

Theoretical study on the formation of H- and O-atoms, HONO, OH, NO, and NO₂
from the lowest-lying singlet and triplet states
in *ortho*-nitrophenol photolysis

- Supporting information -

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Extended potential energy surfaces

Ground state S_0 PES

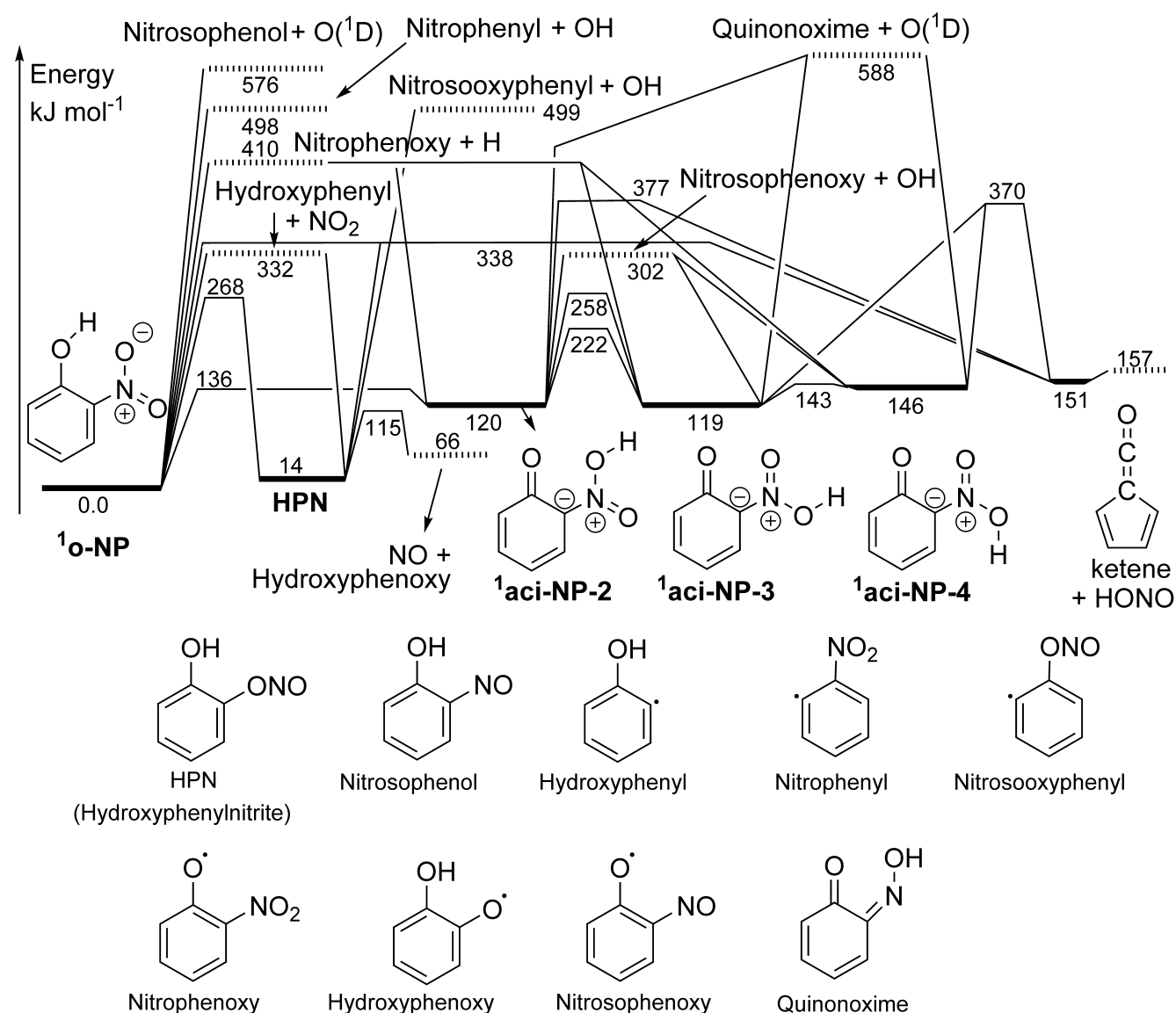


Figure SI-1: S_0 singlet potential energy surface at the G3SX//M06-2X/aug-cc-pVTZ level of theory. The depicted Lewis structures each represent only one of many resonance structures.

The lowest-energy channels are discussed in the main text. The first additional channel shown is the formation of nitrophenoxy by direct H-atom loss, which is possible both from $\mathbf{o}\text{-NP}$ as from $\mathbf{aci}\text{-NP}$. These loss processes are shown here without an exit barrier. However, the relative stability of the nitrophenoxy fragment stems from the delocalization of the phenoxy radical across the aromatic ring.

Constrained optimization along the dissociation pathway show that there might be a shallow, broad exit barrier, with (for **o-NP**) a maximum near 2.1 Å separation with a barrier < 4.0 kJ mol⁻¹ at the M06-2X level of theory. On the other hand, single point calculations at the G3SX level of theory for these geometries do not show this energy maximum. As the calculations are influenced by the proximity of the H-migration pathways between **o-NP** and **aci-NP**, it is not clear how reliable such calculations are. Grygoryeva et al. observe H-atom formation with a minimum appearance energy of ~410 kJ mol⁻¹ but do not discuss the absolute yield, nor the formation of other products. It is therefore not clear whether the current H-formation channel is the one responsible for the observed H-atoms, but if so, it is expected to have a significantly lower yield than some of the other photofragments. These authors also repeatedly refer to the O–H bond as the weakest bond in the system; we find that at least the direct C–N bond scission has a lower BDE, even when disregarding the isomerisation channels or the roaming formation of HONO.

Both **o-NP** and **HPN** can directly lose the OH radical, forming a nitro- or nitrosooxyphenyl radical, respectively. We found no evidence for a post-reactive complex, or an exit barrier for these channels. The highest fragmentation channels examined in this study is the loss of an O(¹D) atom from the NO₂ moiety. For **o-NP** this leads to nitrosophenol, while the same process in **aci-NP** leads to an oxime. Given the high exoergicity, we have not examined these channels in much detail; exploratory constrained optimizations showed no evidence of an exit barrier. Note that o-benzoquinonoxime has several conformers, as the C=N double bond prevents internal rotation, such that oxime formation from the distinct **aci-NP** conformers will lead to different oximes.

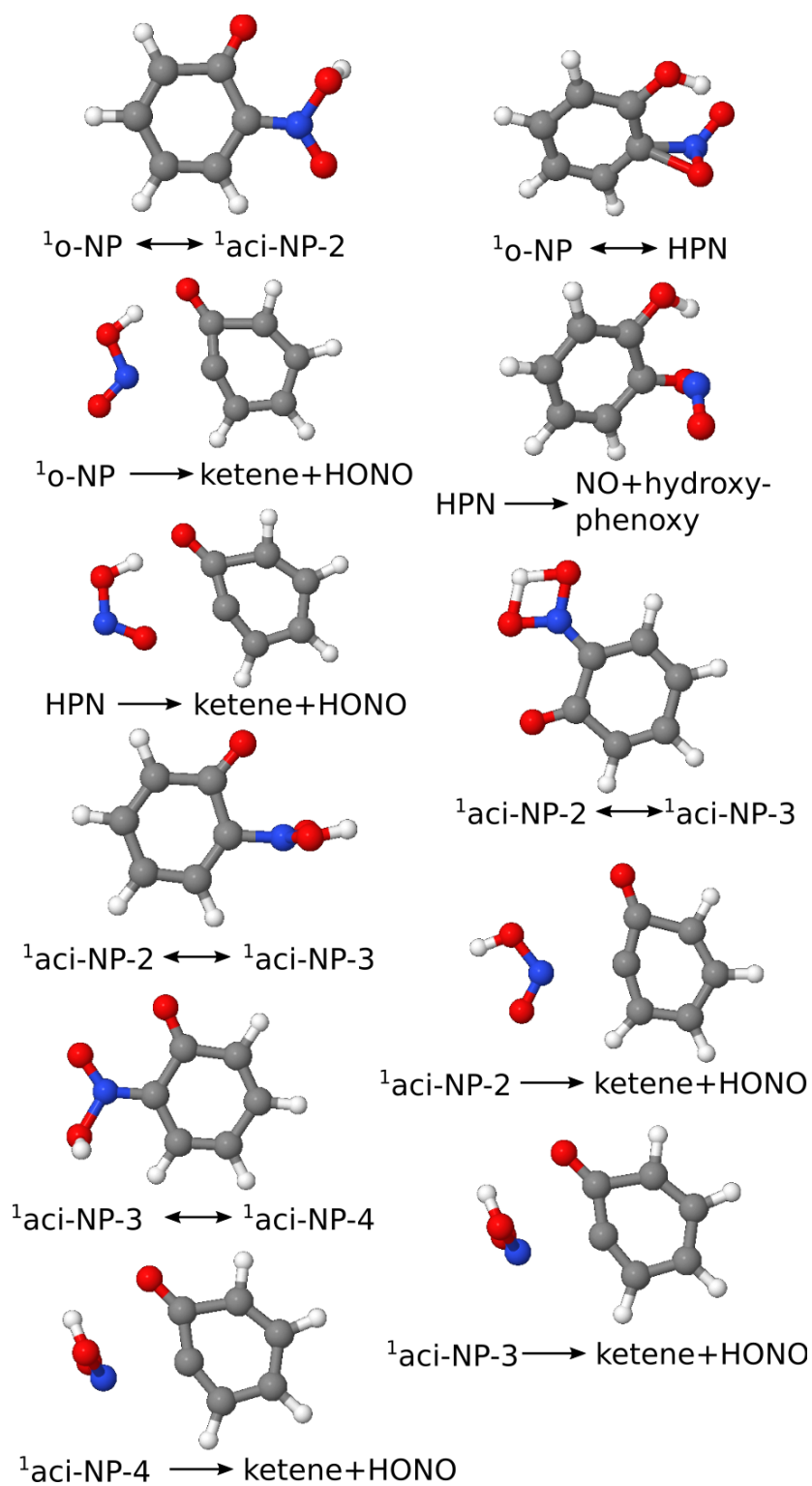


Figure SI-2: Graphical representation of the saddle point geometries on the S_0 PES as obtained from M06-2X/aug-cc-pVTZ optimizations. Only a single conformer is shown for each TS.

First Excited State T_1 PES

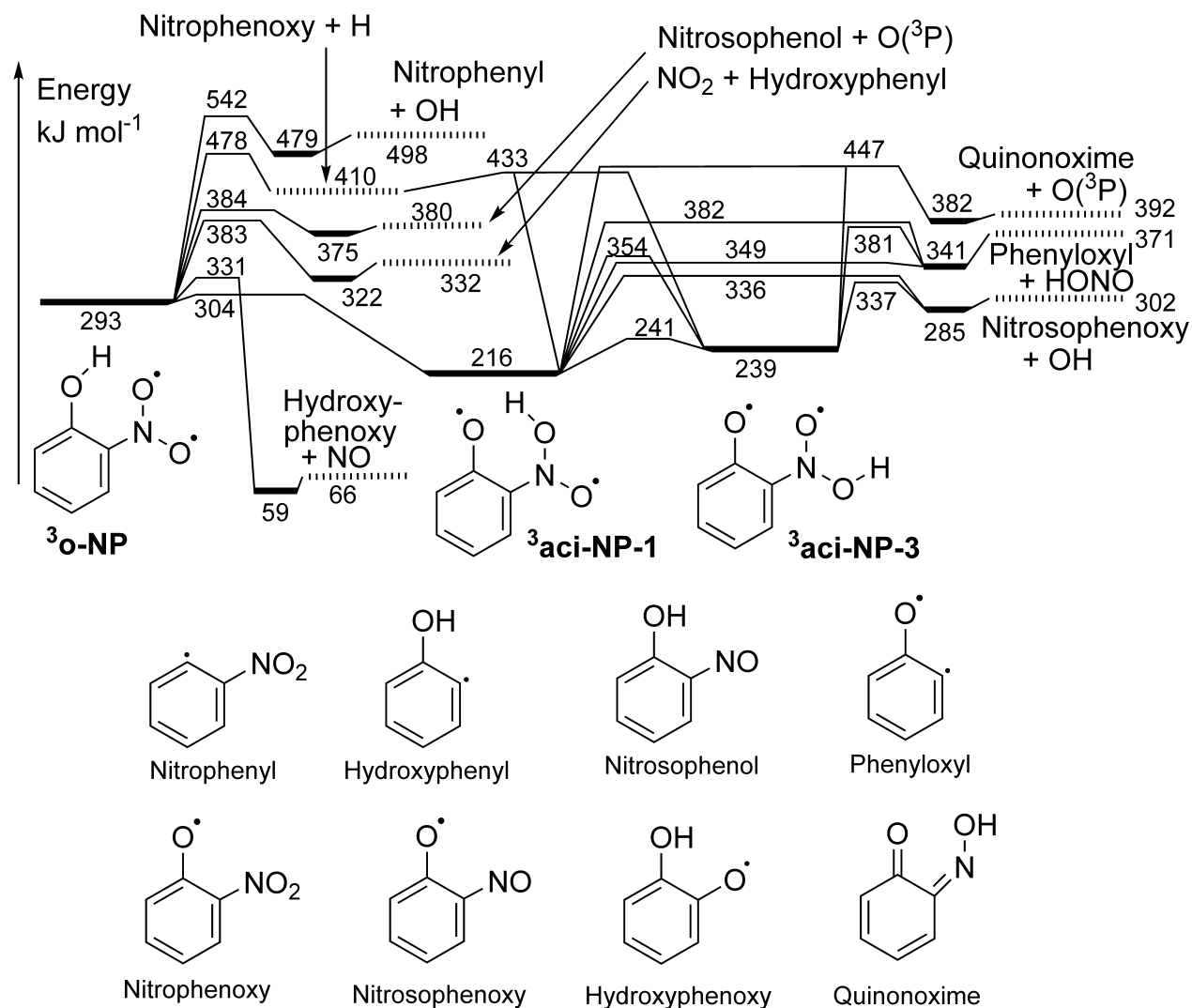


Figure SI-3: T_1 triplet potential energy surface at the G3SX//M06-2X/aug-cc-pVTZ level of theory. The depicted Lewis structures each represent only one of many resonance structures.

The low-lying pathways are discussed in the main text. Contrary to the singlet surface, H-atom loss from **o-NP** or **aci-NP** involves a fairly significant energy barrier, which finds its origin in the rearrangement of one of the free radical electron to the (delocalized) phenoxy radical site in the nitrophenoxyl co-product. This barrier prevents the H-loss to compete effectively with the lower-lying exit channels, even if the product energy is not exceedingly high compared to the other products. Formation of o-benzoquinonoxime + $\text{O}(^3\text{P})$ from **aci-NP** is hindered in a similar manner, with comparatively large exit barriers. Finally, **o-NP** can lose the OH fragment directly, forming nitrophenyl as a coproduct. For all of the above products, we find post-reactive complexes, with the exception of

nitrophenoxy + H, where the optimized geometry for the product complex has a similar or slightly higher energy than the separated products (both before and after ZPE-correction) at all levels of theory used; this complex could thus be an artifact of the methodologies, and suggests that any product complex with H-atoms is very shallow or non-existent.

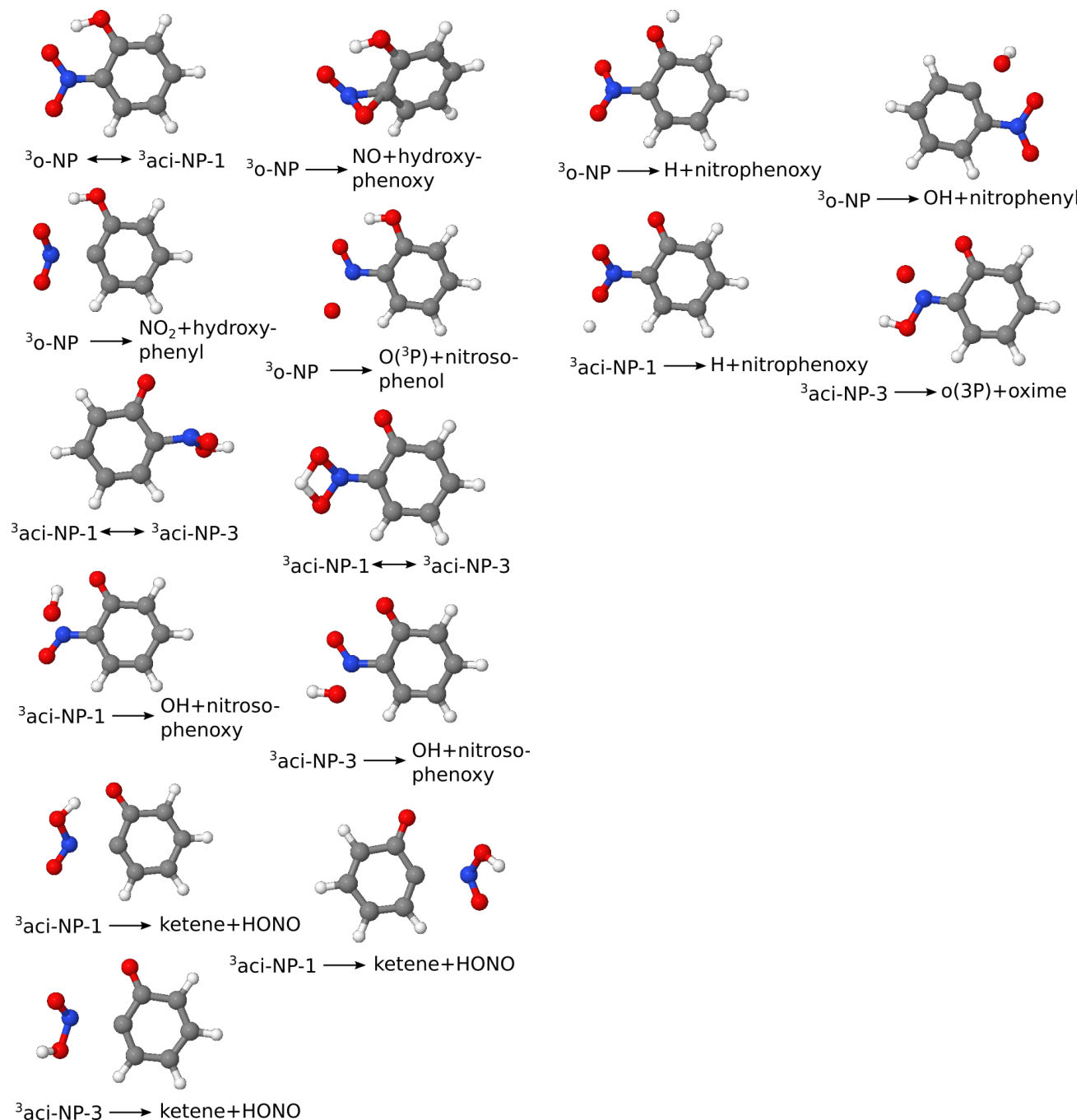


Figure SI-4: Graphical representation of the saddle point geometries on the T_1 PES as obtained from M06-2X/aug-cc-pVTZ optimizations. Only a single conformer is shown for each TS.

Additional product yields graphs.

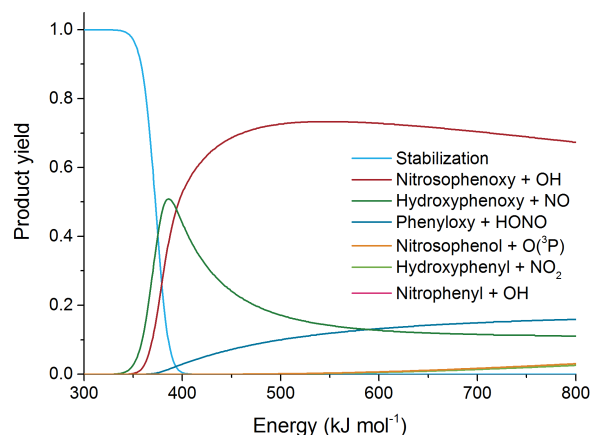


Figure SI-5: Product distribution at 298K and 200 mTorr as a function of the internal energy on the T_1 triplet surface, where the ISC process from the S_1 state forms 100 % $^3\text{o-NP}$. Energies are relative to the $^1\text{o-NP}$ ground state.

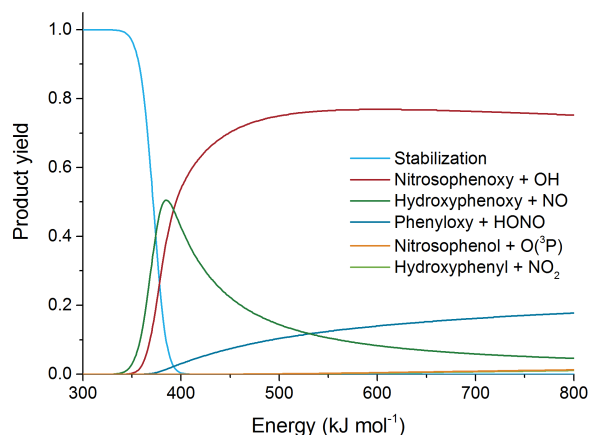


Figure SI-6: Product distribution at 298K and 200 mTorr as a function of the internal energy on the T_1 triplet surface, where the ISC process from the S_1 state forms 100 % $^3\text{aci-NP}$. Energies are relative to the $^1\text{o-NP}$ ground state.

