Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supplementary Information for

Formation of bis-benzimidazole and bis-benzoxazole through organocatalytic depolymerization of poly(ethylene terephthalate) and its mechanism

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Contents

A. Experimental details for the depolymerization of poly(ethylene terephthalate) with *o*-phenylenediamine and 2-aminophenol and the model reaction using methyl benzoate.

A-1. Model reaction operated under milder conditions

Methyl benzoate (0.39 g, 2.86 mmol), 2-aminophenol (1.14 g, 10.4 mmol), 1,5,7-triazabicyclo[4.4.0]dec-5-ene (TBD; 34 mg, 0.24 mmol), and DMF (2 mL) were placed into a 25 ml Schlenk tube. The tube was heated at 110 or 150 °C under a nitrogen atmosphere. Aliquots were taken for NMR analysis to monitor the progress of the reaction.

A-2. NMR data of products and reaction mixtures

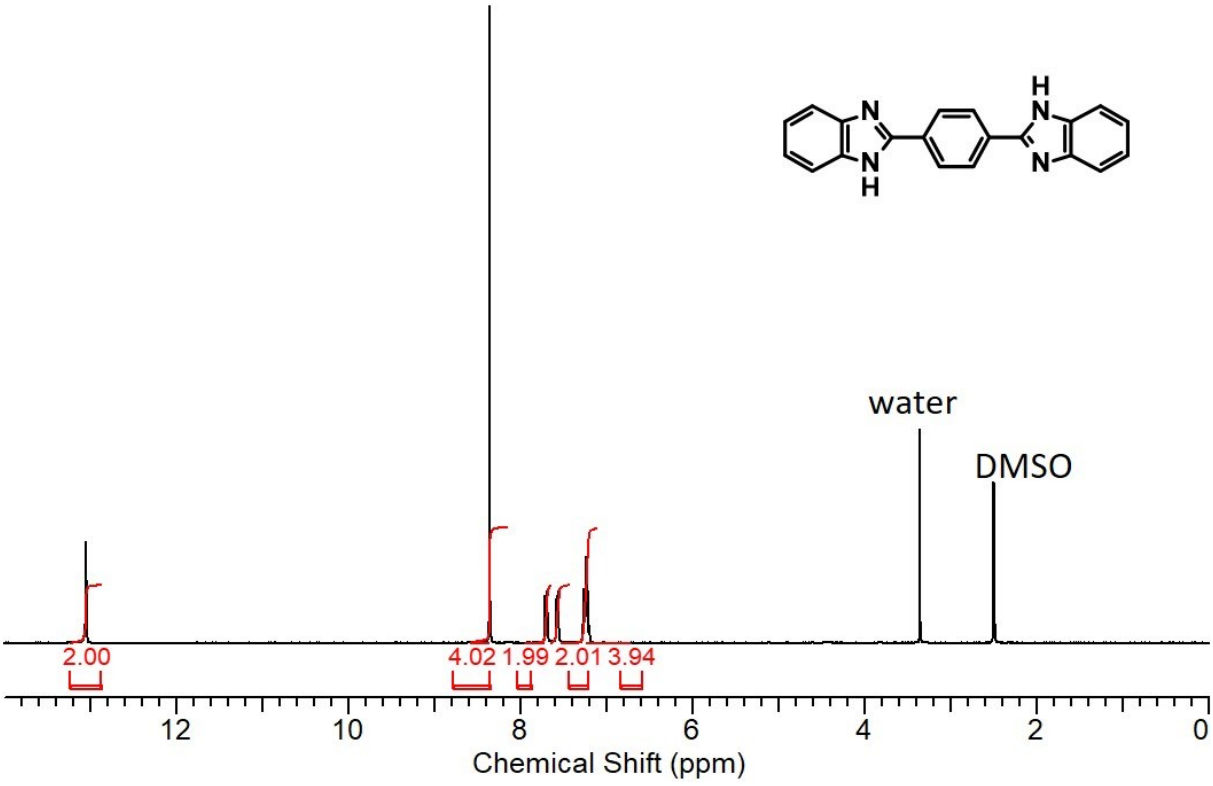

Figure S1. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of 1,4-bis(benzimidazolyl)benzene (BBI; **1**) obtained from PET depolymerization with *o*-phenylenediamine at 190 °C.

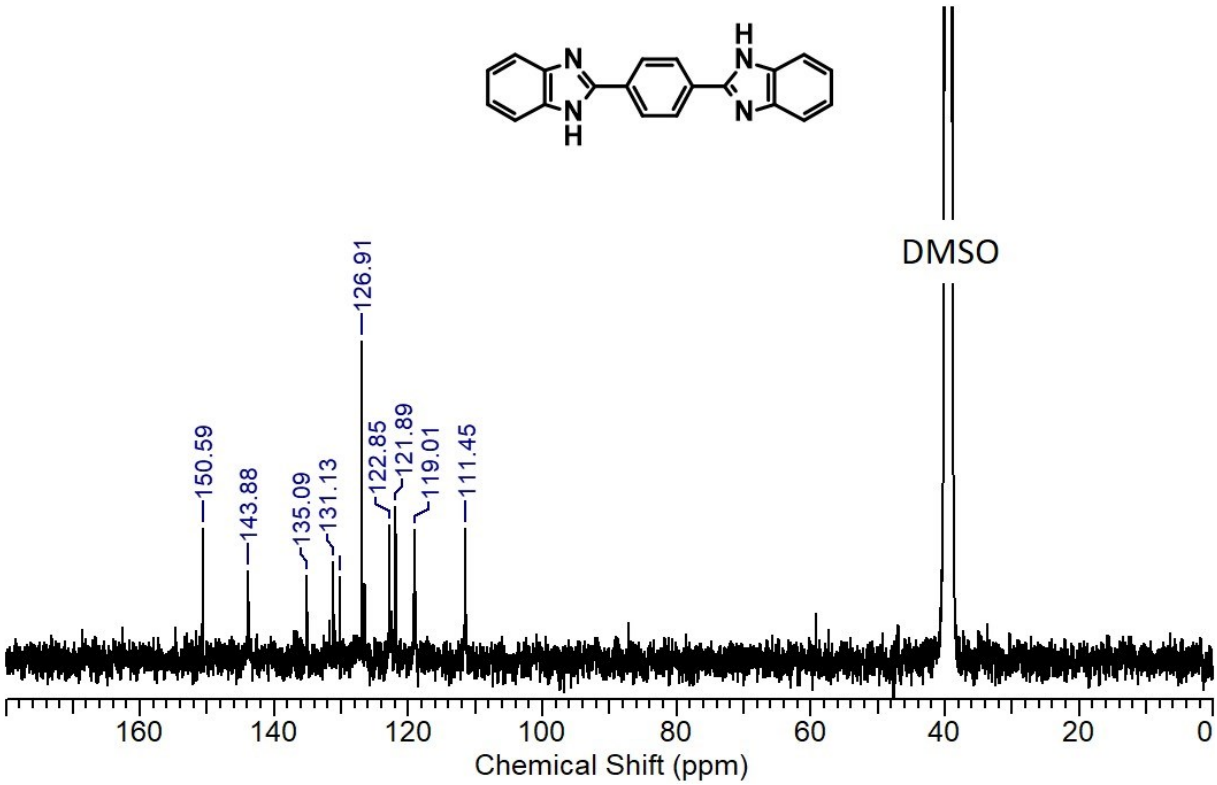

Figure S2. ^{13}C NMR spectrum (100 MHz, DMSO-d_6) of 1,4-bis(benzimidazolyl)benzene (BBI; **1**) obtained from PET depolymerization with *o*-phenylenediamine at 190 °C.

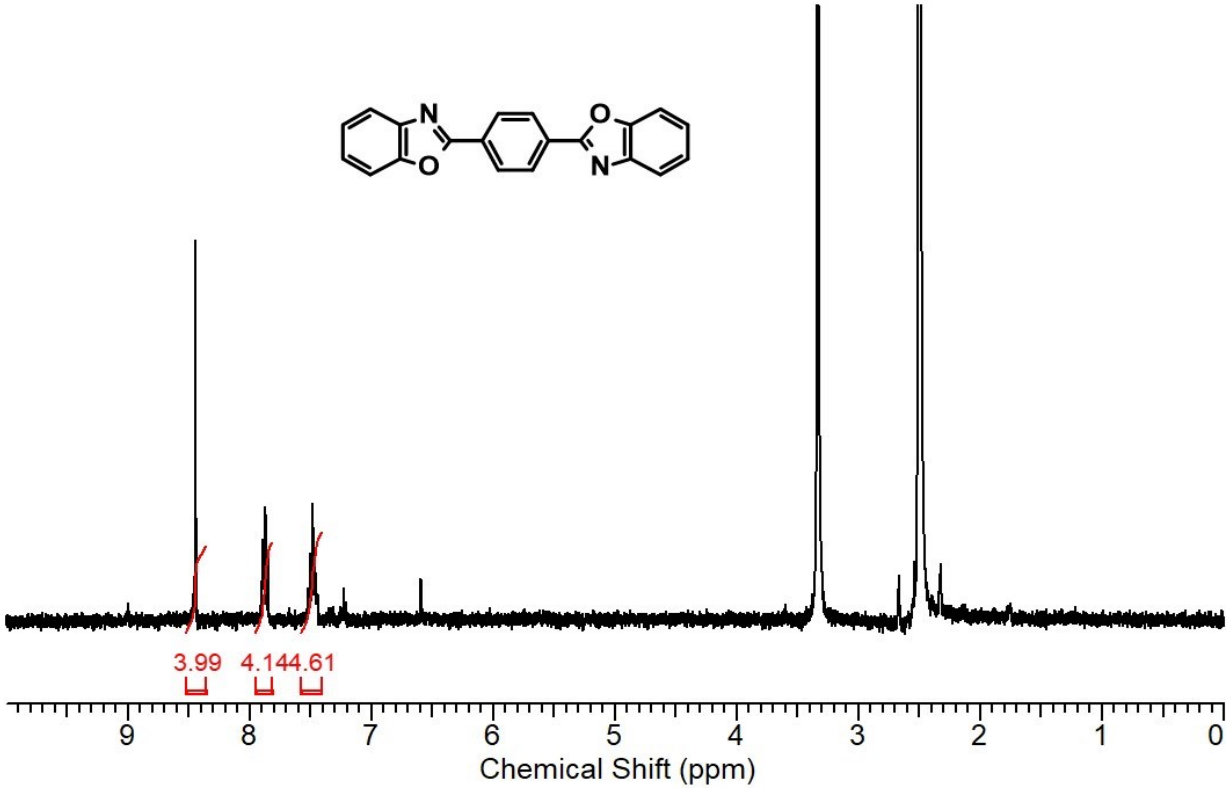

Figure S3. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of 1,4-bis(benzoxazolyl)benzene (BBO; **2**) obtained from PET depolymerization with 2-aminophenol at 190 °C.

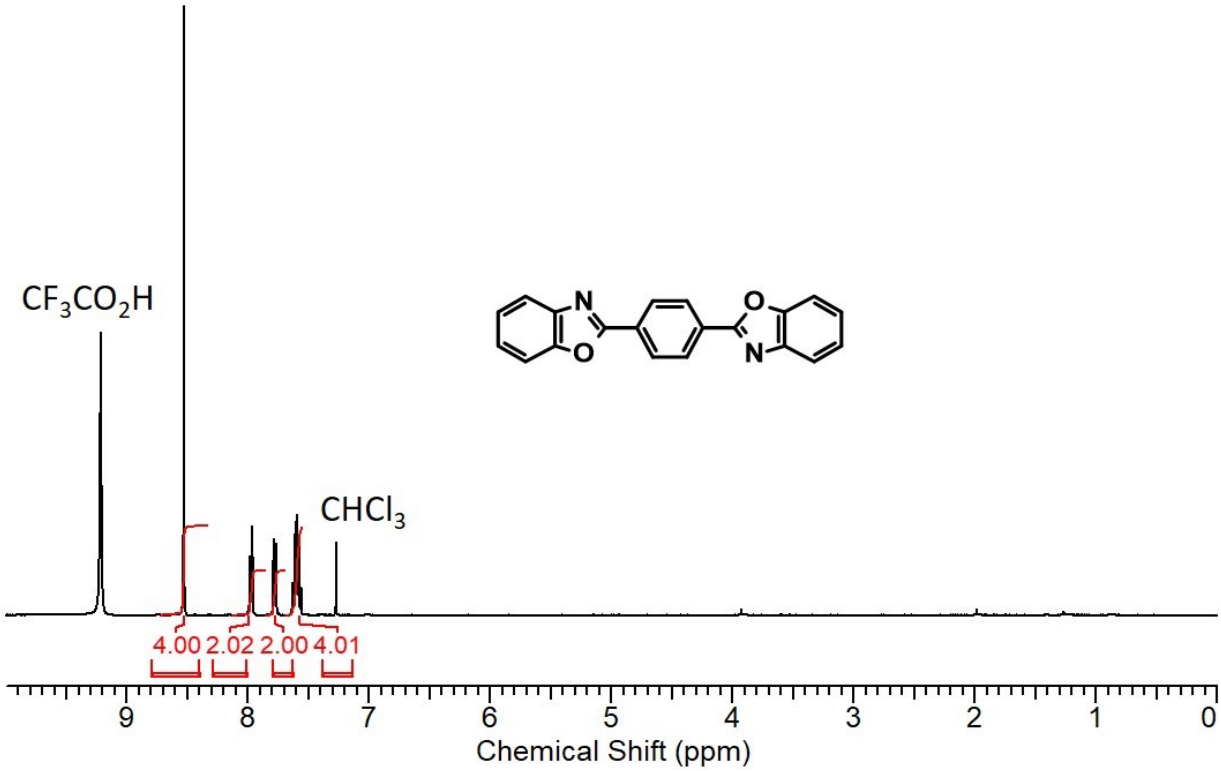

Figure S4. ^{1}H NMR spectrum (400 MHz, $CDCl_3$ with 10% CF_3CO_2D) of 1,4-bis(benzoxazolyl)benzene (BBO; **2**) obtained from PET depolymerization with 2-aminophenol at 190 °C.

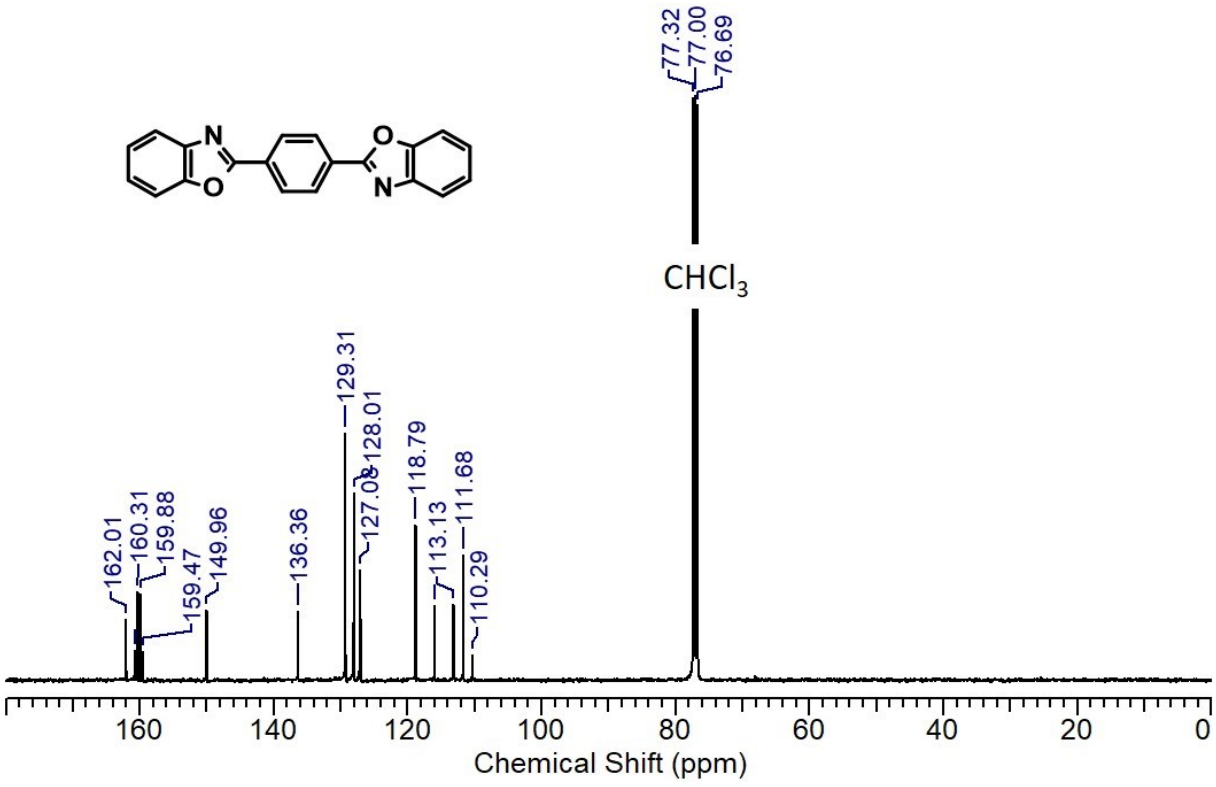

Figure S5. ^{13}C NMR spectrum (100 MHz, $CDCl_3$ with 10% CF_3CO_2D) of 1,4-bis(benzoxazolyl)benzene (BBO; **2**) obtained from PET depolymerization with 2-aminophenol at 190 °C.

