthalpy X-substituted $PHCH_2NO_2$

X = *p*-NH_2, −531.284456

C	1.708937	−0.000313	1.000479
N	2.606312	0.000077	−0.237899
O	2.926589	−1.091340	−0.701705
O	2.926056	1.091790	−0.701375
C	0.257909	−0.000168	0.607026
C	−0.434161	−1.204123	0.410712
C	−1.772750	−1.209524	0.031462
C	−2.465113	0.000049	−0.165988
C	−1.772618	1.209498	0.031661
C	−0.434021	1.203883	0.410923
N	−3.788453	0.000152	−0.599324
H	1.990691	−0.898693	1.550979
H	1.990730	0.897710	1.551551
H	0.081492	−2.150988	0.552228
H	−2.288473	−2.155533	−0.118411
H	−2.288206	2.155602	−0.118073
H	0.081721	2.150677	0.552590
H	−4.321607	−0.841676	−0.421866
H	−4.321620	0.841883	−0.421446

X = *p*-MeO, −590.435670

C	2.168606	0.024556	0.971778
N	3.000895	−0.163919	−0.295464
O	3.197980	−1.316185	−0.672505
O	3.395834	0.849645	−0.865535
C	0.704114	0.113553	0.636066
C	−0.088559	−1.036840	0.586141
C	−1.446115	−0.968125	0.260298
C	−2.026227	0.276100	−0.022461
C	−1.239323	1.438981	0.025999
C	0.108034	1.354101	0.350835
O	−3.336253	0.461713	−0.348140
C	−4.190698	−0.674056	−0.427845
H	2.399879	−0.841118	1.593300
H	2.546798	0.941369	1.425185
H	0.354849	−2.006789	0.797734
H	−2.031526	−1.880091	0.232824
H	−1.706345	2.394182	−0.193635
H	0.708619	2.259920	0.378540
H	−5.171692	−0.285496	−0.705337
H	−4.261088	−1.187407	0.539773
H	−3.845225	−1.378130	−1.195563

X = *p*-OH, −551.160297

C	1.694057	0.018030	1.002743
N	2.589879	−0.011994	−0.234506
O	2.885728	−1.115000	−0.686654
O	2.932803	1.067863	−0.707893
C	0.242259	0.014465	0.605221
C	−0.444569	−1.192320	0.422202
C	−1.785037	−1.200129	0.037414
C	−2.455494	0.011292	−0.169356
C	−1.782666	1.225697	0.011572
C	−0.445022	1.220261	0.395079
O	−3.769304	0.074980	−0.543113
H	1.970403	−0.869277	1.573381
H	1.976001	0.926419	1.535887
H	0.071191	−2.136998	0.574665
H	−2.306554	−2.145679	−0.099088
H	−2.318380	2.155919	−0.150137
H	0.074405	2.165975	0.527975
H	−4.131208	−0.818910	−0.649104

X = *p*-Me, −515.232983

C	1.731061	0.013476	0.996848
N	2.619477	−0.003612	−0.244219
O	2.931006	−1.101754	−0.697169
O	2.943354	1.081554	−0.719042
C	0.275469	0.008973	0.605537
C	−0.408380	−1.200123	0.417958
C	−1.751057	−1.201072	0.042129
C	−2.450550	−0.000015	−0.153867
C	−1.757583	1.204258	0.034153
C	−0.413332	1.212310	0.409858
C	−3.913950	−0.009157	−0.530598
H	2.010814	−0.877734	1.559479
H	2.011358	0.918862	1.535894
H	0.114391	−2.143273	0.557786
H	−2.264018	−2.149816	−0.100797
H	−2.275035	2.149385	−0.114573
H	0.104470	2.159176	0.543004
H	−4.135883	−0.800775	−1.255265
H	−4.546451	−0.187479	0.349524
H	−4.220938	0.946634	−0.967940

X = m-Me, −515.232742

C	−1.556633	0.009311	1.022757
N	−2.466129	−0.324105	−0.155956
O	−3.061105	0.608636	−0.688677
O	−2.523809	−1.499820	−0.505968
C	−0.156787	0.303108	0.543046
C	0.216628	1.610552	0.212870
C	1.513688	1.865788	−0.238855
C	2.433049	0.823260	−0.360930
C	2.077947	−0.495840	−0.035824
C	0.775800	−0.736566	0.416912
C	3.078888	−1.620791	−0.171157
H	−2.017435	0.872032	1.504341
H	−1.596201	−0.866900	1.670570
H	−0.502060	2.421009	0.303069
H	1.807177	2.880567	−0.494515
H	3.441445	1.034321	−0.711444
H	0.477864	−1.751699	0.671005
H	3.431055	−1.715832	−1.205934
H	3.961644	−1.446866	0.456922
H	2.643255	−2.581357	0.121924

X = H, −475.943286

C	1.195716	−0.000144	1.026828
N	2.175298	0.000055	−0.142909
O	2.527376	−1.091698	−0.580817
O	2.526816	1.091946	−0.580914
C	−0.226270	−0.000091	0.522963
C	−0.890642	−1.210599	0.282118
C	−2.202675	−1.210162	−0.195491
C	−2.860399	0.000036	−0.434581
C	−2.202627	1.210167	−0.195311
C	−0.890594	1.210478	0.282317
H	1.431794	−0.898608	1.597613
H	1.431756	0.898159	1.597871
H	−0.377832	−2.152005	0.463232
H	−2.710555	−2.153246	−0.378828
H	−3.882631	0.000081	−0.803797
H	−2.710462	2.153304	−0.378505
H	−0.377746	2.151838	0.463571

X = *p*-Cl, −935.546642

C	−2.146547	0.000137	0.977467
N	−2.986198	−0.000068	−0.296832
O	−3.284851	1.091875	−0.771683
O	−3.284134	−1.092187	−0.771750
C	−0.677697	0.000082	0.637928
C	0.013135	1.208082	0.473185
C	1.370183	1.215644	0.149393
C	2.037783	0.000017	−0.009735
C	1.370168	−1.215574	0.149570
C	0.013141	−1.207949	0.473466
Cl	3.745817	−0.000018	−0.409067
H	−2.445231	0.898299	1.518463
H	−2.445250	−0.897854	1.518742
H	−0.510887	2.152706	0.593059
H	1.903841	2.152109	0.023877
H	1.903810	−2.152066	0.024197
H	−0.510903	−2.152546	0.593449

X = *m*-Cl, −935.546170

C	−1.865829	−0.094482	1.024207
N	−2.718597	−0.531776	−0.162649
O	−3.422482	0.323584	−0.691862
O	−2.624161	−1.702294	−0.519305
C	−0.517838	0.390921	0.550440
C	−0.330289	1.734953	0.202313
C	0.917299	2.172514	−0.245288
C	1.987840	1.280982	−0.347444
C	1.789696	−0.055438	0.002768
C	0.549919	−0.510496	0.449862
Cl	3.127155	−1.187595	−0.114880
H	−2.437088	0.693850	1.514720
H	−1.786943	−0.974516	1.662702
H	−1.159168	2.433593	0.275742
H	1.061649	3.214955	−0.514991
H	2.961352	1.615216	−0.690131

H	0.417092	−1.555586	0.711653

X = *m*−F, −575.191548

C	−1.528428	0.017277	1.026597
N	−2.452322	−0.255014	−0.156494
O	−3.014067	0.711652	−0.663397
O	−2.551620	−1.419137	−0.532627
C	−0.119160	0.260811	0.545513
C	0.305479	1.558158	0.227589
C	1.607092	1.778646	−0.228981
C	2.499324	0.712996	−0.371770
C	2.053638	−0.563620	−0.049933
C	0.766404	−0.816379	0.405568
F	2.911631	−1.607485	−0.180289
H	−1.948689	0.890317	1.525793
H	−1.601913	−0.867586	1.659173
H	−0.383245	2.391892	0.331364
H	1.931570	2.786013	−0.473584
H	3.516690	0.858240	−0.720598
H	0.466559	−1.833874	0.636603

X = *p*−CF_3, −812.993591

C	2.804967	0.012561	0.971668
N	3.612540	−0.009361	−0.322170
O	3.887428	−1.109683	−0.791118
O	3.909749	1.074689	−0.814682
C	1.327752	0.013353	0.664087
C	0.633647	−1.196569	0.523695
C	−0.728639	−1.198252	0.231291
C	−1.407963	0.015504	0.076427
C	−0.725250	1.226971	0.214967
C	0.639031	1.222475	0.507110
C	−2.891509	−0.000171	−0.190705
F	−3.238052	−0.969747	−1.073460
F	−3.602015	−0.241638	0.944967
F	−3.340509	1.175573	−0.689391
H	3.111078	−0.879060	1.519197
H	3.117464	0.917354	1.493165
H	1.161085	−2.139822	0.636890
H	−1.259918	−2.138597	0.121927
H	−1.251942	2.167418	0.092910
H	1.170005	2.165255	0.607229

X = *p*−CN, −568.186591

C	−2.017731	0.000035	0.969774
N	−2.852653	−0.000035	−0.307475
O	−3.148243	1.092408	−0.781666
O	−3.147886	−1.092523	−0.781777
C	−0.548156	0.000026	0.628738
C	0.139107	1.210938	0.464439
C	1.493629	1.217059	0.141610
C	2.177875	0.000027	−0.020194
C	1.493643	−1.217018	0.141724
C	0.139126	−1.210899	0.464535
C	3.576409	−0.000012	−0.344387
N	4.710196	0.000003	−0.606064
H	−2.315317	0.898396	1.510793
H	−2.315299	−0.898287	1.510874
H	−0.388414	2.153169	0.585081
H	2.025091	2.155083	0.016348
H	2.025144	−2.155032	0.016561
H	−0.388389	−2.153125	0.585239