Quantum chemical data based on M06-2X/aug-cc-pVTZ geometries

Product fragments

```
=====
H
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -0.49994519
E(G3SX) excl. ZPE (Hartree): -0.49995454
E(G3X(MP2)) excl. ZPE (Hartree): -0.50182792
E(G3X(MP3)) excl. ZPE (Hartree): -0.50187392
E(G3X) excl. ZPE (Hartree): -0.50096992
E(MP2-Full/G3MP2large) (Hartree): -0.49981792
E(MP2-Full/G3Xlarge) (Hartree): -0.49981792
E(MP2-Full/G3large) (Hartree): -0.49981792
E(MP2/6-31+G(d)) (Hartree): -0.49823291
E(MP2/6-31G(2df,p)) (Hartree): -0.49823291
E(MP2/6-31G(d)) (Hartree): -0.49823291
E(MP2/G3MP2large) (Hartree): -0.49981792
E(MP2/G3Xlarge) (Hartree): -0.49981792
E(MP2/G3large) (Hartree): -0.49981792
E(MP3/6-31+G(d)) (Hartree): -0.49823291
E(MP3/6-31G(2df,p)) (Hartree): -0.49823291
E(MP3/6-31G(d)) (Hartree): -0.49823291
E(MP4/6-31+G(d)) (Hartree): -0.49823291
E(MP4/6-31G(2df,p)) (Hartree): -0.49823291
E(MP4/6-31G(d)) (Hartree): -0.49823291
E(PMP2/G3MP2large) (Hartree): -0.49981792
E(PMP2/G3Xlarge) (Hartree): -0.49981792
E(PMP2/G3large) (Hartree): -0.49981792
E(PUHF/G3MP2large) (Hartree): -0.49981792
E(PUHF/G3Xlarge) (Hartree): -0.49981792
E(PUHF/G3large) (Hartree): -0.49981792
E(QCISD(T)/6-31G(d)) (Hartree): -0.49823291
E(UHF/6-31+G(d)) (Hartree): -0.49823291
E(UHF/6-31G(2df,p)) (Hartree): -0.49823291
E(UHF/6-31G(d)) (Hartree): -0.49823291
E(UHF/G3MP2large) (Hartree): -0.49981792
E(UHF/G3Xlarge) (Hartree): -0.49981792
E(UHF/G3large) (Hartree): -0.49981792
E(UM062X/Aug-CC-pVTZ) (Hartree): -0.49820646
Point group : OH
Electronic state : 2-A1G
Cartesian coordinates (Angs):
      H      0.000000      0.000000      0.000000
```

NO

```
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -129.85518153
E(G3SX) excl. ZPE (Hartree): -129.85719513
E(G3X(MP2)) excl. ZPE (Hartree): -129.76009546
E(G3X(MP3)) excl. ZPE (Hartree): -129.84649812
E(G3X) excl. ZPE (Hartree): -129.84021350
E(MP2-Full/G3Xlarge) (Hartree): -129.77830809
E(MP2-Full/G3large) (Hartree): -129.77830809
E(MP2/6-31+G(d)) (Hartree): -129.56665261
E(MP2/6-31G(2df,p)) (Hartree): -129.63184893
E(MP2/6-31G(d)) (Hartree): -129.55865719
E(MP2/G3MP2large) (Hartree): -129.68698172
E(MP3/6-31+G(d)) (Hartree): -129.56421131
E(MP3/6-31G(2df,p)) (Hartree): -129.63250761
E(MP3/6-31G(d)) (Hartree): -129.55724531
E(MP4/6-31+G(d)) (Hartree): -129.58863028
E(MP4/6-31G(2df,p)) (Hartree): -129.65801005
E(MP4/6-31G(d)) (Hartree): -129.58011312
E(PMP2/6-31+G(d)) (Hartree): -129.57054637
E(PMP2/6-31G(2df,p)) (Hartree): -129.63584332
```

E(PMP2/6-31G(d)) (Hartree): -129.56250537
 E(PMP2/G3MP2large) (Hartree): -129.69116979
 E(PMP2/G3Xlarge) (Hartree): -129.78251976
 E(PMP2/G3large) (Hartree): -129.78251976
 E(PMP3/6-31+G(d)) (Hartree): -129.56669395
 E(PMP3/6-31G(2df,p)) (Hartree): -129.63494565
 E(PMP3/6-31G(d)) (Hartree): -129.55967750
 E(PUHF/6-31+G(d)) (Hartree): -129.25664295
 E(PUHF/6-31G(2df,p)) (Hartree): -129.26552388
 E(PUHF/6-31G(d)) (Hartree): -129.25286301
 E(PUHF/G3MP2large) (Hartree): -129.30026374
 E(PUHF/G3Xlarge) (Hartree): -129.30061830
 E(PUHF/G3large) (Hartree): -129.30061830
 E(QCISD(T)/6-31G(d)) (Hartree): -129.57833766
 E(QCISD/6-31G(d)) (Hartree): -129.56886826
 E(UHF/6-31+G(d)) (Hartree): -129.25139518
 E(UHF/6-31G(2df,p)) (Hartree): -129.25994403
 E(UHF/6-31G(d)) (Hartree): -129.24764099
 E(UHF/G3MP2large) (Hartree): -129.29453296
 E(UHF/G3Xlarge) (Hartree): -129.29485123
 E(UHF/G3large) (Hartree): -129.29485123
 E(UM062X/Aug-CC-pVTZ) (Hartree): -129.89335138
 Point group : C*V
 Cartesian coordinates (Angs):
 N 0.000000 0.000000 -0.606410
 O 0.000000 0.000000 0.530609
 Rotational constants (GHz): 0.00000000 52.3561998 52.3561998
 Vibrational harmonic frequencies (cm-1):
 2066.0391 (SG)
 Zero-point correction (Hartree): 0.004707

NO2

 E(G3SX(MP3)) excl. ZPE (Hartree): -205.01584468
 E(G3SX) excl. ZPE (Hartree): -205.01988276
 E(G3X(MP2)) excl. ZPE (Hartree): -204.86893300
 E(G3X(MP3)) excl. ZPE (Hartree): -204.99985241
 E(G3X) excl. ZPE (Hartree): -204.99176644
 E(MP2-Full/G3Xlarge) (Hartree): -204.90788753
 E(MP2-Full/G3large) (Hartree): -204.90788753
 E(MP2/6-31+G(d)) (Hartree): -204.57037212
 E(MP2/6-31G(2df,p)) (Hartree): -204.67991287
 E(MP2/6-31G(d)) (Hartree): -204.55589789
 E(MP2/G3MP2large) (Hartree): -204.76935316
 E(MP3/6-31+G(d)) (Hartree): -204.54693445
 E(MP3/6-31G(2df,p)) (Hartree): -204.66190042
 E(MP3/6-31G(d)) (Hartree): -204.53461201
 E(MP4/6-31+G(d)) (Hartree): -204.59755518
 E(MP4/6-31G(2df,p)) (Hartree): -204.71435680
 E(MP4/6-31G(d)) (Hartree): -204.58188015
 E(PMP2/6-31+G(d)) (Hartree): -204.57383055
 E(PMP2/6-31G(2df,p)) (Hartree): -204.68351567
 E(PMP2/6-31G(d)) (Hartree): -204.55931932
 E(PMP2/G3MP2large) (Hartree): -204.77307110
 E(PMP2/G3Xlarge) (Hartree): -204.91162314
 E(PMP2/G3large) (Hartree): -204.91162314
 E(PMP3/6-31+G(d)) (Hartree): -204.54858573
 E(PMP3/6-31G(2df,p)) (Hartree): -204.66354541
 E(PMP3/6-31G(d)) (Hartree): -204.53615841
 E(PUHF/6-31+G(d)) (Hartree): -204.04289321
 E(PUHF/6-31G(2df,p)) (Hartree): -204.05823099
 E(PUHF/6-31G(d)) (Hartree): -204.03621263
 E(PUHF/G3MP2large) (Hartree): -204.11401850
 E(PUHF/G3Xlarge) (Hartree): -204.11460323
 E(PUHF/G3large) (Hartree): -204.11460323
 E(QCISD(T)/6-31G(d)) (Hartree): -204.57276734
 E(QCISD/6-31G(d)) (Hartree): -204.55230093
 E(UHF/6-31+G(d)) (Hartree): -204.03721958
 E(UHF/6-31G(2df,p)) (Hartree): -204.05220717
 E(UHF/6-31G(d)) (Hartree): -204.03046970
 E(UHF/G3MP2large) (Hartree): -204.10795218

E(UHF/G3Xlarge) (Hartree): -204.10850757
 E(UHF/G3large) (Hartree): -204.10850757
 E(UM062X/Aug-CC-pVTZ) (Hartree): -205.07463512
 Point group : CS
 Electronic state : 2-A'
 Cartesian coordinates (Angs):
 N 0.000000 0.314436 0.000000
 O 1.090251 -0.137584 0.000000
 O -1.090251 -0.137584 0.000000
 Rotational constants (GHz): 253.9759700 13.2908500 12.6299100
 Vibrational harmonic frequencies (cm-1):
 783.4880 (A') 1465.2746 (A') 1775.5590 (A')
 Zero-point correction (Hartree): 0.009168

OH

 E(G3SX(MP3)) excl. ZPE (Hartree): -75.71102028
 E(G3SX) excl. ZPE (Hartree): -75.71246098
 E(G3X(MP2)) excl. ZPE (Hartree): -75.66442447
 E(G3X(MP3)) excl. ZPE (Hartree): -75.70862620
 E(G3X) excl. ZPE (Hartree): -75.70439979
 E(MP2-Full/G3Xlarge) (Hartree): -75.66086231
 E(MP2-Full/G3large) (Hartree): -75.66086231
 E(MP2/6-31+G(d)) (Hartree): -75.52956768
 E(MP2/6-31G(2df,p)) (Hartree): -75.57415177
 E(MP2/6-31G(d)) (Hartree): -75.52098992
 E(MP2/G3MP2large) (Hartree): -75.61448262
 E(MP3/6-31+G(d)) (Hartree): -75.54094245
 E(MP3/6-31G(2df,p)) (Hartree): -75.58827244
 E(MP3/6-31G(d)) (Hartree): -75.53293272
 E(MP4/6-31+G(d)) (Hartree): -75.54508531
 E(MP4/6-31G(2df,p)) (Hartree): -75.59280077
 E(MP4/6-31G(d)) (Hartree): -75.53605500
 E(PMP2/6-31+G(d)) (Hartree): -75.53124231
 E(PMP2/6-31G(2df,p)) (Hartree): -75.57590848
 E(PMP2/6-31G(d)) (Hartree): -75.52250875
 E(PMP2/G3MP2large) (Hartree): -75.61640846
 E(PMP2/G3Xlarge) (Hartree): -75.66280711
 E(PMP2/G3large) (Hartree): -75.66280711
 E(PMP3/6-31+G(d)) (Hartree): -75.54196412
 E(PMP3/6-31G(2df,p)) (Hartree): -75.58918938
 E(PMP3/6-31G(d)) (Hartree): -75.53376814
 E(PUHF/6-31+G(d)) (Hartree): -75.38932022
 E(PUHF/6-31G(2df,p)) (Hartree): -75.39603434
 E(PUHF/6-31G(d)) (Hartree): -75.38475714
 E(PUHF/G3MP2large) (Hartree): -75.42096812
 E(PUHF/G3Xlarge) (Hartree): -75.42112282
 E(PUHF/G3large) (Hartree): -75.42112282
 E(QCISD(T)/6-31G(d)) (Hartree): -75.53705895
 E(QCISD/6-31G(d)) (Hartree): -75.53582660
 E(UHF/6-31+G(d)) (Hartree): -75.38656153
 E(UHF/6-31G(2df,p)) (Hartree): -75.39287673
 E(UHF/6-31G(d)) (Hartree): -75.38208843
 E(UHF/G3MP2large) (Hartree): -75.41770551
 E(UHF/G3Xlarge) (Hartree): -75.41782333
 E(UHF/G3large) (Hartree): -75.41782333
 E(UM062X/Aug-CC-pVTZ) (Hartree): -75.73381011
 Point group : C*V
 Cartesian coordinates (Angs):
 O 0.000000 0.000000 0.108021
 H 0.000000 0.000000 -0.864170
 Rotational constants (GHz): 0.0000000 563.9825531 563.9825531
 Vibrational harmonic frequencies (cm-1):
 3766.2007 (SG)
 Zero-point correction (Hartree): 0.008580

HONO cis

 E(G3SX(MP3)) excl. ZPE (Hartree): -205.65011379
 E(G3SX) excl. ZPE (Hartree): -205.65412843
 E(G3X(MP2)) excl. ZPE (Hartree): -205.50507485

E(G3X(MP3)) excl. ZPE (Hartree): -205.63497654
 E(G3X) excl. ZPE (Hartree): -205.62643391
 E(MP2-Full/G3Xlarge) (Hartree): -205.52941397
 E(MP2-Full/G3large) (Hartree): -205.52941397
 E(MP2/6-31+G(d)) (Hartree): -205.17909046
 E(MP2/6-31G(2df,p)) (Hartree): -205.29792705
 E(MP2/6-31G(d)) (Hartree): -205.16416932
 E(MP2/G3MP2large) (Hartree): -205.39109721
 E(MP3/6-31+G(d)) (Hartree): -205.17144543
 E(MP3/6-31G(2df,p)) (Hartree): -205.29539172
 E(MP3/6-31G(d)) (Hartree): -205.15852837
 E(MP4/6-31+G(d)) (Hartree): -205.21001448
 E(MP4/6-31G(2df,p)) (Hartree): -205.33632507
 E(MP4/6-31G(d)) (Hartree): -205.19399785
 E(QCISD(T)/6-31G(d)) (Hartree): -205.19047728
 E(QCISD/6-31G(d)) (Hartree): -205.17352729
 E(RHF/6-31+G(d)) (Hartree): -204.64504729
 E(RHF/6-31G(2df,p)) (Hartree): -204.66298651
 E(RHF/6-31G(d)) (Hartree): -204.63841242
 E(RHF/G3MP2large) (Hartree): -204.71965743
 E(RHF/G3Xlarge) (Hartree): -204.72020711
 E(RHF/G3large) (Hartree): -204.72020711
 E(RM062X/Aug-CC-pVTZ) (Hartree): -205.70914802
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):

H	-0.570911	-1.259434	0.000000
N	0.000000	0.540351	0.000000
O	-1.001522	-0.383484	0.000000
O	1.072886	0.068107	0.000000

 Rotational constants (GHz): 86.3096600 13.6583000 11.7922100
 Vibrational harmonic frequencies (cm-1):

687.7319 (A')	703.3714 (A')	969.5133 (A')
1375.1919 (A')	1780.2819 (A')	3665.8048 (A')

 Zero-point correction (Hartree): 0.020918

HONO trans

 E(G3SX(MP3)) excl. ZPE (Hartree): -205.65145884
 E(G3SX) excl. ZPE (Hartree): -205.65515072
 E(G3X(MP2)) excl. ZPE (Hartree): -205.50598728
 E(G3X(MP3)) excl. ZPE (Hartree): -205.63592407
 E(G3X) excl. ZPE (Hartree): -205.62728119
 E(MP2-Full/G3Xlarge) (Hartree): -205.53001596
 E(MP2-Full/G3large) (Hartree): -205.53001596
 E(MP2/6-31+G(d)) (Hartree): -205.17945555
 E(MP2/6-31G(2df,p)) (Hartree): -205.29631327
 E(MP2/6-31G(d)) (Hartree): -205.16195924
 E(MP2/G3MP2large) (Hartree): -205.39172292
 E(MP3/6-31+G(d)) (Hartree): -205.17195116
 E(MP3/6-31G(2df,p)) (Hartree): -205.29445530
 E(MP3/6-31G(d)) (Hartree): -205.15694184
 E(MP4/6-31+G(d)) (Hartree): -205.21026902
 E(MP4/6-31G(2df,p)) (Hartree): -205.33470546
 E(MP4/6-31G(d)) (Hartree): -205.19175280
 E(QCISD(T)/6-31G(d)) (Hartree): -205.18855892
 E(QCISD/6-31G(d)) (Hartree): -205.17168150
 E(RHF/6-31+G(d)) (Hartree): -204.64407758
 E(RHF/6-31G(2df,p)) (Hartree): -204.66124102
 E(RHF/6-31G(d)) (Hartree): -204.63601564
 E(RHF/G3MP2large) (Hartree): -204.71923554
 E(RHF/G3Xlarge) (Hartree): -204.71978022
 E(RHF/G3large) (Hartree): -204.71978022
 E(RM062X/Aug-CC-pVTZ) (Hartree): -205.70918527
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):

H	1.753035	-0.148500	0.000000
N	0.000000	0.507661	0.000000
O	0.882522	-0.566865	0.000000
O	-1.101651	0.141224	0.000000

Rotational constants (GHz): 97.1747900 13.0282200 11.4880200
 Vibrational harmonic frequencies (cm-1):
 578.9048 (A'') 700.9305 (A') 906.1603 (A')
 1343.0818 (A') 1841.5251 (A') 3830.3272 (A')
 Zero-point correction (Hartree): 0.020961

O(1D)

 E(G3SX(MP3)) excl. ZPE (Hartree): -74.96737755
 E(G3SX) excl. ZPE (Hartree): -74.96785098
 E(G3X(MP2)) excl. ZPE (Hartree): -74.91741406
 E(G3X(MP3)) excl. ZPE (Hartree): -74.96003863
 E(G3X) excl. ZPE (Hartree): -74.95736492
 E(MP2-Full/G3Xlarge) (Hartree): -74.89009095
 E(MP2-Full/G3large) (Hartree): -74.89009095
 E(MP2/6-31+G(d)) (Hartree): -74.77644020
 E(MP2/6-31G(2df,p)) (Hartree): -74.80825729
 E(MP2/6-31G(d)) (Hartree): -74.76994637
 E(MP2/G3MP2large) (Hartree): -74.84404122
 E(MP3/6-31+G(d)) (Hartree): -74.79388693
 E(MP3/6-31G(2df,p)) (Hartree): -74.82821011
 E(MP3/6-31G(d)) (Hartree): -74.78753857
 E(MP4/6-31+G(d)) (Hartree): -74.79995640
 E(MP4/6-31G(2df,p)) (Hartree): -74.83462046
 E(MP4/6-31G(d)) (Hartree): -74.79314660
 E(QCISD(T)/6-31G(d)) (Hartree): -74.81275044
 E(QCISD/6-31G(d)) (Hartree): -74.80539056
 E(RHF/6-31+G(d)) (Hartree): -74.66021350
 E(RHF/6-31G(2df,p)) (Hartree): -74.65933634
 E(RHF/6-31G(d)) (Hartree): -74.65660412
 E(RHF/G3MP2large) (Hartree): -74.68183501
 E(RHF/G3Xlarge) (Hartree): -74.68192678
 E(RHF/G3large) (Hartree): -74.68192678
 E(RM062X/Aug-CC-pVTZ) (Hartree): -74.97091207
 Point group : OH
 Cartesian coordinates (Angs):
 O 0.000000 0.000000 0.000000

O(3P)

 E(G3SX(MP3)) excl. ZPE (Hartree): -75.04121425
 E(G3SX) excl. ZPE (Hartree): -75.04248965
 E(G3X(MP2)) excl. ZPE (Hartree): -74.99120012
 E(G3X(MP3)) excl. ZPE (Hartree): -75.03543381
 E(G3X) excl. ZPE (Hartree): -75.03224092
 E(MP2-Full/G3Xlarge) (Hartree): -74.99598547
 E(MP2-Full/G3large) (Hartree): -74.99598547
 E(MP2/6-31+G(d)) (Hartree): -74.88529102
 E(MP2/6-31G(2df,p)) (Hartree): -74.91601431
 E(MP2/6-31G(d)) (Hartree): -74.88003673
 E(MP2/G3MP2large) (Hartree): -74.95003655
 E(MP3/6-31+G(d)) (Hartree): -74.89851523
 E(MP3/6-31G(2df,p)) (Hartree): -74.93124433
 E(MP3/6-31G(d)) (Hartree): -74.89321792
 E(MP4/6-31+G(d)) (Hartree): -74.90172732
 E(MP4/6-31G(2df,p)) (Hartree): -74.93464243
 E(MP4/6-31G(d)) (Hartree): -74.89597297
 E(PMP2/6-31+G(d)) (Hartree): -74.88687490
 E(PMP2/6-31G(2df,p)) (Hartree): -74.91754026
 E(PMP2/6-31G(d)) (Hartree): -74.88131121
 E(PMP2/G3MP2large) (Hartree): -74.95185880
 E(PMP2/G3Xlarge) (Hartree): -74.99783203
 E(PMP2/G3large) (Hartree): -74.99783203
 E(PMP3/6-31+G(d)) (Hartree): -74.89953104
 E(PMP3/6-31G(2df,p)) (Hartree): -74.93199308
 E(PMP3/6-31G(d)) (Hartree): -74.89387061
 E(PUHF/6-31+G(d)) (Hartree): -74.78932427
 E(PUHF/6-31G(2df,p)) (Hartree): -74.78986751
 E(PUHF/6-31G(d)) (Hartree): -74.78631365
 E(PUHF/G3MP2large) (Hartree): -74.81223083
 E(PUHF/G3Xlarge) (Hartree): -74.81233601