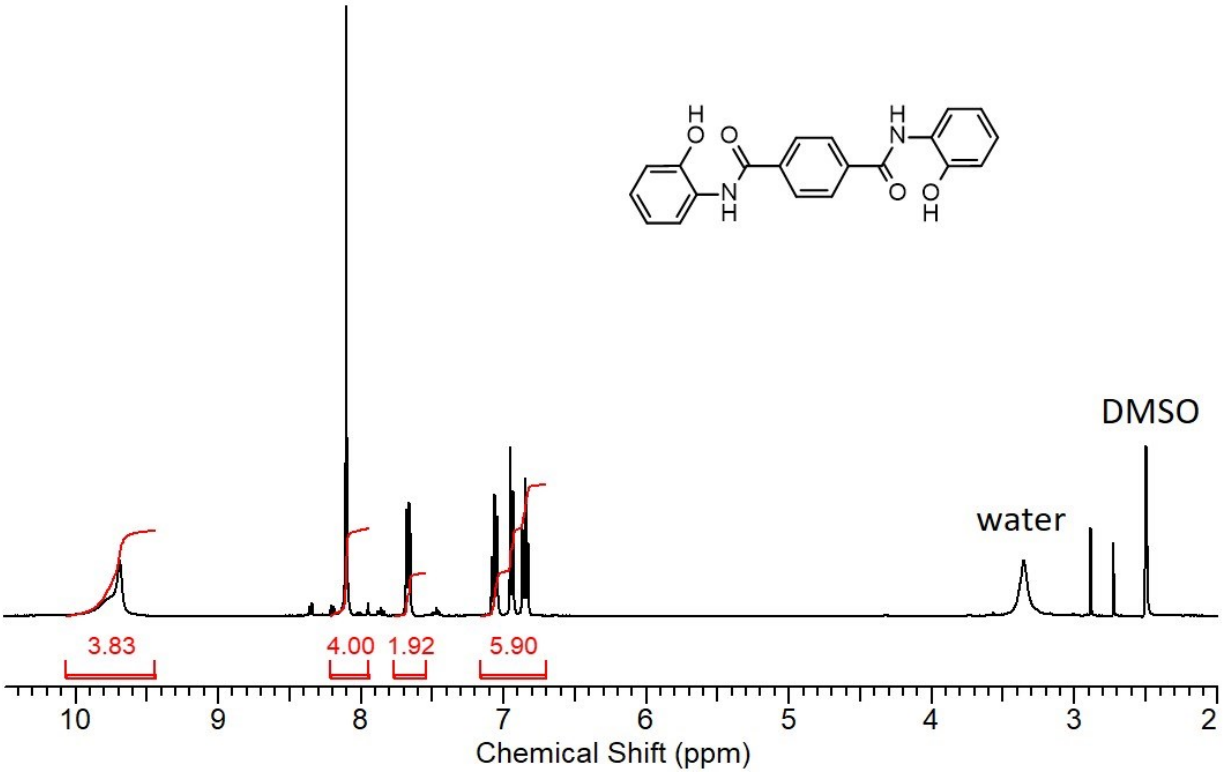

Figure S6. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of *N*,*N*'-bis(2-hydroxyphenyl)terephthalamide (**3**) obtained from PET depolymerization with 2-aminophenol and DMF at 150 °C.

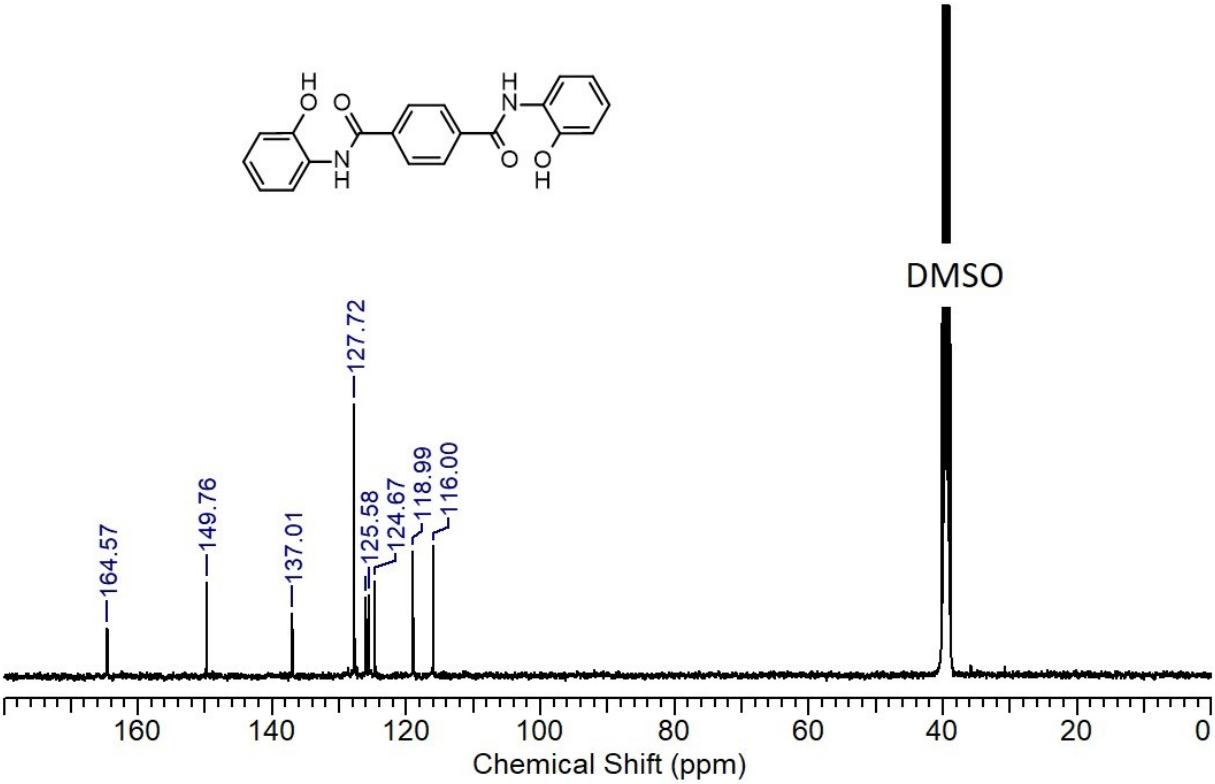

Figure S7. ^{13}C NMR spectrum (100 MHz, DMSO-d_6) of *N*,*N*'-bis(2-hydroxyphenyl)terephthalamide (**3**) obtained from PET depolymerization with 2-aminophenol and DMF at 150 °C.

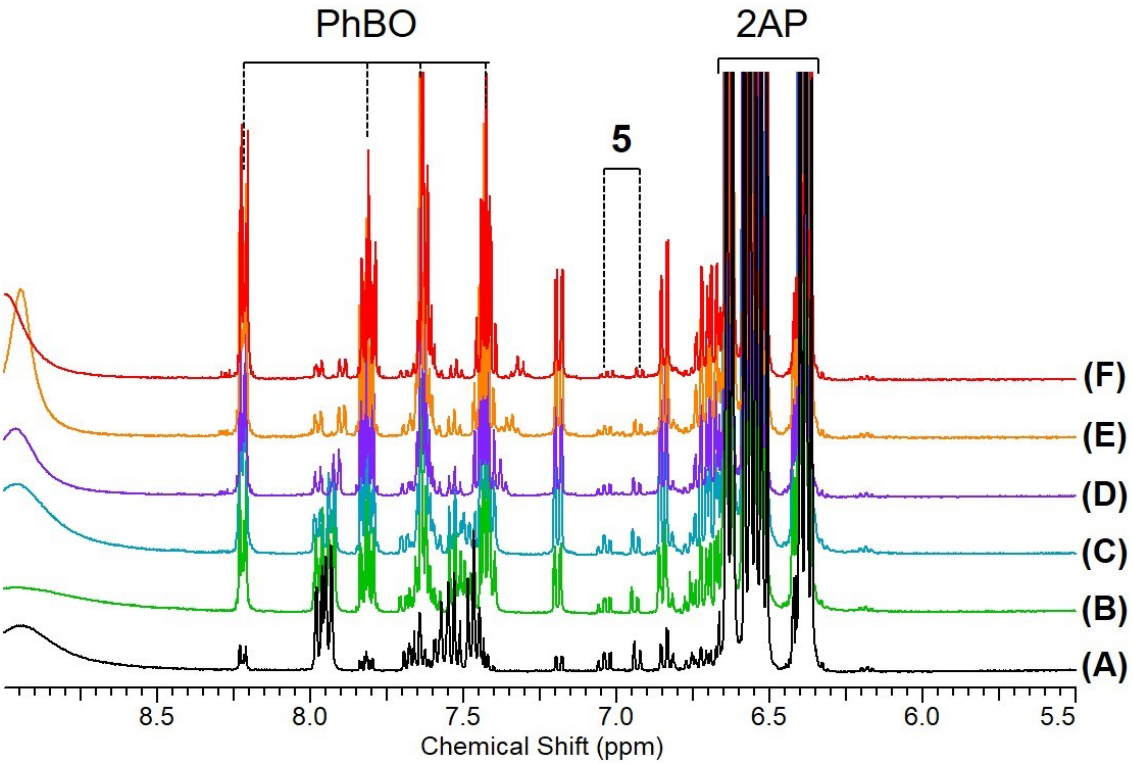

Figure S8. ^{1}H NMR spectra (400 MHz, DMSO-d_6) of the reaction mixture for TBD-catalyzed reaction using methyl benzoate and 2-aminophenol (2AP) at 190 °C. Reaction time: 1 h (A), 4 h (B), 6 h (C), 9 h (D), 12.5 h (E), and 15 h (F). PhBO: 2-phenylbenzoxazole, **5**: amide intermediate.

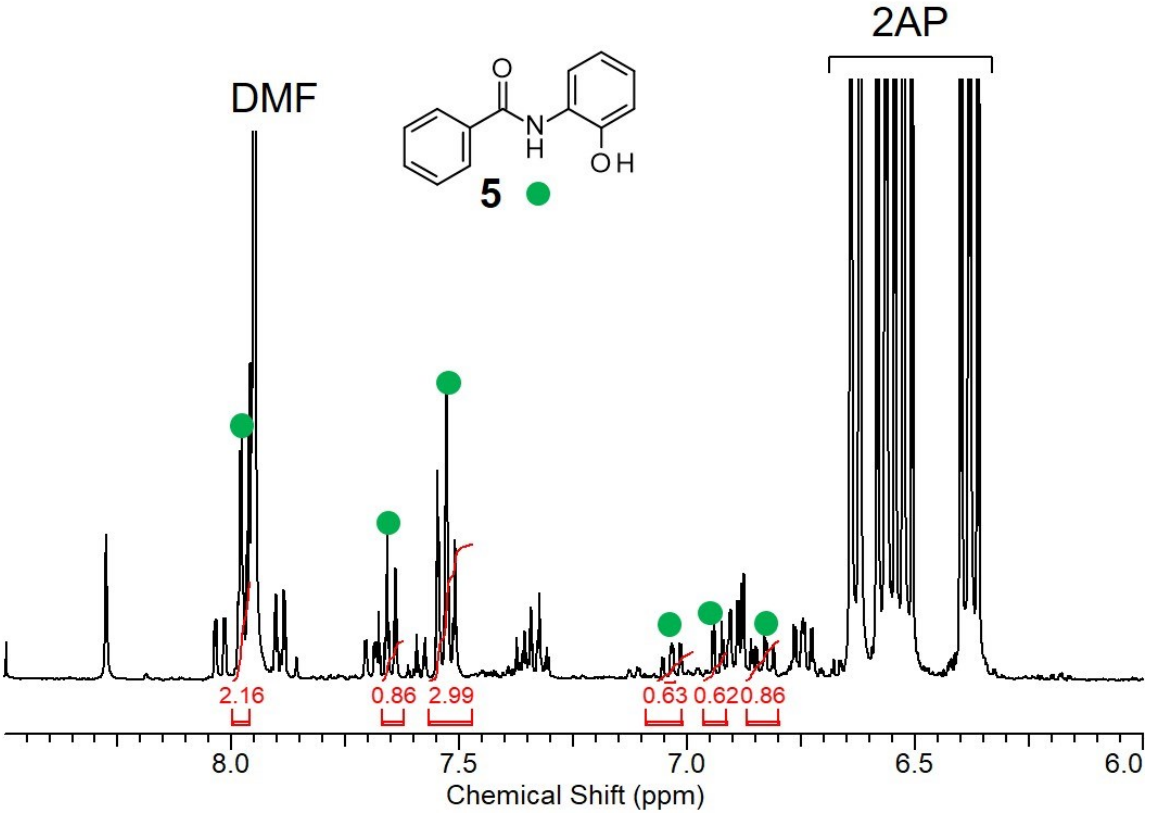

Figure S9. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of the reaction mixture for TBD-catalyzed reaction using methyl benzoate and 2-aminophenol (2AP) performed at 110 °C for 48 h with DMF.

B. Cartesian coordinates and energies for optimized stationary points.

GAMESS/US grid settings:

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$tescav ntsall=240 $end
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Gradient tolerance [a.u.]: 0.0002 for minima, 0.000075 for saddle points

All using PCM (aniline)