X = *m*−CN, −568.186333

C	−1.738859	−0.203446	1.026926
N	−2.625491	−0.537895	−0.168300
O	−3.272136	0.384714	−0.656260
O	−2.611406	−1.696152	−0.571475
C	−0.401385	0.311171	0.554095
C	−0.239277	1.662574	0.215500
C	0.995232	2.135687	−0.233153
C	2.082002	1.269427	−0.344417
C	1.926875	−0.085265	−0.004775
C	0.683628	−0.562255	0.442234
C	3.042026	−0.984041	−0.106315
N	3.948186	−1.709548	−0.185793
H	−2.291122	0.546991	1.593673
H	−1.648197	−1.130158	1.592969
H	−1.083611	2.341724	0.297121
H	1.111346	3.183516	−0.493889
H	3.046535	1.630469	−0.687239
H	0.573068	−1.612051	0.697324

X = *p*−NO_2, −680.446071

C	−2.427821	−0.000193	0.966094
N	−3.238636	0.000044	−0.326431
O	−3.525033	1.092686	−0.805250
O	−3.524926	−1.092417	−0.805716
C	−0.952163	−0.000132	0.650532
C	−0.263360	1.212115	0.498681
C	1.097687	1.220439	0.200341
C	1.756601	−0.000020	0.057567
C	1.097897	−1.220537	0.200843
C	−0.263145	−1.212318	0.499248
N	3.200938	0.000069	−0.250268
O	3.759582	1.090677	−0.368164
O	3.759463	−1.090449	−0.369711
H	−2.734263	0.898023	1.502225
H	−2.734237	−0.898619	1.501886
H	−0.793137	2.154014	0.609613
H	1.645532	2.147528	0.081284
H	1.645873	−2.147584	0.082105
H	−0.792744	−2.154261	0.610665

X-substituted $PHCHNO_2^-$

X = *p*−NH_2, −530.743352

C	−1.660282	0.744495	−0.000647
N	−2.729374	−0.086979	0.007317
O	−2.582204	−1.359361	0.005791
O	−3.907751	0.422002	0.017202
C	−0.269161	0.382915	−0.009609
C	0.691415	1.432560	−0.008381
C	2.063247	1.195108	−0.012152
C	2.566042	−0.114560	−0.010450
C	1.639761	−1.165023	−0.016350
C	0.262743	−0.935405	−0.017398
N	3.975052	−0.360104	−0.067513
H	−1.936558	1.791271	0.002908
H	0.338251	2.463187	−0.003991
H	2.754955	2.038635	−0.022033

H	2.001343	−2.194842	−0.021691
H	−0.434128	−1.763973	−0.017937
H	4.503267	0.333909	0.455226
H	4.210168	−1.280270	0.294870

X = *p*-MeO, −589.898098

C	2.074737	−0.770875	0.000019
N	3.180860	0.013117	0.000051
O	3.091793	1.289716	−0.000015
O	4.333572	−0.549069	−0.000012
C	0.701902	−0.349402	0.000001
C	−0.302781	−1.352700	−0.000024
C	−1.668929	−1.059712	−0.000037
C	−2.093660	0.273840	−0.000026
C	−1.129864	1.289158	−0.000004
C	0.230613	0.995988	0.000008
O	−3.425300	0.682503	−0.000046
C	−4.414578	−0.320483	0.000062
H	2.305765	−1.828416	0.000010
H	0.002797	−2.398234	−0.000031
H	−2.381566	−1.879818	−0.000057
H	−1.466113	2.324220	0.000005
H	0.965175	1.791181	0.000028
H	−5.377524	0.198880	0.000092
H	−4.349800	−0.959811	0.894429
H	−4.349911	−0.959902	−0.894248

X = *p*-OH, −550.623682

C	1.641844	0.749089	0.000026
N	2.717380	−0.075681	0.000017
O	2.579624	−1.348052	0.000005
O	3.890739	0.442508	−0.000038
C	0.253839	0.378051	0.000010
C	−0.710994	1.422818	0.000006
C	−2.082824	1.173743	−0.000008
C	−2.557734	−0.140875	−0.000006
C	−1.641331	−1.193025	0.000001
C	−0.267760	−0.946847	0.000008
O	−3.920786	−0.444090	−0.000029
H	1.911776	1.797399	0.000007
H	−0.365734	2.455725	0.000009
H	−2.784450	2.010346	−0.000023
H	−2.012900	−2.215761	0.000004
H	0.437446	−1.768164	0.000016
H	−4.414646	0.389578	0.000148

X = *p*-Me, −514.698925

C	1.673839	0.739747	0.000041
N	2.747037	−0.092985	0.000040
O	2.602966	−1.362485	0.000127
O	3.921084	0.420044	0.000178
C	0.287079	0.379101	−0.000015
C	−0.670665	1.436457	−0.000076
C	−2.039554	1.199230	−0.000220
C	−2.560683	−0.107993	−0.000331
C	−1.628022	−1.155371	−0.000372
C	−0.248968	−0.938264	−0.000211
C	−4.051565	−0.362133	0.000554
H	1.952723	1.785636	0.000065
H	−0.310333	2.464813	−0.000124
H	−2.723742	2.049612	−0.000315
H	−1.990626	−2.184683	−0.000584
H	0.443101	−1.770650	−0.000358
H	−4.545691	0.062836	0.887774
H	−4.548801	0.076334	−0.878242
H	−4.267066	−1.438119	−0.007166

X = *m*-Me, −514.698769

C	1.410068	−0.785630	0.000137
N	2.650768	−0.229522	−0.000004
O	2.812133	1.036816	0.000136
O	3.668363	−1.007147	−0.000218
C	0.147788	−0.110127	0.000061
C	−1.027797	−0.920994	0.000044
C	−2.316572	−0.395024	−0.000069
C	−2.485338	1.002995	−0.000147
C	−1.350992	1.823025	−0.000028
C	−0.059294	1.297611	0.000046
C	−3.524361	−1.310360	0.000042
H	1.435359	−1.867765	−0.000002
H	−0.903428	−2.004324	0.000112
H	−3.485132	1.436220	−0.000262
H	−1.475639	2.906128	−0.000064
H	0.808876	1.943731	0.000090
H	−3.225351	−2.365376	−0.000895
H	−4.156927	−1.144776	0.883897
H	−4.158132	−1.143509	−0.882711

X = H, −475.410479

C	−1.149208	−0.759019	0.000279
N	−2.269092	0.011848	0.000004
O	−2.199071	1.286622	0.000134
O	−3.410373	−0.568900	−0.000338
C	0.214689	−0.323138	0.000112
C	1.227125	−1.329078	0.000076
C	2.582274	−1.017855	−0.000050
C	3.010917	0.318711	−0.000140
C	2.034407	1.324143	−0.000076
C	0.671915	1.026691	0.000064
H	−1.369399	−1.818786	0.000166
H	0.919850	−2.374440	0.000138
H	3.314672	−1.825194	−0.000080
H	4.070843	0.565704	−0.000234
H	2.340579	2.370475	−0.000122
H	−0.070070	1.814804	0.000145

X = *p*-Cl, −935.021835

C	2.088448	0.731883	0.000010
N	3.140161	−0.132091	0.000003
O	2.959333	−1.395030	0.000000
O	4.324091	0.349135	−0.000014
C	0.696510	0.406769	0.000006
C	−0.234785	1.487673	0.000002
C	−1.611097	1.291216	0.000000
C	−2.116280	−0.011448	−0.000001
C	−1.246544	−1.102107	0.000002
C	0.133452	−0.902622	0.000006
Cl	−3.878000	−0.274877	−0.000004
H	2.395738	1.769519	0.000003
H	0.147653	2.507173	0.000002

H	−2.287952	2.141704	−0.000003
H	−1.645123	−2.113562	0.000002
H	0.808945	−1.748320	0.000008

X = *m*−Cl, −935.022588

C	1.688642	−0.815700	0.000046
N	2.976132	−0.369443	0.000070
O	3.246446	0.876148	−0.000039
O	3.916982	−1.233060	−0.000067
C	0.496855	−0.028518	0.000025
C	−0.746705	−0.732524	0.000019
C	−1.948780	−0.047248	0.000000
C	−2.028706	1.347624	−0.000012
C	−0.811436	2.044908	−0.000004
C	0.419603	1.395437	0.000021
Cl	−3.468088	−0.986711	−0.000014
H	1.618223	−1.895402	0.000038
H	−0.745697	−1.818949	0.000020
H	−2.986689	1.857036	−0.000030
H	−0.831178	3.134186	−0.000014
H	1.345657	1.954730	0.000018

X = *m*−F, −574.666329

C	1.401349	−0.777906	0.000019
N	2.625791	−0.180768	0.000012
O	2.745944	1.088354	−0.000022
O	3.663984	−0.925899	−0.000018
C	0.122298	−0.141430	0.000022
C	−1.027927	−0.988661	0.000012
C	−2.295262	−0.444500	0.000002
C	−2.551949	0.923807	−0.000004
C	−1.426249	1.762960	0.000002
C	−0.126355	1.264026	0.000013
F	−3.373752	−1.307671	−0.000019
H	1.461306	−1.858328	0.000019
H	−0.915076	−2.069763	0.000008
H	−3.569900	1.300569	−0.000015
H	−1.573840	2.842246	−0.000007
H	0.725891	1.930264	0.000011