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E(PUHF/G3large) (Hartree): -74.81233601
E(QCISD(T)/6-31G(d)) (Hartree): -74.89668223
E(QCISD/6-31G(d)) (Hartree): -74.89590031
E(UHF/6-31+G(d)) (Hartree): -74.78676391
E(UHF/6-31G(2df,p)) (Hartree): -74.78703359
E(UHF/6-31G(d)) (Hartree): -74.78393361
E(UHF/G3MP2large) (Hartree): -74.80920713
E(UHF/G3Xlarge) (Hartree): -74.80926720
E(UHF/G3large) (Hartree): -74.80926720
E(UM062X/Aug-CC-pVTZ) (Hartree): -75.06593575
Point group : OH
Cartesian coordinates (Angs):
    O      0.000000      0.000000      0.000000

cycloketene
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E(G3SX(MP3)) excl. ZPE (Hartree): -306.12946163
E(G3SX) excl. ZPE (Hartree): -306.13431900
E(G3X(MP2)) excl. ZPE (Hartree): -305.82320548
E(G3X(MP3)) excl. ZPE (Hartree): -306.10945125
E(G3X) excl. ZPE (Hartree): -306.08913845
E(MP2-Full/G3Xlarge) (Hartree): -305.89300883
E(MP2-Full/G3large) (Hartree): -305.89300883
E(MP2/6-31+G(d)) (Hartree): -305.28435715
E(MP2/6-31G(2df,p)) (Hartree): -305.47633594
E(MP2/6-31G(d)) (Hartree): -305.26589279
E(MP2/G3MP2large) (Hartree): -305.58737277
E(MP3/6-31+G(d)) (Hartree): -305.29510419
E(MP3/6-31G(2df,p)) (Hartree): -305.49120043
E(MP3/6-31G(d)) (Hartree): -305.27852615
E(MP4/6-31+G(d)) (Hartree): -305.36132190
E(MP4/6-31G(2df,p)) (Hartree): -305.56308198
E(MP4/6-31G(d)) (Hartree): -305.34252602
E(QCISD(T)/6-31G(d)) (Hartree): -305.33626708
E(QCISD/6-31G(d)) (Hartree): -305.29487182
E(RHF/6-31+G(d)) (Hartree): -304.34771951
E(RHF/6-31G(2df,p)) (Hartree): -304.37097029
E(RHF/6-31G(d)) (Hartree): -304.33796326
E(RHF/G3MP2large) (Hartree): -304.43964455
E(RHF/G3Xlarge) (Hartree): -304.44054297
E(RHF/G3large) (Hartree): -304.44054297
E(RM062X/Aug-CC-pVTZ) (Hartree): -306.19850137
Electronic state : 1-A
Cartesian coordinates (Angs):
    C      -1.817121      -0.722326      0.000068
    C      -1.817068      0.722399      -0.000004
    C      -0.537850      1.175618      -0.000079
    C      0.315382      -0.000052      -0.000044
    C      -0.537938      -1.175643      0.000038
    H      -2.697855      -1.344855      0.000124
    H      -2.697755      1.344994      -0.000006
    H      -0.188969      2.194185      -0.000155
    H      -0.189139      -2.194238      0.000070
    C      1.641494      0.000004      -0.000002
    O      2.786541      -0.000010      0.000012
Rotational constants (GHz):      8.5593100      1.9565600      1.5925200
Vibrational harmonic frequencies (cm-1):
    129.5800      148.3708      555.1730
    562.2473      581.2457      609.7908
    662.6985      723.4391      761.4507
    846.1682      921.0174      923.8097
    947.7798      1041.6918      1092.2910
    1103.0477      1229.4099      1326.3881
    1365.7197      1466.7307      1501.1935
    1599.4962      2251.6237      3241.2280
    3253.5551      3276.1343      3279.8056
Zero-point correction (Hartree): 0.080650

Hydroxyphenoxy
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E(G3SX(MP3)) excl. ZPE (Hartree): -381.96136394

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E(G3SX) excl. ZPE (Hartree): -381.96770623
E(G3X(MP2)) excl. ZPE (Hartree): -381.60310722
E(G3X(MP3)) excl. ZPE (Hartree): -381.93465971
E(G3X) excl. ZPE (Hartree): -381.91156606
E(MP2-Full/G3Xlarge) (Hartree): -381.63958996
E(MP2-Full/G3large) (Hartree): -381.63958996
E(MP2/6-31+G(d)) (Hartree): -380.90013162
E(MP2/6-31G(2df,p)) (Hartree): -381.13725066
E(MP2/6-31G(d)) (Hartree): -380.87410697
E(MP2/G3MP2large) (Hartree): -381.28695458
E(MP3/6-31+G(d)) (Hartree): -380.93458020
E(MP3/6-31G(2df,p)) (Hartree): -381.17924833
E(MP3/6-31G(d)) (Hartree): -380.91117002
E(MP4/6-31+G(d)) (Hartree): -380.99903069
E(MP4/6-31G(2df,p)) (Hartree): -381.25033716
E(MP4/6-31G(d)) (Hartree): -380.97187377
E(PMP2/6-31+G(d)) (Hartree): -380.93263577
E(PMP2/6-31G(2df,p)) (Hartree): -381.17117237
E(PMP2/6-31G(d)) (Hartree): -380.90799066
E(PMP2/G3MP2large) (Hartree): -381.31928907
E(PMP2/G3Xlarge) (Hartree): -381.67195889
E(PMP2/G3large) (Hartree): -381.67195889
E(PMP3/6-31+G(d)) (Hartree): -380.96027301
E(PMP3/6-31G(2df,p)) (Hartree): -381.20610154
E(PMP3/6-31G(d)) (Hartree): -380.93814035
E(PUHF/6-31+G(d)) (Hartree): -379.87988111
E(PUHF/6-31G(2df,p)) (Hartree): -379.91073412
E(PUHF/6-31G(d)) (Hartree): -379.87057107
E(PUHF/G3MP2large) (Hartree): -379.99750433
E(PUHF/G3Xlarge) (Hartree): -379.99860091
E(PUHF/G3large) (Hartree): -379.99860091
E(QCISD(T)/6-31G(d)) (Hartree): -380.99088810
E(QCISD/6-31G(d)) (Hartree): -380.94815941
E(UHF/6-31+G(d)) (Hartree): -379.84334114
E(UHF/6-31G(2df,p)) (Hartree): -379.87268379
E(UHF/6-31G(d)) (Hartree): -379.83258054
E(UHF/G3MP2large) (Hartree): -379.96112310
E(UHF/G3Xlarge) (Hartree): -379.96217961
E(UHF/G3large) (Hartree): -379.96217961
E(UM062X/Aug-CC-pVTZ) (Hartree): -382.05563576
Electronic state : 2-A
Cartesian coordinates (Angs):
  C      -1.772750      -0.812926      0.000068
  C      -1.881697       0.601472      0.000030
  C      -0.771645       1.388918     -0.000014
  C       0.537065       0.791604      0.000026
  C       0.600607     -0.669841      0.000007
  C      -0.545934     -1.447471      0.000045
  H      -2.675682     -1.407414      0.000094
  H      -2.865868       1.048896      0.000024
  H      -0.826132       2.468340     -0.000069
  H      -0.461446     -2.524614      0.000059
  O       1.813438     -1.198004     -0.000005
  H       2.431176     -0.442001      0.000011
  O       1.612072       1.416287     -0.000131
Rotational constants (GHz):   3.5011400   2.3497500   1.4060800
Vibrational harmonic frequencies (cm-1):
  169.0226      271.4129      340.4343
  448.5077      461.8417      497.2699
  570.5113      579.3797      724.8328
  747.2945      771.2629      798.6241
  879.9564      887.0939      969.6761
  999.1357     1020.6102     1138.1494
 1165.4400     1196.4502     1273.7472
 1360.6921     1388.6846     1447.8328
 1512.0317     1569.2103     1613.2887
 1638.5118     3205.7679     3217.9008
 3229.6687     3233.5231     3636.8693
Zero-point correction (Hartree): 0.097881

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Hydroxyphenyl

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E(G3SX(MP3)) excl. ZPE (Hartree): -306.69859907
E(G3SX) excl. ZPE (Hartree): -306.70306952
E(G3X(MP2)) excl. ZPE (Hartree): -306.39130466
E(G3X(MP3)) excl. ZPE (Hartree): -306.67821148
E(G3X) excl. ZPE (Hartree): -306.65745516
E(MP2-Full/G3Xlarge) (Hartree): -306.41703519
E(MP2-Full/G3large) (Hartree): -306.41703519
E(MP2/6-31+G(d)) (Hartree): -305.80143218
E(MP2/6-31G(2df,p)) (Hartree): -305.99444412
E(MP2/6-31G(d)) (Hartree): -305.77913456
E(MP2/G3MP2large) (Hartree): -306.11174521
E(MP3/6-31+G(d)) (Hartree): -305.83717071
E(MP3/6-31G(2df,p)) (Hartree): -306.03617360
E(MP3/6-31G(d)) (Hartree): -305.81707120
E(MP4/6-31+G(d)) (Hartree): -305.89025956
E(MP4/6-31G(2df,p)) (Hartree): -306.09477282
E(MP4/6-31G(d)) (Hartree): -305.86740584
E(PMP2/6-31+G(d)) (Hartree): -305.83189194
E(PMP2/6-31G(2df,p)) (Hartree): -306.02644615
E(PMP2/6-31G(d)) (Hartree): -305.81134082
E(PMP2/G3MP2large) (Hartree): -306.14171455
E(PMP2/G3Xlarge) (Hartree): -306.44703106
E(PMP2/G3large) (Hartree): -306.44703106
E(PMP3/6-31+G(d)) (Hartree): -305.86230845
E(PMP3/6-31G(2df,p)) (Hartree): -306.06261208
E(PMP3/6-31G(d)) (Hartree): -305.84383911
E(PUHF/6-31+G(d)) (Hartree): -304.95962603
E(PUHF/6-31G(2df,p)) (Hartree): -304.98515257
E(PUHF/6-31G(d)) (Hartree): -304.95179236
E(PUHF/G3MP2large) (Hartree): -305.05168116
E(PUHF/G3Xlarge) (Hartree): -305.05258342
E(PUHF/G3large) (Hartree): -305.05258342
E(QCISD(T)/6-31G(d)) (Hartree): -305.88854701
E(QCISD/6-31G(d)) (Hartree): -305.84914495
E(UHF/6-31+G(d)) (Hartree): -304.92635445
E(UHF/6-31G(2df,p)) (Hartree): -304.95026258
E(UHF/6-31G(d)) (Hartree): -304.91669253
E(UHF/G3MP2large) (Hartree): -305.01892487
E(UHF/G3Xlarge) (Hartree): -305.01979687
E(UHF/G3large) (Hartree): -305.01979687
E(UM062X/Aug-CC-pVTZ) (Hartree): -306.77092246
Electronic state : 2-A
Cartesian coordinates (Angs):
  C      1.107831      1.172085      0.000051
  C      1.834674     -0.011869      0.000010
  C      1.158290     -1.231872     -0.000042
  C     -0.207849     -1.190031     -0.000047
  C     -0.967828     -0.044604     -0.000005
  C     -0.279430      1.166148      0.000044
  H      1.628741      2.119424      0.000090
  H      2.915281      0.006825      0.000017
  H      1.696497     -2.170312     -0.000076
  H     -0.850214      2.085205      0.000076
  O     -2.326822     -0.032739     -0.000014
  H     -2.649864     -0.938365     -0.000060
Rotational constants (GHz):   6.1199100   2.6269600   1.8380000
Vibrational harmonic frequencies (cm-1):
  229.1696           365.9958           392.6757
  418.1752           525.0770           525.8448
  626.5794           687.8485           761.7335
  839.3345           860.2867           952.1943
  992.3656           992.6404          1050.6099
 1117.9574          1163.5723          1182.7939
 1277.5613          1318.9699          1348.2018
 1489.8403          1498.6863          1620.8373
 1673.2861          3200.6705          3207.0746
 3217.4542          3229.0564          3869.4463
Zero-point correction (Hartree): 0.092575
nitrosooxyphenyl.pt

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E(G3SX(MP3)) excl. ZPE (Hartree): -435.93537958
E(G3SX) excl. ZPE (Hartree): -435.94243503
E(G3X(MP2)) excl. ZPE (Hartree): -435.52995065
E(G3X(MP3)) excl. ZPE (Hartree): -435.90293287
E(G3X) excl. ZPE (Hartree): -435.87813172
E(MP2-Full/G3Xlarge) (Hartree): -435.57855871
E(MP2-Full/G3large) (Hartree): -435.57855871
E(MP2/6-31+G(d)) (Hartree): -434.76644614
E(MP2/6-31G(2df,p)) (Hartree): -435.01636489
E(MP2/6-31G(d)) (Hartree): -434.73701263
E(MP2/G3MP2large) (Hartree): -435.18192330
E(MP3/6-31+G(d)) (Hartree): -434.78940552
E(MP3/6-31G(2df,p)) (Hartree): -435.04739038
E(MP3/6-31G(d)) (Hartree): -434.76305652
E(MP4/6-31+G(d)) (Hartree): -434.87754017
E(MP4/6-31G(2df,p)) (Hartree): -435.14246401
E(MP4/6-31G(d)) (Hartree): -434.84653548
E(PMP2/6-31+G(d)) (Hartree): -434.80169860
E(PMP2/6-31G(2df,p)) (Hartree): -435.05319060
E(PMP2/6-31G(d)) (Hartree): -434.77401602
E(PMP2/G3MP2large) (Hartree): -435.21738557
E(PMP2/G3Xlarge) (Hartree): -435.61403887
E(PMP2/G3large) (Hartree): -435.61403887
E(PMP3/6-31+G(d)) (Hartree): -434.81878874
E(PMP3/6-31G(2df,p)) (Hartree): -435.07811917
E(PMP3/6-31G(d)) (Hartree): -434.79410512
E(PUHF/6-31+G(d)) (Hartree): -433.58545490
E(PUHF/6-31G(2df,p)) (Hartree): -433.61568566
E(PUHF/6-31G(d)) (Hartree): -433.57513114
E(PUHF/G3MP2large) (Hartree): -433.71422077
E(PUHF/G3Xlarge) (Hartree): -433.71547784
E(PUHF/G3large) (Hartree): -433.71547784
E(QCISD(T)/6-31G(d)) (Hartree): -434.86612919
E(QCISD/6-31G(d)) (Hartree): -434.81034756
E(UHF/6-31+G(d)) (Hartree): -433.54714507
E(UHF/6-31G(2df,p)) (Hartree): -433.57573518
E(UHF/6-31G(d)) (Hartree): -433.53500158
E(UHF/G3MP2large) (Hartree): -433.67568333
E(UHF/G3Xlarge) (Hartree): -433.67691912
E(UHF/G3large) (Hartree): -433.67691912
E(UM062X/Aug-CC-pVTZ) (Hartree): -436.04594899
Electronic state : 2-A
Cartesian coordinates (Angs):
  C      -2.633368      0.213669      -0.155132
  C      -1.752073      1.273154      0.009417
  C      -0.393779      1.051777      0.197226
  C       0.089086     -0.252168      0.199018
  C      -0.812200     -1.271975      0.029065
  C      -2.157180     -1.098207     -0.139171
  H      -3.689693      0.400149     -0.290661
  H      -2.125073      2.287548      0.003670
  H       0.290305      1.875760      0.347279
  H      -2.827597     -1.938061     -0.261636
  O       1.420951     -0.549516      0.403799
  N       2.272081      0.278086     -0.378804
  O       3.379620      0.040828     -0.152494
Rotational constants (GHz):   5.4163400   0.9995200   0.8631700
Vibrational harmonic frequencies (cm-1):
  63.4169      138.1982      156.0778
  293.7985      382.1172      423.4260
  471.5361      545.8092      615.0109
  662.3159      702.7327      763.2889
  811.0940      870.6370      935.1771
  964.1421     1002.9946     1004.1234
 1055.1692     1134.2142     1169.6612
 1243.9399     1292.4552     1321.0692
 1473.3228     1490.0792     1613.1450
 1670.4694     1848.9509     3201.9827
 3211.0388     3218.4518     3229.5474
Zero-point correction (Hartree): 0.088802

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nitrosophenol.cc

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E(G3SX(MP3)) excl. ZPE (Hartree): -436.65528642
E(G3SX) excl. ZPE (Hartree): -436.66344926
E(G3X(MP2)) excl. ZPE (Hartree): -436.25423412
E(G3X(MP3)) excl. ZPE (Hartree): -436.62574322
E(G3X) excl. ZPE (Hartree): -436.60088099
E(MP2-Full/G3Xlarge) (Hartree): -436.33801309
E(MP2-Full/G3large) (Hartree): -436.33801309
E(MP2/6-31+G(d)) (Hartree): -435.50496173
E(MP2/6-31G(2df,p)) (Hartree): -435.77285512
E(MP2/6-31G(d)) (Hartree): -435.47672049
E(MP2/G3MP2large) (Hartree): -435.94057769
E(MP3/6-31+G(d)) (Hartree): -435.51736069
E(MP3/6-31G(2df,p)) (Hartree): -435.79144984
E(MP3/6-31G(d)) (Hartree): -435.49195552
E(MP4/6-31+G(d)) (Hartree): -435.60204000
E(MP4/6-31G(2df,p)) (Hartree): -435.88431444
E(MP4/6-31G(d)) (Hartree): -435.57244355
E(QCISD(T)/6-31G(d)) (Hartree): -435.56648793
E(QCISD/6-31G(d)) (Hartree): -435.51274329
E(RHF/6-31+G(d)) (Hartree): -434.21766627
E(RHF/6-31G(2df,p)) (Hartree): -434.24986078
E(RHF/6-31G(d)) (Hartree): -434.20479639
E(RHF/G3MP2large) (Hartree): -434.35074294
E(RHF/G3Xlarge) (Hartree): -434.35199193
E(RHF/G3large) (Hartree): -434.35199193
E(RM062X/Aug-CC-pVTZ) (Hartree): -436.76349636
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
  C      1.707771      -1.516577      0.000000
  C      2.244361      -0.223866      0.000000
  C      1.386394       0.848890      0.000000
  C      0.000000       0.650867      0.000000
  C     -0.535393     -0.655291      0.000000
  C      0.345921     -1.736705      0.000000
  H      2.374641     -2.368676      0.000000
  H      3.313990     -0.076757      0.000000
  H      1.741545       1.870840      0.000000
  H     -0.068737     -2.734700      0.000000
  O     -1.844970     -0.893617      0.000000
  H     -2.299885     -0.028683      0.000000
  N     -0.767892       1.827160      0.000000
  O     -1.977610       1.686610      0.000000
Rotational constants (GHz):   3.2209400   1.5713800   1.0561300
Vibrational harmonic frequencies (cm-1):
  145.7649 ( A'')   211.8586 ( A'')   291.6560 ( A')
  313.2100 ( A'')   421.1051 ( A')   446.5262 ( A'')
  446.9569 ( A')    537.6038 ( A'')   574.7158 ( A')
  695.9319 ( A')    731.5500 ( A'')   779.6536 ( A'')
  791.6119 ( A')    794.1299 ( A'')   898.2843 ( A'')
  902.8627 ( A')    994.3363 ( A'')  1014.1770 ( A'')
 1057.7762 ( A')   1132.4559 ( A')   1162.8022 ( A')
 1210.3142 ( A')   1229.4200 ( A')   1337.6026 ( A')
 1354.5357 ( A')   1387.0937 ( A')   1497.7516 ( A')
 1520.9396 ( A')   1615.0592 ( A')   1660.6367 ( A')
 1688.0688 ( A')   3202.5421 ( A')   3216.3499 ( A')
 3226.6476 ( A')   3236.6948 ( A')   3518.2333 ( A')
Zero-point correction (Hartree): 0.103080
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nitrosophenol.ct

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E(RM062X/Aug-CC-pVTZ) (Hartree): -436.76060718
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
  C     -1.025817     -2.011619      0.000000
  C     -1.899989     -0.916524      0.000000
  C     -1.384600      0.357624      0.000000
```

```

C      0.000000      0.539600      0.000000
C      0.872954     -0.555225      0.000000
C      0.343178     -1.845193      0.000000
H     -1.432291     -3.014150      0.000000
H     -2.968060     -1.077342      0.000000
H     -2.016642      1.234766      0.000000
H      1.020042     -2.687168      0.000000
O      2.205601     -0.400158      0.000000
H      2.403476      0.547429      0.000000
N      0.642459      1.803624      0.000000
O     -0.072863      2.770048      0.000000
Rotational constants (GHz):   2.6940100   1.6529300   1.0244000
Vibrational harmonic frequencies (cm-1):
130.5562 ( A'')      220.6655 ( A'')      240.1366 ( A')
277.9934 ( A'')      370.4745 ( A')      453.5190 ( A'')
526.9750 ( A'')      532.2964 ( A')      559.2386 ( A')
606.4125 ( A'')      661.6450 ( A')      739.7804 ( A'')
792.1174 ( A'')      837.7534 ( A')      865.6909 ( A')
897.5134 ( A'')      1001.8824 ( A'')     1013.7027 ( A'')
1054.0556 ( A')      1117.0975 ( A')     1161.2574 ( A')
1200.1252 ( A')      1226.4707 ( A')     1299.1810 ( A')
1360.9066 ( A')      1375.5060 ( A')     1505.5669 ( A')
1537.1702 ( A')      1650.7890 ( A')     1666.8078 ( A')
1712.0466 ( A')      3204.7378 ( A')     3221.0036 ( A')
3230.0587 ( A')      3234.8950 ( A')     3763.4470 ( A')
Zero-point correction (Hartree): 0.103086