Reactants and Products

```
18
MB  # E(6-31+G*)=-460.15452279; E(ACCPVTZ)=-460.30892496 H
   C          0.09020        -0.23331         0.00051
   C          1.10907        -1.19928         0.00015
   C          0.78776        -2.55688        -0.00049
   C         -0.55283        -2.95914        -0.00060
   C         -1.57147        -1.99973         0.00006
   C         -1.25429        -0.64031         0.00065
   C          0.48077         1.20506         0.00043
   O          1.63654         1.60599         0.00029
   O         -0.57918         2.03554         0.00016
   C         -0.29220         3.45046        -0.00093
   H          2.14515        -0.87611         0.00009
   H          1.58083        -3.29966        -0.00102
   H         -0.80289        -4.01691        -0.00117
   H         -2.61282        -2.31021        -0.00001
   H         -2.04393         0.10298         0.00103
   H         -1.26572         3.93987        -0.00076
   H          0.27563         3.72096         0.89251
   H          0.27472         3.71959        -0.89537

23
TBD  # E(6-31+G*)=-438.84879426; E(ACCPVTZ)=-438.99424210 H
   C         -0.69527         1.74095        -0.25009
   C         -1.75160        -0.46558        -0.59505
   N         -0.51728         0.28976        -0.37255
   H          2.30871        -0.10197         1.11254
   C          0.53316        -0.36356         0.25848
   N          1.66826         0.40894         0.51434
   N          0.59636        -1.62938         0.53921
   C         -0.54025        -2.48538         0.20354
   C          1.55034         1.83749         0.81229
   C         -1.42303        -1.92037        -0.91212
   C          0.64228         2.47453        -0.23285
   H         -1.26382         1.97538         0.66723
   H         -2.40674        -0.40503         0.29125
   H         -0.15483        -3.47231        -0.08371
   H          1.14209         2.01248         1.82239
   H         -2.34787        -2.50127        -1.01072
   H          1.11704         2.41121        -1.21960
   H          2.55362         2.27381         0.78073
   H          0.47645         3.53288        -0.00320
   H         -2.28607         0.00850        -1.42669
   H         -1.30508         2.07229        -1.09852
   H         -0.89341        -1.97205        -1.87247
   H         -1.15050        -2.64921         1.10693

16
OPD  # E(6-31+G*)=-342.98312648; E(ACCPVTZ)=-343.10594340 H
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   C          0.70785         0.01556         0.51974
   C          1.39103         0.05042        -0.70178
   C          0.69794         0.03052        -1.91772
   C         -0.69794        -0.03052        -1.91772
   C         -1.39103        -0.05042        -0.70178
   C         -0.70785        -0.01556         0.51974
   N          1.38167         0.08218         1.75838
   N         -1.38167        -0.08218         1.75838
   H          2.47904         0.08290        -0.69574
   H          1.25050         0.05471        -2.85334
   H         -1.25050        -0.05471        -2.85334
   H         -2.47904        -0.08290        -0.69574
   H          1.00084        -0.55163         2.45841
   H          2.38243        -0.07168         1.67651
   H         -2.38243         0.07168         1.67651
   H         -1.00084         0.55163         2.45841

15
2AP  # E(6-31+G*)=-362.84767232; E(ACCPVTZ)=-362.97960218 H
   C          0.69500         0.02084         0.49160
   C          1.38189         0.03102        -0.72037
   C          0.67740         0.00758        -1.93145
   C         -0.71900        -0.02446        -1.91283
   C         -1.40514        -0.03505        -0.69344
   C         -0.71504        -0.01219         0.52705
   O          1.32849         0.04464         1.71795
   N         -1.37551        -0.08861         1.76112
   H          2.47002         0.05954        -0.71714
   H          1.22150         0.01582        -2.87172
   H         -1.28092        -0.04069        -2.84295
   H         -2.49278        -0.06308        -0.68004
   H          2.28789         0.13249         1.59479
   H         -2.32255         0.27522         1.75296
   H         -0.84472         0.28942         2.53881

6
MeOH  # E(6-31+G*)=-115.73187913; E(ACCPVTZ)=-115.78195521 H
   C         -0.07192         0.00769        -0.73186
   O          0.07606        -0.05890         0.69139
   H         -1.06838         0.36906        -1.01743
   H          0.05540        -1.01080        -1.10601
   H          0.69147         0.65158        -1.18746
   H         -0.02884         0.83339         1.05722

3
H2O  # E(6-31+G*)=-76.43186002; E(ACCPVTZ)=-76.47312798 H
   O          0.01189        -0.05592         0.03352
   H         -0.09475         0.04829        -0.92561
   H         -0.09402         0.83934         0.39352

26
TBD_H2O  # E(6-31+G*)=-515.29271543; E(ACCPVTZ)=-515.47859353 H
   O          1.92342        -2.43025        -2.10413
   H          1.69641        -2.31760        -3.04041
   N          1.16131        -0.12014        -0.79048
   C          0.03431        -0.17526        -0.13545
   N         -0.73201        -1.32539        -0.27434
   N         -0.51371         0.84899         0.61137
   H         -0.20034        -2.07832        -0.69914
   C          1.96947         1.09665        -0.73456
   H          2.46507         1.22434        -1.70509
   H          2.77432         0.96656         0.00670
   C          1.15207         2.34260        -0.38970
   H          0.50206         2.61064        -1.23264
   H          1.80893         3.19731        -0.19062
   C          0.29348         2.05058         0.83640
   H         -0.39548         2.87829         1.03967
   H          0.92736         1.92504         1.73018
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   C         -1.69581        -1.73123         0.74892
   H         -2.33823        -2.50567         0.31898
   H         -1.19341        -2.16510         1.62939
   C         -2.50897        -0.51007         1.16093
   H         -3.18977        -0.76270         1.98101
   H         -3.11232        -0.16549         0.31238
   C         -1.56037         0.59754         1.60881
   H         -2.10690         1.53571         1.75627
   H         -1.10140         0.33386         2.57698
   H          1.70111        -1.55255        -1.66718

29
TBD_MeOH  # E(6-31+G*)=-554.59245348; E(ACCPVTZ)=-554.78721449 H
   C          1.57586        -2.20650        -3.14452
   O          1.72638        -2.27361        -1.73093
   H          0.58569        -1.82395        -3.43337
   H          1.68277        -3.22101        -3.54160
   H          2.34446        -1.57045        -3.60851
   N          1.02412         0.10792        -0.52332
   C         -0.10050         0.03629         0.13406
   N         -0.85983        -1.11669        -0.01832
   N         -0.65297         1.04736         0.89714
   H         -0.32532        -1.85938        -0.45917
   C          1.82375         1.32973        -0.45938
   H          2.30172         1.47895        -1.43577
   H          2.64251         1.19191         0.26501
   C          1.00489         2.56446        -0.07839
   H          0.34558         2.84934        -0.90845
   H          1.66083         3.41677         0.13368
   C          0.15890         2.24057         1.14829
   H         -0.52604         3.06328         1.38267
   H          0.80248         2.08806         2.03106
   C         -1.81331        -1.54525         1.00525
   H         -2.45346        -2.31735         0.56769
   H         -1.30173        -1.98983         1.87512
   C         -2.63232        -0.33700         1.44309
   H         -3.30286        -0.60778         2.26589
   H         -3.24725         0.01513         0.60604
   C         -1.68887         0.77144         1.89951
   H         -2.24155         1.70272         2.06657
   H         -1.21925         0.49621         2.85944
   H          1.55758        -1.36433        -1.34233

25
benzimidazole  # E(6-31+G*)=-610.96382225; E(ACCPVTZ)=-611.15663125 H
   C          1.40645        -2.98572         0.31338
   C          0.73657        -4.11921         0.77045
   C         -0.62507        -4.06890         1.14555
   C         -1.35780        -2.88324         1.07680
   C         -0.67783        -1.75105         0.61801
   C          0.68611        -1.78360         0.23399
   N         -1.06443        -0.43907         0.41904
   N          1.09286        -0.52723        -0.18368
   C          0.02843         0.25137        -0.06403
   C          1.08375         2.25867        -1.07258
   C         -0.00776         1.68197        -0.39701
   C         -1.10241         2.49668        -0.05734
   C         -1.10625         3.85338        -0.38806
   C         -0.01772         4.41759        -1.06012
   C          1.07727         3.61397        -1.39975
   H          2.45313        -3.02345         0.02401
   H          1.26931        -5.06387         0.84132
   H         -1.11322        -4.97428         1.49636
   H         -2.40414        -2.84817         1.36686
   H         -1.99493        -0.06961         0.55924
   H          1.92908         1.63198        -1.33706
   H         -1.95491         2.08873         0.47866
   H         -1.95931         4.46896        -0.11551
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   H         -0.02201         5.47368        -1.31639
   H          1.92730         4.04372        -1.92327

24
benzoxazole  # E(6-31+G*)=-630.81904820; E(ACCPVTZ)=-631.01827635 H
   C          1.36497        -3.04760         0.23988
   C          0.63989        -4.12119         0.76293
   C         -0.68946        -3.96979         1.20848
   C         -1.34760        -2.73546         1.14886
   C         -0.60501        -1.68699         0.62579
   C          0.71716        -1.80874         0.17476
   O         -0.98030        -0.37663         0.44614
   N          1.14802        -0.56395        -0.28209
   C          0.13006         0.23011        -0.10357
   C          1.14094         2.31228        -0.98310
   C          0.03533         1.65468        -0.41316
   C         -1.14129         2.37811        -0.14911
   C         -1.20695         3.73902        -0.45171
   C         -0.10550         4.38928        -1.01812
   C          1.06748         3.67140        -1.28283
   H          2.38872        -3.16518        -0.10293
   H          1.10967        -5.09868         0.82908
   H         -1.21732        -4.83107         1.60822
   H         -2.37044        -2.60790         1.48864
   H          2.04753         1.75097        -1.18530
   H         -1.99762         1.87712         0.29061
   H         -2.11903         4.29195        -0.24408
   H         -0.15987         5.44923        -1.25173
   H          1.92556         4.17189        -1.72340
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o-phenylenediamine (OPD)

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57
RC_OPD  # E(6-31+G*)=-1241.99219117; E(ACCPVTZ)=-1242.41375116 H
   C          2.87887        -3.42489         1.34735
   C          2.92153        -4.50820         2.23214
   C          2.02499        -4.60275         3.30408
   C          1.06647        -3.60282         3.48932
   C          1.02402        -2.50786         2.61862
   C          1.92924        -2.39160         1.55312
   N          3.80253        -3.28854         0.28539
   N          1.87576        -1.31925         0.64867
   H          3.66032        -5.29145         2.06998
   H          2.07453        -5.45510         3.97687
   H          0.35726        -3.66437         4.31120
   H          0.29281        -1.71678         2.76714
   H          4.32426        -4.14115         0.10337
   H          3.36965        -2.97193        -0.58046
   H          1.32025        -0.51937         0.97543
   H          2.79379        -1.00603         0.34175
   C         -2.69831        -2.81474        -2.26284
   O         -2.02966        -1.91212        -3.17111
   C         -1.63539        -0.72976        -2.66527
   O         -1.83017        -0.41250        -1.49933
   C         -0.95003         0.13313        -3.66834
   C         -0.48734         1.39396        -3.25834
   C          0.16004         2.23129        -4.16714
   C          0.34904         1.81670        -5.49045
   C         -0.11135         0.56135        -5.90336
   C         -0.75926        -0.28010        -4.99748
   H          0.85385         2.46969        -6.19771
   H         -2.03760        -3.06987        -1.43116
   H         -2.92834        -3.69853        -2.85726
   H         -3.61434        -2.35646        -1.88265
   H         -0.63666         1.70793        -2.22998
   H          0.51719         3.20538        -3.84402
   H          0.03463         0.23780        -6.93040
   H         -1.11566        -1.25347        -5.31628
   N          0.51217         1.19597         1.86655
   C         -0.48791         2.01228         1.69710
   N         -1.28326         1.84007         0.57024
   N         -0.77992         3.11660         2.48752
   H         -1.12208         0.94681         0.11447
   C          1.41459         1.40543         2.99866
   H          2.42599         1.10932         2.69113
   H          1.13581         0.72400         3.81866
   C          1.42350         2.84476         3.51588
   H          1.91234         3.50391         2.78651
   H          1.98135         2.91822         4.45703
   C         -0.01594         3.30060         3.72235
   H         -0.05889         4.36444         3.98367
   H         -0.48119         2.74125         4.55232
   C         -2.67604         2.28576         0.54590
   H         -3.02149         2.25074        -0.49145
   H         -3.32691         1.61570         1.13326
   C         -2.74932         3.70017         1.10716
   H         -3.79103         4.03335         1.17364
   H         -2.21343         4.39008         0.44379
   C         -2.11855         3.71683         2.49533
   H         -2.01634         4.74522         2.86045
   H         -2.76810         3.18303         3.21113

57
TS1_OPD  # E(6-31+G*)=-1241.95352819; E(ACCPVTZ)=-1242.37105590 H
   C          1.04589        -3.18299         1.35416
   C          0.83079        -3.92780         2.52462
   C         -0.05241        -3.47842         3.50873
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   C         -0.74207        -2.27483         3.33709
   C         -0.51599        -1.51080         2.18778
   C          0.37894        -1.94557         1.20719
   N          1.94304        -3.60609         0.35543
   N          0.65615        -1.10884         0.06117
   H          1.34805        -4.87708         2.64800
   H         -0.20982        -4.07830         4.40172
   H         -1.44165        -1.92565         4.09158
   H         -1.02641        -0.56398         2.05227
   H          2.32222        -4.53146         0.53356
   H          1.61012        -1.30226        -0.25663
   H          0.59664         0.08478         0.37069
   C         -1.05791        -3.23016        -2.43930
   O         -0.14873        -2.70384        -1.47807
   C         -0.33537        -1.27011        -1.20331
   O         -1.53506        -0.92106        -0.88980
   C          0.34936        -0.46988        -2.34007
   C         -0.24651         0.70604        -2.80990
   C          0.34654         1.45002        -3.83523
   C          1.55075         1.02548        -4.40604
   C          2.15266        -0.15140        -3.94745
   C          1.55332        -0.89286        -2.92424
   H          2.01314         1.60228        -5.20344
   H         -0.86997        -4.30628        -2.48959
   H         -0.88997        -2.78998        -3.43283
   H         -2.09490        -3.05148        -2.13617
   H         -1.18201         1.02954        -2.36544
   H         -0.13234         2.36064        -4.18817
   H          3.08389        -0.49701        -4.39032
   H          2.01750        -1.81916        -2.59555
   N          0.58645         1.40526         0.76117
   C         -0.53035         2.09417         0.92925
   N         -1.69535         1.54186         0.49802
   N         -0.56793         3.35434         1.47675
   H         -1.63296         0.63589         0.00276
   C          1.87464         1.94242         1.19516
   H          2.64263         1.60590         0.48720
   H          2.14387         1.51783         2.17560
   C          1.87007         3.46714         1.28374
   H          1.82900         3.90363         0.27778
   H          2.78382         3.82819         1.76911
   C          0.64590         3.91224         2.07696
   H          0.54791         5.00294         2.06373
   H          0.73367         3.60279         3.13116
   C         -3.01890         2.08989         0.76727
   H         -3.68398         1.77612        -0.04325
   H         -3.42862         1.67928         1.70369
   C         -2.94164         3.60987         0.85719
   H         -3.89723         4.02180         1.19891
   H         -2.72394         4.03199        -0.13153
   C         -1.83677         3.99546         1.83583
   H         -1.67246         5.07822         1.82260
   H         -2.12454         3.72125         2.86397
   H          1.50785        -3.57857        -0.56773

57
INT1_OPD  # E(6-31+G*)=-1241.96789434; E(ACCPVTZ)=-1242.38568700 H
   C          1.63448        -1.65324         0.14346
   C          2.61481        -0.77271        -0.32828
   C          3.95903        -1.14843        -0.41138
   C          4.33742        -2.42802         0.00762
   C          3.37368        -3.32342         0.47625
   C          2.01656        -2.96202         0.53406