X = *p*−CF_3, −812.478165

C	−2.750197	−0.728445	0.000040
N	−3.799236	0.149117	0.000056
O	−3.608334	1.405832	0.000111
O	−4.981413	−0.326149	0.000350
C	−1.362789	−0.418613	−0.000133
C	−0.443512	−1.516665	−0.000158
C	0.926439	−1.334979	−0.000393
C	1.477444	−0.037144	−0.000632
C	0.598534	1.058921	−0.000487
C	−0.779711	0.884702	−0.000312
C	2.949514	0.130785	0.000006
F	3.567499	−0.446970	1.088061
F	3.569135	−0.455274	−1.082500
F	3.351147	1.432365	−0.004495
H	−3.071391	−1.761638	0.000150
H	−0.843580	−2.529040	−0.000041
H	1.584144	−2.201829	−0.000415
H	1.000910	2.068446	−0.000630
H	−1.441803	1.740306	−0.000333

X = *p*−CN, −567.677505

C	1.938098	0.725076	0.000525
N	3.001128	−0.140655	0.000235
O	2.827915	−1.397891	0.000368
O	4.173273	0.353228	−0.000206
C	0.558856	0.397942	0.000116
C	−0.375919	1.484389	0.000029
C	−1.741775	1.286455	−0.000443
C	−2.281450	−0.023263	−0.000684
C	−1.376525	−1.110743	−0.000726
C	−0.005812	−0.916961	−0.000221
C	−3.688172	−0.234051	−0.000992
N	−4.846112	−0.404101	0.001739
H	2.247393	1.761881	0.000544
H	0.011318	2.501654	0.000318
H	−2.415184	2.140545	−0.000525
H	−1.771438	−2.124333	−0.001018
H	0.669484	−1.762213	−0.000064

X = *m*−CN, −567.671532

C	1.566855	−0.840476	−0.000083
N	2.852168	−0.383576	−0.000026
O	3.109176	0.864178	−0.000175
O	3.798344	−1.237745	0.000243
C	0.373160	−0.059459	−0.000071
C	−0.867571	−0.759129	−0.000129
C	−2.093999	−0.087610	−0.000029
C	−2.151820	1.322607	0.000088
C	−0.940733	2.019534	0.000092
C	0.289952	1.365981	−0.000001
C	−3.314066	−0.844414	−0.000001
N	−4.312654	−1.447255	0.000016
H	1.503058	−1.920464	0.000183
H	−0.862498	−1.846308	−0.000186
H	−3.108893	1.834948	0.000214
H	−0.955219	3.108351	0.000202
H	1.216122	1.925619	−0.000082

X = *p*−NO_2, −679.945598

C	2.342043	0.730289	0.000082
N	3.409159	−0.142599	0.000111
O	3.232535	−1.394497	−0.000065
O	4.576011	0.353911	−0.000110
C	0.968013	0.411823	0.000045
C	0.042207	1.511099	0.000009
C	−1.321892	1.328264	−0.000026
C	−1.853210	0.020381	−0.000030
C	−0.976932	−1.084120	0.000006
C	0.391935	−0.901780	0.000043
N	−3.262663	−0.177082	−0.000068
O	−4.013940	0.824980	−0.000001
O	−3.712237	−1.344672	0.000030
H	2.660085	1.764220	0.000061
H	0.441256	2.523453	0.000008
H	−2.000384	2.173834	−0.000053
H	−1.396951	−2.083892	0.000006
H	1.058600	−1.753368	0.000074

TS of deprotonation of X-substituted $PhCH_2NO_2$ with $HO^-(H_2O)_2$

$(H_2O)_3$
−229.217070

O	0.117128	1.588161	0.112304
H	0.049976	2.222187	−0.616704
H	−0.680535	1.013493	0.057013
O	−1.445480	−0.687070	−0.086893
H	−1.980776	−1.103226	0.604131
H	−0.561244	−1.116941	−0.058656
O	1.323504	−0.893602	−0.091693
H	1.219953	0.082533	−0.012780
H	1.991416	−1.157956	0.557258

$OH(H_2O)_2^-$
−228.662484

O	0.003717	0.872283	0.076315
H	−0.004452	1.586577	−0.578889
O	−2.268383	−0.401922	0.035975
H	−1.395021	0.157641	0.077624
H	−1.952884	−1.250258	−0.308679
O	2.203158	−0.492648	−0.099561
H	1.307905	0.041140	−0.091272
H	2.536510	−0.356801	0.799384

X = *p*−NH_2, −759.970094

C	−0.570299	−0.348391	0.548880
N	−1.078699	−1.698236	0.354860
O	−0.564134	−2.441777	−0.497009
C	0.886379	−0.124230	0.303775
O	−2.094060	−2.025923	1.001562
H	−0.888358	−0.039244	1.544591
C	1.665717	0.493997	1.295018
C	3.014604	0.795841	1.095080
C	3.640782	0.476772	−0.116728
C	2.871230	−0.131327	−1.120197
C	1.521932	−0.417131	−0.916670
H	1.206352	0.747432	2.248460
H	3.583891	1.280513	1.887541
N	4.996568	0.815903	−0.347949
H	3.333061	−0.374067	−2.076753
H	0.952271	−0.889578	−1.708863
H	−1.277427	0.354945	−0.228024
O	−2.153819	1.152118	−0.957100
H	−1.821192	1.258515	−1.861831
O	−3.987898	2.823176	0.273777
H	−3.204246	2.423411	−0.181575
H	−4.583871	2.055596	0.320260
O	−4.468486	−0.200640	−0.484233
H	−3.636415	0.259156	−0.792633
H	−4.126554	−0.902924	0.092669
H	5.452077	0.211857	−1.024160
H	5.550431	0.861907	0.501027

X = *p*−MeO, −819.123825

C	1.007465	−0.392530	−0.496164
N	1.603810	−1.718556	−0.405548
O	1.146170	−2.554153	0.391058
C	−0.459255	−0.281776	−0.233871
O	2.629546	−1.930758	−1.081662
H	1.296485	0.008958	−1.467423
C	−1.272390	0.375484	−1.165936
C	−2.639439	0.592491	−0.944724
C	−3.222837	0.134839	0.239163
C	−2.428992	−0.522587	1.188927
C	−1.071222	−0.718141	0.959303
H	−0.831252	0.737187	−2.092415
H	−3.222394	1.109348	−1.700035
O	−4.556394	0.282418	0.563642
H	−2.894149	−0.866810	2.108991
H	−0.471618	−1.226110	1.705730
H	1.667671	0.297162	0.323343
O	2.501745	1.122120	1.087515
H	2.246431	1.084017	2.022223
O	3.907894	3.132561	−0.185821
H	3.256771	2.589102	0.326410
H	4.598743	2.471577	−0.364819
O	4.900556	0.154380	0.254279
H	4.056852	0.467539	0.689937
H	4.591405	−0.556627	−0.330200
C	−5.392441	0.957121	−0.356818
H	−6.388502	0.967843	0.092720
H	−5.436137	0.433600	−1.322831
H	−5.058446	1.991148	−0.524173

X = *p*−OH, −779.849346

C	−0.604792	−0.371374	0.480699
N	−1.100264	−1.736355	0.361426
O	−0.545042	−2.535947	−0.409545
C	0.858869	−0.153482	0.272505
O	−2.139818	−2.022704	0.987038
H	−0.957260	0.000457	1.442838
C	1.588557	0.552119	1.241376
C	2.939966	0.864631	1.063042
C	3.594211	0.462979	−0.102145
C	2.891123	−0.238433	−1.084665
C	1.540901	−0.532274	−0.900107
H	1.090428	0.871987	2.154010
H	3.478401	1.415579	1.834434
O	4.931257	0.734861	−0.334737
H	3.408472	−0.539991	−1.991569
H	1.004329	−1.073835	−1.670495
H	−1.282306	0.278832	−0.353848
O	−2.147980	1.065533	−1.128137
H	−1.868197	1.070071	−2.056518
O	−3.635151	2.945346	0.245801
H	−2.964656	2.461732	−0.300111
H	−4.292350	2.243425	0.393476
O	−4.493058	−0.048544	−0.323683
H	−3.671878	0.319935	−0.758260
H	−4.138977	−0.751039	0.245637
H	5.281160	1.243976	0.412299

X = *p*−Me, −743.921914

C	−0.598560	−0.393190	0.528491
N	−1.100320	−1.751259	0.343144
O	−0.578003	−2.498750	−0.498726
C	0.860175	−0.164198	0.300190
O	−2.111449	−2.077379	0.993054
H	−0.926947	−0.079575	1.519368
C	1.606547	0.504956	1.283098
C	2.954219	0.821800	1.088446
C	3.614486	0.475367	−0.095847
C	2.867840	−0.186897	−1.083297
C	1.520534	−0.494394	−0.898727

H	1.122041	0.789088	2.215139
H	3.498212	1.343769	1.874785
C	5.079641	0.789280	-0.305296
H	3.348941	-0.460438	-2.022115
H	0.970832	-1.002911	-1.682373
H	-1.286159	0.295040	-0.253979
O	-2.169769	1.113349	-1.000899
H	-1.868154	1.180418	-1.920098
O	-3.796265	2.950180	0.258183
H	-3.075496	2.467083	-0.222702
H	-4.461995	2.247143	0.347741
O	-4.537500	-0.083427	-0.432636
H	-3.685528	0.321635	-0.767477
H	-4.227400	-0.802822	0.140293
H	5.695692	-0.120956	-0.282587
H	5.254793	1.271668	-1.275932
H	5.457998	1.461539	0.473766