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nitrosophenol.tc

E(RM062X/Aug-CC-pVTZ) (Hartree): -436.74863949

Point group : CS

Electronic state : 1-A'

Cartesian coordinates (Angs):

```

C      1.676165     -1.555084      0.000000
C      2.231755     -0.280137      0.000000
C      1.384190      0.808906      0.000000
C      0.000000      0.653226      0.000000
C     -0.558452     -0.636524      0.000000
C      0.303606     -1.730875      0.000000
H      2.317875     -2.425743      0.000000
H      3.303250     -0.146964      0.000000
H      1.760107      1.823642      0.000000
H     -0.118530     -2.729128      0.000000
O     -1.894067     -0.796639      0.000000
H     -2.104000     -1.735758      0.000000
N     -0.710242      1.901623      0.000000
O     -1.907256      1.839830      0.000000

```

Rotational constants (GHz): 3.1164200 1.5603400 1.0397500

Vibrational harmonic frequencies (cm-1):

```

77.8585 ( A'')      189.4154 ( A'')      252.8930 ( A')
271.4155 ( A'')      416.6793 ( A')      426.8200 ( A'')
429.6941 ( A')      465.0304 ( A'')      552.9965 ( A'')
579.3489 ( A')      691.9504 ( A')      731.2035 ( A'')
769.5582 ( A')      788.7370 ( A'')      882.7701 ( A'')
891.4586 ( A')      992.2197 ( A'')      1008.9135 ( A'')
1075.6724 ( A')      1117.4406 ( A')      1174.6795 ( A')
1187.7077 ( A')      1194.0057 ( A')      1322.8431 ( A')
1340.7234 ( A')      1360.3691 ( A')      1504.1366 ( A')
1527.3060 ( A')      1635.7368 ( A')      1679.6454 ( A')
1715.7405 ( A')      3182.0056 ( A')      3209.3997 ( A')
3214.4754 ( A')      3235.9775 ( A')      3853.5430 ( A')

```

Zero-point correction (Hartree): 0.102404

nitrosophenol.tt

E(RM062X/Aug-CC-pVTZ) (Hartree): -436.75108060

Point group : CS

Electronic state : 1-A'

Cartesian coordinates (Angs):

```

C     -0.955492     -2.034275      0.000000
C     -1.856774     -0.969981      0.000000

```

C	-1.372270	0.320176	0.000000
C	0.000000	0.559129	0.000000
C	0.903572	-0.507566	0.000000
C	0.407952	-1.811175	0.000000
H	-1.323456	-3.051360	0.000000
H	-2.920435	-1.157923	0.000000
H	-2.032576	1.176194	0.000000
H	1.101305	-2.643367	0.000000
O	2.225135	-0.243231	0.000000
H	2.722425	-1.065809	0.000000
N	0.559370	1.885563	0.000000
O	-0.253233	2.768914	0.000000
Rotational constants (GHz):		2.6441600	1.6566400
Vibrational harmonic frequencies (cm-1):			1.0185100
99.8149 (A'')	165.8255 (A'')	245.0690 (A')	
264.5866 (A'')	365.7154 (A'')	372.8823 (A')	
457.0968 (A'')	511.0419 (A')	536.9676 (A'')	
563.9545 (A')	657.1371 (A')	731.4310 (A')	
787.2240 (A'')	828.3244 (A')	857.9135 (A')	
881.7377 (A'')	995.7410 (A'')	1010.5256 (A'')	
1069.8945 (A')	1105.8568 (A')	1166.8086 (A')	
1187.0057 (A')	1193.2641 (A')	1305.0167 (A')	
1341.2644 (A')	1358.7116 (A')	1500.6121 (A')	
1535.6754 (A')	1647.3617 (A')	1676.5881 (A')	
1706.9228 (A')	3189.9309 (A')	3211.2739 (A')	
3221.7518 (A')	3233.3699 (A')	3874.4223 (A')	
Zero-point correction (Hartree):		0.102196	

nitrophenyl

E(G3SX(MP3)) excl. ZPE (Hartree): -435.93776531
E(G3SX) excl. ZPE (Hartree): -435.94518374
E(G3X(MP2)) excl. ZPE (Hartree): -435.53180456
E(G3X(MP3)) excl. ZPE (Hartree): -435.90537862
E(G3X) excl. ZPE (Hartree): -435.88089321
E(MP2-Full/G3Xlarge) (Hartree): -435.59303972
E(MP2-Full/G3large) (Hartree): -435.59303972
E(MP2/6-31+G(d)) (Hartree): -434.77747185
E(MP2/6-31G(2df,p)) (Hartree): -435.03061866
E(MP2/6-31G(d)) (Hartree): -434.74861203
E(MP2/G3MP2large) (Hartree): -435.19581462
E(MP3/6-31+G(d)) (Hartree): -434.79068639
E(MP3/6-31G(2df,p)) (Hartree): -435.05200730
E(MP3/6-31G(d)) (Hartree): -434.76499870
E(MP4/6-31+G(d)) (Hartree): -434.88178745
E(MP4/6-31G(2df,p)) (Hartree): -435.15057262
E(MP4/6-31G(d)) (Hartree): -434.85150503
E(PMP2/6-31+G(d)) (Hartree): -434.81014434
E(PMP2/6-31G(2df,p)) (Hartree): -435.06467135
E(PMP2/6-31G(d)) (Hartree): -434.78271860
E(PMP2/G3MP2large) (Hartree): -435.22815081
E(PMP2/G3Xlarge) (Hartree): -435.62540531
E(PMP2/G3large) (Hartree): -435.62540531
E(PMP3/6-31+G(d)) (Hartree): -434.81786549
E(PMP3/6-31G(2df,p)) (Hartree): -435.08035097
E(PMP3/6-31G(d)) (Hartree): -434.79353175
E(PUHF/6-31+G(d)) (Hartree): -433.57850394
E(PUHF/6-31G(2df,p)) (Hartree): -433.60975686
E(PUHF/6-31G(d)) (Hartree): -433.56779801
E(PUHF/G3MP2large) (Hartree): -433.70744082
E(PUHF/G3Xlarge) (Hartree): -433.70872813
E(PUHF/G3large) (Hartree): -433.70872813
E(QCISD(T)/6-31G(d)) (Hartree): -434.86567295
E(QCISD/6-31G(d)) (Hartree): -434.80821038
E(UHF/6-31+G(d)) (Hartree): -433.54295598
E(UHF/6-31G(2df,p)) (Hartree): -433.57276825
E(UHF/6-31G(d)) (Hartree): -433.53075644
E(UHF/G3MP2large) (Hartree): -433.67224455
E(UHF/G3Xlarge) (Hartree): -433.67349856
E(UHF/G3large) (Hartree): -433.67349856
E(UM062X/Aug-CC-pVTZ) (Hartree): -436.04805275

Electronic state : 2-A
 Cartesian coordinates (Angs):

C	2.498879	-0.036361	0.000042
C	1.808999	1.171245	0.000040
C	0.422288	1.195166	-0.000029
C	-0.255702	-0.014143	-0.000097
C	0.446845	-1.187183	-0.000092
C	1.812306	-1.251625	-0.000026
H	3.580636	-0.037440	0.000096
H	2.357302	2.102123	0.000092
H	-0.140542	2.117381	-0.000033
H	2.340837	-2.194702	-0.000025
N	-1.725631	-0.044817	-0.000177
O	-2.250559	-1.133981	0.000104
O	-2.307003	1.016953	0.000157

Rotational constants (GHz): 4.2021900 1.2948100 0.9898200
 Vibrational harmonic frequencies (cm-1):

65.6815	167.5151	229.9335
390.7270	416.4802	457.1553
537.8760	615.5546	664.7650
694.6609	749.7153	819.8779
884.0300	889.0658	985.9317
997.1176	1012.0486	1048.2878
1126.6586	1162.3045	1189.5429
1263.9437	1331.4002	1460.5776
1477.4360	1482.7539	1615.9552
1667.3723	1691.8636	3205.2373
3219.6247	3227.4527	3239.2225

Zero-point correction (Hartree): 0.091099

nitrosophenoxy_cis

 E(G3SX(MP3)) excl. ZPE (Hartree): -436.01216970
 E(G3SX) excl. ZPE (Hartree): -436.01926550
 E(G3X(MP2)) excl. ZPE (Hartree): -435.60615043
 E(G3X(MP3)) excl. ZPE (Hartree): -435.97937085
 E(G3X) excl. ZPE (Hartree): -435.95429047
 E(MP2-Full/G3Xlarge) (Hartree): -435.66643334
 E(MP2-Full/G3large) (Hartree): -435.66643334
 E(MP2/6-31+G(d)) (Hartree): -434.84988774
 E(MP2/6-31G(2df,p)) (Hartree): -435.10378084
 E(MP2/6-31G(d)) (Hartree): -434.82214387
 E(MP2/G3MP2large) (Hartree): -435.26896288
 E(MP3/6-31+G(d)) (Hartree): -434.86831208
 E(MP3/6-31G(2df,p)) (Hartree): -435.12948414
 E(MP3/6-31G(d)) (Hartree): -434.84346874
 E(MP4/6-31+G(d)) (Hartree): -434.95711456
 E(MP4/6-31G(2df,p)) (Hartree): -435.22596186
 E(MP4/6-31G(d)) (Hartree): -434.92821527
 E(PMP2/6-31+G(d)) (Hartree): -434.86689489
 E(PMP2/6-31G(2df,p)) (Hartree): -435.12193886
 E(PMP2/6-31G(d)) (Hartree): -434.84012232
 E(PMP2/G3MP2large) (Hartree): -435.28590013
 E(PMP2/G3Xlarge) (Hartree): -435.68340302
 E(PMP2/G3large) (Hartree): -435.68340302
 E(PMP3/6-31+G(d)) (Hartree): -434.88177364
 E(PMP3/6-31G(2df,p)) (Hartree): -435.14387622
 E(PMP3/6-31G(d)) (Hartree): -434.85778637
 E(PUHF/6-31+G(d)) (Hartree): -433.62421175
 E(PUHF/6-31G(2df,p)) (Hartree): -433.65402559
 E(PUHF/6-31G(d)) (Hartree): -433.61342870
 E(PUHF/G3MP2large) (Hartree): -433.75299004
 E(PUHF/G3Xlarge) (Hartree): -433.75425668
 E(PUHF/G3large) (Hartree): -433.75425668
 E(QCISD(T)/6-31G(d)) (Hartree): -434.94042695
 E(QCISD/6-31G(d)) (Hartree): -434.88428606
 E(UHF/6-31+G(d)) (Hartree): -433.60533673
 E(UHF/6-31G(2df,p)) (Hartree): -433.63392001
 E(UHF/6-31G(d)) (Hartree): -433.59353875
 E(UHF/G3MP2large) (Hartree): -433.73416303
 E(UHF/G3Xlarge) (Hartree): -433.73539250

E(UHF/G3large) (Hartree): -433.73539250
 E(UM062X/Aug-CC-pVTZ) (Hartree): -436.11674554
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-2.228626	0.355821	-0.000027
C	-1.942614	-1.062397	0.000026
C	-0.671936	-1.498880	0.000044
C	0.397726	-0.539190	0.000025
C	0.149528	0.932594	-0.000028
C	-1.266304	1.296503	-0.000053
H	-3.266688	0.663028	-0.000043
H	-2.764289	-1.763145	0.000053
H	-0.418306	-2.549693	0.000082
H	-1.490603	2.353635	-0.000089
O	1.064573	1.729204	-0.000049
N	1.635711	-0.946251	0.000045
O	2.668334	-0.352552	0.000019

 Rotational constants (GHz): 3.2780700 1.5716700 1.0623300
 Vibrational harmonic frequencies (cm-1):

109.9301	200.5074	205.5468
375.2095	413.3316	445.3096
473.9478	511.7894	557.2960
618.4378	723.9689	743.8915
783.8970	875.9816	889.3405
992.8368	996.6270	1021.3235
1155.7990	1169.3824	1214.4984
1312.2044	1368.6640	1430.5786
1492.2713	1576.7009	1674.3114
1718.9452	1779.7970	3198.9632
3218.7501	3229.3205	3236.6376

 Zero-point correction (Hartree): 0.090480

nitrosophenoxy_trans

 E(G3SX(MP3)) excl. ZPE (Hartree): -436.00647783
 E(G3SX) excl. ZPE (Hartree): -436.01349905
 E(G3X(MP2)) excl. ZPE (Hartree): -435.60057169
 E(G3X(MP3)) excl. ZPE (Hartree): -435.97386159
 E(G3X) excl. ZPE (Hartree): -435.94871563
 E(MP2-Full/G3Xlarge) (Hartree): -435.66200914
 E(MP2-Full/G3large) (Hartree): -435.66200914
 E(MP2/6-31+G(d)) (Hartree): -434.84561162
 E(MP2/6-31G(2df,p)) (Hartree): -435.09865043
 E(MP2/6-31G(d)) (Hartree): -434.81765542
 E(MP2/G3MP2large) (Hartree): -435.26455917
 E(MP3/6-31+G(d)) (Hartree): -434.86456679
 E(MP3/6-31G(2df,p)) (Hartree): -435.12511017
 E(MP3/6-31G(d)) (Hartree): -434.83964433
 E(MP4/6-31+G(d)) (Hartree): -434.95220030
 E(MP4/6-31G(2df,p)) (Hartree): -435.22023845
 E(MP4/6-31G(d)) (Hartree): -434.92309783
 E(PMP2/6-31+G(d)) (Hartree): -434.86518004
 E(PMP2/6-31G(2df,p)) (Hartree): -435.11917566
 E(PMP2/6-31G(d)) (Hartree): -434.83806511
 E(PMP2/G3MP2large) (Hartree): -435.28400043
 E(PMP2/G3Xlarge) (Hartree): -435.68149000
 E(PMP2/G3large) (Hartree): -435.68149000
 E(PMP3/6-31+G(d)) (Hartree): -434.88027264
 E(PMP3/6-31G(2df,p)) (Hartree): -435.14158171
 E(PMP3/6-31G(d)) (Hartree): -434.85610024
 E(PUHF/6-31+G(d)) (Hartree): -433.62406615
 E(PUHF/6-31G(2df,p)) (Hartree): -433.65351865
 E(PUHF/6-31G(d)) (Hartree): -433.61318216
 E(PUHF/G3MP2large) (Hartree): -433.75264282
 E(PUHF/G3Xlarge) (Hartree): -433.75391916
 E(PUHF/G3large) (Hartree): -433.75391916
 E(QCISD(T)/6-31G(d)) (Hartree): -434.93476104
 E(QCISD/6-31G(d)) (Hartree): -434.87966075
 E(UHF/6-31+G(d)) (Hartree): -433.60249409
 E(UHF/6-31G(2df,p)) (Hartree): -433.63091858
 E(UHF/6-31G(d)) (Hartree): -433.59072858

E(UHF/G3MP2large) (Hartree): -433.73117780
 E(UHF/G3Xlarge) (Hartree): -433.73240969
 E(UHF/G3large) (Hartree): -433.73240969
 E(UM062X/Aug-CC-pVTZ) (Hartree): -436.11179985
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	2.188435	-0.489789	0.000018
C	1.281312	-1.622721	-0.000008
C	-0.047408	-1.437889	-0.000014
C	-0.567152	-0.088463	-0.000037
C	0.326033	1.104528	-0.000171
C	1.757375	0.781937	-0.000008
H	3.251532	-0.693223	0.000077
H	1.693466	-2.621637	0.000026
H	-0.750121	-2.259550	0.000017
H	2.436353	1.622798	0.000048
O	-0.101681	2.239110	0.000056
N	-1.845685	0.139868	0.000010
O	-2.816194	-0.553245	0.000079

 Rotational constants (GHz): 2.7799500 1.6101500 1.0196000
 Vibrational harmonic frequencies (cm-1):

86.9370	197.6686	200.1280
343.1112	356.7996	434.4052
491.4410	526.6348	564.9417
593.9027	749.4950	759.9435
780.7286	874.7827	879.3059
992.1931	999.0513	1024.7867
1143.8152	1171.3494	1208.5305
1308.5353	1373.9854	1437.1164
1466.2410	1598.4011	1692.1327
1723.6916	1790.3207	3197.4008
3214.3267	3227.6168	3231.5042

 Zero-point correction (Hartree): 0.090309

phenyloxyl

 E(G3SX(MP3)) excl. ZPE (Hartree): -306.04673816
 E(G3SX) excl. ZPE (Hartree): -306.05125308
 E(G3X(MP2)) excl. ZPE (Hartree): -305.73912986
 E(G3X(MP3)) excl. ZPE (Hartree): -306.02711940
 E(G3X) excl. ZPE (Hartree): -306.00648429
 E(MP2-Full/G3Xlarge) (Hartree): -305.76162050
 E(MP2-Full/G3large) (Hartree): -305.76162050
 E(MP2/6-31+G(d)) (Hartree): -305.16688001
 E(MP2/6-31G(2df,p)) (Hartree): -305.34568633
 E(MP2/6-31G(d)) (Hartree): -305.14719840
 E(MP2/G3MP2large) (Hartree): -305.45681755
 E(MP3/6-31+G(d)) (Hartree): -305.20861325
 E(MP3/6-31G(2df,p)) (Hartree): -305.39374565
 E(MP3/6-31G(d)) (Hartree): -305.19056374
 E(MP4/6-31+G(d)) (Hartree): -305.26087252
 E(MP4/6-31G(2df,p)) (Hartree): -305.45101948
 E(MP4/6-31G(d)) (Hartree): -305.24035680
 E(PMP2/6-31+G(d)) (Hartree): -305.19879639
 E(PMP2/6-31G(2df,p)) (Hartree): -305.37865603
 E(PMP2/6-31G(d)) (Hartree): -305.18007712
 E(PMP2/G3MP2large) (Hartree): -305.48870378
 E(PMP2/G3Xlarge) (Hartree): -305.79355176
 E(PMP2/G3large) (Hartree): -305.79355176
 E(PMP3/6-31+G(d)) (Hartree): -305.23442764
 E(PMP3/6-31G(2df,p)) (Hartree): -305.42043062
 E(PMP3/6-31G(d)) (Hartree): -305.21731553
 E(PUHF/6-31+G(d)) (Hartree): -304.37493721
 E(PUHF/6-31G(2df,p)) (Hartree): -304.39431006
 E(PUHF/6-31G(d)) (Hartree): -304.36786548
 E(PUHF/G3MP2large) (Hartree): -304.45922320
 E(PUHF/G3Xlarge) (Hartree): -304.46011614
 E(PUHF/G3large) (Hartree): -304.46011614
 E(QCISD(T)/6-31G(d)) (Hartree): -305.26435933
 E(QCISD/6-31G(d)) (Hartree): -305.22792570
 E(UHF/6-31+G(d)) (Hartree): -304.33928786

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E(UHF/6-31G(2df,p)) (Hartree): -304.35756005
E(UHF/6-31G(d)) (Hartree): -304.33123128
E(UHF/G3MP2large) (Hartree): -304.42358266
E(UHF/G3Xlarge) (Hartree): -304.42442404
E(UHF/G3large) (Hartree): -304.42442404
E(UM062X/Aug-CC-pVTZ) (Hartree): -306.12101719
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      0.986681      1.223011      0.000013
  C      1.763994      0.042465      0.000078
  C      1.152866     -1.215501      0.000041
  C     -0.206639     -1.249537     -0.000003
  C     -1.082856     -0.106489      0.000095
  C     -0.374377      1.169426     -0.000028
  H      1.490060      2.179985     -0.000020
  H      2.843026      0.112869      0.000110
  H      1.746964     -2.119609      0.000031
  H     -0.988520      2.059956     -0.000112
  O     -2.316193     -0.176681     -0.000148
Rotational constants (GHz):   5.9461300   2.7881900   1.8981400
Vibrational harmonic frequencies (cm-1):
  181.0803      390.5785      433.9507
  484.3666      515.0795      588.3134
  684.6253      784.0338      817.2482
  863.8564      956.4563      963.6124
 1001.4379     1017.7171     1117.1893
 1144.4376     1204.0657     1308.0816
 1371.0607     1415.6588     1493.9954
 1551.7033     1606.4897     3199.6906
 3207.4530     3217.1244     3226.4088
Zero-point correction (Hartree): 0.079157