   N          0.28378        -1.19435         0.30900
   N          1.04281        -3.84755         1.02676
   H          2.30686         0.22549        -0.62801
   H          4.69975        -0.44573        -0.78418
   H          5.37962        -2.73563        -0.03573
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   H          3.66665        -4.32515         0.78609
   H         -0.13931        -1.68275         1.10096
   H          1.37784        -4.80250         1.11016
   H          0.18848        -3.81359         0.46779
   C         -1.86764        -3.26706        -1.82637
   O         -0.77987        -2.80912        -1.03444
   C         -0.76302        -1.33769        -0.78247
   O         -1.92222        -0.89865        -0.33165
   C         -0.26589        -0.64244        -2.07372
   C         -0.65676         0.67835        -2.33251
   C         -0.22835         1.34478        -3.48509
   C          0.59405         0.69110        -4.40953
   C          0.98345        -0.62981        -4.16613
   C          0.56028        -1.28662        -3.00531
   H          0.92208         1.20338        -5.31111
   H         -1.80132        -4.35955        -1.85185
   H         -1.80662        -2.88515        -2.85605
   H         -2.82797        -2.96759        -1.39204
   H         -1.31246         1.17977        -1.62726
   H         -0.54369         2.37031        -3.66565
   H          1.61752        -1.15155        -4.87981
   H          0.86468        -2.31193        -2.82205
   N          0.01204         1.46322         1.55569
   C         -1.22628         1.96799         1.72007
   N         -2.24700         1.35335         1.11250
   N         -1.41755         3.09834         2.44729
   H         -2.05174         0.47593         0.55305
   C          1.18617         1.95385         2.27672
   H          2.06351         1.77075         1.65031
   H          1.32259         1.38964         3.21059
   C          1.02293         3.44014         2.57223
   H          1.08022         4.01506         1.64027
   H          1.82604         3.78509         3.23120
   C         -0.32645         3.67913         3.24250
   H         -0.52653         4.75096         3.33372
   H         -0.33750         3.25332         4.25695
   C         -3.63842         1.78601         1.23076
   H         -4.13930         1.55932         0.28519
   H         -4.14439         1.20899         2.01784
   C         -3.70131         3.27726         1.54223
   H         -4.72616         3.56914         1.79282
   H         -3.39033         3.85745         0.66509
   C         -2.77672         3.58865         2.71518
   H         -2.70632         4.66862         2.87568
   H         -3.16036         3.13962         3.64349
   H          0.10081         0.55973         1.05084

57
INT2_OPD  # E(6-31+G*)=-1241.96410911; E(ACCPVTZ)=-1242.38273979 H
   C         -0.47504         0.13610        -2.03084
   C         -1.83777         0.37717        -1.81998
   C         -2.40044         1.63313        -2.06818
   C         -1.59500         2.66412        -2.56231
   C         -0.23000         2.44543        -2.76762
   C          0.34854         1.19859        -2.48329
   N          0.06353        -1.17159        -1.87194
   N          1.72364         0.95817        -2.68893
   H         -2.45105        -0.44594        -1.46846
   H         -3.46171         1.79653        -1.89747
   H         -2.02186         3.64014        -2.78159
   H          0.40220         3.25313        -3.13341
   H          0.87023        -1.28943        -2.48039
   H          2.25725         1.80490        -2.86075
   H          2.13747         0.42876        -1.92074
   C          2.20698        -1.10565         1.13281
   O          1.58954        -0.74848        -0.09833
   C          0.39081        -1.68147        -0.51514
   O         -0.57437        -1.60844         0.35565
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C          0.99893        -3.09076        -0.71807
C          0.31262        -4.20575        -0.22525
C          0.80574        -5.50008        -0.42559
C          2.00147        -5.69641        -1.12410
C          2.70040        -4.58748        -1.61476
C          2.20148        -3.29698        -1.41165
H          2.38761        -6.70076        -1.28114
H          2.89894        -0.29991         1.40348
H          2.77720        -2.04015         1.04294
H          1.46153        -1.22119         1.93082
H         -0.61273        -4.04166         0.31767
H          0.25586        -6.35446        -0.03685
H          3.63663        -4.72637        -2.15088
H          2.76668        -2.44331        -1.77809
N          0.47357         1.71153         1.07363
C         -0.62418         1.64575         1.84951
N         -1.31348         0.50196         1.87393
N         -1.02014         2.72561         2.56957
H         -0.99841        -0.27944         1.23904
C          1.33216         2.88723         0.94763
H          1.68105         2.93791        -0.08783
H          2.21524         2.77829         1.59314
C          0.55335         4.14378         1.32138
H         -0.17946         4.37596         0.53986
H          1.23510         4.99549         1.41028
C         -0.16966         3.91999         2.64661
H         -0.82061         4.76805         2.87810
H          0.55061         3.81908         3.47247
C         -2.50453         0.29048         2.69372
H         -3.17749        -0.36969         2.13896
H         -2.23109        -0.22529         3.62517
C         -3.17812         1.62401         3.00330
H         -3.95954         1.48641         3.75756
H         -3.64978         2.02467         2.09817
C         -2.13683         2.61442         3.51720
H         -2.57274         3.61208         3.62501
H         -1.76141         2.30733         4.50483
H          0.74271         0.86313         0.55978

57
TS2_OPD  # E(6-31+G*)=-1241.96298283; E(ACCPVTZ)=-1242.38209910 H
C         -0.61516         0.04558        -2.03809
C         -2.00266         0.19807        -1.95248
C         -2.61552         1.42173        -2.23858
C         -1.82778         2.50444        -2.64470
C         -0.43994         2.37031        -2.72753
C          0.18679         1.15506        -2.40420
N         -0.01237        -1.23126        -1.84616
N          1.58006         0.99134        -2.48598
H         -2.59548        -0.66708        -1.67103
H         -3.69551         1.52100        -2.16570
H         -2.28976         3.45773        -2.89161
H          0.17279         3.21996        -3.02481
H          0.80294        -1.34076        -2.44228
H          2.08385         1.86729        -2.58366
H          1.94844         0.43827        -1.70542
C          2.36290        -1.18889         1.06157
O          1.66334        -0.73405        -0.07353
C          0.23893        -1.76137        -0.52868
O         -0.65010        -1.59244         0.36819
C          0.88579        -3.14591        -0.63926
C          0.29084        -4.21641         0.03847
C          0.81416        -5.51041        -0.06215
C          1.94788        -5.75023        -0.84398
C          2.55388        -4.68513        -1.52119
C          2.02785        -3.39502        -1.41605
H          2.35786        -6.75413        -0.92396
H          2.98640        -0.37562         1.46589
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   H          3.02995        -2.03454         0.82965
   H          1.67186        -1.50998         1.85936
   H         -0.58992        -4.02179         0.64226
   H          0.33568        -6.32950         0.47011
   H          3.44249        -4.85727        -2.12417
   H          2.53047        -2.57399        -1.92061
   N          0.70184         1.61287         1.18739
   C         -0.50491         1.73583         1.76418
   N         -1.38382         0.73727         1.62066
   N         -0.83272         2.86011         2.45194
   H         -1.08826        -0.09861         1.07085
   C          1.77599         2.59267         1.33210
   H          2.36075         2.58634         0.40768
   H          2.44881         2.29787         2.15044
   C          1.19093         3.97469         1.60116
   H          0.69559         4.35443         0.69987
   H          1.98750         4.67586         1.86981
   C          0.18013         3.88369         2.74043
   H         -0.34537         4.83509         2.86586
   H          0.68460         3.65530         3.69139
   C         -2.72778         0.73576         2.19404
   H         -3.39146         0.22841         1.48761
   H         -2.73375         0.15698         3.12842
   C         -3.19273         2.16521         2.45161
   H         -4.11052         2.16177         3.04820
   H         -3.40932         2.66667         1.50100
   C         -2.09934         2.92990         3.19212
   H         -2.36340         3.98758         3.28456
   H         -1.96413         2.53134         4.20885
   H          0.92222         0.73550         0.67337

57
PC1_OPD  # E(6-31+G*)=-1241.99445801; E(ACCPVTZ)=-1242.41692808 H
   C         -1.22373         2.39684        -3.67344
   C         -0.41915         1.35283        -3.17453
   N          0.95545         1.51134        -2.99257
   H          1.25563         2.47979        -3.04287
   C         -1.03632         0.10754        -2.91996
   C         -2.40812        -0.06449        -3.12264
   C         -3.19715         0.98677        -3.59302
   C         -2.59077         2.21691        -3.87747
   N         -0.22299        -0.99296        -2.50477
   H         -2.84692        -1.03609        -2.91446
   H         -4.26313         0.84481        -3.74643
   H         -3.18683         3.04478        -4.25384
   H         -0.76342         3.35986        -3.88454
   H          0.47568        -1.31104        -3.16600
   H          1.34159         1.07062        -2.15110
   C          3.36503         0.00430        -0.08855
   O          2.19959         0.75413        -0.40885
   C         -0.31849        -1.63304        -1.30633
   O         -1.13633        -1.29634        -0.43763
   C          0.60067        -2.80531        -1.09256
   C          0.22509        -3.75446        -0.12886
   C          1.02269        -4.87363         0.11424
   C          2.21519        -5.05218        -0.59530
   C          2.60446        -4.10467        -1.54730
   C          1.80177        -2.98909        -1.79653
   H          2.83911        -5.92165        -0.40539
   H          4.04069         0.56607         0.57309
   H          3.89468        -0.20606        -1.02317
   H          3.11618        -0.95243         0.39105
   H         -0.69960        -3.60557         0.41929
   H          0.71390        -5.60545         0.85610
   H          3.53635        -4.22850        -2.09241
   H          2.14460        -2.25587        -2.52111
   N          1.06475         1.49177         2.01392
   C         -0.12606         1.39993         2.54576
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   N         -1.10783         0.73686         1.83322
   N         -0.51898         2.00005         3.73004
   H         -0.75363         0.18797         1.05422
   C          2.10669         2.24533         2.71258
   H          2.74836         2.71888         1.95865
   H          2.75241         1.54781         3.27096
   C          1.55352         3.30105         3.66957
   H          1.09770         4.12222         3.10132
   H          2.35393         3.72589         4.28670
   C          0.49744         2.65306         4.55650
   H         -0.01060         3.40192         5.17484
   H          0.96383         1.92512         5.24188
   C         -2.29585         0.17958         2.47655
   H         -3.02577        -0.04391         1.69359
   H         -2.06691        -0.76657         2.99506
   C         -2.84223         1.19435         3.47244
   H         -3.68528         0.77040         4.02898
   H         -3.19940         2.08339         2.93848
   C         -1.73133         1.58200         4.44209
   H         -2.04605         2.42001         5.07423
   H         -1.50382         0.73688         5.11445
   H          1.70684         0.96854         0.43807

28
product1_OPD [N-(2-aminophenyl)benzamide] # E(6-31+G*)=-687.39906257; E(ACCPVTZ)=-
687.62805940 H
   C         -1.95099         0.55503        -1.69002
   C         -2.60776         1.27866        -2.70606
   C         -2.20364         2.56109        -3.06852
   C         -1.10936         3.16020        -2.43339
   C         -0.43555         2.45194        -1.43900
   C         -0.84112         1.16533        -1.05934
   N         -0.15611         0.55682         0.03953
   C          0.39695        -0.68771         0.08382
   N         -2.43965        -0.68459        -1.26836
   O          0.25216        -1.51362        -0.83253
   C          1.17816        -1.02820         1.32023
   C          1.86781        -0.06828         2.07921
   C          1.23973        -2.37740         1.70304
   C          1.95877        -2.75850         2.83653
   C          2.63972        -1.79680         3.59120
   C          2.59810        -0.45307         3.20617
   H         -3.45928         0.81770        -3.20213
   H         -2.74078         3.09029        -3.85149
   H         -0.77944         4.15662        -2.71244
   H          0.42324         2.89485        -0.94013
   H          0.00666         1.16086         0.83587
   H         -1.70144        -1.36767        -1.09912
   H         -3.14505        -1.06725        -1.89051
   H          1.87468         0.97709         1.78253
   H          0.71551        -3.11828         1.10769
   H          1.98971        -3.80461         3.12919
   H          3.20556        -2.09320         4.47048
   H          3.13878         0.29598         3.77833

51
INT3_OPD  # E(6-31+G*)=-1126.25132988; E(ACCPVTZ)=-1126.62505382 H
   H         -2.58974        -2.08426         0.53098
   H          2.52571        -2.53968        -0.67310
   H         -1.63048        -4.44490        -0.33141
   H          0.97726        -4.68990        -0.91243
   H          1.06991        -0.55156        -1.14772
   C         -2.51365        -1.80162        -0.53222
   N         -1.18476        -1.25309        -0.79274
   C          2.17155        -2.26073        -1.68049
   H          2.75957        -4.18147        -2.49163
   H         -3.78569        -3.48783        -1.06505
   C         -1.70480        -4.00593        -1.34157
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C	0.69254	-4.24426	-1.88206
H	-3.25094	-1.00261	-0.68519
H	2.95683	-1.65879	-2.14890
C	-0.27499	-2.02124	-1.31753
N	-0.45188	-3.34405	-1.70740
N	0.95653	-1.44888	-1.61816
H	0.36890	-5.06693	-2.53018
H	-1.86017	-4.83387	-2.04348
C	-2.85806	-3.01104	-1.40388
C	1.88716	-3.51851	-2.49205
H	-3.00732	-2.69429	-2.44456
H	1.66831	-3.24668	-3.53201
C	-1.39016	2.93371	-0.83203
C	-1.75198	4.02242	-1.65778
C	-1.32591	5.31899	-1.38352
C	-0.51289	5.58225	-0.27348
C	-0.13314	4.51667	0.54395
C	-0.56053	3.21122	0.28017
N	-0.18123	2.16666	1.18634
C	0.79995	1.25525	0.93036
N	-1.90750	1.67285	-1.07411
O	1.39042	1.21122	-0.15947
C	1.14206	0.31269	2.04715
C	0.22092	-0.06223	3.03855
C	2.44391	-0.20991	2.08755
C	2.82581	-1.07730	3.11200
C	1.90516	-1.44315	4.10040
C	0.60147	-0.93830	4.05810
H	-2.38919	3.83167	-2.51894
H	-1.63064	6.12897	-2.04201
H	-0.17389	6.59085	-0.05573
H	0.50843	4.68500	1.40581
H	-0.50489	2.25304	2.14262
H	-1.39110	0.83259	-0.79263
H	-2.31048	1.55401	-1.99664
H	-0.80465	0.29499	3.00402
H	3.14963	0.07569	1.31373
H	3.83983	-1.46756	3.13924
H	2.20049	-2.12166	4.89652
H	-0.12269	-1.23146	4.81353

51
TS3_OPD # E(6-31+G*)=-1126.21285322; E(ACCPVTZ)=-1126.58390613 H

N	0.89540	1.12301	-1.15377
C	0.46901	0.71021	-2.33810
N	-0.42902	-0.30878	-2.37384
N	0.93401	1.21264	-3.53013
H	-0.78766	-0.62945	-1.45712
C	1.86822	2.20966	-1.05825
H	2.48688	2.03935	-0.16767
H	1.34918	3.16937	-0.90146
C	2.74816	2.31231	-2.30194
H	3.41582	1.44365	-2.36372
H	3.37097	3.21312	-2.26299
C	1.85112	2.35435	-3.53399
H	2.44666	2.29570	-4.45168
H	1.28764	3.30086	-3.56935
C	-1.16723	-0.70403	-3.56671
H	-1.45982	-1.75226	-3.45016
H	-2.09303	-0.11518	-3.66939
C	-0.29100	-0.51370	-4.79920
H	-0.87237	-0.68252	-5.71198
H	0.53510	-1.23514	-4.78449
C	0.26610	0.90642	-4.79984
H	1.00666	1.02825	-5.59742
H	-0.54034	1.63348	-4.98952
H	0.42302	0.64462	0.07333
C	-0.80675	-1.05384	1.19518

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   C          0.16646        -2.19318         1.56046
   C          0.56404        -2.44457         2.88225
   C          1.45522        -3.48282         3.17410
   C          1.96456        -4.28196         2.14527
   C          1.57475        -4.03568         0.82417
   C          0.68092        -2.99949         0.53648
   H          0.36361        -2.81137        -0.48458
   H          1.96332        -4.65350         0.01783
   H          2.65485        -5.09104         2.37138
   H          1.74555        -3.67032         4.20529
   H          0.15871        -1.83608         3.68517
   N          0.10378         0.32561         1.21078
   C         -0.71435         1.30267         1.89385
   C         -1.79085         0.65671         2.52142
   N         -1.70239        -0.72201         2.36698
   H         -2.58864        -1.21276         2.27808
   C         -2.74108         1.41124         3.21886
   C         -2.57439         2.80140         3.28410
   C         -1.48899         3.43617         2.66739
   C         -0.54566         2.67807         1.95294
   H          0.29657         3.15881         1.46293
   H         -1.37564         4.51439         2.73504
   H         -3.30529         3.39556         3.82731