X = *m*-Me, -743.921993

C	0.464963	-0.366389	-0.462056
N	1.036102	-1.700632	-0.633771
O	0.651891	-2.640180	0.079298
C	-0.963755	-0.278332	-0.031084
O	1.967572	-1.816854	-1.451425
H	0.659694	0.168073	-1.391708
C	-1.829704	0.559317	-0.753396
C	-3.162288	0.770551	-0.372979
C	-3.643636	0.108408	0.762697
C	-2.796870	-0.727722	1.499031
C	-1.468974	-0.915764	1.117909
H	-1.448650	1.065900	-1.639345
C	-4.046109	1.708610	-1.166890
H	-4.677974	0.248366	1.073600
H	-3.177040	-1.234875	2.383933
H	-0.820711	-1.564609	1.694596
H	1.211723	0.179278	0.365873
O	2.160716	0.885176	1.169842
H	1.992819	0.725562	2.111452
O	3.452223	3.093706	0.153705
H	2.847735	2.449085	0.605813
H	4.145986	2.497196	-0.175061
O	4.482879	0.052257	0.051593
H	3.664695	0.300996	0.573429
H	4.137058	-0.555634	-0.621142
H	-3.912288	1.570200	-2.246998
H	-5.106344	1.550365	-0.936091
H	-3.813419	2.759602	-0.945442

X = H, -704.633467

C	-0.123099	0.313303	-0.528719
N	-0.523722	1.710458	-0.371532
O	0.023164	2.421896	0.484822
C	1.304937	-0.022379	-0.242707
O	-1.478633	2.107790	-1.064002
H	-0.435218	0.019250	-1.530746
C	2.042461	-0.730080	-1.208361
C	3.355805	-1.140661	-0.965113
C	3.967793	-0.845749	0.256021
C	3.244433	-0.147299	1.229127
C	1.928578	0.252298	0.988857
H	1.575896	-0.963602	-2.163240
H	3.900475	-1.686786	-1.732920
H	4.991638	-1.159138	0.449451
H	3.705662	0.082306	2.187827
H	1.377011	0.790263	1.751238
H	-0.888403	-0.306210	0.229409
O	-1.873194	-1.036097	0.961002
H	-1.601945	-1.131734	1.887153
O	-3.698226	-2.696628	-0.272846
H	-2.925762	-2.288910	0.197777
H	-4.284510	-1.926459	-0.366099
O	-4.104362	0.395065	0.389487
H	-3.293684	-0.092914	0.718372
H	-3.730533	1.077918	-0.189842

X = *p*-Cl, -1164.241164

C	-0.994581	-0.436238	0.536006
N	-1.522404	-1.791138	0.326520
O	-1.009498	-2.527700	-0.527905
C	0.474281	-0.250808	0.327205
O	-2.532261	-2.110034	0.974349
H	-1.319893	-0.137226	1.532257
C	1.237682	0.348619	1.342467
C	2.598268	0.621275	1.177826
C	3.210305	0.281690	-0.025795
C	2.483387	-0.308233	-1.059376
C	1.122695	-0.562090	-0.881676
H	0.758892	0.613287	2.282442
H	3.171270	1.085011	1.975026
Cl	4.937328	0.608143	-0.249330
H	2.972146	-0.558742	-1.996090
H	0.556492	-1.016628	-1.686063
H	-1.636605	0.259345	-0.230783
O	-2.523218	1.146319	-1.002770
H	-2.231342	1.242057	-1.922475
O	-3.914540	3.096976	0.325302
H	-3.271656	2.534180	-0.184288
H	-4.675355	2.496846	0.395131
O	-4.968575	0.106516	-0.513401
H	-4.078622	0.464969	-0.807708
H	-4.730581	-0.645462	0.050989

X = *m*-Cl, -1164.241002

C	0.739575	-0.334942	-0.490089
N	1.359648	-1.637662	-0.767480
O	1.083132	-2.615824	-0.059213
C	-0.645385	-0.368031	0.072287
O	2.213268	-1.674968	-1.668254
H	0.809922	0.236282	-1.415434
C	-1.667908	0.323138	-0.600077
C	-2.950705	0.374321	-0.058532
C	-3.265172	-0.250260	1.145672
C	-2.245247	-0.934948	1.815856
C	-0.952715	-0.989940	1.295983
H	-1.459614	0.820686	-1.542516
Cl	-4.219809	1.249507	-0.932776
H	-4.271800	-0.199152	1.548626
H	-2.466534	-1.423824	2.761993
H	-0.173183	-1.521046	1.829172
H	1.513538	0.204548	0.288768

O	2.511926	0.911447	1.089733
H	2.382125	0.750729	2.037243
O	3.782372	3.178507	0.195749
H	3.184541	2.493564	0.597189
H	4.503506	2.621529	-0.142167
O	4.855208	0.126985	-0.006630
H	4.015847	0.358544	0.492125
H	4.538965	-0.445048	-0.723130

X = *m*-F, -803.885534

C	0.429075	-0.395259	-0.491435
N	0.932551	-1.773753	-0.540545
O	0.534126	-2.606447	0.286099
C	-0.987673	-0.215350	-0.048103
O	1.817087	-2.021665	-1.376099
C	-1.862557	0.513571	-0.872731
C	-3.158521	0.764202	-0.444469
C	-3.650180	0.321661	0.774785
C	-2.775807	-0.400981	1.595889
C	-1.463926	-0.661372	1.199563
F	-3.992863	1.473245	-1.269154
H	0.620815	0.029935	-1.476229
H	1.198714	0.179252	0.266490
H	-1.539097	0.887102	-1.839908
H	-4.672862	0.540783	1.065992
H	-3.125179	-0.756674	2.562518
H	-0.800341	-1.218935	1.849200
O	2.200646	0.918373	1.034115
H	2.033818	0.842807	1.986432
O	3.559392	3.061682	-0.017889
H	2.931185	2.431590	0.425196
H	4.276208	2.459285	-0.277881
O	4.556255	-0.025080	0.116158
H	3.702416	0.275947	0.550993
H	4.259710	-0.687763	-0.526661

X = *p*-CN, -796.891330

C	1.103679	-0.466592	-0.383295
N	1.765605	-1.746601	-0.178303
O	1.363672	-2.515918	0.709425
C	-0.378822	-0.372101	-0.208878
O	2.784621	-1.974467	-0.853439
H	1.426684	-0.104446	-1.360883
C	-0.933374	0.913689	-0.396387
C	-2.303612	1.123633	-0.303944
C	-3.168433	0.050253	-0.013781
C	-2.622970	-1.229386	0.189282
C	-1.248275	-1.434468	0.098452
H	-0.276698	1.759023	-0.596457
H	-2.709644	2.121113	-0.446032
C	-4.582495	0.256560	0.079452
H	-3.281100	-2.062893	0.419351
H	-0.845447	-2.423948	0.275626
H	1.675608	0.314426	0.382826
O	2.412865	1.370516	1.035276
H	2.310173	1.302962	1.997245
O	1.296151	3.427138	-0.230013
H	1.728272	2.705888	0.328580
H	2.016566	3.758394	-0.785411
O	4.878009	0.695518	0.025966
H	4.034551	1.009480	0.453926
H	4.630488	-0.163448	-0.351240
N	-5.735059	0.419688	0.152495

X = m-CN, -796.887023

C	0.612731	-0.359703	-0.533923
N	1.162677	-1.712410	-0.725550
O	0.868853	-2.610441	0.075586
C	-0.760244	-0.302253	0.055444
O	1.970975	-1.867337	-1.652076
C	-1.794312	0.319044	-0.656092
C	-3.079719	0.445915	-0.099817
C	-3.347011	-0.054989	1.185629
C	-2.317220	-0.668041	1.898383
C	-1.039864	-0.784559	1.347737
C	-4.128178	1.077687	-0.848886
N	-4.988665	1.584131	-1.449536
H	0.682358	0.136586	-1.501453
H	1.411226	0.190495	0.195609
H	-1.606029	0.709644	-1.652225
H	-4.342068	0.042855	1.609339
H	-2.509505	-1.051412	2.897371
H	-0.246166	-1.258151	1.913844
O	2.435253	0.916123	0.980616
H	2.311138	0.798761	1.935294
O	3.667777	3.191513	0.060338
H	3.081292	2.494823	0.459305
H	4.424374	2.656156	-0.231082
O	4.828487	0.148066	0.005783
H	3.956485	0.376870	0.450001
H	4.570947	-0.460666	-0.703235

X = *p*-NO_2, -909.153472

C	1.454311	-0.566119	-0.470323
N	2.066583	-1.881510	-0.300426
O	1.716636	-2.598561	0.650159
C	-0.018409	-0.430807	-0.263208
O	2.984794	-2.189600	-1.075587
H	1.762751	-0.205957	-1.453010
C	-0.553348	0.856726	-0.502140
C	-1.913788	1.102947	-0.374296
C	-2.765824	0.056683	0.000441
C	-2.263153	-1.221747	0.257222
C	-0.897424	-1.458255	0.131784
H	0.114523	1.674659	-0.766938
H	-2.318265	2.092458	-0.551797
N	-4.195124	0.302237	0.129841
H	-2.940259	-2.015651	0.550081
H	-0.507996	-2.445207	0.348076
H	2.053559	0.179322	0.297233
O	2.789603	1.230483	0.993911
H	2.579837	1.198143	1.940419
O	1.753289	3.246791	-0.407341
H	2.151361	2.542640	0.195730
H	2.516548	3.624902	-0.867349
O	5.456751	1.124712	0.480830
H	4.486687	1.204166	0.714599
H	5.522553	0.246205	0.077716
O	-4.925578	-0.636599	0.478697
O	-4.622458	1.438107	-0.116612