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nitrophenoxy

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-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.17704730
E(G3SX) excl. ZPE (Hartree): -511.18642888
E(G3X(MP2)) excl. ZPE (Hartree): -510.72000143
E(G3X(MP3)) excl. ZPE (Hartree): -511.13837585
E(G3X) excl. ZPE (Hartree): -511.11184270
E(MP2-Full/G3Xlarge) (Hartree): -510.78719671
E(MP2-Full/G3large) (Hartree): -510.78719671
E(MP2/6-31+G(d)) (Hartree): -509.84933354
E(MP2/6-31G(2df,p)) (Hartree): -510.14462260
E(MP2/6-31G(d)) (Hartree): -509.81510754
E(MP2/G3MP2large) (Hartree): -510.34276229
E(MP3/6-31+G(d)) (Hartree): -509.86414285
E(MP3/6-31G(2df,p)) (Hartree): -510.16959960
E(MP3/6-31G(d)) (Hartree): -509.83365804
E(MP4/6-31+G(d)) (Hartree): -509.96645922
E(MP4/6-31G(2df,p)) (Hartree): -510.27979178
E(MP4/6-31G(d)) (Hartree): -509.92980779
E(PMP2/6-31+G(d)) (Hartree): -509.89054418
E(PMP2/6-31G(2df,p)) (Hartree): -510.18692696
E(PMP2/6-31G(d)) (Hartree): -509.85727624
E(PMP2/G3MP2large) (Hartree): -510.38400112
E(PMP2/G3Xlarge) (Hartree): -510.82848326
E(PMP2/G3large) (Hartree): -510.82848326
E(PMP3/6-31+G(d)) (Hartree): -509.89765617
E(PMP3/6-31G(2df,p)) (Hartree): -510.20402006
E(PMP3/6-31G(d)) (Hartree): -509.86811370
E(PUHF/6-31+G(d)) (Hartree): -508.48850099
E(PUHF/6-31G(2df,p)) (Hartree): -508.52465239
E(PUHF/6-31G(d)) (Hartree): -508.47572393
E(PUHF/G3MP2large) (Hartree): -508.64308003
E(PUHF/G3Xlarge) (Hartree): -508.64456504
E(PUHF/G3large) (Hartree): -508.64456504
E(QCISD(T)/6-31G(d)) (Hartree): -509.94420118
E(QCISD/6-31G(d)) (Hartree): -509.88409581
E(UHF/6-31+G(d)) (Hartree): -508.44274321
E(UHF/6-31G(2df,p)) (Hartree): -508.47775437
E(UHF/6-31G(d)) (Hartree): -508.42898385

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E(UHF/G3MP2large) (Hartree): -508.59727529
 E(UHF/G3Xlarge) (Hartree): -508.59870580
 E(UHF/G3large) (Hartree): -508.59870580
 E(UM062X/Aug-CC-pVTZ) (Hartree): -511.30517954
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-2.538708	-0.241489	0.061721
C	-1.806491	-1.435320	0.129145
C	-0.403793	-1.421943	0.090161
C	0.248690	-0.230868	0.007977
C	-0.446525	1.044803	-0.105183
C	-1.894034	0.958426	-0.052026
H	-3.618631	-0.278302	0.091994
H	-2.322627	-2.380779	0.212910
H	0.165777	-2.339565	0.132379
H	-2.426609	1.895927	-0.130330
O	0.133454	2.117037	-0.286160
N	1.715075	-0.242455	0.037476
O	2.253496	0.559411	0.757502
O	2.268266	-1.081667	-0.641348

 Rotational constants (GHz): 2.4870200 1.2283000 0.8724000
 Vibrational harmonic frequencies (cm-1):

50.3947	115.5963	205.7602
209.8908	343.5227	364.8243
470.5941	480.3759	554.3197
561.9466	640.8944	698.8528
782.7753	802.9063	842.9460
896.5397	905.7784	985.7002
1010.3474	1038.6513	1097.2312
1139.8729	1157.1405	1254.3518
1332.9067	1424.4210	1447.7243
1461.2979	1521.8603	1566.1201
1626.5925	1686.7505	3211.8894
3222.6004	3229.5336	3235.0486

 Zero-point correction (Hartree): 0.094722

quinonoxime

 E(G3SX(MP3)) excl. ZPE (Hartree): -436.65021348
 E(G3SX) excl. ZPE (Hartree): -436.65850242
 E(G3X(MP2)) excl. ZPE (Hartree): -436.24857993
 E(G3X(MP3)) excl. ZPE (Hartree): -436.62054254
 E(G3X) excl. ZPE (Hartree): -436.59575800
 E(MP2-Full/G3Xlarge) (Hartree): -436.32896626
 E(MP2-Full/G3large) (Hartree): -436.32896626
 E(MP2/6-31+G(d)) (Hartree): -435.49623428
 E(MP2/6-31G(2df,p)) (Hartree): -435.76365794
 E(MP2/6-31G(d)) (Hartree): -435.46840940
 E(MP2/G3MP2large) (Hartree): -435.93163188
 E(MP3/6-31+G(d)) (Hartree): -435.50946195
 E(MP3/6-31G(2df,p)) (Hartree): -435.78370571
 E(MP3/6-31G(d)) (Hartree): -435.48453767
 E(MP4/6-31+G(d)) (Hartree): -435.59667856
 E(MP4/6-31G(2df,p)) (Hartree): -435.87915123
 E(MP4/6-31G(d)) (Hartree): -435.56751370
 E(QCISD(T)/6-31G(d)) (Hartree): -435.56146318
 E(QCISD/6-31G(d)) (Hartree): -435.50722568
 E(RHF/6-31+G(d)) (Hartree): -434.20482620
 E(RHF/6-31G(2df,p)) (Hartree): -434.23771308
 E(RHF/6-31G(d)) (Hartree): -434.19221660
 E(RHF/G3MP2large) (Hartree): -434.33892657
 E(RHF/G3Xlarge) (Hartree): -434.34018083
 E(RHF/G3large) (Hartree): -434.34018083
 E(RM062X/Aug-CC-pVTZ) (Hartree): -436.75522567
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-2.239267	0.436274	0.000057
C	-2.021365	-0.989898	-0.000033
C	-0.768843	-1.478196	-0.000023
C	0.357441	-0.577966	-0.000177
C	0.143950	0.881716	-0.000367

C	-1.229392	1.332246	0.000039	
H	-3.260727	0.795222	0.000181	
H	-2.874828	-1.651534	-0.000003	
H	-0.552690	-2.537637	0.000009	
H	-1.399079	2.399353	0.000197	
O	1.110231	1.658952	0.000152	
N	1.543856	-1.127183	-0.000040	
O	2.586286	-0.329686	0.000208	
H	2.253047	0.625693	0.000050	
Rotational constants (GHz):			3.2709400	1.5671600 1.0595300
Vibrational harmonic frequencies (cm-1):				
124.8604	207.3719	305.5901		
380.2751	419.9885	443.6391		
500.0096	500.5237	560.7174		
646.6861	761.5832	762.7206		
792.5473	890.1929	908.0127		
1003.4360	1005.0658	1008.4846		
1024.2586	1164.9476	1169.6457		
1203.2730	1230.4997	1329.4051		
1413.1792	1472.6942	1485.9830		
1605.7192	1643.3678	1689.5533		
1736.7062	2851.0603	3198.8126		
3217.4423	3230.4024	3235.1689		
Zero-point correction (Hartree): 0.102800				

===== Singlet surface =====

nitrophenol cis

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-----
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.97720176
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -2.538637      -0.171398      -0.000083
  C      -1.891888      -1.410072      -0.000041
  C      -0.518117      -1.449200       0.000007
  C       0.210808      -0.261185       0.000016
  C      -0.424219       0.990537       0.000016
  C      -1.822756       1.003805      -0.000060
  H      -3.619370      -0.130496      -0.000121
  H      -2.461416      -2.327151      -0.000066
  H       0.024579      -2.381968       0.000000
  H      -2.310616       1.967797      -0.000060
  O       0.204083       2.165227       0.000175
  H       1.163843       1.991994       0.000425
  N       1.661165      -0.359742      -0.000075
  O       2.310751       0.684391      -0.000248
  O       2.170626      -1.451730       0.000226
Rotational constants (GHz):   2.3939800   1.2895000   0.8380700
Vibrational harmonic frequencies (cm-1):
  74.2198      147.3617      251.7325
 291.2318      381.0905      433.3021
 437.0305      538.3031      558.6470
 573.1640      688.3326      705.3213
 731.6665      778.2254      828.4526
 854.0870      894.6948      901.1200
 994.6629     1022.7424     1064.2168
1112.8408     1164.2160     1187.7677
1232.2156     1305.5224     1349.5093
1380.3124     1438.0726     1511.4013
1538.0241     1646.3634     1656.1628
1707.1555     3210.3500     3231.5291
3235.7406     3251.7395     3572.1614
Zero-point correction (Hartree): 0.109080

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nitrophenol trans

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.83173960
E(G3SX) excl. ZPE (Hartree): -511.84184556
E(G3X(MP2)) excl. ZPE (Hartree): -511.37933329
E(G3X(MP3)) excl. ZPE (Hartree): -511.79518579
E(G3X) excl. ZPE (Hartree): -511.76864169
E(MP2-Full/G3Xlarge) (Hartree): -511.48289383
E(MP2-Full/G3large) (Hartree): -511.48289383
E(MP2/6-31+G(d)) (Hartree): -510.52321211
E(MP2/6-31G(2df,p)) (Hartree): -510.83592476
E(MP2/6-31G(d)) (Hartree): -510.48790843
E(MP2/G3MP2large) (Hartree): -511.03820127
E(MP3/6-31+G(d)) (Hartree): -510.52005466
E(MP3/6-31G(2df,p)) (Hartree): -510.84113504
E(MP3/6-31G(d)) (Hartree): -510.48879733
E(MP4/6-31+G(d)) (Hartree): -510.62410720
E(MP4/6-31G(2df,p)) (Hartree): -510.95391917
E(MP4/6-31G(d)) (Hartree): -510.58665054
E(QCISD(T)/6-31G(d)) (Hartree): -510.57589301
E(QCISD/6-31G(d)) (Hartree): -510.51457670
E(RHF/6-31+G(d)) (Hartree): -509.03269217
E(RHF/6-31G(2df,p)) (Hartree): -509.07312540
E(RHF/6-31G(d)) (Hartree): -509.01723994
E(RHF/G3MP2large) (Hartree): -509.19525532
E(RHF/G3Xlarge) (Hartree): -509.19672276
E(RHF/G3large) (Hartree): -509.19672276
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.96160508
Electronic state : 1-A

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Cartesian coordinates (Angs):

C	-2.523130	-0.260408	0.040176
C	-1.833620	-1.465611	0.101469
C	-0.453137	-1.451140	0.075530
C	0.231289	-0.247120	0.012036
C	-0.445883	0.972239	-0.058175
C	-1.840032	0.937717	-0.045104
H	-3.604255	-0.252237	0.054002
H	-2.365961	-2.402640	0.166052
H	0.125549	-2.362125	0.108132
H	-2.382065	1.873521	-0.106918
O	0.230170	2.129759	-0.173257
H	-0.391914	2.856333	-0.272319
N	1.698285	-0.308362	0.021788
O	2.301625	0.629329	0.485747
O	2.207921	-1.317635	-0.419621

Rotational constants (GHz): 2.3702200 1.2686000 0.8470200

Vibrational harmonic frequencies (cm-1):

48.0635	134.4509	241.2119
248.5117	367.9545	376.3883
402.2516	451.8663	533.6764
563.0343	579.3621	681.0236
705.4662	779.3952	816.4781
847.6270	883.7251	896.0323
988.4733	1005.6639	1078.8490
1111.4356	1178.7457	1186.0045
1197.5283	1310.2072	1344.3555
1357.5157	1459.4836	1504.5053
1548.7856	1655.8214	1667.5353
1705.4361	3190.2081	3216.5953
3232.3568	3245.6621	3867.9372

Zero-point correction (Hartree): 0.108463

hydroxyphenylnitrite.pc

E(G3SX(MP3)) excl. ZPE (Hartree): -511.83822279

E(G3SX) excl. ZPE (Hartree): -511.84815773

E(G3X(MP2)) excl. ZPE (Hartree): -511.38696588

E(G3X(MP3)) excl. ZPE (Hartree): -511.80199594

E(G3X) excl. ZPE (Hartree): -511.77517381

E(MP2-Full/G3Xlarge) (Hartree): -511.48295803

E(MP2-Full/G3large) (Hartree): -511.48295803

E(MP2/6-31+G(d)) (Hartree): -510.52688344

E(MP2/6-31G(2df,p)) (Hartree): -510.83674154

E(MP2/6-31G(d)) (Hartree): -510.49244683

E(MP2/G3MP2large) (Hartree): -511.03884515

E(MP3/6-31+G(d)) (Hartree): -510.52975523

E(MP3/6-31G(2df,p)) (Hartree): -510.84740651

E(MP3/6-31G(d)) (Hartree): -510.49907293

E(MP4/6-31+G(d)) (Hartree): -510.63281951

E(MP4/6-31G(2df,p)) (Hartree): -510.95914224

E(MP4/6-31G(d)) (Hartree): -510.59619285

E(QCISD(T)/6-31G(d)) (Hartree): -510.58745988

E(QCISD/6-31G(d)) (Hartree): -510.52721336

E(RHF/6-31+G(d)) (Hartree): -509.04343331

E(RHF/6-31G(2df,p)) (Hartree): -509.08244199

E(RHF/6-31G(d)) (Hartree): -509.02871431

E(RHF/G3MP2large) (Hartree): -509.20428675

E(RHF/G3Xlarge) (Hartree): -509.20571444

E(RHF/G3large) (Hartree): -509.20571444

E(RM062X/Aug-CC-pVTZ) (Hartree): -511.96799732

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-2.440631	-0.326996	0.323437
C	-1.761919	-1.473145	-0.074161
C	-0.437421	-1.379256	-0.469177
C	0.190660	-0.146574	-0.464887
C	-0.483825	1.004362	-0.063125
C	-1.812246	0.907412	0.327624
H	-3.474880	-0.394327	0.631170
H	-2.261002	-2.431022	-0.077443

H	0.121695	-2.248387	-0.788342
H	-2.330276	1.806888	0.628475
O	0.128586	2.210572	-0.052958
H	1.004340	2.119290	-0.445668
O	1.505738	-0.003623	-0.870782
N	2.518574	-0.338003	0.130713
O	2.088477	-0.707103	1.131058
Rotational constants (GHz):	2.2825100	1.2184500	0.9163200
Vibrational harmonic frequencies (cm-1):			
37.8531	114.1480		199.9548
206.1740	320.9654		359.7248
450.1255	453.2066		473.2135
522.8112	567.6609		584.4582
612.4085	754.3162		770.6553
785.5781	856.8576		892.8753
952.9276	981.2709		1012.0113
1060.9287	1120.2059		1170.7026
1195.7060	1246.5395		1299.8665
1329.8848	1370.8506		1516.0127
1544.0435	1670.6951		1680.5806
1852.9296	3207.5848		3215.4443
3226.2403	3234.4272		3833.7576
Zero-point correction (Hartree):	0.106358		