   H         -3.58417         0.92900         3.70681
   H          0.96778         0.14650         1.73044
   O         -1.43920        -1.18423         0.06827

51
INT4_OPD  # E(6-31+G*)=-1126.22881177; E(ACCPVTZ)=-1126.60205833 H
   N          1.19498         1.31089        -1.36670
   C          0.66727         0.63727        -2.45227
   N         -0.11299        -0.38320        -2.20965
   N          1.08572         1.04306        -3.70594
   H         -0.90531        -0.66538        -0.69198
   C          1.65877         2.69287        -1.46482
   H          2.26675         2.90974        -0.58063
   H          0.81566         3.40395        -1.47081
   C          2.47752         2.84800        -2.74117
   H          3.39275         2.24814        -2.66785
   H          2.76819         3.89424        -2.88586
   C          1.64353         2.38133        -3.93029
   H          2.25845         2.33414        -4.83609
   H          0.83050         3.10087        -4.12735
   C         -0.64080        -1.17287        -3.32113
   H         -0.70076        -2.22072        -2.99958
   H         -1.67513        -0.85803        -3.53431
   C          0.20020        -1.05984        -4.59346
   H         -0.31846        -1.51615        -5.44463
   H          1.15410        -1.58702        -4.46241
   C          0.47371         0.41302        -4.87762
   H          1.16893         0.52924        -5.71671
   H         -0.45991         0.93307        -5.15098
   H          0.75392         1.04236        -0.48529
   C         -0.81345        -0.84659         1.32375
   C          0.03645        -2.11022         1.50105
   C          0.13611        -2.74720         2.74556
   C          0.93975        -3.88193         2.90191
   C          1.66314        -4.38638         1.81745
   C          1.57487        -3.74980         0.57465
   C          0.76518        -2.62161         0.41576
   H          0.69984        -2.13832        -0.55568
   H          2.13422        -4.13352        -0.27522
   H          2.28815        -5.26778         1.93797
   H          0.99849        -4.36960         3.87197
   H         -0.42452        -2.35475         3.58783
   N          0.03715         0.37526         1.43612
   C         -0.72235         1.32110         2.19046
   C         -1.87233         0.69243         2.69639
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   N         -1.81545        -0.67515         2.38773
   H         -2.69551        -1.13797         2.17975
   C         -2.81003         1.41000         3.43474
   C         -2.56365         2.77469         3.66839
   C         -1.40891         3.39487         3.18092
   C         -0.47277         2.66547         2.42345
   H          0.41872         3.14522         2.02753
   H         -1.23497         4.44964         3.37597
   H         -3.28499         3.35245         4.24081
   H         -3.70141         0.92958         3.82973
   H          0.94375         0.16762         1.85188
   O         -1.51267        -0.84281         0.09943

51
INT5_OPD  # E(6-31+G*)=-1126.22364832; E(ACCPVTZ)=-1126.59742662 H
   C          1.84596         0.34855         0.10777
   C          2.71585        -0.65276         0.87072
   C          2.46737        -0.95244         2.21546
   C          3.29007        -1.84839         2.90644
   C          4.37770        -2.44632         2.26378
   C          4.63692        -2.14540         0.92199
   C          3.80967        -1.25802         0.22945
   H          4.01966        -1.03650        -0.81397
   H          5.48197        -2.60208         0.41298
   H          5.01897        -3.13950         2.80215
   H          3.07985        -2.07582         3.94857
   H          1.62985        -0.47835         2.71636
   N          2.53375         1.61275        -0.13622
   C          1.58208         2.64632        -0.08031
   C          0.42147         2.11771         0.51723
   N          0.65255         0.76896         0.82097
   H         -0.15074         0.11662         0.75118
   C         -0.68625         2.92406         0.75448
   C         -0.61245         4.28015         0.38092
   C          0.54304         4.80266        -0.20816
   C          1.66562         3.98383        -0.44340
   H          2.56472         4.38768        -0.90215
   H          0.58113         5.85162        -0.49058
   H         -1.46974         4.92590         0.55405
   H         -1.58543         2.51765         1.20941
   H          3.19120         1.59746        -0.90866
   O          1.50553        -0.22758        -1.19762
   H          1.49819        -1.19672        -1.11566
   N         -1.70420        -0.99974         0.43468
   C         -2.29238        -1.02701        -0.72839
   N         -1.62997        -0.44174        -1.79923
   N         -3.56967        -1.50414        -0.97865
   H         -0.65357        -0.25165        -1.58582
   C         -2.40522        -1.52377         1.60538
   H         -2.13016        -0.91029         2.47347
   H         -2.04094        -2.54095         1.82404
   C         -3.92626        -1.55151         1.44249
   H         -4.32477        -0.52883         1.46268
   H         -4.39729        -2.10886         2.26084
   C         -4.26817        -2.19811         0.10478
   H         -5.34314        -2.13501        -0.10007
   H         -3.99921        -3.26832         0.11446
   C         -1.90213        -0.83590        -3.18084
   H         -1.46387        -0.07974        -3.83982
   H         -1.43232        -1.80334        -3.42789
   C         -3.41017        -0.92825        -3.37900
   H         -3.64315        -1.30109        -4.38243
   H         -3.85851         0.06722        -3.27360
   C         -3.99445        -1.87278        -2.33328
   H         -5.08971        -1.84130        -2.35498
   H         -3.69622        -2.91239        -2.55513

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TS4_OPD # E(6-31+G*)=-1126.20652502; E(ACCPVTZ)=-1126.58287575 H

C	1.82764	0.60013	0.39671
C	2.53400	-0.61186	0.86239
C	1.95758	-1.42733	1.84806
C	2.64204	-2.54891	2.32421
C	3.91255	-2.86060	1.83283
C	4.49572	-2.04526	0.85516
C	3.81167	-0.93070	0.37120
H	4.26215	-0.32611	-0.41087
H	5.48165	-2.28158	0.46389
H	4.44594	-3.73019	2.20746
H	2.18277	-3.17301	3.08626
H	0.97855	-1.18299	2.24657
N	2.48773	1.76800	0.12787
C	1.57503	2.81573	0.06939
C	0.33969	2.26367	0.46253
N	0.55302	0.91860	0.74981
H	-0.24116	0.18923	0.71910
C	-0.80906	3.05219	0.53158
C	-0.68220	4.40510	0.19572
C	0.55474	4.95164	-0.19070
C	1.70972	4.16268	-0.25878
H	2.66446	4.58441	-0.55890
H	0.61743	6.00628	-0.44414
H	-1.55897	5.04576	0.23480
H	-1.76374	2.62989	0.82982
H	3.45222	1.81172	-0.17013
O	1.44092	-0.15141	-1.59416
H	1.85757	-1.02803	-1.63214
N	-1.52574	-0.84575	0.55855
C	-2.05076	-1.07175	-0.62625
N	-1.33169	-0.69556	-1.73175
N	-3.31991	-1.58958	-0.82748
H	-0.31990	-0.49156	-1.57458
C	-2.26096	-1.21455	1.76424
H	-2.00685	-0.49624	2.55564
H	-1.91881	-2.19967	2.12446
C	-3.77501	-1.25392	1.55715
H	-4.16162	-0.23699	1.41093
H	-4.27951	-1.68154	2.43178
C	-4.07530	-2.09261	0.32030
H	-5.13980	-2.04463	0.06324
H	-3.83327	-3.15262	0.50815
C	-1.64836	-1.16015	-3.07818
H	-1.20746	-0.45462	-3.78990
H	-1.19408	-2.14623	-3.27590
C	-3.15795	-1.24902	-3.26088
H	-3.40120	-1.69944	-4.22971
H	-3.59897	-0.24467	-3.23327
C	-3.73981	-2.09719	-2.13599
H	-4.83520	-2.07531	-2.16133
H	-3.43358	-3.15069	-2.25686

51
PC2_OPD # E(6-31+G*)=-1126.26194925; E(ACCPVTZ)=-1126.63901787 H

C	2.18405	0.66104	0.64266
C	2.65754	-0.72952	0.63838
C	2.45439	-1.53183	-0.49945
C	2.90177	-2.85269	-0.51881
C	3.55681	-3.39470	0.59296
C	3.75966	-2.60484	1.72908
C	3.31287	-1.28255	1.75370
H	3.46215	-0.69626	2.65640
H	4.26064	-3.01800	2.60040
H	3.90474	-4.42408	0.57465
H	2.74123	-3.45879	-1.40650
H	1.95277	-1.11410	-1.36630
N	2.61412	1.59254	1.55921

C	1.98152	2.79037	1.28011
C	1.15694	2.50858	0.16481
N	1.30379	1.17890	-0.20590
H	-0.87408	0.07890	-0.21677
C	0.35475	3.51857	-0.38769
C	0.40956	4.78315	0.19502
C	1.24041	5.04788	1.30704
C	2.04289	4.05577	1.87106
H	2.67998	4.26114	2.72648
H	1.25500	6.04759	1.73274
H	-0.19928	5.58587	-0.21227
H	-0.28347	3.31566	-1.24280
H	3.32518	1.44876	2.26359
O	0.34569	0.35007	-2.92534
H	0.73130	0.66830	-2.08299
N	-1.77699	-0.24471	0.11851
C	-2.46762	-0.98211	-0.83474
N	-2.04091	-0.93592	-2.06525
N	-3.61641	-1.62439	-0.40338
H	-0.49627	-0.10127	-2.64308
C	-1.81968	-0.59203	1.53832
H	-1.41901	0.25466	2.10437
H	-1.18927	-1.46929	1.76109
C	-3.26415	-0.87842	1.92966
H	-3.85995	0.03788	1.83859
H	-3.31947	-1.21767	2.96982
C	-3.82528	-1.95779	1.00972
H	-4.90416	-2.07223	1.16487
H	-3.35964	-2.93129	1.24179
C	-2.78455	-1.63468	-3.11224
H	-2.70985	-1.04653	-4.03577
H	-2.29652	-2.59994	-3.32393
C	-4.25275	-1.87197	-2.75531
H	-4.72752	-2.54322	-3.48058
H	-4.80192	-0.92156	-2.77128
C	-4.33031	-2.47549	-1.35735
H	-5.36991	-2.55233	-1.01877
H	-3.90886	-3.49517	-1.35449

2-aminophenol (2AP)

(X) indicates that X is the nucleophilic atom, e.g. TS2_2AP(N)

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56
RC_2AP(N)  # E(6-31+G*)=-1261.85913130; E(ACCPVTZ)=-1262.28878766 H
   C          0.11502        -2.11267         2.58659
   C         -0.36400        -2.89400         3.63920
   C          0.48666        -3.28508         4.67980
   C          1.82722        -2.88974         4.65867
   C          2.30040        -2.08771         3.61446
   C          1.45869        -1.67211         2.57041
   O         -0.76084        -1.77333         1.58427
   N          1.91521        -0.90738         1.48007
   H         -1.40511        -3.20627         3.61906
   H          0.10291        -3.89892         5.49045
   H          2.50365        -3.19084         5.45464
   H          3.33934        -1.76245         3.60690
   H          2.89850        -0.66690         1.57054
   H          1.38324        -0.04003         1.30757
   C         -0.19482        -3.87373        -1.19260
   O         -0.01156        -3.08876        -2.39236
   C         -0.08478        -1.75610        -2.27804
   O         -0.29935        -1.18918        -1.20955
   C          0.11830        -1.05112        -3.57315
   C          0.10999         0.35321        -3.58601
   C          0.29892         1.04297        -4.78365
   C          0.49659         0.33736        -5.97590
   C          0.50574        -1.06191        -5.96771
   C          0.31846        -1.75672        -4.77207
   H          0.64349         0.87638        -6.90820
   H         -0.16049        -4.91071        -1.52469
   H         -1.15892        -3.64499        -0.73424
   H          0.61346        -3.67121        -0.48651
   H         -0.04297         0.89775        -2.66005
   H          0.29362         2.12950        -4.78661
   H          0.65908        -1.61200        -6.89208
   H          0.32768        -2.84098        -4.76559
   N          0.70048         1.89814         1.21706
   C         -0.43406         2.38022         0.79893
   N         -1.06727         1.72084        -0.24859
   N         -1.02621         3.55918         1.22975
   H         -0.66958         0.79993        -0.41055
   C          1.44149         2.61583         2.25363
   H          2.51456         2.50279         2.04987
   H          1.26484         2.13192         3.22798
   C          1.08056         4.09960         2.34952
   H          1.47154         4.64043         1.47780
   H          1.52122         4.55094         3.24644
   C         -0.43736         4.23567         2.38666
   H         -0.74072         5.28820         2.34518
   H         -0.83774         3.81630         3.32570
   C         -2.51497         1.80874        -0.43941
   H         -2.74903         1.41203        -1.43237
   H         -3.06049         1.19711         0.29868
   C         -2.93734         3.26755        -0.31595
   H         -4.02738         3.35817        -0.37875
   H         -2.49997         3.85010        -1.13600
   C         -2.45663         3.81323         1.02477
   H         -2.60988         4.89722         1.07696
   H         -3.04172         3.36340         1.84588
   H         -0.29171        -1.55670         0.75152

56
TS1_2AP(N)  # E(6-31+G*)=-1261.83006176; E(ACCPVTZ)=-1262.25433597 H
   C         -0.45875        -2.27187         1.82128
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   C         -0.38113        -3.06604         2.97879
   C          0.83111        -3.59993         3.41322
   C          2.00504        -3.35465         2.69296
   C          1.94219        -2.55883         1.54789
   C          0.73351        -2.00754         1.11094
   O         -1.67363        -1.80667         1.45522
   N          0.76539        -1.09165        -0.02680
   H         -1.30284        -3.26068         3.52043
   H          0.85602        -4.21462         4.30940
   H          2.95548        -3.77005         3.01478
   H          2.85074        -2.35069         0.98586
   H          1.71813        -1.09673        -0.39787
   H          0.57405         0.00741         0.35270
   C         -1.05613        -3.34192        -2.30069
   O         -0.12409        -2.76993        -1.38279
   C         -0.23326        -1.34032        -1.24384
   O         -1.43073        -0.90203        -0.91753
   C          0.41494        -0.65029        -2.46216
   C         -0.15048         0.50918        -3.00399
   C          0.43414         1.13614        -4.10997
   C          1.59415         0.60952        -4.68584
   C          2.16305        -0.55298        -4.15338
   C          1.57493        -1.17823        -3.05073
   H          2.04871         1.09632        -5.54507
   H         -0.87421        -4.41918        -2.28435
   H         -0.89693        -2.96457        -3.31994
   H         -2.08668        -3.13677        -1.99393
   H         -1.05148         0.91541        -2.55831
   H         -0.01828         2.03567        -4.52048
   H          3.05923        -0.97675        -4.59984
   H          2.00692        -2.09604        -2.66005
   N          0.49824         1.34433         0.95520
   C         -0.53163         2.16718         0.89351
   N         -1.58550         1.81671         0.09590
   N         -0.57937         3.38823         1.52324
   H         -1.54570         0.85884        -0.27087
   C          1.65759         1.67978         1.78266
   H          2.55286         1.26177         1.30523
   H          1.56938         1.18761         2.76429
   C          1.82097         3.18522         1.97890
   H          2.11490         3.65839         1.03336
   H          2.60255         3.39695         2.71720
   C          0.49240         3.76691         2.44761
   H          0.53261         4.86126         2.47449
   H          0.25768         3.42239         3.46780
   C         -2.89843         2.44922         0.17509
   H         -3.41811         2.26802        -0.77104
   H         -3.50745         2.00142         0.97693
   C         -2.72356         3.94203         0.42596
   H         -3.69508         4.41755         0.59771
   H         -2.26449         4.41524        -0.45066
   C         -1.83278         4.14193         1.64754
   H         -1.56915         5.19882         1.76149
   H         -2.36558         3.83815         2.56331
   H         -1.65416        -1.43440         0.49591

56
INT1_2AP(N)  # E(6-31+G*)=-1261.84746187; E(ACCPVTZ)=-1262.27421354 H
   C         -0.43049        -2.31229         1.79875
   C         -0.35550        -3.05669         2.98700
   C          0.85187        -3.58295         3.45037
   C          2.02044        -3.37617         2.71234
   C          1.95438        -2.64553         1.52294
   C          0.75390        -2.09506         1.04632
   O         -1.64415        -1.82826         1.43955
   N          0.80966        -1.24239        -0.10363
   H         -1.27842        -3.20945         3.54116
   H          0.87389        -4.15309         4.37583
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   H          2.97208        -3.77984         3.04789
   H          2.86315        -2.48245         0.94493
   H          1.75120        -1.28046        -0.48675
   H          0.56953         0.53137         0.55181
   C         -1.23592        -3.21264        -2.41119
   O         -0.24772        -2.79958        -1.47519
   C         -0.19088        -1.36176        -1.22102
   O         -1.37971        -0.84799        -0.87050
   C          0.43908        -0.67277        -2.45715
   C         -0.13309         0.48299        -2.99889
   C          0.43874         1.11358        -4.11027
   C          1.59657         0.59323        -4.69543
   C          2.17117        -0.56912        -4.16802
   C          1.59287        -1.19692        -3.06123
   H          2.04360         1.08286        -5.55720
   H         -1.16924        -4.30341        -2.46530
   H         -1.04634        -2.79448        -3.41054
   H         -2.24047        -2.92231        -2.08444
   H         -1.03574         0.88104        -2.54849
   H         -0.02214         2.01067        -4.51753
   H          3.06520        -0.99011        -4.62201
   H          2.03094        -2.11494        -2.67703
   N          0.56920         1.46333         1.00296
   C         -0.55395         2.19872         0.94959
   N         -1.58143         1.73735         0.21994
   N         -0.62400         3.39624         1.57883
   H         -1.48179         0.79214        -0.20713
   C          1.72411         1.79795         1.83472
   H          2.61696         1.40874         1.33710
   H          1.64265         1.29965         2.81073
   C          1.80619         3.30916         2.00945
   H          2.08144         3.78091         1.05873
   H          2.57401         3.56271         2.74703
   C          0.45393         3.83958         2.47624