X-substituted PhCH=N(O)OH

X = *p*-NH_2, −531.271383

C	−1.584768	0.733426	−0.000076
N	−2.581717	−0.112415	0.003178
O	−2.597279	−1.369049	0.003649
O	−3.865837	0.515335	0.006859
C	−0.181377	0.379180	−0.003970
C	0.754645	1.436984	−0.002526
C	2.121506	1.198981	−0.003164
C	2.616381	−0.119423	−0.004083
C	1.690646	−1.179198	−0.008006
C	0.321441	−0.940883	−0.007653
N	3.986248	−0.366047	−0.060522
H	−1.884484	1.773328	0.000178
H	−4.449784	−0.268871	0.005243
H	0.398303	2.464908	0.000300
H	2.816219	2.036204	−0.008454
H	2.052733	−2.205277	−0.016189
H	−0.371572	−1.773054	−0.008456
H	4.590564	0.376543	0.268364
H	4.290394	−1.279237	0.253222

X = *p*-MeO, −590.422274

C	2.002721	−0.754704	−0.000159
N	3.033741	0.049313	0.000096
O	3.102201	1.302505	−0.000043
O	4.288822	−0.632242	0.000555
C	0.614040	−0.340887	−0.000169
C	−0.360999	−1.357050	−0.000204
C	−1.724288	−1.067111	−0.000144
C	−2.144638	0.270896	−0.000056
C	−1.185940	1.297082	−0.000038
C	0.169903	1.002861	−0.000099
O	−3.447449	0.672507	0.000028
C	−4.469561	−0.317057	0.000265
H	2.258708	−1.806084	−0.000328
H	4.907124	0.125328	−0.001530
H	−0.047315	−2.398672	−0.000253
H	−2.439513	−1.881897	−0.000179
H	−1.529369	2.327322	0.000057
H	0.897968	1.804250	−0.000116
H	−5.412239	0.232433	0.000470
H	−4.413576	−0.947105	0.897437
H	−4.413989	−0.947114	−0.896926

X = *p*-OH, −551.146933

C	1.568437	0.737122	0.000346
N	2.568998	−0.104498	0.000132
O	2.590024	−1.359066	0.000062
O	3.847924	0.529776	−0.000744
C	0.165322	0.374297	0.000212
C	−0.771159	1.429280	0.000141
C	−2.139926	1.182605	−0.000005
C	−2.607041	−0.137886	−0.000081
C	−1.695170	−1.199595	0.000010
C	−0.327220	−0.950812	0.000155
O	−3.938921	−0.451206	−0.000285
H	1.863042	1.778304	0.000488
H	4.438291	−0.249859	0.001262
H	−0.419706	2.458521	0.000180
H	−2.842458	2.014143	−0.000057
H	−2.073459	−2.217383	−0.000078
H	0.372005	−1.777459	0.000272
H	−4.472375	0.359123	0.000073

X = *p*-Me, −515.219655

C	1.604615	0.730112	0.000576
N	2.598777	−0.119566	0.003205
O	2.611568	−1.372798	0.003066
O	3.881690	0.505655	0.006933
C	0.197628	0.378290	−0.002593
C	−0.729150	1.443323	−0.003797
C	−2.098623	1.202160	−0.008351
C	−2.604187	−0.107934	−0.009949
C	−1.681014	−1.163754	−0.013615
C	−0.305026	−0.939684	−0.008663
C	−4.091676	−0.368463	0.019311
H	1.907657	1.768833	0.001914
H	4.467360	−0.277552	0.008883
H	−0.365506	2.468723	−0.004592
H	−2.787777	2.044121	−0.012326
H	−2.044959	−2.189159	−0.021890
H	0.384356	−1.774647	−0.012863
H	−4.646818	0.411538	−0.513817
H	−4.338969	−1.333284	−0.436676
H	−4.468244	−0.388769	1.051419

X = *m*-Me, −515.219282

C	−1.355360	−0.754079	−0.000027
N	−2.517672	−0.154171	−0.000006
O	−2.817986	1.061649	−0.000036
O	−3.622322	−1.057608	0.000071
C	−0.064841	−0.090231	−0.000061
C	1.074724	−0.926553	0.000034
C	2.370183	−0.409888	0.000113
C	2.527261	0.986698	0.000139
C	1.413723	1.827553	−0.000008
C	0.118759	1.306719	−0.000108
C	3.576594	−1.321709	−0.000083
H	−1.413524	−1.834446	0.000015
H	−4.372830	−0.430562	0.000095
H	0.935296	−2.006232	0.000081
H	3.528053	1.413910	0.000300
H	1.552613	2.905780	0.000021
H	−0.741684	1.963418	−0.000171
H	3.282088	−2.376314	−0.000760
H	4.205082	−1.149395	−0.882893
H	4.204821	−1.150359	0.883073

X = H, −475.930025

C	1.085231	−0.744533	0.000051
N	2.124400	0.049888	0.000019
O	2.205855	1.299561	0.000063
O	3.369861	−0.645003	−0.000157
C	−0.301481	−0.316313	0.000026
C	−1.280499	−1.334663	0.000034
C	−2.636934	−1.022513	0.000008
C	−3.047745	0.315117	−0.000032

C	-2.088044	1.331432	-0.000040
C	-0.725770	1.029887	-0.000007
H	1.331194	-1.798126	0.000060
H	3.999120	0.103736	0.000368
H	-0.966865	-2.376279	0.000060
H	-3.373633	-1.821594	0.000016
H	-4.106304	0.561451	-0.000053
H	-2.400607	2.372542	-0.000069
H	0.012017	1.822109	-0.000005

X = *p*-Cl, -935.53412

C	2.017474	0.724663	0.000230
N	2.989466	-0.151333	-0.000111
O	2.965920	-1.403013	0.000126
O	4.285338	0.438992	-0.000717
C	0.603050	0.404945	0.000211
C	-0.297650	1.492328	0.000196
C	-1.673815	1.292025	0.000075
C	-2.170001	-0.013863	-0.000016
C	-1.304658	-1.108518	0.000041
C	0.074195	-0.903413	0.000169
Cl	-3.905909	-0.278295	-0.000166
H	2.345746	1.755459	0.000429
H	4.853469	-0.357425	0.001931
H	0.088286	2.508965	0.000246
H	-2.355481	2.136262	0.000048
H	-1.705145	-2.117145	-0.000005
H	0.745687	-1.752612	0.000246

X = *m*-Cl, -935.533400

C	-1.638861	-0.775404	0.000000
N	-2.848555	-0.276250	0.000000
O	-3.248103	0.909119	-0.000002
O	-3.869190	-1.268450	0.000001
C	-0.412876	0.001780	0.000000
C	0.792950	-0.733245	0.000000
C	2.012175	-0.067064	0.000000
C	2.078604	1.327823	0.000000
C	0.884355	2.052625	0.000001
C	-0.354087	1.411267	0.000001
Cl	3.500968	-1.003875	0.000000
H	-1.602479	-1.856469	0.000001
H	-4.672917	-0.710739	-0.000003
H	0.772484	-1.818890	0.000000
H	3.040270	1.829565	0.000000
H	0.922090	3.138639	0.000001
H	-1.271242	1.985462	0.000001

X = *m*-F, -575.178779

C	-1.346639	-0.748802	-0.000016
N	-2.489234	-0.110622	-0.000020
O	-2.747027	1.113211	0.000004
O	-3.619393	-0.976472	0.000017
C	-0.037433	-0.122447	-0.000005
C	1.073624	-0.994564	-0.000001
C	2.351141	-0.462086	0.000003
C	2.595754	0.906922	0.000005
C	1.492975	1.765441	0.000002
C	0.187959	1.270990	-0.000002
F	3.409022	-1.316619	0.000003
H	-1.438024	-1.826603	-0.000011
H	-4.352097	-0.328371	0.000047
H	0.945597	-2.072910	-0.000003
H	3.616011	1.276572	0.000007
H	1.654470	2.839868	0.000003
H	-0.655438	1.948733	-0.000005

X = *p*-CF_3, -812.981613

C	-2.685965	-0.722926	0.000565
N	-3.646761	0.167004	0.000318
O	-3.606003	1.415806	-0.000105
O	-4.947389	-0.406825	-0.000398
C	-1.267486	-0.420586	0.000090
C	-0.383123	-1.523686	-0.000251
C	0.991828	-1.337930	-0.000673
C	1.520167	-0.039204	-0.000683
C	0.660492	1.061493	-0.000387
C	-0.722396	0.879652	-0.000011
C	3.014726	0.134209	-0.000010
F	3.589556	-0.442198	1.090874
F	3.591623	-0.451835	-1.084275
F	3.392881	1.433218	-0.005571
H	-3.028075	-1.749092	0.000916
H	-5.508289	0.394888	0.001334
H	-0.785848	-2.533436	-0.000228
H	1.655906	-2.197277	-0.000998
H	1.066605	2.067459	-0.000532
H	-1.381827	1.737796	0.000201

X = *p*-CN, -568.175337

C	1.879206	0.719075	0.000531
N	2.852856	-0.158225	0.000438
O	2.828489	-1.406871	0.000027
O	4.143859	0.433379	0.000060
C	0.466423	0.397704	-0.000003
C	-0.432985	1.488416	-0.000165
C	-1.805333	1.287446	-0.000632
C	-2.320938	-0.022325	-0.000846
C	-1.436609	-1.115106	-0.000801
C	-0.060649	-0.912779	-0.000324
C	-3.738355	-0.237661	-0.000896
N	-4.889692	-0.410705	0.002159
H	2.207542	1.749685	0.000888
H	4.717367	-0.359511	0.001003
H	-0.043668	2.503342	0.000071
H	-2.484292	2.134391	-0.000762
H	-1.834203	-2.125326	-0.001051
H	0.611762	-1.760746	-0.000199

X = *m*-CN, -568.174404

C	1.517845	-0.800819	0.000197
N	2.725108	-0.294932	-0.000139
O	3.114664	0.893113	-0.000489
O	3.749621	-1.279023	0.000143
C	0.289725	-0.026835	0.000144
C	-0.914715	-0.757053	0.000167
C	-2.149272	-0.097517	0.000107
C	-2.200560	1.308403	0.000115
C	-1.009184	2.031479	0.000117
C	0.226999	1.383920	0.000110