hydroxyphenylnitrite.pt

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-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.83873876
E(G3SX) excl. ZPE (Hartree): -511.84855514
E(G3X(MP2)) excl. ZPE (Hartree): -511.38730497
E(G3X(MP3)) excl. ZPE (Hartree): -511.80254339
E(G3X) excl. ZPE (Hartree): -511.77557932
E(MP2-Full/G3Xlarge) (Hartree): -511.48277546
E(MP2-Full/G3large) (Hartree): -511.48277546
E(MP2/6-31+G(d)) (Hartree): -510.52658344
E(MP2/6-31G(2df,p)) (Hartree): -510.83534234
E(MP2/6-31G(d)) (Hartree): -510.49115431
E(MP2/G3MP2large) (Hartree): -511.03865582
E(MP3/6-31+G(d)) (Hartree): -510.53157932
E(MP3/6-31G(2df,p)) (Hartree): -510.84845091
E(MP3/6-31G(d)) (Hartree): -510.50000904
E(MP4/6-31+G(d)) (Hartree): -510.63235607
E(MP4/6-31G(2df,p)) (Hartree): -510.95766718
E(MP4/6-31G(d)) (Hartree): -510.59474416
E(QCISD(T)/6-31G(d)) (Hartree): -510.58668239
E(QCISD/6-31G(d)) (Hartree): -510.52731186
E(RHF/6-31+G(d)) (Hartree): -509.04756931
E(RHF/6-31G(2df,p)) (Hartree): -509.08576002
E(RHF/6-31G(d)) (Hartree): -509.03187146
E(RHF/G3MP2large) (Hartree): -509.20866774
E(RHF/G3Xlarge) (Hartree): -509.21010881
E(RHF/G3large) (Hartree): -509.21010881
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.96933495
Electronic state : 1-A
Cartesian coordinates (Angs):
C      2.588877      -0.550211      -0.188941
C      1.736995      -1.627453      0.015655
C      0.386378      -1.401542      0.235131
C     -0.094671     -0.105564      0.228963
C      0.752962      0.980795      0.022299
C      2.104999      0.748788     -0.181158
H      3.643694     -0.720971     -0.352609
H      2.120731     -2.637101      0.013829
H     -0.299553     -2.217842      0.414528
H      2.755847      1.597455     -0.336654
O      0.284908      2.250637      0.020026
H     -0.660749      2.237918      0.205440
O     -1.428626      0.191227      0.457336
N     -2.296755     -0.532825     -0.429429
O     -3.398273     -0.291683     -0.193640
Rotational constants (GHz):      2.6124100      0.9989600      0.7419300
Vibrational harmonic frequencies (cm-1):

```

62.4385	122.2215	149.2181
219.1563	304.5634	334.6515
434.6019	439.5524	485.2106
507.0532	568.5915	581.1507
649.5063	741.7329	771.2141
788.0357	859.1452	888.5934
938.6362	970.5267	1002.5820
1063.9254	1124.6592	1171.3164
1201.3265	1258.5546	1312.6011
1328.0848	1375.9413	1517.5340
1549.1145	1675.1352	1681.4462
1858.7914	3208.3759	3217.3496
3226.4788	3234.4471	3838.6905

Zero-point correction (Hartree): 0.106304

aci-NP-2

E(G3SX(MP3)) excl. ZPE (Hartree): -511.79922358
E(G3SX) excl. ZPE (Hartree): -511.80966400
E(G3X(MP2)) excl. ZPE (Hartree): -511.34723228
E(G3X(MP3)) excl. ZPE (Hartree): -511.76289225
E(G3X) excl. ZPE (Hartree): -511.73651410
E(MP2-Full/G3Xlarge) (Hartree): -511.44627190
E(MP2-Full/G3large) (Hartree): -511.44627190
E(MP2/6-31+G(d)) (Hartree): -510.48851392
E(MP2/6-31G(2df,p)) (Hartree): -510.79980672
E(MP2/6-31G(d)) (Hartree): -510.45431307
E(MP2/G3MP2large) (Hartree): -511.00173953
E(MP3/6-31+G(d)) (Hartree): -510.48987195
E(MP3/6-31G(2df,p)) (Hartree): -510.80904641
E(MP3/6-31G(d)) (Hartree): -510.45927745
E(MP4/6-31+G(d)) (Hartree): -510.59376404
E(MP4/6-31G(2df,p)) (Hartree): -510.92273667
E(MP4/6-31G(d)) (Hartree): -510.55764053
E(QCISD(T)/6-31G(d)) (Hartree): -510.54667212
E(QCISD/6-31G(d)) (Hartree): -510.48496717
E(RHF/6-31+G(d)) (Hartree): -508.99744286
E(RHF/6-31G(2df,p)) (Hartree): -509.03599895
E(RHF/6-31G(d)) (Hartree): -508.98173669
E(RHF/G3MP2large) (Hartree): -509.15891202
E(RHF/G3Xlarge) (Hartree): -509.16036572
E(RHF/G3large) (Hartree): -509.16036572
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.928864996

Electronic state : 1-A

Cartesian coordinates (Angs):

C	2.564020	-0.185722	0.000182
C	1.854220	-1.444298	-0.000306
C	0.511409	-1.468237	-0.000432
C	-0.230739	-0.235285	-0.000294
C	0.453415	1.087497	-0.000566
C	1.918041	0.990966	0.000289
H	3.646291	-0.203712	0.000543
H	2.413794	-2.368190	-0.000335
H	-0.045739	-2.392472	-0.000529
H	2.439824	1.937491	0.000792
O	-0.113301	2.161887	0.000634
H	-3.190439	0.449486	0.000261
N	-1.554980	-0.349086	0.000001
O	-2.282529	0.795487	0.000062
O	-2.204303	-1.388439	0.000057

Rotational constants (GHz): 2.3982900 1.2601600 0.8261000

Vibrational harmonic frequencies (cm-1):

72.0737	114.1696	210.6680
264.9154	379.3236	384.1650
414.5597	480.4341	498.6473
550.8525	591.0696	618.7837
687.8394	736.7097	778.6020
779.9696	873.5986	878.9176
997.9786	1006.5041	1021.5010
1082.6207	1145.9609	1175.6311
1214.9976	1311.6986	1360.4934

1368.9618	1430.6793	1481.3749
1619.1708	1680.0586	1713.4300
1776.4677	3199.5758	3226.1662
3231.3471	3249.2880	3748.1066

Zero-point correction (Hartree): 0.107888

aci-NP-3

E(G3SX(MP3)) excl. ZPE (Hartree): -511.79901089
 E(G3SX) excl. ZPE (Hartree): -511.80947269
 E(G3X(MP2)) excl. ZPE (Hartree): -511.34693581
 E(G3X(MP3)) excl. ZPE (Hartree): -511.76264777
 E(G3X) excl. ZPE (Hartree): -511.73629619
 E(MP2-Full/G3Xlarge) (Hartree): -511.44744218
 E(MP2-Full/G3large) (Hartree): -511.44744218
 E(MP2/6-31+G(d)) (Hartree): -510.48975196
 E(MP2/6-31G(2df,p)) (Hartree): -510.80070952
 E(MP2/6-31G(d)) (Hartree): -510.45534790
 E(MP2/G3MP2large) (Hartree): -511.00290456
 E(MP3/6-31+G(d)) (Hartree): -510.48925452
 E(MP3/6-31G(2df,p)) (Hartree): -510.80819758
 E(MP3/6-31G(d)) (Hartree): -510.45851608
 E(MP4/6-31+G(d)) (Hartree): -510.59443260
 E(MP4/6-31G(2df,p)) (Hartree): -510.92306113
 E(MP4/6-31G(d)) (Hartree): -510.55806587
 E(QCISD(T)/6-31G(d)) (Hartree): -510.54624760
 E(QCISD/6-31G(d)) (Hartree): -510.48411581
 E(RHF/6-31+G(d)) (Hartree): -508.99462594
 E(RHF/6-31G(2df,p)) (Hartree): -509.03310061
 E(RHF/6-31G(d)) (Hartree): -508.97893215
 E(RHF/G3MP2large) (Hartree): -509.15611450
 E(RHF/G3Xlarge) (Hartree): -509.15756605
 E(RHF/G3large) (Hartree): -509.15756605
 E(RM062X/Aug-CC-pVTZ) (Hartree): -511.92828001

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.534201	1.092371	-0.000050
C	-0.243544	-0.175474	-0.000005
C	0.401806	-1.459924	-0.000016
C	1.744932	-1.528809	-0.000006
C	2.544035	-0.326769	0.000029
C	1.987110	0.895661	0.000031
O	0.029885	2.197514	0.000055
N	-1.570018	-0.093533	0.000018
O	-2.283369	0.883382	-0.000004
O	-2.233113	-1.310504	-0.000062
H	-3.159848	-1.024382	-0.000048
H	-0.204334	-2.351296	-0.000015
H	2.236420	-2.490614	0.000001
H	3.621927	-0.425367	0.000060
H	2.577485	1.800933	0.000069

Rotational constants (GHz): 2.3758100 1.2627000 0.8245000

Vibrational harmonic frequencies (cm-1):

83.6410	105.2548	209.9037
253.0398	371.2420	379.9300
419.4681	437.4177	494.7285
554.4346	564.2312	630.3238
685.4430	727.7346	766.2719
783.9585	855.7284	878.2736
994.4686	999.7263	1013.4288
1022.2774	1160.5974	1194.4433
1224.0746	1297.3572	1346.9508
1402.0289	1430.0573	1481.5375
1601.5064	1679.6669	1712.7617
1791.3783	3198.9830	3226.6859
3231.5197	3259.5832	3772.6630

Zero-point correction (Hartree): 0.107627

aci-NP-4

E(G3SX(MP3)) excl. ZPE (Hartree): -511.78873906

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E(G3SX) excl. ZPE (Hartree): -511.79925682
E(G3X(MP2)) excl. ZPE (Hartree): -511.33637971
E(G3X(MP3)) excl. ZPE (Hartree): -511.75201636
E(G3X) excl. ZPE (Hartree): -511.72580063
E(MP2-Full/G3Xlarge) (Hartree): -511.43757059
E(MP2-Full/G3large) (Hartree): -511.43757059
E(MP2/6-31+G(d)) (Hartree): -510.47811087
E(MP2/6-31G(2df,p)) (Hartree): -510.79035785
E(MP2/6-31G(d)) (Hartree): -510.44356397
E(MP2/G3MP2large) (Hartree): -510.99310282
E(MP3/6-31+G(d)) (Hartree): -510.47602151
E(MP3/6-31G(2df,p)) (Hartree): -510.79632224
E(MP3/6-31G(d)) (Hartree): -510.44521338
E(MP4/6-31+G(d)) (Hartree): -510.58221934
E(MP4/6-31G(2df,p)) (Hartree): -510.91208265
E(MP4/6-31G(d)) (Hartree): -510.54561698
E(QCISD(T)/6-31G(d)) (Hartree): -510.53370876
E(QCISD/6-31G(d)) (Hartree): -510.47055520
E(RHF/6-31+G(d)) (Hartree): -508.97838435
E(RHF/6-31G(2df,p)) (Hartree): -509.01810415
E(RHF/6-31G(d)) (Hartree): -508.96260072
E(RHF/G3MP2large) (Hartree): -509.14146747
E(RHF/G3Xlarge) (Hartree): -509.14291957
E(RHF/G3large) (Hartree): -509.14291957
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.91718528
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.512887      1.097790      0.001299
  C       0.255742     -0.170576     -0.069440
  C      -0.403895     -1.443465     -0.138174
  C      -1.747965     -1.511446     -0.081105
  C      -2.533110     -0.312454      0.061826
  C      -1.963103      0.904158      0.101479
  O      -0.005813      2.202030      0.010079
  N       1.593825     -0.089422     -0.026153
  O       2.285387      0.877570     -0.138205
  O       2.311150     -1.271225      0.170059
  H       1.775758     -1.823219      0.756114
  H       0.171781     -2.341941     -0.310612
  H      -2.245037     -2.466347     -0.167562
  H      -3.609644     -0.404803      0.122814
  H      -2.544125      1.811223      0.191550
Rotational constants (GHz):   2.3572700   1.2632000   0.8280300
Vibrational harmonic frequencies (cm-1):
  89.6142      109.2360      209.6658
  236.6854      299.7551      383.5756
  399.7461      440.3805      507.7854
  556.7047      564.2343      637.2417
  685.7480      740.9805      761.3023
  786.0177      850.0230      879.1783
  983.8006      992.8486     1018.8017
 1028.7415     1158.2228     1198.6147
 1225.7459     1314.6571     1331.7090
 1386.9969     1425.6959     1490.3008
 1584.6297     1664.6774     1707.7246
 1781.4124     3200.9996     3213.6600
 3227.4558     3235.0434     3804.1091
Zero-point correction (Hartree): 0.107333

complex.cycloketene.HONO_cis
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E(G3SX(MP3)) excl. ZPE (Hartree): -511.78325672
E(G3SX) excl. ZPE (Hartree): -511.79249908
E(G3X(MP2)) excl. ZPE (Hartree): -511.33188705
E(G3X(MP3)) excl. ZPE (Hartree): -511.74789541
E(G3X) excl. ZPE (Hartree): -511.71945142
E(MP2-Full/G3Xlarge) (Hartree): -511.42668185
E(MP2-Full/G3large) (Hartree): -511.42668185
E(MP2/6-31+G(d)) (Hartree): -510.46745524
E(MP2/6-31G(2df,p)) (Hartree): -510.77962077
E(MP2/6-31G(d)) (Hartree): -510.43447271

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E(MP2/G3MP2large) (Hartree): -510.98258315
E(MP3/6-31+G(d)) (Hartree): -510.46957330
E(MP3/6-31G(2df,p)) (Hartree): -510.79039399
E(MP3/6-31G(d)) (Hartree): -510.44020504
E(MP4/6-31+G(d)) (Hartree): -510.57553489
E(MP4/6-31G(2df,p)) (Hartree): -510.90463491
E(MP4/6-31G(d)) (Hartree): -510.54090715
E(QCISD(T)/6-31G(d)) (Hartree): -510.53065938
E(QCISD/6-31G(d)) (Hartree): -510.47171080
E(RHF/6-31+G(d)) (Hartree): -508.99190228
E(RHF/6-31G(2df,p)) (Hartree): -509.03393963
E(RHF/6-31G(d)) (Hartree): -508.97627738
E(RHF/G3MP2large) (Hartree): -509.15832698
E(RHF/G3Xlarge) (Hartree): -509.15976420
E(RHF/G3large) (Hartree): -509.15976420
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.91037975
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      3.221709      -0.401901      0.049704
  C      2.266752      -1.483057     -0.013572
  C      1.007203      -0.977020     -0.052566
  C      1.143072      0.467220     -0.014340
  C      0.180287      1.381413     -0.037530
  C      2.561011      0.783872      0.049748
  H      4.293312      -0.517501      0.090599
  H      2.515144      -2.532586     -0.027618
  H      0.076004      -1.513421     -0.103349
  H      2.971813      1.778510      0.088420
  O     -0.615015      2.204367     -0.056572
  H     -4.143714     -0.232216      0.089748
  N     -2.275284     -0.458956      0.002108
  O     -3.359701      0.349760      0.074005
  O     -2.533507     -1.603285     -0.022586
Rotational constants (GHz):   2.4189200   0.7156800   0.5526300
Vibrational harmonic frequencies (cm-1):
  110.5880      29.9313      48.2052
   58.1069      84.8012     100.2191
  131.9764     160.6396     558.3139
  562.9739     583.1374     612.0377
  656.7539     700.0402     711.8807
  725.5669     761.8010     846.5618
  920.0331     922.9107     945.6837
  994.5390    1042.9596    1095.8000
 1107.5548    1229.4908    1326.3368
 1365.8724    1378.1265    1466.3165
 1498.9470    1597.7627    1778.7921
 2250.1377    3241.2827    3254.0834
 3274.8359    3288.8728    3659.4800
Zero-point correction (Hartree): 0.102455

complex.cycloketene.HONO_trans
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.78607749
E(G3SX) excl. ZPE (Hartree): -511.79513966
E(G3X(MP2)) excl. ZPE (Hartree): -511.33440604
E(G3X(MP3)) excl. ZPE (Hartree): -511.75039247
E(G3X) excl. ZPE (Hartree): -511.72199293
E(MP2-Full/G3Xlarge) (Hartree): -511.42801494
E(MP2-Full/G3large) (Hartree): -511.42801494
E(MP2/6-31+G(d)) (Hartree): -510.46926127
E(MP2/6-31G(2df,p)) (Hartree): -510.77974657
E(MP2/6-31G(d)) (Hartree): -510.43435522
E(MP2/G3MP2large) (Hartree): -510.98392145
E(MP3/6-31+G(d)) (Hartree): -510.47260408
E(MP3/6-31G(2df,p)) (Hartree): -510.79205331
E(MP3/6-31G(d)) (Hartree): -510.44164654
E(MP4/6-31+G(d)) (Hartree): -510.57783911
E(MP4/6-31G(2df,p)) (Hartree): -510.90538243
E(MP4/6-31G(d)) (Hartree): -510.54134013
E(QCISD(T)/6-31G(d)) (Hartree): -510.53173132
E(QCISD/6-31G(d)) (Hartree): -510.47266449

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E(RHF/6-31+G(d)) (Hartree): -508.99330745
E(RHF/6-31G(2df,p)) (Hartree): -509.03449925
E(RHF/6-31G(d)) (Hartree): -508.97663298
E(RHF/G3MP2large) (Hartree): -509.15944679
E(RHF/G3Xlarge) (Hartree): -509.16087528
E(RHF/G3large) (Hartree): -509.16087528
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.91303302
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -3.240888      -0.273273      0.003269
  C      -2.360075      -1.420924     -0.000814
  C      -1.069805      -1.006171     -0.003526
  C      -1.106523       0.448754     -0.001148
  C      -0.077688       1.277487     -0.002645
  C      -2.503740       0.863730      0.003101
  H      -4.318656      -0.315156      0.006017
  H      -2.680924      -2.450615     -0.001541
  H      -0.172891      -1.600518     -0.006693
  H      -2.845834       1.884530      0.005552
  O       0.792520       2.031095     -0.003799
  H       2.817282       1.211182      0.003700
  N       2.244400      -0.560034     -0.000825
  O       3.270780       0.355142      0.005043
  O       2.642016      -1.654588     -0.000080
Rotational constants (GHz):   2.5509800   0.7200200   0.5615300
Vibrational harmonic frequencies (cm-1):
  i11.1574      41.7092      42.3666
   95.9878     106.3890     123.0078
  131.5026     176.6452     550.8634
  563.0499     576.7736     606.8017
  624.6458     658.3356     720.5857
  727.0325     764.3873     844.4978
  914.9550     928.8819     940.3025
  950.7708    1038.2234    1095.6542
 1105.4849    1223.1402    1318.7558
 1366.3735    1375.3725    1465.9296
 1504.9309    1605.0596    1828.5603
 2224.9103    3243.5014    3256.5761
 3279.0395    3289.9361    3779.9242
Zero-point correction (Hartree): 0.102725

TS.aci-NP-2.aci-NP-3.H-shift
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E(G3SX(MP3)) excl. ZPE (Hartree): -511.75567739
E(G3SX) excl. ZPE (Hartree): -511.76622389
E(G3X(MP2)) excl. ZPE (Hartree): -511.30298726
E(G3X(MP3)) excl. ZPE (Hartree): -511.71867869
E(G3X) excl. ZPE (Hartree): -511.69256844
E(MP2-Full/G3Xlarge) (Hartree): -511.40146467
E(MP2-Full/G3large) (Hartree): -511.40146467
E(MP2/6-31+G(d)) (Hartree): -510.44187631
E(MP2/6-31G(2df,p)) (Hartree): -510.75584425
E(MP2/6-31G(d)) (Hartree): -510.40894810
E(MP2/G3MP2large) (Hartree): -510.95692575
E(MP3/6-31+G(d)) (Hartree): -510.44094150
E(MP3/6-31G(2df,p)) (Hartree): -510.76294606
E(MP3/6-31G(d)) (Hartree): -510.41171184
E(MP4/6-31+G(d)) (Hartree): -510.54728916
E(MP4/6-31G(2df,p)) (Hartree): -510.87891434
E(MP4/6-31G(d)) (Hartree): -510.51226166
E(QCISD(T)/6-31G(d)) (Hartree): -510.50183805
E(QCISD/6-31G(d)) (Hartree): -510.43956315
E(RHF/6-31+G(d)) (Hartree): -508.94015289
E(RHF/6-31G(2df,p)) (Hartree): -508.98192066
E(RHF/6-31G(d)) (Hartree): -508.92562111
E(RHF/G3MP2large) (Hartree): -509.10346260
E(RHF/G3Xlarge) (Hartree): -509.10495416
E(RHF/G3large) (Hartree): -509.10495416
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.88548074
Point group : CS
Electronic state : 1-A'

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Cartesian coordinates (Angs):
  C      1.959095    -1.682239    0.000000
  C      2.329649    -0.280691    0.000000
  C      1.392011     0.678105    0.000000
  C      0.000000     0.301255    0.000000
  C     -0.433858    -1.128041    0.000000
  C      0.679354    -2.084262    0.000000
  H      2.751577    -2.419016    0.000000
  H      3.376598    -0.015511    0.000000
  H      1.635395     1.729634    0.000000
  H      0.398740    -3.127657    0.000000
  O     -1.594721    -1.471274    0.000000
  N     -0.896944     1.249779    0.000000
  O     -2.186173     1.165819    0.000000
  O     -0.659548     2.536748    0.000000
  H     -1.917676     2.408992    0.000000
Rotational constants (GHz):   2.4530000   1.2277100   0.8182000
Vibrational harmonic frequencies (cm-1):
  i1916.6707 ( A' )      75.0630 ( A'')      139.2556 ( A'')
    203.7929 ( A'')      227.1611 ( A')      361.3814 ( A')
    375.2887 ( A'')      426.7497 ( A')      481.8158 ( A'')
    554.2691 ( A')      581.0706 ( A')      635.3400 ( A'')
    656.2752 ( A')      762.5759 ( A'')      784.5506 ( A'')
    847.0093 ( A')      879.9371 ( A'')      967.3269 ( A')
    998.8135 ( A')      998.8792 ( A'')     1021.7344 ( A'')
   1091.8353 ( A'')     1107.4451 ( A')     1168.5274 ( A')
   1192.3430 ( A')     1225.4871 ( A')     1298.7523 ( A')
   1394.1411 ( A')     1417.3259 ( A')     1470.3874 ( A')
   1560.1844 ( A')     1641.2444 ( A')     1713.6503 ( A')
   1795.4622 ( A')     2343.3852 ( A')     3202.7812 ( A')
   3228.1574 ( A')     3235.3058 ( A')     3248.8877 ( A')
Zero-point correction (Hartree): 0.103232

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TS.aci-NP-2.aci-NP-3.introt

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-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.74494246
E(G3SX) excl. ZPE (Hartree): -511.75515669
E(G3X(MP2)) excl. ZPE (Hartree): -511.29216942
E(G3X(MP3)) excl. ZPE (Hartree): -511.70761859
E(G3X) excl. ZPE (Hartree): -511.68141329
E(MP2-Full/G3Xlarge) (Hartree): -511.39098114
E(MP2-Full/G3large) (Hartree): -511.39098114
E(MP2/6-31+G(d)) (Hartree): -510.43117068
E(MP2/6-31G(2df,p)) (Hartree): -510.74104281
E(MP2/6-31G(d)) (Hartree): -510.39202255
E(MP2/G3MP2large) (Hartree): -510.94645417
E(MP3/6-31+G(d)) (Hartree): -510.42890021
E(MP3/6-31G(2df,p)) (Hartree): -510.74696059
E(MP3/6-31G(d)) (Hartree): -510.39386048
E(MP4/6-31+G(d)) (Hartree): -510.53546287
E(MP4/6-31G(2df,p)) (Hartree): -510.86238475
E(MP4/6-31G(d)) (Hartree): -510.49408834
E(QCISD(T)/6-31G(d)) (Hartree): -510.48459416
E(QCISD/6-31G(d)) (Hartree): -510.42387408
E(RHF/6-31+G(d)) (Hartree): -508.93928480
E(RHF/6-31G(2df,p)) (Hartree): -508.97720869
E(RHF/6-31G(d)) (Hartree): -508.92093781
E(RHF/G3MP2large) (Hartree): -509.10267698
E(RHF/G3Xlarge) (Hartree): -509.10414062
E(RHF/G3large) (Hartree): -509.10414062
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.87496615

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Electronic state : 1-A

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Cartesian coordinates (Angs):
  C      -2.553976     0.025170     0.045961
  C      -2.053358    -1.290020    -0.005052
  C      -0.692664    -1.469388    -0.053604
  C       0.112310    -0.338136    -0.056142
  C      -0.311601     1.056271    -0.012514
  C      -1.748179     1.131306     0.045338
  H      -3.626177     0.169939     0.088129
  H      -2.718566    -2.139090    -0.004793

```

H	-0.247471	-2.454667	-0.090534	
H	-2.163033	2.129168	0.086766	
O	0.485819	2.001464	-0.031431	
N	1.530642	-0.404622	-0.105020	
O	2.124063	-0.385997	1.086158	
O	2.197557	-0.287488	-1.060771	
H	3.066053	-0.188038	0.920002	
Rotational constants (GHz):		2.5349300	1.1715800	0.9110900
Vibrational harmonic frequencies (cm-1):				
i333.0517		117.1080		146.6778
161.4093		343.3179		364.0505
448.6946		470.7327		545.4507
554.8006		591.1964		653.9613
689.8436		719.6810		742.0403
781.4608		850.4297		870.5340
941.7446		1005.6296		1032.2588
1039.6523		1110.2272		1144.7546
1173.8105		1206.0077		1311.9027
1420.8537		1427.8685		1476.7262
1557.3924		1613.2541		1681.7753
1785.6309		3193.2252		3206.9660
3217.9890		3241.5360		3676.9024
Zero-point correction (Hartree):		0.105975		

TS.aci-NP-4.aci-NP-3

E(G3SX(MP3)) excl. ZPE (Hartree): -511.78885619
E(G3SX) excl. ZPE (Hartree): -511.79927745
E(G3X(MP2)) excl. ZPE (Hartree): -511.33653868
E(G3X(MP3)) excl. ZPE (Hartree): -511.75220786
E(G3X) excl. ZPE (Hartree): -511.72587073
E(MP2-Full/G3Xlarge) (Hartree): -511.43685984
E(MP2-Full/G3large) (Hartree): -511.43685984
E(MP2/6-31+G(d)) (Hartree): -510.47811219
E(MP2/6-31G(2df,p)) (Hartree): -510.78953510
E(MP2/6-31G(d)) (Hartree): -510.44343021
E(MP2/G3MP2large) (Hartree): -510.99240198
E(MP3/6-31+G(d)) (Hartree): -510.47672918
E(MP3/6-31G(2df,p)) (Hartree): -510.79627584
E(MP3/6-31G(d)) (Hartree): -510.44582114
E(MP4/6-31+G(d)) (Hartree): -510.58297747
E(MP4/6-31G(2df,p)) (Hartree): -510.91204850
E(MP4/6-31G(d)) (Hartree): -510.54629921
E(QCISD(T)/6-31G(d)) (Hartree): -510.53444242
E(QCISD/6-31G(d)) (Hartree): -510.47136072
E(RHF/6-31+G(d)) (Hartree): -508.97947131
E(RHF/6-31G(2df,p)) (Hartree): -509.01848575
E(RHF/6-31G(d)) (Hartree): -508.96351746
E(RHF/G3MP2large) (Hartree): -509.14202791
E(RHF/G3Xlarge) (Hartree): -509.14347239
E(RHF/G3large) (Hartree): -509.14347239
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.91657106
Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.531008	1.094016	0.001318	
C	-0.256696	-0.167908	-0.048123	
C	0.387381	-1.451508	-0.089140	
C	1.730165	-1.529066	-0.049498	
C	2.533871	-0.334884	0.039984	
C	1.981269	0.889082	0.064123	
O	0.033208	2.201989	0.010788	
N	-1.587839	-0.070184	-0.024691	
O	-2.274993	0.908268	-0.083360	
O	-2.301835	-1.287196	0.047962	
H	-2.163489	-1.610910	0.948979	
H	-0.215157	-2.339864	-0.190733	
H	2.216503	-2.491934	-0.099951	
H	3.610134	-0.439842	0.078758	
H	2.573857	1.790956	0.120678	
Rotational constants (GHz):		2.3488200	1.2649400	0.8257700
Vibrational harmonic frequencies (cm-1):				

i275.4890	86.9634	119.4905
209.8006	252.5658	370.4554
395.5333	438.1985	500.0790
553.9965	562.4232	634.9136
664.6021	730.1247	757.5512
785.2845	843.5531	879.4939
972.8764	996.6442	1013.4292
1024.8389	1158.7472	1193.0770
1224.6930	1310.9836	1331.7808
1386.0098	1427.8785	1484.0425
1581.1612	1656.6129	1708.3268
1780.4574	3202.5689	3228.2385
3232.8611	3254.4953	3801.8134