   H          0.44852         4.93349         2.47264
   H          0.23996         3.51011         3.50348
   C         -2.88668         2.39543         0.15888
   H         -3.32165         2.18780        -0.82288
   H         -3.55878         1.96865         0.91651
   C         -2.72011         3.89558         0.37837
   H         -3.69947         4.37203         0.48774
   H         -2.22039         4.34800        -0.48647
   C         -1.89072         4.14059         1.63551
   H         -1.63915         5.20106         1.73016
   H         -2.45034         3.85051         2.53674
   H         -1.60922        -1.42525         0.48440

56
INT2_2AP(N)  # E(6-31+G*)=-1261.83418207; E(ACCPVTZ)=-1262.26073986 H
   C         -0.60824         0.02922        -1.92659
   C         -1.99509         0.22111        -1.91140
   C         -2.55883         1.47197        -2.17636
   C         -1.72378         2.55146        -2.48687
   C         -0.33707         2.38589        -2.49599
   C          0.22550         1.13966        -2.19329
   N         -0.06519        -1.28559        -1.76403
   O          1.58980         1.02107        -2.18776
   H         -2.62511        -0.64021        -1.70851
   H         -3.63851         1.59681        -2.16249
   H         -2.14948         3.52563        -2.71595
   H          0.32573         3.21897        -2.71569
   H          0.65217        -1.46515        -2.46361
   H          1.83433         0.30376        -1.54000
   C          2.57407        -1.14604         0.85503
   O          1.73074        -0.79381        -0.23165
   C          0.39267        -1.74260        -0.44575
   O         -0.41694        -1.55597         0.54065
   C          0.94764        -3.16948        -0.61912
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C          0.29860        -4.22687         0.02819
C          0.72616        -5.54715        -0.15009
C          1.81793        -5.82679        -0.97817
C          2.48035        -4.77508        -1.62161
C          2.04658        -3.45808        -1.44264
H          2.15210        -6.85194        -1.11878
H          3.23483        -0.29734         1.07101
H          3.19717        -2.01948         0.61979
H          1.97862        -1.36707         1.75163
H         -0.54850        -4.00003         0.66793
H          0.20493        -6.35694         0.35565
H          3.33756        -4.97887        -2.25926
H          2.58329        -2.64846        -1.93141
N          0.67021         1.59174         1.26275
C         -0.56447         1.73307         1.78155
N         -1.41371         0.70717         1.67518
N         -0.92968         2.89241         2.37923
H         -1.06783        -0.14448         1.17314
C          1.70802         2.62153         1.30853
H          2.28500         2.55431         0.38206
H          2.39216         2.42697         2.14624
C          1.06645         3.99754         1.45478
H          0.56654         4.27828         0.52052
H          1.83339         4.74903         1.66716
C          0.04726         3.96883         2.59050
H         -0.50945         4.90954         2.63107
H          0.54805         3.83707         3.56108
C         -2.78335         0.72326         2.18369
H         -3.40654         0.15860         1.48384
H         -2.82612         0.20956         3.15423
C         -3.27767         2.16008         2.31919
H         -4.22238         2.18369         2.87163
H         -3.45557         2.58991         1.32641
C         -2.23099         2.99417         3.05363
H         -2.51314         4.05094         3.05722
H         -2.13782         2.67109         4.10104
H          0.87435         0.72587         0.75345

56
TS2_2AP(N)  # E(6-31+G*)=-1261.83430573; E(ACCPVTZ)=-1262.26091125 H
C         -0.46048         0.14323        -2.11732
C         -1.84221         0.33975        -2.22433
C         -2.37616         1.59883        -2.51310
C         -1.51444         2.68143        -2.72337
C         -0.13306         2.51125        -2.60615
C          0.39592         1.25698        -2.27829
N          0.06927        -1.17478        -1.94282
O          1.75353         1.13276        -2.14096
H         -2.49027        -0.52304        -2.10296
H         -3.45233         1.72729        -2.59679
H         -1.91565         3.66122        -2.97176
H          0.54889         3.34618        -2.74592
H          0.86278        -1.32249        -2.56246
H          1.92873         0.41181        -1.47361
C          2.38605        -1.05507         0.96842
O          1.65526        -0.68034        -0.18798
C          0.37689        -1.68097        -0.60247
O         -0.54692        -1.56870         0.28551
C          1.01812        -3.07287        -0.75672
C          0.38558        -4.17109        -0.16358
C          0.89555        -5.46447        -0.32155
C          2.05420        -5.67536        -1.07544
C          2.70117        -4.58204        -1.66305
C          2.18688        -3.29207        -1.50202
H          2.45199        -6.67944        -1.20167
H          3.00868        -0.20613         1.27812
H          3.04324        -1.91380         0.77432
H          1.70538        -1.31075         1.79288
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   H         -0.51327        -3.99551         0.41892
   H          0.38698        -6.30638         0.14286
   H          3.60928        -4.73242        -2.24234
   H          2.71549        -2.45026        -1.94299
   N          0.43942         1.64239         1.21546
   C         -0.72089         1.60190         1.89502
   N         -1.48373         0.51001         1.77754
   N         -1.11055         2.65540         2.65350
   H         -1.13534        -0.25355         1.15308
   C          1.37854         2.76344         1.24447
   H          1.82626         2.84895         0.25040
   H          2.18632         2.55627         1.96044
   C          0.64489         4.04330         1.63033
   H         -0.00000         4.37008         0.80629
   H          1.36588         4.84172         1.83195
   C         -0.20377         3.79022         2.87318
   H         -0.82455         4.66173         3.10023
   H          0.43350         3.59859         3.74933
   C         -2.72338         0.30434         2.52330
   H         -3.39424        -0.29238         1.89891
   H         -2.52050        -0.27233         3.43688
   C         -3.35143         1.65029         2.87113
   H         -4.18543         1.50983         3.56606
   H         -3.74392         2.12539         1.96432
   C         -2.30122         2.55545         3.50947
   H         -2.69358         3.56827         3.64012
   H         -2.01475         2.17960         4.50290
   H          0.70294         0.81245         0.67127

56
PC1_2AP(N)  # E(6-31+G*)=-1261.85695478; E(ACCPVTZ)=-1262.28822452 H
   C         -0.40120         0.18520        -2.19200
   C         -1.76781         0.43677        -2.34435
   C         -2.22347         1.73661        -2.57560
   C         -1.30241         2.78595        -2.67727
   C          0.06299         2.54300        -2.51727
   C          0.52179         1.24812        -2.25198
   N          0.10414        -1.13904        -2.04790
   O          1.86580         1.03450        -2.10298
   H         -2.46344        -0.39536        -2.29707
   H         -3.28708         1.92512        -2.69320
   H         -1.64751         3.79875        -2.86988
   H          0.78804         3.35038        -2.57018
   H          0.83160        -1.39924        -2.70216
   H          2.03904         0.44671        -1.31827
   C          2.79874        -1.07672         1.18455
   O          2.16968        -0.16481         0.29335
   C         -0.14490        -1.99472        -1.01540
   O         -0.97992        -1.75862        -0.13197
   C          0.63812        -3.28016        -1.03325
   C          0.09351        -4.39280        -0.37403
   C          0.77749        -5.60956        -0.35325
   C          2.02086        -5.72719        -0.98435
   C          2.57758        -4.62017        -1.63198
   C          1.89046        -3.40476        -1.65765
   H          2.55582        -6.67314        -0.96651
   H          3.33344        -0.54835         1.98688
   H          3.52166        -1.66822         0.61534
   H          2.06937        -1.76299         1.63733
   H         -0.86875        -4.29224         0.11803
   H          0.34119        -6.46556         0.15461
   H          3.54986        -4.69712        -2.11133
   H          2.36435        -2.55348        -2.13828
   N          0.58413         1.66560         1.45360
   C         -0.59056         1.64549         2.02833
   N         -1.28757         0.46307         2.03873
   N         -1.20929         2.74610         2.59500
   H         -0.96017        -0.25001         1.39399
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   C          1.31605         2.92336         1.31975
   H          1.79269         2.93560         0.33119
   H          2.13551         2.94687         2.05665
   C          0.43980         4.16390         1.49312
   H         -0.20453         4.29510         0.61436
   H          1.05753         5.06421         1.59338
   C         -0.43472         3.97945         2.72905
   H         -1.14557         4.80622         2.83517
   H          0.18522         3.95875         3.64142
   C         -2.49431         0.20878         2.81387
   H         -3.07355        -0.56255         2.29749
   H         -2.24340        -0.18492         3.81245
   C         -3.30166         1.49571         2.95989
   H         -4.12442         1.35175         3.66919
   H         -3.73172         1.77961         1.99168
   C         -2.38285         2.60684         3.45878
   H         -2.90823         3.56842         3.45831
   H         -2.07523         2.40564         4.49952
   H          1.51765         0.43234         0.79496

27
product1_2AP(N) [N-(2-hydroxyphenyl)benzamide]  # E(6-31+G*)=-707.26753196;
E(ACCPVTZ)=-707.50564531 H
   C         -1.87985         0.52459        -1.74268
   C         -2.58258         1.24071        -2.72298
   C         -2.28303         2.57292        -2.99844
   C         -1.25307         3.21480        -2.30049
   C         -0.53941         2.50960        -1.33460
   C         -0.83928         1.16959        -1.03835
   N         -0.10654         0.56807         0.02708
   C          0.34044        -0.71174         0.13835
   O         -2.28172        -0.75176        -1.48379
   O          0.08651        -1.58314        -0.71932
   C          1.17016        -1.03402         1.33952
   C          1.07267        -0.32686         2.54981
   C          2.06759        -2.10985         1.24093
   C          2.87160        -2.45776         2.32628
   C          2.77606        -1.74531         3.52699
   C          1.87144        -0.68462         3.63805
   H         -3.37723         0.72282        -3.25246
   H         -2.84869         3.10648        -3.75739
   H         -1.00327         4.25126        -2.50736
   H          0.26532         2.99762        -0.78910
   H          0.26377         1.23039         0.69851
   H         -1.48492        -1.27695        -1.20879
   H          0.35409         0.47960         2.66926
   H          2.12952        -2.66096         0.30818
   H          3.57065        -3.28477         2.23636
   H          3.39850        -2.01994         4.37445
   H          1.77980        -0.14018         4.57379

50
INT3_2AP(N)  # E(6-31+G*)=-1146.13465127; E(ACCPVTZ)=-1146.51512712 H
   N          1.34522         2.22962        -1.45177
   C          0.78720         1.41146        -2.35460
   N          0.08571         0.35679        -1.90248
   N          0.95512         1.61169        -3.68419
   H         -0.00363         0.25217        -0.88664
   C          2.07874         3.44447        -1.79740
   H          2.86383         3.58945        -1.04917
   H          1.40914         4.31500        -1.74895
   C          2.67334         3.30969        -3.19579
   H          3.49492         2.58349        -3.18485
   H          3.07822         4.27085        -3.52814
   C          1.59304         2.84398        -4.16865
   H          2.02742         2.62110        -5.14764
   H          0.83323         3.62642        -4.31266
   C         -0.65955        -0.55472        -2.76883
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H	-0.68290	-1.52747	-2.27476
H	-1.69776	-0.20906	-2.87442
C	0.01861	-0.62661	-4.13253
H	-0.60366	-1.18989	-4.83519
H	0.98134	-1.14437	-4.04448
C	0.24161	0.78505	-4.66846
H	0.85222	0.76173	-5.57614
H	-0.71721	1.25939	-4.92523
H	1.09449	2.02401	-0.45496
C	-0.62765	-1.60450	1.49945
C	-0.04482	-2.92899	1.91203
C	0.85891	-3.06132	2.97891
C	1.37895	-4.31524	3.31270
C	0.99772	-5.44916	2.58886
C	0.10133	-5.32335	1.52094
C	-0.40956	-4.07023	1.18022
H	-1.09883	-3.96251	0.34842
H	-0.19757	-6.20111	0.95372
H	1.40094	-6.42395	2.85103
H	2.08701	-4.40325	4.13253
H	1.18765	-2.18604	3.53291
O	0.53800	1.24205	0.92647
C	-0.57004	1.56628	1.53083
C	-1.30714	0.62891	2.32832
N	-0.80822	-0.70058	2.49795
H	-0.69212	-1.03045	3.44864
C	-2.47269	0.99767	3.00615
C	-2.98079	2.29781	2.92303
C	-2.29649	3.23277	2.13209
C	-1.13116	2.87777	1.45607
H	-0.59803	3.61813	0.86241
H	-2.67312	4.25099	2.04817
H	-3.88817	2.57039	3.45507
H	-2.98833	0.24654	3.60280
O	-0.93478	-1.38291	0.31757

50

TS3_2AP(N) # E(6-31+G*)=-1146.09545831; E(ACCPVTZ)=-1146.47658296 H

N	-2.18435	-0.63411	0.11384
C	-1.93125	-1.39503	-0.99875
N	-0.90196	-1.06240	-1.75130
N	-2.80081	-2.40903	-1.30064
H	-0.13930	-0.01126	-1.48613
C	-3.05759	-1.07876	1.19880
H	-3.37849	-0.19395	1.75687
H	-2.51608	-1.73559	1.89770
C	-4.25362	-1.81439	0.60768
H	-4.87862	-1.11345	0.04141
H	-4.86623	-2.24611	1.40606
C	-3.75638	-2.92450	-0.31231
H	-4.59125	-3.36774	-0.86502
H	-3.28901	-3.73042	0.27604
C	-0.58838	-1.81007	-2.96746
H	-0.15365	-1.11000	-3.69000
H	0.18537	-2.56253	-2.75093
C	-1.82389	-2.48959	-3.55323
H	-1.54392	-3.16474	-4.36938
H	-2.50868	-1.73572	-3.96147
C	-2.52846	-3.27522	-2.45234
H	-3.48980	-3.66399	-2.80488
H	-1.91851	-4.13823	-2.14152
H	-1.42618	-0.00659	0.37469
C	1.20014	1.03236	-0.20799
C	2.14514	-0.14812	0.03924
C	2.48520	-0.55971	1.33661
C	3.39604	-1.60141	1.53397
C	3.98893	-2.23560	0.43654
C	3.66109	-1.82368	-0.85894

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   C          2.74263        -0.78733        -1.05543
   H          2.48027        -0.47243        -2.06058
   H          4.11667        -2.31018        -1.71801
   H          4.69917        -3.04415         0.59073
   H          3.64274        -1.91669         2.54483
   H          2.02872        -0.07233         2.19251
   N          1.91403         2.32904        -0.09126
   C          1.30819         3.08352         0.92989
   C          0.27347         2.33028         1.50112
   O          0.21750         1.07921         0.95203
   C         -0.53193         2.83300         2.51209
   C         -0.26793         4.14014         2.96492
   C          0.76981         4.89544         2.41018
   C          1.56906         4.37491         1.37531
   H          2.36833         4.96588         0.93580
   H          0.96037         5.90147         2.77442
   H         -0.88026         4.56086         3.75821
   H         -1.32498         2.23279         2.94893
   H          2.92350         2.23532        -0.02661
   O          0.50766         0.96790        -1.35728

50
INT4_2AP(N)  # E(6-31+G*)=-1146.09765270; E(ACCPVTZ)=-1146.47841785 H
   N         -2.18884        -0.68556         0.15867
   C         -1.96520        -1.40396        -1.00355
   N         -0.95261        -1.05092        -1.75101
   N         -2.88954        -2.37826        -1.32333
   H          0.08568         0.22286        -1.44043
   C         -2.94216        -1.24576         1.27983
   H         -3.21233        -0.42344         1.94959
   H         -2.33309        -1.95968         1.85893
   C         -4.18530        -1.94117         0.73891
   H         -4.85638        -1.20028         0.28773
   H         -4.72721        -2.44093         1.54904
   C         -3.76751        -2.96955        -0.30720
   H         -4.64622        -3.36977        -0.82504
   H         -3.26181        -3.82110         0.17895
   C         -0.71326        -1.73869        -3.01893
   H         -0.29823        -1.01245        -3.72893
   H          0.06182        -2.50870        -2.87713
   C         -1.97460        -2.38086        -3.59659
   H         -1.72955        -3.02003        -4.45275
   H         -2.66545        -1.60333        -3.94716
   C         -2.65256        -3.20592        -2.50834
   H         -3.62436        -3.58130        -2.84841
   H         -2.03575        -4.08225        -2.24781
   H         -1.39839        -0.09827         0.41117
   C          1.33016         1.04655        -0.12363
   C          2.21831        -0.17374         0.10223
   C          2.45230        -0.67411         1.39109
   C          3.31416        -1.75800         1.58106
   C          3.96023        -2.34352         0.48689
   C          3.73751        -1.84077        -0.79871
   C          2.86843        -0.76243        -0.99063
   H          2.68623        -0.37863        -1.98944
   H          4.23550        -2.28975        -1.65445
   H          4.63131        -3.18569         0.63581
   H          3.48013        -2.14444         2.58351
   H          1.95241        -0.22339         2.24270
   N          2.06696         2.31068         0.01460
   C          1.35293         3.11696         0.92836
   C          0.28168         2.37599         1.43887
   O          0.30029         1.09374         0.94688
   C         -0.62201         2.90648         2.34519