C	-3.364709	-0.862646	-0.000084
N	-4.350579	-1.480880	-0.000347
H	1.485130	-1.881948	0.000559
H	4.551730	-0.718633	0.000000
H	-0.892777	-1.843035	0.000152
H	-3.161148	1.813518	0.000041
H	-1.040814	3.117308	0.000086
H	1.145120	1.957164	0.000090

X = *p*-NO_2, -680.435299,

C	2.376165	-0.378382	0.019640
N	3.200837	0.641359	0.024477
O	2.980869	1.869314	0.020111
O	4.566820	0.258476	0.036506
C	0.931159	-0.281337	0.007806
C	0.214960	-1.501336	0.004538
C	-1.172306	-1.520434	-0.006398
C	-1.859113	-0.304037	-0.014304
C	-1.185274	0.917640	-0.011404
C	0.206103	0.931782	-0.000419
N	-3.328731	-0.314210	-0.025956
O	-3.894896	-1.409852	-0.028242
O	-3.911500	0.771928	-0.032771
H	2.862065	-1.344644	0.025355
H	5.011773	1.130148	0.037388
H	0.759114	-2.442057	0.010766
H	-1.724557	-2.452499	-0.008874
H	-1.750555	1.842059	-0.017773
H	0.736911	1.874652	0.001887

TS for isomerization from phenylnitromethane to phenyl-*aci*-nitromethane with H_2O

X = H, -552.288328

C	0.850214	-0.395473	-0.349545
N	1.787581	0.640385	-0.431638
O	1.528452	1.834168	-0.313294
O	3.048395	0.258313	-0.509070
C	-0.594521	-0.155228	-0.173189
C	-1.466660	-1.163664	-0.631417
C	-2.844293	-1.069636	-0.440454
C	-3.386873	0.038072	0.217387
C	-2.533684	1.044888	0.677438
C	-1.153295	0.956182	0.488029
H	1.116353	-1.178941	-1.059733
H	-1.056229	-2.031795	-1.143577
H	-3.493096	-1.859899	-0.809607
H	-4.460701	0.117767	0.364576
H	-2.944178	1.914419	1.184781
H	-0.512921	1.757432	0.835716
O	2.675810	-1.537685	1.059815
H	2.862144	-1.259459	1.973979
H	1.623606	-1.145363	0.717651
H	3.105378	-0.766062	0.328587

TS for isomerization from phenylnitromethane to phenyl-*aci*-nitromethane with $(H_2O)_2$

X = *p*-NH_2, -684.050007

C	0.834100	-0.551391	-0.731762
N	1.839140	0.375100	-0.864335
O	1.760162	1.530769	-0.371310
O	2.971735	-0.036386	-1.350222
C	-0.568230	-0.239684	-0.417496
C	-1.511099	-1.270301	-0.625490
C	-2.859119	-1.105866	-0.330089
C	-3.334371	0.110792	0.190975
C	-2.405978	1.142081	0.404776
C	-1.053227	0.974342	0.113514
N	-4.681295	0.265146	0.543910
H	1.034117	-1.434420	-1.331183
H	-1.177851	-2.220793	-1.037721
H	-3.552937	-1.925472	-0.507082
H	-2.747475	2.094539	0.806436
H	-0.365274	1.794285	0.275369
H	-5.013965	1.221917	0.569105
H	-5.329622	-0.338135	0.051530
O	4.158438	0.052987	0.918847
H	3.908904	0.093257	-0.079920
H	4.173700	0.981156	1.208305
O	2.123309	-1.145783	1.586139
H	1.634776	-0.743024	2.325821
H	1.517479	-1.002305	0.682586
H	3.091623	-0.575258	1.385526

X = *p*-MeO, -743.201579 -869.46

C	1.239099	-0.499709	-0.760606
N	2.277686	0.397322	-0.834953
O	2.235409	1.526291	-0.282117
O	3.397753	-0.028177	-1.334304
C	-0.155834	-0.153811	-0.447508
C	-1.131670	-1.125840	-0.740879
C	-2.483575	-0.934358	-0.450881
C	-2.899052	0.260598	0.151127
C	-1.944316	1.242281	0.451309
C	-0.598434	1.042381	0.163538
O	-4.193187	0.558818	0.479740
C	-5.204995	-0.393670	0.183546
H	1.414792	-1.354474	-1.406620
H	-0.829625	-2.056926	-1.216266
H	-3.193646	-1.713710	-0.705155
H	-2.278783	2.168569	0.909925
H	0.119694	1.819821	0.390281
H	-6.141198	0.052151	0.524085
H	-5.034771	-1.337624	0.718519
H	-5.265720	-0.589989	-0.895161
O	4.568932	-0.104353	0.944739
H	4.332252	-0.000044	-0.051688
H	4.612631	0.805049	1.286482
O	2.491290	-1.269019	1.529295
H	2.013229	-0.897207	2.291660
H	1.895545	-1.053201	0.635788
H	3.482895	-0.719393	1.366123

X = *p*-OH, -703.926366

C	0.817279	-0.555745	-0.721537
N	1.823632	0.369558	-0.865198
O	1.750083	1.526690	-0.378309
O	2.949611	-0.046743	-1.357432

C	-0.584770	-0.236185	-0.410668
C	-1.530363	-1.259815	-0.630260
C	-2.880192	-1.088032	-0.332846
C	-3.326927	0.127870	0.196355
C	-2.410346	1.157785	0.422877
C	-1.059477	0.979747	0.129308
O	-4.642119	0.364994	0.510601
H	1.012623	-1.440497	-1.319760
H	-1.202716	-2.208808	-1.049428
H	-3.583934	-1.897337	-0.521644
H	-2.767806	2.100906	0.826151
H	-0.363876	1.791670	0.297535
H	-5.179262	-0.412107	0.290984
O	4.161922	0.046500	0.900017
H	3.905328	0.089285	-0.095462
H	4.189799	0.973633	1.191959
O	2.131013	-1.143693	1.588813
H	1.653706	-0.741686	2.336194
H	1.514036	-1.002970	0.695165
H	3.101371	-0.574740	1.375794

X = *p*-Me, -667.999662

C	0.847285	-0.518359	-0.753921
N	1.853639	0.414255	-0.845048
O	1.774394	1.547183	-0.306663
O	2.983177	0.023186	-1.347881
C	-0.555769	-0.219981	-0.432087
C	-1.492074	-1.248811	-0.682514
C	-2.840499	-1.093415	-0.379565
C	-3.326999	0.096229	0.187454
C	-2.399845	1.114460	0.439067
C	-1.041004	0.970951	0.144754
C	-4.797514	0.270977	0.488917
H	1.050441	-1.375353	-1.388648
H	-1.151066	-2.181404	-1.128073
H	-3.530059	-1.908238	-0.593258
H	-2.743268	2.051029	0.874761
H	-0.355488	1.784831	0.342692
H	-4.974111	1.148381	1.120351
H	-5.380548	0.405593	-0.432376
H	-5.209845	-0.604292	1.005894
O	4.172328	0.016487	0.927529
H	3.928960	0.101256	-0.067544
H	4.192290	0.930571	1.258722
O	2.138372	-1.209472	1.543284
H	1.651201	-0.842355	2.302258
H	1.530817	-1.032135	0.652772
H	3.107550	-0.629043	1.365000

X = *m*-Me, -667.999674

C	0.655466	-0.445484	-0.682044
N	1.788075	0.306201	-0.890994
O	1.929069	1.461652	-0.417997
O	2.802031	-0.287754	-1.438718
C	-0.657250	0.088789	-0.291948
C	-1.748896	-0.803872	-0.403733
C	-3.046958	-0.447879	-0.036269
C	-3.267786	0.846607	0.464279
C	-2.206072	1.742597	0.581871
C	-0.906646	1.379244	0.216097
C	-4.193642	-1.423302	-0.182603
H	0.677522	-1.356440	-1.271984
H	-1.570582	-1.802657	-0.799680
H	-4.271775	1.149616	0.754785
H	-2.387394	2.745566	0.961631
H	-0.094037	2.088653	0.300662
H	-3.849636	-2.394338	-0.554117
H	-4.699906	-1.591347	0.776473
H	-4.948909	-1.046335	-0.884115
H	3.011896	-0.809809	1.300358
O	4.133173	-0.373524	0.756713
H	3.837169	-0.299648	-0.224352
H	4.326853	0.539658	1.029200
O	1.976695	-1.210080	1.575779
H	1.609404	-0.721864	2.334107
H	1.345815	-0.987013	0.713868

X = H, -628.710562

C	0.361132	-0.385034	-0.793681
N	1.389356	0.528603	-0.795173
O	1.369728	1.568872	-0.091069
O	2.480898	0.192169	-1.407245
C	-1.016721	-0.112080	-0.360403
C	-1.982182	-1.088223	-0.697898
C	-3.311752	-0.958880	-0.304895
C	-3.721356	0.153925	0.438244
C	-2.779999	1.128776	0.776182
C	-1.442144	1.003893	0.391835
H	0.511586	-1.143211	-1.555849
H	-1.679345	-1.954149	-1.283354
H	-4.031030	-1.724525	-0.585322
H	-4.759136	0.260027	0.743232
H	-3.085938	2.003574	1.345310
H	-0.727172	1.773767	0.651477
H	2.717059	-0.863496	1.168674
O	3.777908	-0.183180	0.779047
H	3.491443	0.059554	-0.176813
H	3.846439	0.667547	1.245086
O	1.740361	-1.443246	1.305690
H	1.301984	-1.192003	2.138115
H	1.095585	-1.118479	0.487962