Zero-point correction (Hartree): 0.106519

TS.nitrophenol.acinitrophenol

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-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.79199467
E(G3SX) excl. ZPE (Hartree): -511.80232406
E(G3X(MP2)) excl. ZPE (Hartree): -511.33985024
E(G3X(MP3)) excl. ZPE (Hartree): -511.75554708
E(G3X) excl. ZPE (Hartree): -511.72925446
E(MP2-Full/G3Xlarge) (Hartree): -511.43830588
E(MP2-Full/G3large) (Hartree): -511.43830588
E(MP2/6-31+G(d)) (Hartree): -510.48151421
E(MP2/6-31G(2df,p)) (Hartree): -510.79087155
E(MP2/6-31G(d)) (Hartree): -510.44607212
E(MP2/G3MP2large) (Hartree): -510.99383920
E(MP3/6-31+G(d)) (Hartree): -510.48247976
E(MP3/6-31G(2df,p)) (Hartree): -510.80013979
E(MP3/6-31G(d)) (Hartree): -510.45097266
E(MP4/6-31+G(d)) (Hartree): -510.58731672
E(MP4/6-31G(2df,p)) (Hartree): -510.91428256
E(MP4/6-31G(d)) (Hartree): -510.54982734
E(QCISD(T)/6-31G(d)) (Hartree): -510.53895962
E(QCISD/6-31G(d)) (Hartree): -510.47661202
E(RHF/6-31+G(d)) (Hartree): -508.98841682
E(RHF/6-31G(2df,p)) (Hartree): -509.02629987
E(RHF/6-31G(d)) (Hartree): -508.97234688
E(RHF/G3MP2large) (Hartree): -509.14984303
E(RHF/G3Xlarge) (Hartree): -509.15128657
E(RHF/G3large) (Hartree): -509.15128657
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.92011326
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -2.554080    -0.153186     0.086177
  C      -1.869327    -1.423624    -0.001833
  C      -0.527800    -1.472758    -0.051382
  C       0.236966    -0.255291    -0.000797
  C      -0.429255     1.077770    -0.049549
  C      -1.888719     1.012814     0.082742
  H      -3.634481    -0.153949     0.150753
  H      -2.447351    -2.336093    -0.007679
  H       0.012843    -2.406260    -0.091846
  H      -2.393230     1.967511     0.127718
  O       0.145723     2.129839    -0.251506
  H       2.694624     1.058470    -0.452968
  N       1.560974    -0.379939     0.020104
  O       2.278296     0.744621     0.363378
  O       2.205239    -1.397518    -0.144229
Rotational constants (GHz):   2.3777400   1.2610100   0.8347300
Vibrational harmonic frequencies (cm-1):
  i455.2813           84.0121       110.5876
  208.5923           264.7442       375.8297
  384.3860           433.4045       499.6236
  551.3784           590.6360       618.1637
  670.6140           739.3683       775.4055
  784.2501           875.8732       881.7447
  1002.7878          1011.3536       1031.0776
  1054.7310          1146.7761       1176.6776
  1215.8215          1319.0944       1363.0780

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1392.1798	1437.3157	1480.7524
1580.6596	1638.4979	1708.5670
1769.4973	3200.7179	3225.8602
3231.7647	3245.7832	3784.5345

Zero-point correction (Hartree): 0.106769

TS.nitrophenol_cis.introtNO2

E(G3SX(MP3)) excl. ZPE (Hartree): -511.83080174
 E(G3SX) excl. ZPE (Hartree): -511.84077785
 E(G3X(MP2)) excl. ZPE (Hartree): -511.37796102
 E(G3X(MP3)) excl. ZPE (Hartree): -511.79403213
 E(G3X) excl. ZPE (Hartree): -511.76753093
 E(MP2-Full/G3Xlarge) (Hartree): -511.48224718
 E(MP2-Full/G3large) (Hartree): -511.48224718
 E(MP2/6-31+G(d)) (Hartree): -510.52306984
 E(MP2/6-31G(2df,p)) (Hartree): -510.83298031
 E(MP2/6-31G(d)) (Hartree): -510.48539873
 E(MP2/G3MP2large) (Hartree): -511.03747334
 E(MP3/6-31+G(d)) (Hartree): -510.51909807
 E(MP3/6-31G(2df,p)) (Hartree): -510.83785519
 E(MP3/6-31G(d)) (Hartree): -510.48581986
 E(MP4/6-31+G(d)) (Hartree): -510.62333931
 E(MP4/6-31G(2df,p)) (Hartree): -510.95033621
 E(MP4/6-31G(d)) (Hartree): -510.58342114
 E(QCISD(T)/6-31G(d)) (Hartree): -510.57274393
 E(QCISD/6-31G(d)) (Hartree): -510.51138913
 E(RHF/6-31+G(d)) (Hartree): -509.02954532
 E(RHF/6-31G(2df,p)) (Hartree): -509.06925710
 E(RHF/6-31G(d)) (Hartree): -509.01260310
 E(RHF/G3MP2large) (Hartree): -509.19265334
 E(RHF/G3Xlarge) (Hartree): -509.19411583
 E(RHF/G3large) (Hartree): -509.19411583
 E(RM062X/Aug-CC-pVTZ) (Hartree): -511.95890754

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-2.540547	-0.120619	0.000032
C	-1.935101	-1.372382	0.000029
C	-0.554332	-1.458991	-0.000012
C	0.183922	-0.292336	-0.000038
C	-0.396448	0.967417	-0.000044
C	-1.785159	1.037941	-0.000034
H	-3.618722	-0.045903	0.000066
H	-2.532362	-2.271637	0.000049
H	-0.044574	-2.412116	-0.000025
H	-2.245427	2.015387	-0.000065
N	1.655348	-0.373307	0.000036
O	2.208592	-0.387719	-1.076263
O	2.208496	-0.387399	1.076377
O	0.303523	2.123204	0.000006
H	1.254753	1.976562	-0.000843

Rotational constants (GHz): 2.4245200 1.1874800 0.9026000

Vibrational harmonic frequencies (cm-1):

i128.8005	121.4238	175.8126
200.0769	242.9166	339.3441
378.9446	476.7595	512.0321
559.1498	591.8323	681.1988
753.3170	782.9823	783.9553
848.3976	889.5252	893.1590
971.7267	1004.8971	1064.4341
1110.5584	1169.8461	1179.5470
1221.4551	1302.3177	1339.2071
1359.8805	1494.0914	1518.8069
1542.7348	1670.2955	1673.0924
1685.7699	3214.4413	3223.3103
3231.9045	3241.0528	3856.3575

Zero-point correction (Hartree): 0.107772

TS.nitrophenol_trans.introtNO2

E(G3SX(MP3)) excl. ZPE (Hartree): -511.83051546

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E(G3SX) excl. ZPE (Hartree): -511.84047936
E(G3X(MP2)) excl. ZPE (Hartree): -511.37771255
E(G3X(MP3)) excl. ZPE (Hartree): -511.79376885
E(G3X) excl. ZPE (Hartree): -511.76724112
E(MP2-Full/G3Xlarge) (Hartree): -511.48194711
E(MP2-Full/G3large) (Hartree): -511.48194711
E(MP2/6-31+G(d)) (Hartree): -510.52267874
E(MP2/6-31G(2df,p)) (Hartree): -510.83261465
E(MP2/6-31G(d)) (Hartree): -510.48511828
E(MP2/G3MP2large) (Hartree): -511.03716469
E(MP3/6-31+G(d)) (Hartree): -510.51877018
E(MP3/6-31G(2df,p)) (Hartree): -510.83751543
E(MP3/6-31G(d)) (Hartree): -510.48558674
E(MP4/6-31+G(d)) (Hartree): -510.62304066
E(MP4/6-31G(2df,p)) (Hartree): -510.94997474
E(MP4/6-31G(d)) (Hartree): -510.58321299
E(QCISD(T)/6-31G(d)) (Hartree): -510.57252170
E(QCISD/6-31G(d)) (Hartree): -510.51131961
E(RHF/6-31+G(d)) (Hartree): -509.02975647
E(RHF/6-31G(2df,p)) (Hartree): -509.06931980
E(RHF/6-31G(d)) (Hartree): -509.01286169
E(RHF/G3MP2large) (Hartree): -509.19285118
E(RHF/G3Xlarge) (Hartree): -509.19431561
E(RHF/G3large) (Hartree): -509.19431561
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.95825904
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      2.534418      -0.162102      -0.000002
  C      1.907063      -1.399616      -0.000007
  C      0.521777      -1.462118      -0.000006
  C     -0.198352      -0.287731      -0.000002
  C      0.407273       0.959419       0.000003
  C      1.795115       1.010791       0.000003
  H      3.613592      -0.104569      -0.000002
  H      2.488656      -2.309077      -0.000010
  H     -0.002378      -2.407439      -0.000010
  H      2.289657       1.973895       0.000007
  N     -1.670633      -0.344098       0.000000
  O     -2.217261      -0.370438       1.076891
  O     -2.217265      -0.370429      -1.076890
  O     -0.394234       2.047400       0.000008
  H      0.131226       2.851760       0.000006
Rotational constants (GHz):   2.4377700   1.1884100   0.9051000
Vibrational harmonic frequencies (cm-1):
  i60.1387      124.8442      173.9779
  222.4337      297.8125      337.7440
  378.7591      462.7024      511.4001
  559.6031      595.2857      683.1453
  758.1593      777.6375      781.0176
  849.4590      876.1945      894.1177
  965.9508      998.5389     1070.3337
 1112.3750     1175.6867     1180.4329
 1195.4144     1321.6625     1334.6056
 1345.6660     1495.8726     1514.0120
 1555.8035     1673.7990     1687.2362
 1690.9672     3198.1461     3219.0790
 3225.1487     3240.9570     3883.7063
Zero-point correction (Hartree): 0.107916

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TS.nitrophenol_cis.hydroxyphenylnitrite

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-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.73935805
E(G3SX) excl. ZPE (Hartree): -511.74970781
E(G3X(MP2)) excl. ZPE (Hartree): -511.28723824
E(G3X(MP3)) excl. ZPE (Hartree): -511.70151273
E(G3X) excl. ZPE (Hartree): -511.67630366
E(MP2-Full/G3Xlarge) (Hartree): -511.39205377
E(MP2-Full/G3large) (Hartree): -511.39205377
E(MP2/6-31+G(d)) (Hartree): -510.43389601
E(MP2/6-31G(2df,p)) (Hartree): -510.74460151
E(MP2/6-31G(d)) (Hartree): -510.39621597

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E(MP2/G3MP2large) (Hartree): -510.94795148
E(MP3/6-31+G(d)) (Hartree): -510.41773676
E(MP3/6-31G(2df,p)) (Hartree): -510.73666411
E(MP3/6-31G(d)) (Hartree): -510.38498472
E(MP4/6-31+G(d)) (Hartree): -510.53633709
E(MP4/6-31G(2df,p)) (Hartree): -510.86368687
E(MP4/6-31G(d)) (Hartree): -510.49612280
E(QCISD(T)/6-31G(d)) (Hartree): -510.48239508
E(QCISD/6-31G(d)) (Hartree): -510.41524535
E(RHF/6-31+G(d)) (Hartree): -508.90854431
E(RHF/6-31G(2df,p)) (Hartree): -508.94873694
E(RHF/6-31G(d)) (Hartree): -508.89219825
E(RHF/G3MP2large) (Hartree): -509.07070179
E(RHF/G3Xlarge) (Hartree): -509.07212945
E(RHF/G3large) (Hartree): -509.07212945
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.86453024
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -2.519944      0.234736      -0.126910
  C      -2.153822     -1.112917     -0.112695
  C      -0.823759     -1.466054     -0.022480
  C       0.105632     -0.445406      0.059046
  C      -0.212132      0.908039      0.084433
  C      -1.565701      1.227146     -0.042215
  H      -3.562792      0.507048     -0.201960
  H      -2.904850     -1.885575     -0.186945
  H      -0.493612     -2.493615     -0.025369
  H      -1.832005      2.274689     -0.038443
  O       0.685508      1.898785      0.195567
  H       1.591751      1.559789      0.231361
  N       1.692458     -0.732789     -0.271590
  O       2.498026     -0.032211     -0.824602
  O       1.613048     -0.729834      1.014962
Rotational constants (GHz):   2.6221100   1.2150200   0.9198000
Vibrational harmonic frequencies (cm-1):
  1899.1999      99.6996      145.5547
  200.3002      246.8255      304.8465
  327.1959      404.1669      450.8852
  496.9753      545.6385      558.2814
  636.8758      704.1680      765.2690
  789.6697      846.0299      865.6358
  966.0787      971.6372     1005.4923
 1055.5581     1144.0529     1169.9027
 1224.8307     1251.3496     1296.5101
 1350.1950     1375.2504     1493.0098
 1517.2615     1570.8412     1634.6781
 1678.5910     3214.9144     3226.3023
 3234.5336     3246.7606     3756.9652
Zero-point correction (Hartree): 0.104278

TS.nitrophenol_cis.nitrophenol_trans
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E(G3SX(MP3)) excl. ZPE (Hartree): -511.82842984
E(G3SX) excl. ZPE (Hartree): -511.83850131
E(G3X(MP2)) excl. ZPE (Hartree): -511.37610431
E(G3X(MP3)) excl. ZPE (Hartree): -511.79191484
E(G3X) excl. ZPE (Hartree): -511.76553000
E(MP2-Full/G3Xlarge) (Hartree): -511.47983096
E(MP2-Full/G3large) (Hartree): -511.47983096
E(MP2/6-31+G(d)) (Hartree): -510.52138113
E(MP2/6-31G(2df,p)) (Hartree): -510.83212266
E(MP2/6-31G(d)) (Hartree): -510.48507036
E(MP2/G3MP2large) (Hartree): -511.03518152
E(MP3/6-31+G(d)) (Hartree): -510.51843328
E(MP3/6-31G(2df,p)) (Hartree): -510.83776913
E(MP3/6-31G(d)) (Hartree): -510.48640455
E(MP4/6-31+G(d)) (Hartree): -510.62196562
E(MP4/6-31G(2df,p)) (Hartree): -510.94978005
E(MP4/6-31G(d)) (Hartree): -510.58341358
E(QCISD(T)/6-31G(d)) (Hartree): -510.57285596
E(QCISD/6-31G(d)) (Hartree): -510.51165016

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E(RHF/6-31+G(d)) (Hartree): -509.03067042
 E(RHF/6-31G(2df,p)) (Hartree): -509.07018270
 E(RHF/6-31G(d)) (Hartree): -509.01496555
 E(RHF/G3MP2large) (Hartree): -509.19284337
 E(RHF/G3Xlarge) (Hartree): -509.19430055
 E(RHF/G3large) (Hartree): -509.19430055
 E(RM062X/Aug-CC-pVTZ) (Hartree): -511.95782009
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-2.531698	-0.205736	0.067564
C	-1.867999	-1.424610	0.130417
C	-0.485901	-1.452541	0.079804
C	0.212137	-0.260738	-0.006168
C	-0.433744	0.967805	-0.096740
C	-1.822799	0.977328	-0.061938
H	-3.611965	-0.176839	0.099764
H	-2.423488	-2.346935	0.215890
H	0.069235	-2.378350	0.119335
H	-2.332059	1.926289	-0.161379
O	0.277431	2.106179	-0.326778
H	0.191937	2.720254	0.407906
N	1.679875	-0.328414	0.034365
O	2.259267	0.503215	0.692393
O	2.204207	-1.241215	-0.565578

 Rotational constants (GHz): 2.3774200 1.2515300 0.8626400
 Vibrational harmonic frequencies (cm-1):

i386.8939	68.7323	134.8518
227.3382	242.9277	353.7202
398.8273	456.8476	514.4736
559.3191	588.5490	679.2827
717.6693	774.5652	820.2699
848.0792	895.8561	901.1943
990.6330	1017.3830	1071.1060
1116.6900	1171.9940	1184.6290
1196.5915	1296.5311	1309.7559
1336.2060	1471.9984	1497.5260
1544.5211	1655.2884	1662.8811
1701.9522	3208.2307	3219.8799
3229.1269	3240.1052	3870.6840

 Zero-point correction (Hartree): 0.107475

TS.nitrophenol_trans.hydroxyphenylnitrite

 E(G3SX(MP3)) excl. ZPE (Hartree): -511.73667200
 E(G3SX) excl. ZPE (Hartree): -511.74672281
 E(G3X(MP2)) excl. ZPE (Hartree): -511.28423412
 E(G3X(MP3)) excl. ZPE (Hartree): -511.69882147
 E(G3X) excl. ZPE (Hartree): -511.67310104
 E(MP2-Full/G3Xlarge) (Hartree): -511.38895611
 E(MP2-Full/G3large) (Hartree): -511.38895611
 E(MP2/6-31+G(d)) (Hartree): -510.42993208
 E(MP2/6-31G(2df,p)) (Hartree): -510.73950305
 E(MP2/6-31G(d)) (Hartree): -510.39069296
 E(MP2/G3MP2large) (Hartree): -510.94479215
 E(MP3/6-31+G(d)) (Hartree): -510.41382760
 E(MP3/6-31G(2df,p)) (Hartree): -510.73199374
 E(MP3/6-31G(d)) (Hartree): -510.37962354
 E(MP4/6-31+G(d)) (Hartree): -510.53311853
 E(MP4/6-31G(2df,p)) (Hartree): -510.85930474
 E(MP4/6-31G(d)) (Hartree): -510.49145319
 E(QCISD(T)/6-31G(d)) (Hartree): -510.47701221
 E(QCISD/6-31G(d)) (Hartree): -510.41061507
 E(RHF/6-31+G(d)) (Hartree): -508.90643841
 E(RHF/6-31G(2df,p)) (Hartree): -508.94584808
 E(RHF/6-31G(d)) (Hartree): -508.88867921
 E(RHF/G3MP2large) (Hartree): -509.06960695
 E(RHF/G3Xlarge) (Hartree): -509.07104967
 E(RHF/G3large) (Hartree): -509.07104967
 E(UM062X/Aug-CC-pVTZ) (Hartree): -511.86157381
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-2.492496	-0.429344	-0.122931
C	-1.707102	-1.558911	0.008939
C	-0.324737	-1.441140	0.132424
C	0.221113	-0.177291	0.109353
C	-0.540556	0.984626	-0.022881
C	-1.908052	0.836817	-0.139870
H	-3.564701	-0.519115	-0.217231
H	-2.155037	-2.541779	0.017967
H	0.321546	-2.301859	0.220086
H	-2.521082	1.723402	-0.248247
O	0.126644	2.158967	-0.032949
H	-0.485785	2.884381	-0.184557
N	1.826970	-0.050035	-0.227029
O	2.703879	-0.660637	-0.744372
O	1.685383	-0.021245	1.053692
Rotational constants (GHz): 2.4053600 1.2033000 0.8812500			
Vibrational harmonic frequencies (cm-1):			
i871.1625	108.0677	145.5031	
193.0723	235.0374	272.4320	
356.4323	406.7466	468.1579	
481.7446	552.6213	558.8355	
638.5691	702.4678	760.8384	
785.0169	847.5672	854.6340	
940.2338	994.7497	998.4329	
1065.2948	1128.5508	1173.6110	
1183.9033	1277.9950	1318.2557	
1322.2836	1364.2115	1488.9826	
1531.3611	1638.6118	1643.8640	
1679.9668	3192.2433	3218.9649	
3233.3509	3240.7869	3874.7359	
Zero-point correction (Hartree): 0.104518			