   C         -0.41882         4.23888         2.75111
   C          0.65341         4.98719         2.25400
   C          1.55415         4.43329         1.32582
   H          2.38164         5.01673         0.93141
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   H          0.79153         6.01432         2.58079
   H         -1.10842         4.68791         3.46078
   H         -1.44409         2.31416         2.73584
   H          3.05500         2.18952         0.21812
   O          0.68625         1.04955        -1.34057

56
RC_2AP(O)  # E(6-31+G*)=-1261.87277350; E(ACCPVTZ)=-1262.30088086 H
   C          2.74265        -0.87093         2.06174
   C          3.81999        -1.48421         1.41807
   C          4.21064        -1.09631         0.12510
   C          3.51110        -0.07377        -0.52094
   C          2.42685         0.54816         0.11683
   C          2.00520         0.17536         1.41387
   N          2.36765        -1.20453         3.38244
   O          0.97537         0.72860         2.03582
   H          4.36439        -2.27433         1.93540
   H          5.05168        -1.58784        -0.35853
   H          3.80082         0.24242        -1.52162
   H          1.87555         1.33854        -0.39069
   H          2.48366        -2.18765         3.60938
   H          0.83690         2.52276         2.17887
   C          0.18662        -5.34478         0.45813
   O          0.12303        -4.64618        -0.80380
   C         -1.08699        -4.19895        -1.18570
   O         -2.09834        -4.36791        -0.51798
   C         -1.05601        -3.48806        -2.49552
   C         -2.26749        -3.01243        -3.02204
   C         -2.28499        -2.34175        -4.24507
   C         -1.09256        -2.14116        -4.95036
   C          0.11709        -2.61331        -4.42906
   C          0.13873        -3.28591        -3.20590
   H         -1.10619        -1.61826        -5.90317
   H          1.23316        -5.62365         0.57751
   H         -0.44829        -6.23359         0.42969
   H         -0.13133        -4.68629         1.26982
   H         -3.18557        -3.17422        -2.46615
   H         -3.22596        -1.97719        -4.64824
   H          1.04383        -2.45768        -4.97464
   H          1.07631        -3.65046        -2.80085
   N          0.32916         3.41750         2.04875
   C         -0.83506         3.29507         1.38989
   N         -1.15116         2.07840         0.91879
   N         -1.63804         4.36238         1.17776
   H         -0.46621         1.33838         1.16733
   C          0.77670         4.65075         2.68978
   H          1.86896         4.68160         2.64029
   H          0.49160         4.64952         3.75136
   C          0.16189         5.85001         1.97301
   H          0.61584         5.96485         0.98151
   H          0.35453         6.76654         2.53955
   C         -1.34516         5.64970         1.82412
   H         -1.77640         6.43481         1.19593
   H         -1.84410         5.69633         2.80332
   C         -2.41170         1.76714         0.25142
   H         -2.22121         0.97864        -0.48221
   H         -3.13794         1.37636         0.97816
   C         -2.95487         3.02390        -0.42350
   H         -3.97141         2.84651        -0.78835
   H         -2.32813         3.28456        -1.28473
   C         -2.96499         4.18375         0.57048
   H         -3.21994         5.12013         0.06535
   H         -3.71463         4.01617         1.35772
   H          1.41535        -0.89894         3.56880

56
RCx_2AP(O)  # E(6-31+G*)=-1261.86864660; E(ACCPVTZ)=-1262.29701753 H
   C          0.20057        -3.26887         1.11605
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   C          0.45523        -4.56721         1.56410
   C          1.75124        -4.97413         1.92657
   C          2.80233        -4.05841         1.83201
   C          2.55759        -2.75132         1.38513
   C          1.26295        -2.30642         1.02383
   N         -1.10528        -2.83101         0.79555
   O          1.01093        -1.07892         0.61151
   H         -0.37220        -5.27423         1.63173
   H          1.92583        -5.99145         2.26948
   H          3.81515        -4.35543         2.09978
   H          3.37599        -2.03714         1.30407
   H         -1.71497        -3.58002         0.48112
   H         -1.09031        -2.07485         0.11388
   H          1.14875         0.14944         1.72510
   C         -1.59874        -2.80157        -3.15664
   O         -0.95679        -1.60350        -3.64471
   C         -0.95603        -0.54125        -2.81863
   O         -1.47460        -0.56267        -1.71101
   C         -0.26297         0.64337        -3.39939
   C          0.04273         1.72161        -2.55354
   C          0.68404         2.85118        -3.06250
   C          1.01538         2.91656        -4.42070
   C          0.71116         1.84483        -5.26730
   C          0.07955         0.70791        -4.75978
   H          1.51125         3.79878        -4.81729
   H         -1.06394        -3.18237        -2.28343
   H         -1.54197        -3.51288        -3.97993
   H         -2.63895        -2.59477        -2.89449
   H         -0.21033         1.65878        -1.50017
   H          0.92789         3.67815        -2.40091
   H          0.96621         1.89374        -6.32237
   H         -0.15420        -0.12432        -5.41472
   N          0.91534         0.99497         2.30485
   C         -0.28593         1.52897         2.05509
   N         -0.98828         1.02905         1.01812
   N         -0.76315         2.56872         2.77885
   H         -0.58885         0.18659         0.58953
   C          1.76433         1.39373         3.42354
   H          2.80696         1.28163         3.11149
   H          1.59955         0.72223         4.27787
   C          1.46021         2.83749         3.81137
   H          1.82581         3.51820         3.03324
   H          1.96739         3.09211         4.74720
   C         -0.04641         3.01798         3.98086
   H         -0.29321         4.07321         4.13056
   H         -0.40996         2.46421         4.85898
   C         -2.37174         1.40680         0.72967
   H         -2.53473         1.26795        -0.34066
   H         -3.06748         0.74264         1.26214
   C         -2.59473         2.85596         1.14951
   H         -3.65495         3.11437         1.06304
   H         -2.03099         3.52826         0.49150
   C         -2.14016         3.04951         2.59347
   H         -2.15308         4.10973         2.86369
   H         -2.81256         2.52228         3.28624

56
INT1_2AP(O)  # E(6-31+G*)=-1261.84240300; E(ACCPVTZ)=-1262.26772957 H
   C          1.14407        -2.36194         1.65179
   C          1.99552        -3.14603         2.45323
   C          3.35734        -3.27278         2.16712
   C          3.90664        -2.61049         1.06476
   C          3.07014        -1.83304         0.25475
   C          1.70703        -1.70200         0.53020
   N         -0.19937        -2.18147         1.98338
   O          0.96347        -0.84030        -0.25473
   H          1.57315        -3.65557         3.31796
   H          3.98434        -3.88793         2.80843
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   H          4.96485        -2.69862         0.83262
   H          3.46564        -1.30892        -0.61172
   H         -0.59505        -2.93498         2.53565
   H          0.40511         0.74263         0.57114
   C         -0.82999        -3.49412        -2.01096
   O          0.17715        -2.70252        -1.39027
   C         -0.22852        -1.34616        -1.11970
   O         -1.35506        -1.22508        -0.48205
   C         -0.08533        -0.50657        -2.40489
   C         -1.12111         0.33899        -2.81403
   C         -1.00941         1.09282        -3.98961
   C          0.14406         1.00313        -4.77302
   C          1.18380         0.15219        -4.37460
   C          1.06734        -0.59437        -3.20027
   H          0.23339         1.58542        -5.68711
   H         -0.40546        -4.49530        -2.12632
   H         -1.09429        -3.10101        -3.00357
   H         -1.73311        -3.54541        -1.39343
   H         -2.01922         0.39679        -2.20705
   H         -1.82526         1.74539        -4.29266
   H          2.08430         0.07245        -4.97952
   H          1.87338        -1.25372        -2.89290
   N          0.19904         1.64030         1.02839
   C         -1.08913         1.92756         1.29195
   N         -2.03384         1.10200         0.82374
   N         -1.41720         3.05022         1.97662
   H         -1.73099         0.24393         0.30813
   C          1.33283         2.41438         1.53484
   H          2.13267         2.36205         0.79085
   H          1.71056         1.96438         2.46339
   C          0.90252         3.85635         1.77751
   H          0.72474         4.36140         0.82064
   H          1.69229         4.40072         2.30453
   C         -0.37581         3.87193         2.61004
   H         -0.77055         4.88886         2.69125
   H         -0.18180         3.50822         3.62987
   C         -3.46066         1.26542         1.09744
   H         -4.01142         0.87737         0.23581
   H         -3.74709         0.66356         1.97145
   C         -3.77815         2.73758         1.33589
   H         -4.80620         2.85025         1.69444
   H         -3.68488         3.29726         0.39757
   C         -2.81048         3.30550         2.37007
   H         -2.93007         4.38960         2.45514
   H         -3.00101         2.87133         3.36263
   H         -0.79371        -1.92600         1.18690

56
INT2_2AP(O)  # E(6-31+G*)=-1261.83980318; E(ACCPVTZ)=-1262.26536949 H
   C          2.61870        -0.40520         0.73233
   C          2.93581        -1.20789         1.84084
   C          2.39670        -0.93617         3.10189
   C          1.53092         0.14754         3.27882
   C          1.21633         0.96109         2.18336
   C          1.74944         0.69720         0.92007
   N          3.19152        -0.62264        -0.52810
   O          1.54822         1.55566        -0.13658
   H          3.61471        -2.04886         1.70821
   H          2.65832        -1.57314         3.94384
   H          1.11150         0.36578         4.25785
   H          0.55904         1.81755         2.29066
   H          3.53503        -1.56656        -0.67115
   H         -0.10536        -1.22875        -0.42627
   C         -0.49678        -0.04017        -2.68150
   O          0.47742         0.20636        -1.66902
   C          0.25712         1.49287        -0.90628
   O         -0.81511         1.46433        -0.19373
   C          0.40592         2.67273        -1.88415
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C         -0.58444         3.65827        -1.93169
C         -0.46997         4.74688        -2.80480
C          0.64270         4.85892        -3.64373
C          1.63726         3.87336        -3.60504
C          1.51800         2.78960        -2.73105
H          0.73573         5.70383        -4.32204
H         -0.31191        -1.04820        -3.06552
H         -0.40300         0.67621        -3.50747
H         -1.51468         0.01217        -2.27505
H         -1.44267         3.56136        -1.27410
H         -1.24864         5.50611        -2.82768
H          2.50650         3.95127        -4.25435
H          2.29076         2.02733        -2.70487
N         -0.51366        -2.06698        -0.00056
C         -1.61668        -1.90431         0.75433
N         -2.07150        -0.66330         0.94991
N         -2.22840        -2.97675         1.31431
H         -1.53299         0.12957         0.52164
C          0.09719        -3.35861        -0.31057
H          1.18144        -3.21814        -0.33976
H         -0.22364        -3.69525        -1.30637
C         -0.29075        -4.38306         0.74972
H          0.22545        -4.16163         1.69105
H          0.00704        -5.38605         0.42841
C         -1.79944        -4.33970         0.97358
H         -2.08379        -4.98768         1.80764
H         -2.33761        -4.69155         0.08076
C         -3.29747        -0.35777         1.68475
H         -3.15787         0.60836         2.17774
H         -4.13808        -0.25379         0.98422
C         -3.58477        -1.45696         2.70265
H         -4.58013        -1.31992         3.13710
H         -2.85208        -1.41372         3.51708
C         -3.50885        -2.81922         2.01845
H         -3.57572        -3.62498         2.75547
H         -4.34131        -2.94613         1.31062
H          2.57988        -0.32797        -1.28637

56
TS2_2AP(O)  # E(6-31+G*)=-1261.83334589; E(ACCPVTZ)=-1262.25988993 H
C          2.41051        -0.36841         1.08802
C          2.69248        -1.01116         2.30888
C          2.34872        -0.42626         3.52921
C          1.71089         0.81918         3.56462
C          1.43108         1.47500         2.36070
C          1.77277         0.89043         1.14348
N          2.79632        -0.90091        -0.14165
O          1.62191         1.59346        -0.04586
H          3.19181        -1.97831         2.28983
H          2.58191        -0.94746         4.45491
H          1.44411         1.27950         4.51219
H          0.95345         2.45019         2.35185
H          2.98212        -1.89795        -0.11312
H         -0.25528        -1.21258        -0.77535
C         -0.16247        -0.04133        -2.89414
O          0.53726         0.00884        -1.68085
C          0.36461         1.68807        -0.66486
O         -0.68151         1.55216        -0.00176
C          0.45291         2.66973        -1.80485
C         -0.71640         3.32039        -2.21805
C         -0.68195         4.24950        -3.26248
C          0.52647         4.53838        -3.90387
C          1.69863         3.89057        -3.49478
C          1.66264         2.96126        -2.45293
H          0.55651         5.26202        -4.71490
H         -0.20557        -1.07778        -3.27358
H          0.31116         0.57217        -3.67931
H         -1.20668         0.30908        -2.79026
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   H         -1.64858         3.09554        -1.70910
   H         -1.59713         4.74913        -3.57130
   H          2.64240         4.10997        -3.98843
   H          2.57073         2.45780        -2.13989
   N         -0.71387        -2.07994        -0.39228
   C         -1.60702        -1.96642         0.59976
   N         -1.82913        -0.75028         1.12377
   N         -2.24838        -3.05668         1.09271
   H         -1.31741         0.05006         0.72066
   C         -0.42616        -3.33732        -1.07991
   H          0.62498        -3.31840        -1.38259
   H         -1.03011        -3.41221        -1.99557
   C         -0.71265        -4.51836        -0.15979
   H          0.03045        -4.55757         0.64551
   H         -0.65318        -5.45706        -0.71980
   C         -2.10771        -4.36443         0.43813
   H         -2.28829        -5.12953         1.19897
   H         -2.87890        -4.47968        -0.33817
   C         -2.82104        -0.47137         2.16067
   H         -2.43919         0.34831         2.77559
   H         -3.76055        -0.13314         1.70103
   C         -3.05959        -1.72205         2.99948
   H         -3.91536        -1.57244         3.66541
   H         -2.18053        -1.93046         3.62063
   C         -3.32798        -2.90848         2.07857
   H         -3.37338        -3.83872         2.65259
   H         -4.29203        -2.79052         1.56155
   H          2.15755        -0.64845        -0.90582

56
PC1_2AP(O)  # E(6-31+G*)=-1261.85681622; E(ACCPVTZ)=-1262.28618746 H
   C          3.07241         0.19261         1.45590
   C          3.62116        -0.18923         2.69856
   C          3.55739         0.65013         3.80990
   C          2.94339         1.90567         3.72215
   C          2.39701         2.30608         2.50003
   C          2.46285         1.45996         1.39796
   N          3.19099        -0.61086         0.32855
   O          2.00241         1.92008         0.14964
   H          4.10142        -1.16216         2.77848
   H          3.99016         0.31956         4.75085
   H          2.89265         2.56331         4.58495
   H          1.92201         3.27703         2.38943
   H          3.43425        -1.57362         0.53495
   H          0.19893        -1.44544        -1.31940
   C          0.95862        -0.74849        -3.02856
   O          1.02460        -0.96224        -1.62422
   C          0.66620         1.93368        -0.10497
   O         -0.16189         1.46816         0.66012
   C          0.34466         2.60023        -1.39471
   C         -1.00136         2.66704        -1.78854
   C         -1.35177         3.29805        -2.98170
   C         -0.36038         3.86833        -3.78898
   C          0.98198         3.80561        -3.39932
   C          1.33678         3.17467        -2.20587
   H         -0.63347         4.36131        -4.71843
   H          0.94903        -1.69756        -3.58494
   H          1.84802        -0.18322        -3.32298
   H          0.07002        -0.16611        -3.30934
   H         -1.76132         2.22356        -1.15320
   H         -2.39504         3.34644        -3.28188