X = *p*-Cl, -1088.315058

C	-1.244462	0.540221	-0.746789
N	-2.235978	-0.411045	-0.837430
O	-2.121887	-1.552719	-0.326748
O	-3.379179	-0.031489	-1.309263
C	0.170302	0.256274	-0.471142
C	1.081924	1.308295	-0.713701
C	2.442666	1.174458	-0.454019
C	2.922527	-0.032080	0.059476
C	2.051813	-1.091246	0.308514
C	0.686634	-0.948576	0.051126
Cl	4.640935	-0.214913	0.390814
H	-1.476779	1.405620	-1.359533
H	0.716332	2.248033	-1.121860
H	3.125213	1.994326	-0.654247
H	2.434952	-2.028572	0.699989
H	0.017943	-1.778899	0.236642
H	-3.476842	0.582717	1.413853
O	-4.539707	-0.073755	0.987372
H	-4.314584	-0.150697	-0.009394
H	-4.556278	-0.988493	1.316740
O	-2.515786	1.177828	1.582219

H	-2.015705	0.823588	2.338974
H	-1.914260	1.020208	0.687575

X = *m*-Cl, -1088.314917

C	0.949207	-0.394040	-0.670202
N	2.129398	0.281994	-0.887029
O	2.349095	1.423540	-0.413533
O	3.092371	-0.375732	-1.446155
C	-0.320366	0.233791	-0.279125
C	-1.466866	-0.587627	-0.373670
C	-2.712313	-0.103777	0.007864
C	-2.877262	1.196281	0.489098
C	-1.745871	2.009306	0.580391
C	-0.480731	1.546821	0.211989
Cl	-4.117117	-1.158671	-0.127529
H	0.904011	-1.301587	-1.263859
H	-1.380551	-1.601943	-0.752530
H	-3.858962	1.557462	0.777005
H	-1.852534	3.028079	0.944649
H	0.379880	2.198329	0.282145
H	3.304459	-0.953058	1.281064
O	4.447968	-0.590694	0.731613
H	4.151715	-0.472688	-0.241996
H	4.727356	0.293715	1.023568
O	2.246860	-1.285295	1.561042
H	1.926219	-0.804318	2.344705
H	1.618471	-0.999621	0.720626

X = *m*-F, -727.960155

C	0.643059	-0.418893	-0.699365
N	1.755277	0.375825	-0.868499
O	1.860468	1.510705	-0.343037
O	2.782770	-0.162303	-1.441478
C	-0.684220	0.064202	-0.295975
C	-1.748250	-0.853246	-0.452565
C	-3.026555	-0.494237	-0.061033
C	-3.329503	0.746904	0.487540
C	-2.277491	1.653296	0.639845
C	-0.971453	1.328208	0.264428
F	-4.031068	-1.399284	-0.226610
H	0.691002	-1.297132	-1.335309
H	-1.583959	-1.836499	-0.884242
H	-4.348403	0.984613	0.775031
H	-2.478947	2.636344	1.057734
H	-0.175131	2.050513	0.381782
H	3.018939	-0.844227	1.258704
O	4.126600	-0.346967	0.745247
H	3.831604	-0.214653	-0.227279
H	4.311692	0.546979	1.080123
O	1.995166	-1.290704	1.506568
H	1.620406	-0.880351	2.306218
H	1.351912	-1.026054	0.670562

X = *p*-CF_3, -965.763801

C	-1.909159	0.532396	-0.765569
N	-2.891941	-0.433800	-0.825541
O	-2.754608	-1.565775	-0.303124
O	-4.043667	-0.074121	-1.284765
C	-0.488717	0.269888	-0.512371
C	0.402166	1.337513	-0.774242
C	1.764720	1.222526	-0.533023
C	2.285894	0.027807	-0.017861
C	1.424022	-1.040617	0.241791
C	0.053621	-0.925110	0.006733
C	3.765977	-0.105295	0.197719
F	4.433011	-0.372391	-0.960938
F	4.316630	1.035102	0.694014
F	4.079577	-1.103975	1.060302
H	-2.164186	1.386482	-1.384912
H	0.012766	2.268998	-1.178512
H	2.424130	2.058926	-0.744910
H	1.819172	-1.972142	0.634765
H	-0.599740	-1.763385	0.208372
O	-5.175382	-0.084057	1.034349
H	-4.969424	-0.182374	0.038299
H	-5.188178	-0.990442	1.386185
O	-3.155020	1.198295	1.574990
H	-2.642999	0.870322	2.335758
H	-2.562222	1.031591	0.680778
H	-4.110434	0.590619	1.431899

X = *p*-CN, -720.957858

C	-1.098302	0.471961	-0.779321
N	-2.093576	-0.485465	-0.798066
O	-1.978416	-1.584883	-0.206513
O	-3.230470	-0.140710	-1.298996
C	0.311934	0.209822	-0.484252
C	1.219997	1.252284	-0.789404
C	2.575360	1.139951	-0.517194
C	3.079111	-0.033702	0.075363
C	2.191561	-1.079732	0.379865
C	0.830690	-0.961945	0.111695
C	4.476838	-0.158227	0.363330
N	5.612917	-0.256815	0.600654
H	-1.332202	1.289743	-1.453535
H	0.848328	2.161760	-1.255587
H	3.252360	1.951808	-0.765269
H	2.574479	-1.991451	0.828913
H	0.163099	-1.780707	0.344494
H	-3.340729	0.702273	1.368191
O	-4.409855	0.010444	0.997953
H	-4.191349	-0.157708	0.016288
H	-4.444053	-0.869182	1.410898
O	-2.384002	1.307541	1.485613
H	-1.893231	1.036233	2.281956
H	-1.773279	1.071584	0.620583

X = m-CN, -720.956476

C	0.826085	-0.397152	-0.669048
N	1.998166	0.299079	-0.875476
O	2.201965	1.433916	-0.380585
O	2.964945	-0.333170	-1.451325
C	-0.450593	0.212937	-0.274708
C	-1.590418	-0.610445	-0.379552
C	-2.855836	-0.147252	0.001385
C	-3.016650	1.160357	0.494211
C	-1.894139	1.978531	0.595749
C	-0.626301	1.521453	0.226903
C	-3.993659	-1.015952	-0.115170
N	-4.916706	-1.719446	-0.204056

H	0.789963	−1.291679	−1.282875
H	−1.494095	−1.621325	−0.766375
H	−4.000629	1.515296	0.783115
H	−2.003021	2.994045	0.967176
H	0.231167	2.176415	0.307261
H	3.205392	−0.999788	1.250226
O	4.342036	−0.606800	0.710618
H	4.043619	−0.453845	−0.255128
H	4.625412	0.264203	1.036851
O	2.152841	−1.355273	1.521195
H	1.834783	−0.925300	2.334921
H	1.511946	−1.039702	0.703711

X = *p*-NO_2, −833.218531

C	1.509766	−0.642231	−0.666548
N	2.502801	0.295984	−0.883165
O	2.375302	1.496181	−0.547634
O	3.644158	−0.142975	−1.285423
C	0.097120	−0.331858	−0.453960
C	−0.801471	−1.425683	−0.527627
C	−2.161009	−1.268005	−0.304893
C	−2.651943	0.005595	−0.001729
C	−1.799763	1.107917	0.074136
C	−0.435142	0.941772	−0.144308
N	−4.084466	0.183438	0.239524
O	−4.811439	−0.811624	0.159598
O	−4.489286	1.317402	0.512283
H	1.757317	−1.586958	−1.139883
H	−0.418129	−2.413256	−0.772250
H	−2.842903	−2.107829	−0.367353
H	−2.209217	2.085300	0.301740
H	0.224695	1.797303	−0.094596
O	4.807800	0.213193	1.003663
H	4.601713	0.169375	0.008337
H	4.850442	1.159836	1.221355
O	2.772129	−0.945427	1.743975
H	2.274074	−0.504113	2.455386
H	2.170322	−0.911937	0.844025
H	3.728683	−0.382715	1.506606

Protonation TS on PhCH=NO_2^-

$CH_2(NO_2)_2$, C-protonation TS
X = H, −924.880849

C	0.316338	1.141836	−0.549802
N	0.161994	2.421906	0.051633
O	0.778702	2.712883	1.099962
C	1.545798	0.336636	−0.394122
O	−0.683398	3.194229	−0.458305
C	1.838926	−0.575391	−1.432491
C	2.945089	−1.420521	−1.370518
C	3.802500	−1.379809	−0.265723
C	3.522751	−0.486873	0.772587
C	2.410393	0.356333	0.720189
H	−0.061398	1.196904	−1.568027
H	1.175193	−0.625914	−2.293107
H	3.135954	−2.113807	−2.187339
H	4.667059	−2.038053	−0.212233
H	4.172557	−0.448823	1.645026
H	2.202689	1.035715	1.536411
H	−0.812640	0.426994	0.044118
C	−1.931328	−0.184604	0.485044
N	−2.759247	−0.393180	−0.693971
O	−3.838669	0.224517	−0.731923
O	−2.322383	−1.082082	−1.620521
N	−1.522527	−1.389487	1.186706
O	−1.479201	−2.484872	0.620065
O	−1.193637	−1.203850	2.372820
H	−2.435058	0.480059	1.176806