   H          1.75242         4.24897        -4.02438
   H          2.37677         3.12662        -1.90281
   N         -1.19739        -2.41707        -0.83753
   C         -1.96781        -2.25404         0.20495
   N         -1.70822        -1.18214         1.04129
   N         -2.96868        -3.12228         0.60254
   H         -1.07598        -0.49880         0.63523
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   C         -1.39526        -3.57847        -1.70450
   H         -0.41509        -3.89037        -2.08723
   H         -1.98861        -3.28263        -2.58500
   C         -2.08111        -4.74841        -0.99875
   H         -1.39967        -5.19663        -0.26415
   H         -2.35820        -5.52908        -1.71679
   C         -3.32452        -4.23109        -0.28486
   H         -3.77890        -5.01519         0.33145
   H         -4.08388        -3.91010        -1.01788
   C         -2.72885        -0.62297         1.92610
   H         -2.22511         0.01739         2.65587
   H         -3.44378         0.00662         1.37033
   C         -3.46813        -1.76590         2.61010
   H         -4.29447        -1.37912         3.21640
   H         -2.78244        -2.30566         3.27451
   C         -4.01440        -2.71215         1.54619
   H         -4.41500        -3.62143         2.00822
   H         -4.84605        -2.23113         1.00316
   H          2.43850        -0.56588        -0.36421

27
product1_2AP(O) [2-aminophenyl benzoate]  # E(6-31+G*)=-707.25860507; E(ACCPVTZ)=-
707.49433651 H
   C         -1.97618         0.48214        -1.58753
   C         -2.64462         1.20068        -2.59692
   C         -2.23460         2.47919        -2.97451
   C         -1.13133         3.08033        -2.35909
   C         -0.45454         2.38592        -1.35362
   C         -0.87430         1.11268        -0.97920
   O         -0.22336         0.53775         0.12805
   C          0.51243        -0.59529        -0.01636
   N         -2.43631        -0.76749        -1.15521
   O          0.57627        -1.21155        -1.06834
   C          1.20177        -0.98817         1.23969
   C          1.09073        -0.23535         2.42095
   C          1.99038        -2.15051         1.22419
   C          2.66104        -2.55579         2.37751
   C          2.54799        -1.80431         3.55325
   C          1.76286        -0.64616         3.57289
   H         -3.49942         0.73781        -3.08519
   H         -2.77653         3.00259        -3.75784
   H         -0.80241         4.07300        -2.65181
   H          0.39819         2.82372        -0.84248
   H         -1.69933        -1.45067        -1.00559
   H          0.48228         0.66206         2.43548
   H          2.07048        -2.72434         0.30652
   H          3.27064        -3.45499         2.36090
   H          3.07054        -2.12121         4.45202
   H          1.67439        -0.06271         4.48516
   H         -3.14889        -1.16084        -1.76203

50
INT3_2AP(O)  # E(6-31+G*)=-1146.11341745; E(ACCPVTZ)=-1146.49372112 H
   H         -2.83627        -1.60635        -0.19635
   H         -2.75179        -2.74181        -2.36469
   H         -2.86198        -4.00197        -1.12482
   C         -2.22119        -3.20629        -1.52320
   C         -1.92092        -2.15625        -0.45148
   H         -1.59832        -2.65686         0.47592
   N         -0.90499        -1.18778        -0.85635
   H         -1.07078        -4.46054        -2.87602
   H          0.95016         0.17868        -1.45667
   C         -0.03509        -1.52500        -1.76370
   C         -0.90589        -3.79594        -2.01985
   H          1.35758        -1.58983        -4.62174
   N         -0.00615        -2.72619        -2.45594
   N          0.89054        -0.55931        -2.15316
   H         -0.43105        -4.39771        -1.22608
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H	0.87811	-3.89131	-3.93178
H	2.62841	-0.04154	-3.17385
C	1.19686	-3.17736	-3.16360
C	1.94486	-2.00823	-3.79517
C	2.17858	-0.93838	-2.73618
H	2.90013	-2.35871	-4.20120
H	1.86281	-3.72187	-2.47157
H	2.87528	-1.31861	-1.96992
C	-1.69715	2.70134	-0.26475
C	-2.06975	3.91365	-0.88497
C	-1.56755	5.13934	-0.45068
C	-0.66901	5.20291	0.62141
C	-0.29006	4.01615	1.25422
C	-0.79657	2.79831	0.81276
O	-0.48157	1.63263	1.53897
C	0.68768	0.98987	1.28119
N	-2.24845	1.48608	-0.65037
O	1.43065	1.30631	0.36573
C	0.95677	-0.10979	2.24471
C	0.07284	-0.41929	3.29106
C	2.14584	-0.84176	2.09842
C	2.44689	-1.87417	2.98609
C	1.56167	-2.18332	4.02574
C	0.37642	-1.45505	4.17624
H	-2.76666	3.87700	-1.71973
H	-1.87879	6.05008	-0.95626
H	-0.27469	6.15510	0.96378
H	0.39450	4.02425	2.09810
H	-1.65585	0.64498	-0.58663
H	-0.84502	0.14611	3.40763
H	2.82446	-0.59215	1.28915
H	3.36904	-2.43691	2.86872
H	1.79638	-2.98847	4.71721
H	-0.31087	-1.69257	4.98370
H	-2.71416	1.52274	-1.55110

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TS3_2AP(O) # E(6-31+G*)=-1146.08507348; E(ACCPVTZ)=-1146.46315647 H

N	0.89648	1.13518	-1.19719
C	0.48101	0.72011	-2.38200
N	-0.41252	-0.30762	-2.42235
N	0.94982	1.21902	-3.57335
H	-0.78820	-0.60045	-1.51049
C	1.87123	2.21994	-1.09690
H	2.48842	2.04572	-0.20590
H	1.35242	3.17906	-0.93648
C	2.75398	2.32674	-2.33803
H	3.42432	1.46011	-2.39898
H	3.37403	3.22924	-2.29611
C	1.85937	2.36707	-3.57186
H	2.45661	2.31583	-4.48868
H	1.28881	3.30937	-3.60422
C	-1.16228	-0.68600	-3.61459
H	-1.46701	-1.73128	-3.50363
H	-2.08043	-0.08439	-3.71077
C	-0.28497	-0.49887	-4.84669
H	-0.86806	-0.66087	-5.75952
H	0.53514	-1.22709	-4.83394
C	0.28285	0.91698	-4.84489
H	1.02632	1.03377	-5.64048
H	-0.51767	1.65017	-5.03587
H	0.42437	0.65173	0.06402
C	-0.76371	-1.02705	1.16935
C	0.15387	-2.18168	1.57648
C	0.54572	-2.41116	2.90332
C	1.41218	-3.46496	3.21210
C	1.90286	-4.29372	2.19744
C	1.51648	-4.06743	0.87221

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   C          0.64404        -3.01930         0.56599
   H          0.33142        -2.84346        -0.45869
   H          1.89164        -4.70732         0.07713
   H          2.57839        -5.11083         2.43812
   H          1.70070        -3.63995         4.24566
   H          0.16083        -1.77790         3.69684
   N          0.13052         0.34330         1.18358
   C         -0.69948         1.30436         1.87248
   C         -1.72491         0.62422         2.53827
   O         -1.66426        -0.71652         2.38224
   C         -2.67355         1.32545         3.28240
   C         -2.55970         2.72232         3.33941
   C         -1.53489         3.40083         2.66797
   C         -0.58771         2.68629         1.91634
   H          0.21358         3.20140         1.39439
   H         -1.47049         4.48365         2.72413
   H         -3.28872         3.28787         3.91425
   H         -3.47155         0.79988         3.79822
   H          1.00171         0.17870         1.69742
   O         -1.42917        -1.12997         0.09175

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INT4_2AP(O)  # E(6-31+G*)=-1146.09602237; E(ACCPVTZ)=-1146.47650018 H
   N          1.21903         1.41174        -1.41549
   C          0.69382         0.73238        -2.49780
   N         -0.06931        -0.30084        -2.25046
   N          1.09284         1.14575        -3.75324
   H         -0.80051        -0.62265        -0.78308
   C          1.66515         2.79951        -1.51480
   H          2.27713         3.02229        -0.63493
   H          0.81343         3.50001        -1.51416
   C          2.47376         2.96430        -2.79637
   H          3.39629         2.37508        -2.72929
   H          2.75124         4.01383        -2.94262
   C          1.63813         2.48889        -3.98093
   H          2.24890         2.44647        -4.88966
   H          0.81742         3.20024        -4.17478
   C         -0.59758        -1.09559        -3.35856
   H         -0.64111        -2.14456        -3.03868
   H         -1.63738        -0.79346        -3.56228
   C          0.23228        -0.96943        -4.63653
   H         -0.28663        -1.43226        -5.48390
   H          1.19431        -1.48332        -4.51308
   C          0.48265         0.50730        -4.92161
   H          1.17122         0.63373        -5.76457
   H         -0.45954         1.01457        -5.18868
   H          0.78825         1.13160        -0.53352
   C         -0.75467        -0.85897         1.21622
   C          0.03048        -2.13170         1.52406
   C          0.51391        -2.36220         2.82140
   C          1.25351        -3.51162         3.10731
   C          1.52005        -4.44347         2.09707
   C          1.03931        -4.21900         0.80447
   C          0.29469        -3.06875         0.52007
   H         -0.08400        -2.89956        -0.48222
   H          1.23944        -4.93875         0.01482
   H          2.09576        -5.33852         2.31861
   H          1.61645        -3.68215         4.11763
   H          0.30148        -1.64886         3.61361
   N          0.08521         0.36153         1.35192
   C         -0.68829         1.27292         2.12822
   C         -1.82109         0.60518         2.60278
   O         -1.81036        -0.71159         2.22201
   C         -2.77538         1.23338         3.38827
   C         -2.56012         2.58902         3.69635
   C         -1.42842         3.26647         3.22976
   C         -0.47497         2.61143         2.42887
   H          0.40385         3.13664         2.06465
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   H         -1.28384         4.31359         3.48114
   H         -3.28930         3.11502         4.30675
   H         -3.64615         0.69689         3.75290
   H          0.99644         0.15848         1.76021
   O         -1.40983        -0.87670         0.00252

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INT5_2AP  # E(6-31+G*)=-1146.09151384; E(ACCPVTZ)=-1146.47260503 H
   C          1.70469         0.61905         0.01890
   C          2.48860        -0.57338         0.54090
   C          1.85769        -1.54106         1.33242
   C          2.55255        -2.68680         1.72975
   C          3.88285        -2.87427         1.34107
   C          4.51827        -1.90538         0.55769
   C          3.82480        -0.75935         0.15785
   H          4.32753        -0.00721        -0.44396
   H          5.55401        -2.03965         0.25670
   H          4.42107        -3.76718         1.64845
   H          2.05282        -3.43252         2.34284
   H          0.82445        -1.40058         1.63499
   O          2.54516         1.79117        -0.01042
   C          1.71996         2.87096         0.25113
   C          0.48769         2.40736         0.72849
   N          0.55202         1.01202         0.79125
   H         -0.31666         0.45375         0.64610
   C         -0.50988         3.31196         1.07878
   C         -0.23200         4.68463         0.92964
   C          1.00415         5.12978         0.45178
   C          2.01532         4.21099         0.09972
   H          2.97772         4.53902        -0.28170
   H          1.19141         6.19435         0.34168
   H         -0.99940         5.40901         1.19032
   H         -1.47232         2.97345         1.45184
   O          1.26082         0.34773        -1.32472
   H          1.98736        -0.06765        -1.82315
   N         -1.87367        -0.57647         0.45710
   C         -2.24886        -1.15300        -0.65261
   N         -1.45078        -0.97638        -1.76947
   N         -3.42936        -1.85127        -0.83782
   H         -0.54347        -0.57350        -1.54761
   C         -2.73504        -0.65863         1.63518
   H         -2.65047         0.28553         2.18972
   H         -2.36082        -1.44359         2.31286
   C         -4.20035        -0.93690         1.29469
   H         -4.64864        -0.05610         0.81658
   H         -4.77823        -1.15516         2.20041
   C         -4.26637        -2.11827         0.33254
   H         -5.29042        -2.28076        -0.02245
   H         -3.94390        -3.04465         0.83777
   C         -1.48253        -1.88949        -2.90836
   H         -0.99434        -1.39192        -3.75263
   H         -0.92301        -2.81802        -2.70309
   C         -2.93470        -2.21921        -3.23092
   H         -2.99174        -2.96501        -4.03111
   H         -3.45048        -1.31312        -3.57190
   C         -3.61176        -2.75902        -1.97492
   H         -4.68958        -2.87192        -2.13663
   H         -3.21333        -3.75932        -1.73186

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TS4_2AP  # E(6-31+G*)=-1146.07882661; E(ACCPVTZ)=-1146.46085619 H
   C          1.66240         0.67899         0.25470
   C          2.41917        -0.55911         0.59743
   C          1.81557        -1.56153         1.37070
   C          2.51710        -2.72496         1.69498
   C          3.83531        -2.89893         1.25893
   C          4.44616        -1.89749         0.49660
   C          3.74410        -0.73526         0.16713
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   H          4.22586         0.03911        -0.42214
   H          5.47251        -2.01870         0.15901
   H          4.38261        -3.80251         1.51529
   H          2.03574        -3.49310         2.29542
   H          0.79890        -1.42060         1.72269
   O          2.47994         1.78737        -0.02026
   C          1.67653         2.88134         0.21355
   C          0.46813         2.41253         0.76450
   N          0.52337         1.03319         0.88030
   H         -0.98484        -0.00448         0.55691
   C         -0.51606         3.34222         1.12208
   C         -0.24777         4.70478         0.91111
   C          0.96743         5.13999         0.36123
   C          1.96734         4.21510         0.00012
   H          2.91522         4.53388        -0.42426
   H          1.14345         6.20168         0.21024
   H         -1.00231         5.44019         1.18067
   H         -1.46079         3.02000         1.55282
   O          1.11704         0.23283        -1.49217
   H          1.83874        -0.27101        -1.90626
   N         -1.87548        -0.53522         0.47576
   C         -2.13347        -1.20590        -0.66079
   N         -1.24597        -1.13654        -1.66121
   N         -3.28934        -1.90567        -0.79891
   H         -0.34506        -0.60829        -1.52140
   C         -2.72038        -0.59489         1.66719
   H         -2.63702         0.36588         2.18337
   H         -2.35221        -1.37096         2.35354
   C         -4.16266        -0.88349         1.26779
   H         -4.59114        -0.01462         0.75413
   H         -4.76864        -1.08294         2.15730
   C         -4.19600        -2.09548         0.34198
   H         -5.20142        -2.24299        -0.06335
   H         -3.92183        -3.01018         0.88861
   C         -1.38679        -1.86777        -2.91951
   H         -0.92507        -1.26491        -3.70697
   H         -0.83606        -2.81788        -2.86483
   C         -2.85959        -2.12571        -3.21505
   H         -2.96191        -2.80510        -4.06727
   H         -3.36173        -1.18491        -3.47064
   C         -3.52031        -2.74132        -1.98552
   H         -4.60301        -2.81386        -2.12506
   H         -3.14030        -3.75829        -1.80680

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PC_2AP  # E(6-31+G*)=-1146.11556855; E(ACCPVTZ)=-1146.49939506 H
   C          2.15066         0.66543         0.57559
   C          2.65662        -0.70402         0.61685
   C          2.36624        -1.58655        -0.44050
   C          2.84750        -2.89430        -0.40790
   C          3.61835        -3.33650         0.67425
   C          3.90761        -2.46221         1.72747
   C          3.43230        -1.15067         1.70229
   H          3.65711        -0.47526         2.52119
   H          4.50457        -2.80122         2.56988
   H          3.99266        -4.35657         0.69505
   H          2.62297        -3.56841        -1.23002
   H          1.77615        -1.24288        -1.28432
   O          2.57462         1.52827         1.55756
   C          1.95249         2.72234         1.27244
   C          1.17515         2.52496         0.12439
   N          1.32658         1.19911        -0.28741
   H         -0.92715         0.08492        -0.25590
   C          0.42264         3.58078        -0.40149
   C          0.49143         4.80546         0.26666
   C          1.28211         4.97626         1.42142
   C          2.03883         3.92648         1.95511
   H          2.65132         4.04674         2.84264
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H	1.30648	5.94626	1.90984
H	-0.07853	5.64954	-0.11125
H	-0.18626	3.45091	-1.29070
O	0.30609	0.28553	-3.00176
H	0.71548	0.63686	-2.18721
N	-1.82546	-0.23632	0.09047
C	-2.51146	-0.98727	-0.85736
N	-2.08452	-0.94560	-2.08759
N	-3.65295	-1.63545	-0.41958
H	-0.53690	-0.14236	-2.68607
C	-1.85500	-0.58342	1.51143
H	-1.45816	0.26683	2.07485
H	-1.21714	-1.45606	1.73019
C	-3.29547	-0.87923	1.91041
H	-3.89762	0.03298	1.82143
H	-3.34249	-1.21714	2.95137
C	-3.85480	-1.96434	0.99599
H	-4.93235	-2.08351	1.15586
H	-3.38340	-2.93473	1.22884
C	-2.82426	-1.65655	-3.12970
H	-2.75364	-1.07412	-4.05704
H	-2.33021	-2.62006	-3.33444
C	-4.29072	-1.89965	-2.76963
H	-4.76251	-2.57763	-3.49041
H	-4.84495	-0.95230	-2.79090
C	-4.36436	-2.49518	-1.36799
H	-5.40318	-2.57463	-1.02783
H	-3.93829	-3.51277	-1.35913