$CH_2(NO_2)_2$, O-protonation TS
X = H, −924.892879

C	−1.539393	0.319872	−0.856362
N	−0.447766	−0.306085	−0.437971
O	−0.383285	−1.145319	0.500384
O	0.686159	−0.012176	−1.118024
C	−2.881668	0.129377	−0.352869
C	−3.912605	0.881482	−0.969300
C	−5.238605	0.769641	−0.561995
C	−5.586606	−0.099903	0.479578
C	−4.581180	−0.848340	1.100041
C	−3.247884	−0.742800	0.700387
H	−1.358879	1.019883	−1.660502
H	1.632677	−0.107902	−0.372656
H	−3.655355	1.560584	−1.780071
H	−6.004421	1.362904	−1.058039
H	−6.621826	−0.189262	0.801262
H	−4.835228	−1.526236	1.912776
H	−2.475036	−1.321623	1.189139
C	2.792576	−0.140655	0.431679
N	3.774707	−0.955403	−0.263633
O	3.900421	−2.120092	0.161030
O	4.364153	−0.524876	−1.257059
N	3.156822	1.236863	0.709402
O	3.960840	1.856859	0.010061
O	2.547733	1.744494	1.670504
H	2.495745	−0.629139	1.351404

CH_2NO_2, C-protonation TS
−720.369996

C	−0.056966	0.766212	−0.926213
N	−0.353045	2.160862	−0.698125
O	−0.026978	2.693894	0.382974
C	1.237255	0.216783	−0.430047
O	−1.032523	2.755413	−1.560111
C	1.941133	−0.663298	−1.274889
C	3.125973	−1.274953	−0.864312
C	3.644575	−1.019490	0.408910
C	2.952354	−0.154411	1.261697
C	1.760099	0.450352	0.856576
C	−2.232159	−0.573141	0.326774
H	−0.227681	0.571304	−1.983485
H	1.544852	−0.875570	−2.265610
H	3.643414	−1.952074	−1.541006
H	4.568851	−1.492925	0.733513
H	3.337423	0.047116	2.259678
H	1.232317	1.116897	1.527192
H	−1.030000	0.159266	−0.342874
H	−3.035773	0.141586	0.175661
N	−2.417814	−1.748919	−0.401419

O	-3.116534	-1.716939	-1.451552
O	-1.815741	-2.798446	-0.044925
H	-1.900936	-0.760583	1.343658

CH_3COCH_3, C-protonation TS
-668.459576

C	-0.104954	0.617928	-0.507445
N	-0.327717	2.034415	-0.324274
O	0.223735	2.633355	0.623566
C	1.260539	0.072480	-0.247843
O	-1.172592	2.582741	-1.064552
C	1.767495	-0.881164	-1.151408
C	3.003872	-1.495236	-0.944932
C	3.772057	-1.168921	0.177130
C	3.276155	-0.231491	1.088840
C	2.034128	0.376171	0.889292
C	-1.943563	-0.791892	1.244083
C	-2.920501	-1.297180	0.341213
O	-2.817725	-2.367113	-0.309842
H	-0.473864	0.365802	-1.500623
H	1.176182	-1.148485	-2.024548
H	3.366160	-2.228555	-1.662852
H	4.737870	-1.642387	0.341728
H	3.857398	0.025586	1.972673
H	1.659539	1.098899	1.603470
H	-0.925515	0.069512	0.254983
H	-2.227524	-0.001168	1.938827
C	-4.162361	-0.430686	0.073943
H	-5.061549	-1.007805	0.328442
H	-4.167320	0.508608	0.639187
H	-4.219373	-0.197315	-0.996917
H	-1.192540	-1.495543	1.604935

$CH_2(COCH_3)_2$, O-protonation TS
-821.097498

C	1.465563	-0.568319	-0.674517
N	0.423112	0.244863	-0.595323
O	0.412611	1.402417	-0.096133
O	-0.729390	-0.232162	-1.137457
C	2.818937	-0.267516	-0.261623
C	3.792341	-1.276854	-0.465287
C	5.124179	-1.084916	-0.110492
C	5.535075	0.125920	0.461662
C	4.586514	1.131961	0.671377
C	3.247425	0.948698	0.322196
H	1.234956	-1.532174	-1.106529
H	3.484978	-2.222053	-0.908620
H	5.845207	-1.882386	-0.279361
H	6.575059	0.278876	0.741296
H	4.890084	2.076707	1.118485
H	2.517464	1.729045	0.494093
H	-1.585931	-0.062956	-0.397613
C	-2.761476	0.029389	0.595250
C	-3.513913	1.115679	-0.009555
O	-4.462706	1.000024	-0.805458
C	-3.220088	-1.353456	0.679751
O	-2.781658	-2.134600	1.541967
H	-2.154967	0.318261	1.457374
C	-3.036286	2.522123	0.370519
H	-3.315439	2.744202	1.410425
H	-1.944959	2.598835	0.297359
H	-3.510311	3.257139	-0.287306
C	-4.221276	-1.876412	-0.344623
H	-5.174494	-1.343913	-0.253136
H	-3.874202	-1.686665	-1.366898
H	-4.362058	-2.950177	-0.183600

$CH_2(COCH_3)_2$, C-protonation TS
-821.087875

C	0.326745	0.978451	-0.940088
N	-0.119679	2.301595	-0.685909
O	0.119413	2.856598	0.412332
C	1.546870	0.431204	-0.308101
O	-0.852589	2.838906	-1.553527
C	2.246936	-0.560891	-1.030443
C	3.373874	-1.190193	-0.503381
C	3.843457	-0.846721	0.769147
C	3.157532	0.128511	1.499688
C	2.022654	0.755683	0.980088
C	-1.961910	-0.575196	-0.356876
C	-1.516418	-1.918781	-0.761752
O	-1.521870	-2.249135	-1.957186
C	-2.466918	-0.257728	0.983422
O	-2.243228	-0.912228	2.010814
H	0.254908	0.793879	-2.009497
H	1.889908	-0.844033	-2.018537
H	3.885709	-1.951186	-1.089605
H	4.722554	-1.334760	1.184892
H	3.502127	0.401999	2.495477
H	1.498167	1.503055	1.561013
H	-0.780840	0.207576	-0.522856
H	-2.517029	-0.085027	-1.161424
C	-3.329517	1.003180	1.076544
H	-2.951083	1.809410	0.439004
H	-4.350902	0.768254	0.743338
H	-3.371034	1.340374	2.116061
C	-0.978730	-2.887338	0.279618
H	-0.170988	-2.427814	0.859870
H	-1.758959	-3.141099	1.005626
H	-0.616037	-3.786006	-0.228664

$CH_2(CN)_2$, C-protonation TS
-700.359838

C	-0.134054	0.908423	-0.660833
N	-0.438148	2.207126	-0.168348
O	0.070003	2.622338	0.897372
C	1.151477	0.238230	-0.365109
O	-1.318673	2.859069	-0.781793
C	1.629156	-0.676389	-1.329705
C	2.795759	-1.412244	-1.125196
C	3.529680	-1.256011	0.055319
C	3.066873	-0.359010	1.022778
C	1.894276	0.373955	0.826444
C	-2.387436	-0.493135	0.303337
H	-0.426263	0.868901	-1.708609
H	1.068579	-0.810437	-2.252963
H	3.131772	-2.108244	-1.891568
H	4.440570	-1.827630	0.220119

H	3.619117	−0.231585	1.952093
H	1.546279	1.059143	1.588338
H	−1.192545	0.159699	−0.112435
H	−3.027079	0.382118	0.451980
C	−2.166507	−1.216326	1.526143
N	−1.948337	−1.772428	2.529687
C	−2.819490	−1.291319	−0.811440
N	−3.117727	−1.897592	−1.764483

$CH_2(CHO)_2$, O-protonation TS
−742.511576

C	−0.974471	0.468325	−0.734278
N	0.095090	−0.291475	−0.528391
O	0.125967	−1.356184	0.149673
O	1.232645	0.122516	−1.122874
C	−2.319055	0.199386	−0.277267
C	−3.321311	1.135668	−0.636747
C	−4.647817	0.967656	−0.251371
C	−5.027407	−0.145546	0.509982
C	−4.051353	−1.078763	0.874331
C	−2.717453	−0.918864	0.495315
H	−0.770793	1.356450	−1.316456
H	−3.039852	2.005030	−1.228146
H	−5.389769	1.708010	−0.544829
H	−6.063192	−0.279389	0.814153
H	−4.329504	−1.947716	1.468098
H	−1.967176	−1.642470	0.786405
H	2.163921	−0.002816	−0.346498
C	3.269506	−0.045000	0.569464
C	3.981319	−1.221494	0.093478
O	4.943949	−1.259355	−0.680186
C	3.896413	1.262094	0.462867
O	3.607704	2.261520	1.129597
H	2.678276	−0.202704	1.476128
H	3.555268	−2.183899	0.459755
H	4.684849	1.341093	−0.314205

$CH_2(CHO)_2$, C-protonation TS
−742.501870

C	−0.055751	0.902758	−0.821119
N	−0.448130	2.208218	−0.450465
O	−0.079014	2.699128	0.644162
C	1.199713	0.281703	−0.361009
O	−1.265825	2.801312	−1.199041
C	1.715441	−0.764882	−1.159981
C	2.868170	−1.460252	−0.798983
C	3.551221	−1.132815	0.377605
C	3.049342	−0.106075	1.183101
C	1.889589	0.588608	0.831749
C	−2.304379	−0.555144	0.064687
C	−2.096854	−1.887906	−0.501196
O	−2.272970	−2.189521	−1.684500
C	−2.467660	−0.431614	1.514948
O	−2.109302	−1.242812	2.370522
H	−0.283881	0.752583	−1.873213
H	1.193982	−1.034876	−2.076130
H	3.233277	−2.260705	−1.439935
H	4.451420	−1.672723	0.663867
H	3.560885	0.156467	2.107568
H	1.508063	1.375219	1.469510
H	−1.155824	0.128661	−0.260326
H	−2.981514	0.077654	−0.517666
H	−1.721450	−2.651041	0.208876
H	−2.944150	0.520099	1.842740