TS.aci-NP-2.cycloketene+HONO

E(G3SX(MP3)) excl. ZPE (Hartree): -511.69382077
E(G3SX) excl. ZPE (Hartree): -511.70358988
E(G3X(MP2)) excl. ZPE (Hartree): -511.24239378
E(G3X(MP3)) excl. ZPE (Hartree): -511.65730458
E(G3X) excl. ZPE (Hartree): -511.62997513
E(MP2-Full/G3Xlarge) (Hartree): -511.33270877
E(MP2-Full/G3large) (Hartree): -511.33270877
E(MP2/6-31+G(d)) (Hartree): -510.37338608
E(MP2/6-31G(2df,p)) (Hartree): -510.68606163
E(MP2/6-31G(d)) (Hartree): -510.33839563
E(MP2/G3MP2large) (Hartree): -510.88897981
E(MP3/6-31+G(d)) (Hartree): -510.37202249
E(MP3/6-31G(2df,p)) (Hartree): -510.69267713
E(MP3/6-31G(d)) (Hartree): -510.34069385
E(MP4/6-31+G(d)) (Hartree): -510.48541565
E(MP4/6-31G(2df,p)) (Hartree): -510.81491310
E(MP4/6-31G(d)) (Hartree): -510.44852824
E(QCISD(T)/6-31G(d)) (Hartree): -510.43868817
E(QCISD/6-31G(d)) (Hartree): -510.37678826
E(RHF/6-31+G(d)) (Hartree): -508.88937311
E(RHF/6-31G(2df,p)) (Hartree): -508.93036765
E(RHF/6-31G(d)) (Hartree): -508.87309650
E(RHF/G3MP2large) (Hartree): -509.05419085
E(RHF/G3Xlarge) (Hartree): -509.05563229
E(RHF/G3large) (Hartree): -509.05563229
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.82167200
Electronic state : 1-A

Cartesian coordinates (Angs):

C	2.778219	-0.368720	-0.000009
C	2.057457	-1.570454	0.000078
C	0.686483	-1.389065	0.000220
C	0.306834	-0.085533	0.000321
C	0.616698	1.218871	-0.000130
C	2.113486	0.825007	0.000017
H	3.859348	-0.358456	-0.000068
H	2.506861	-2.550159	-0.000008
H	-0.053031	-2.176224	0.000174

H	2.629856	1.778222	0.000098
O	0.202062	2.356560	-0.000379
H	-3.790096	0.371271	0.000321
N	-2.056624	-0.338565	0.000006
O	-2.876329	0.719157	0.000600
O	-2.589686	-1.385134	-0.000662
Rotational constants (GHz):		2.2509700	0.9180000 0.6520700
Vibrational harmonic frequencies (cm-1):			
i305.5470	25.6031	46.8816	
60.2533	72.9067	113.0839	
167.5456	184.8580	424.0061	
424.2742	486.4401	582.8770	
641.9976	704.3742	708.0449	
725.1553	740.6975	752.6469	
810.5152	909.5921	953.7566	
966.0250	1045.2983	1076.0849	
1107.7734	1169.8509	1261.3388	
1391.3427	1396.4445	1440.1955	
1518.0514	1614.9580	1772.1910	
1921.1955	3185.9520	3220.4279	
3237.6312	3259.0051	3645.5230	
Zero-point correction (Hartree): 0.099704			

TS.aci-NP-3.cycloketene+HONO_cis

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.69681480
E(G3SX) excl. ZPE (Hartree): -511.70697851
E(G3X(MP2)) excl. ZPE (Hartree): -511.24541784
E(G3X(MP3)) excl. ZPE (Hartree): -511.65991297
E(G3X) excl. ZPE (Hartree): -511.63357857
E(MP2-Full/G3Xlarge) (Hartree): -511.33515317
E(MP2-Full/G3large) (Hartree): -511.33515317
E(MP2/6-31+G(d)) (Hartree): -510.37745712
E(MP2/6-31G(2df,p)) (Hartree): -510.68941357
E(MP2/6-31G(d)) (Hartree): -510.34201116
E(MP2/G3MP2large) (Hartree): -510.89138997
E(MP3/6-31+G(d)) (Hartree): -510.37451743
E(MP3/6-31G(2df,p)) (Hartree): -510.69420907
E(MP3/6-31G(d)) (Hartree): -510.34296390
E(MP4/6-31+G(d)) (Hartree): -510.49001272
E(MP4/6-31G(2df,p)) (Hartree): -510.81866649
E(MP4/6-31G(d)) (Hartree): -510.45234724
E(QCISD(T)/6-31G(d)) (Hartree): -510.44294219
E(QCISD/6-31G(d)) (Hartree): -510.38094465
E(RHF/6-31+G(d)) (Hartree): -508.88721037
E(RHF/6-31G(2df,p)) (Hartree): -508.92790049
E(RHF/6-31G(d)) (Hartree): -508.87175282
E(RHF/G3MP2large) (Hartree): -509.05052654
E(RHF/G3Xlarge) (Hartree): -509.05194337
E(RHF/G3large) (Hartree): -509.05194337
E(RM062X/Aug-CC-pVTZ) (Hartree): -511.82496752

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Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.131371	0.926381	-0.035128
C	0.306830	-0.417139	0.020254
C	1.169816	-1.453723	0.057686
C	2.501033	-1.059309	0.038250
C	2.692847	0.323493	-0.017343
C	1.624849	1.179822	-0.048351
O	-0.736225	1.782960	-0.070046
N	-1.951365	-0.840133	-0.053921
O	-2.413553	-0.427447	-1.049638
O	-2.320431	-0.173610	1.057301
H	-2.693254	0.679387	0.750728
H	0.818995	-2.473494	0.096655
H	3.302091	-1.780249	0.063069
H	3.687416	0.746888	-0.036575
H	1.745499	2.256022	-0.089571
Rotational constants (GHz):		2.7302700	0.9634200 0.7933000
Vibrational harmonic frequencies (cm-1):			
i296.7882	67.3497	84.8010	

104.6780	125.5960	168.5174
172.6319	317.7412	415.6548
447.4191	472.6270	548.3744
577.4294	646.8332	692.8515
731.4848	754.9890	771.5993
834.0129	904.3320	956.5314
969.9273	1020.6567	1060.5273
1109.5465	1175.4782	1258.7329
1381.9205	1407.8439	1436.8504
1516.1186	1611.5524	1762.0152
1837.6121	3189.8173	3219.8252
3246.9342	3261.1187	3617.3398

Zero-point correction (Hartree): 0.099964

TS.hydroxyphenylnitrite_pt.cycloketene+HONO_cis

E(G3SX(MP3)) excl. ZPE (Hartree): -511.70882297
 E(G3SX) excl. ZPE (Hartree): -511.71896902
 E(G3X(MP2)) excl. ZPE (Hartree): -511.25765473
 E(G3X(MP3)) excl. ZPE (Hartree): -511.67269669
 E(G3X) excl. ZPE (Hartree): -511.64583074
 E(MP2-Full/G3Xlarge) (Hartree): -511.35046218
 E(MP2-Full/G3large) (Hartree): -511.35046218
 E(MP2/6-31+G(d)) (Hartree): -510.39458201
 E(MP2/6-31G(2df,p)) (Hartree): -510.70559907
 E(MP2/6-31G(d)) (Hartree): -510.36019497
 E(MP2/G3MP2large) (Hartree): -510.90667048
 E(MP3/6-31+G(d)) (Hartree): -510.39149936
 E(MP3/6-31G(2df,p)) (Hartree): -510.71044544
 E(MP3/6-31G(d)) (Hartree): -510.36066436
 E(MP4/6-31+G(d)) (Hartree): -510.50500095
 E(MP4/6-31G(2df,p)) (Hartree): -510.83286671
 E(MP4/6-31G(d)) (Hartree): -510.46846875
 E(QCISD(T)/6-31G(d)) (Hartree): -510.45806650
 E(QCISD/6-31G(d)) (Hartree): -510.39480979
 E(RHF/6-31+G(d)) (Hartree): -508.90427204
 E(RHF/6-31G(2df,p)) (Hartree): -508.94507130
 E(RHF/6-31G(d)) (Hartree): -508.88879128
 E(RHF/G3MP2large) (Hartree): -509.06727335
 E(RHF/G3Xlarge) (Hartree): -509.06870608
 E(RHF/G3large) (Hartree): -509.06870608
 E(RM062X/Aug-CC-pVTZ) (Hartree): -511.83963856

Electronic state : 1-A

Cartesian coordinates (Angs):

C	2.848415	0.387625	-0.009256
C	2.715919	-1.004424	-0.064899
C	1.395974	-1.411945	0.001953
C	0.539747	-0.369535	0.173111
C	0.203240	0.884011	-0.052063
C	1.715684	1.158712	0.085239
H	3.812009	0.876229	0.006734
H	3.534824	-1.691909	-0.203111
H	1.019116	-2.413492	-0.141735
H	1.760778	2.216504	0.321765
O	-0.685144	1.721789	-0.118674
H	-2.100886	0.943964	-0.035605
O	-3.015732	0.504495	0.011292
N	-2.920782	-0.808859	0.021242
O	-1.810904	-1.243277	-0.005275

Rotational constants (GHz): 3.0330700 0.8287400 0.6524400

Vibrational harmonic frequencies (cm-1):

i346.8521	40.1945	72.0713
79.9022	151.7476	186.8545
237.5913	253.2024	423.5913
457.0375	499.5171	577.1621
668.3477	700.7205	754.4769
771.6291	774.9926	831.5554
918.8738	961.7334	969.3661
1018.6312	1072.4624	1104.7399
1128.5923	1162.7496	1257.3878
1383.0246	1432.2273	1499.7410

1508.6981	1591.3438	1680.1788
1949.9586	2873.2323	3180.6833
3228.3903	3244.1871	3261.5500

Zero-point correction (Hartree): 0.100031

TS.nitrophenol_cis.cycloketene+HONO_trans

E(G3SX(MP3)) excl. ZPE (Hartree): -511.70956571
 E(G3SX) excl. ZPE (Hartree): -511.71935879
 E(G3X(MP2)) excl. ZPE (Hartree): -511.25785552
 E(G3X(MP3)) excl. ZPE (Hartree): -511.67303692
 E(G3X) excl. ZPE (Hartree): -511.64598327
 E(MP2-Full/G3Xlarge) (Hartree): -511.35114263
 E(MP2-Full/G3large) (Hartree): -511.35114263
 E(MP2/6-31+G(d)) (Hartree): -510.39420134
 E(MP2/6-31G(2df,p)) (Hartree): -510.70388932
 E(MP2/6-31G(d)) (Hartree): -510.35773739
 E(MP2/G3MP2large) (Hartree): -510.90735257
 E(MP3/6-31+G(d)) (Hartree): -510.39129328
 E(MP3/6-31G(2df,p)) (Hartree): -510.70954673
 E(MP3/6-31G(d)) (Hartree): -510.35887031
 E(MP4/6-31+G(d)) (Hartree): -510.50400074
 E(MP4/6-31G(2df,p)) (Hartree): -510.83066848
 E(MP4/6-31G(d)) (Hartree): -510.46547725
 E(QCISD(T)/6-31G(d)) (Hartree): -510.45512119
 E(QCISD/6-31G(d)) (Hartree): -510.39206841
 E(RHF/6-31+G(d)) (Hartree): -508.90193404
 E(RHF/6-31G(2df,p)) (Hartree): -508.94281257
 E(RHF/6-31G(d)) (Hartree): -508.88539146
 E(RHF/G3MP2large) (Hartree): -509.06602250
 E(RHF/G3Xlarge) (Hartree): -509.06746165
 E(RHF/G3large) (Hartree): -509.06746165
 E(RM062X/Aug-CC-pVTZ) (Hartree): -511.83888296

Electronic state : 1-A

Cartesian coordinates (Angs):

C	2.861753	0.025733	-0.003443
C	2.460074	-1.313223	-0.080769
C	1.086436	-1.456639	-0.019326
C	0.444810	-0.271292	0.170857
C	0.364681	1.029791	-0.045559
C	1.901709	1.001423	0.102802
H	3.902540	0.315403	0.021046
H	3.129468	-2.144947	-0.230545
H	0.525265	-2.365594	-0.177295
H	2.149742	2.026744	0.357069
O	-0.345111	2.022442	-0.108135
H	-1.906029	1.314011	-0.058881
N	-2.129705	-0.538886	0.010803
O	-2.678949	0.690657	-0.027361
O	-2.927169	-1.396622	0.043697

Rotational constants (GHz): 2.5608300 0.8651400 0.6483600

Vibrational harmonic frequencies (cm-1):

i365.0210	54.2701	67.2983
78.8048	146.5742	156.0667
194.4508	239.5658	415.1367
457.3918	497.5366	575.9965
662.5724	697.9604	751.7852
764.9671	774.4425	826.0466
915.1943	918.4356	959.7625
970.0136	1029.3263	1074.9055
1104.7656	1161.3096	1257.1174
1383.6632	1431.7482	1509.5162
1524.5971	1591.8105	1804.1055
1941.2840	3176.3199	3227.6073
3241.1403	3242.3014	3260.3334

Zero-point correction (Hartree): 0.100436

TS.aci-NP-2.nitrosophenoxy+OH

E(UM062X/Aug-CC-pVTZ) (Hartree): -511.83968434

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-2.933290	0.227107	0.006343
C	-2.459964	-1.139193	0.009895
C	-1.119396	-1.407751	0.007044
C	-0.179617	-0.305579	-0.002006
C	-0.609991	1.105266	-0.004559
C	-2.076049	1.272046	-0.000252
H	-4.009882	0.405753	0.008942
H	-3.182260	-1.956956	0.013365
H	-0.733814	-2.422795	0.009191
H	-2.416520	2.307159	-0.002421
O	0.163770	2.042636	-0.010471
N	1.154232	-0.600296	-0.005530
O	1.677999	-1.674575	-0.019027
O	4.767437	0.537600	0.021703
H	5.659049	0.112252	-0.026798

Rotational constants (GHz): 2.3867300 0.6828300 0.5309600

Vibrational harmonic frequencies (cm-1):

17.2329	46.3033	54.3499
122.3279	229.0789	233.8693
357.0215	367.8450	468.0675
476.1809	478.3599	491.6135
556.8839	565.2779	591.5764
757.9518	761.9000	804.6939
862.0285	898.4087	1003.8397
1012.0583	1045.7281	1081.5378
1156.1196	1189.2992	1216.7733
1357.8648	1404.2690	1452.0185
1524.3370	1620.2251	1659.5123
1746.0074	3115.2372	3130.0633
3148.6732	3182.4163	3551.2938

Zero-point correction (Hartree): 0.099643

TS.hydroxyphenylnitrite_pt.nitritephenyl+OH

E(G3SX(MP3)) excl. ZPE (Hartree): -511.66027259
 E(G3SX) excl. ZPE (Hartree): -511.66692705
 E(G3X(MP2)) excl. ZPE (Hartree): -511.21307525
 E(G3X(MP3)) excl. ZPE (Hartree): -511.62396256
 E(G3X) excl. ZPE (Hartree): -511.60100027
 E(MP2-Full/G3Xlarge) (Hartree): -511.27803970
 E(MP2-Full/G3large) (Hartree): -511.27803970
 E(MP2/6-31+G(d)) (Hartree): -510.33338006
 E(MP2/6-31G(2df,p)) (Hartree): -510.63272092
 E(MP2/6-31G(d)) (Hartree): -510.29763556
 E(MP2/G3MP2large) (Hartree): -510.83549398
 E(MP3/6-31+G(d)) (Hartree): -510.30707524
 E(MP3/6-31G(2df,p)) (Hartree): -510.62246500
 E(MP3/6-31G(d)) (Hartree): -510.28600516
 E(MP4/6-31+G(d)) (Hartree): -510.49740901
 E(MP4/6-31G(2df,p)) (Hartree): -510.80962785
 E(MP4/6-31G(d)) (Hartree): -510.45708341
 E(QCISD(T)/6-31G(d)) (Hartree): -510.42219794
 E(QCISD/6-31G(d)) (Hartree): -510.32302813
 E(RHF/6-31+G(d)) (Hartree): -508.74823986
 E(RHF/6-31G(2df,p)) (Hartree): -508.77343884
 E(RHF/6-31G(d)) (Hartree): -508.71979034
 E(RHF/G3MP2large) (Hartree): -508.90789076
 E(RHF/G3Xlarge) (Hartree): -508.90922965
 E(RHF/G3large) (Hartree): -508.90922965
 E(UM062X/Aug-CC-pVTZ) (Hartree): -511.78866880

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-2.883089	0.096019	0.146813
C	-2.311555	-1.139084	-0.127368
C	-0.939050	-1.272521	-0.295219
C	-0.130972	-0.149932	-0.163835
C	-0.733250	1.049486	0.113154
C	-2.078096	1.230237	0.264707
H	-3.954101	0.184695	0.264856
H	-2.941524	-2.011829	-0.224147

H	-0.494598	-2.230052	-0.530045
H	-2.501691	2.203068	0.472439
O	1.962377	2.756642	-0.130195
H	2.059571	1.812869	-0.352710
O	1.240047	-0.196460	-0.337698
N	1.838005	-1.280091	0.393364
O	2.975373	-1.295600	0.216211
Rotational constants (GHz):	1.9103300	0.9163200	0.6325400
Vibrational harmonic frequencies (cm-1):			
178.4736	45.4161	55.9528	
102.2602	142.1222	157.5833	
289.9166	322.9824	352.3456	
388.1013	423.3644	472.2803	
544.3219	614.3947	653.2981	
699.4154	761.4661	797.5099	
871.5539	932.8248	966.2269	
1001.1198	1006.1978	1053.0672	
1134.2096	1169.9754	1242.1070	
1289.9353	1322.1431	1475.0367	
1491.3043	1612.6710	1675.5868	
1865.3119	3205.3907	3213.5701	
3220.6247	3231.1793	3725.7504	
Zero-point correction (Hartree):	0.099165		

TS.nitrophenol_cis.nitrophenyl+OH

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.65769662
E(G3SX) excl. ZPE (Hartree): -511.66600081
E(G3X(MP2)) excl. ZPE (Hartree): -511.20212576
E(G3X(MP3)) excl. ZPE (Hartree): -511.62020698
E(G3X) excl. ZPE (Hartree): -511.59195889
E(MP2-Full/G3Xlarge) (Hartree): -511.23006760
E(MP2-Full/G3large) (Hartree): -511.23006760
E(MP2/6-31+G(d)) (Hartree): -510.28437343
E(MP2/6-31G(2df,p)) (Hartree): -510.58133897
E(MP2/6-31G(d)) (Hartree): -510.24635610
E(MP2/G3MP2large) (Hartree): -510.78614770
E(MP3/6-31+G(d)) (Hartree): -510.32374134
E(MP3/6-31G(2df,p)) (Hartree): -510.63120669
E(MP3/6-31G(d)) (Hartree): -510.28901451
E(MP4/6-31+G(d)) (Hartree): -510.41116381
E(MP4/6-31G(2df,p)) (Hartree): -510.72652640
E(MP4/6-31G(d)) (Hartree): -510.37105040
E(PMP2/6-31+G(d)) (Hartree): -527.38900999
E(PMP2/6-31G(2df,p)) (Hartree): -502.68506189
E(PMP2/6-31G(d)) (Hartree): -504.13478777
E(PMP2/G3MP2large) (Hartree): -526.44301681
E(PMP2/G3Xlarge) (Hartree): -526.11054305
E(PMP2/G3large) (Hartree): -526.11054305
E(PMP3/6-31+G(d)) (Hartree): -527.42353961
E(PMP3/6-31G(2df,p)) (Hartree): -502.72990876
E(PMP3/6-31G(d)) (Hartree): -504.17258447
E(PUHF/6-31+G(d)) (Hartree): -526.04789168
E(PUHF/6-31G(2df,p)) (Hartree): -501.08288326
E(PUHF/6-31G(d)) (Hartree): -502.81523463
E(PUHF/G3MP2large) (Hartree): -524.75960329
E(PUHF/G3Xlarge) (Hartree): -523.98456883
E(PUHF/G3large) (Hartree): -523.98456883
E(QCISD(T)/6-31G(d)) (Hartree): -510.40930017
E(QCISD/6-31G(d)) (Hartree): -510.35020860
E(UHF/6-31+G(d)) (Hartree): -508.94080705
E(UHF/6-31G(2df,p)) (Hartree): -508.97664015
E(UHF/6-31G(d)) (Hartree): -508.92432794
E(UHF/G3MP2large) (Hartree): -509.10024566
E(UHF/G3Xlarge) (Hartree): -509.10159965
E(UHF/G3large) (Hartree): -509.10159965
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.78956755
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -2.506063      -1.213119      0.000075
C      -2.643647      0.171189      0.001089

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C	-1.528659	0.995012	0.000925
C	-0.274664	0.401830	-0.000277
C	-0.170291	-0.961185	-0.001272
C	-1.242919	-1.806847	-0.001129
H	-3.387092	-1.840618	0.000227
H	-3.629913	0.611914	0.002011
H	-1.606752	2.072553	0.001702
H	-1.124784	-2.881277	-0.001904
O	3.495427	-1.962437	0.001822
H	3.006577	-1.117837	0.000308
N	0.936326	1.232089	-0.000507
O	2.006996	0.658690	-0.001582
O	0.795719	2.429917	0.000352
Rotational constants (GHz): 1.7794700 0.9592800 0.6232800			
Vibrational harmonic frequencies (cm-1):			
143.3526	24.2877	68.3703	
115.2443	168.2579	232.3177	
292.3095	375.9442	391.7058	
416.0313	455.0303	537.6598	
615.5032	644.8932	695.1322	
753.3160	819.2637	886.4757	
893.1192	989.3637	996.4917	
1014.2563	1048.7838	1128.3209	
1162.5930	1190.2998	1264.6561	
1332.7501	1460.7684	1477.6880	
1482.7053	1613.6928	1667.7581	
1689.6680	3206.1598	3221.2196	
3227.4276	3239.2929	3702.6763	
Zero-point correction (Hartree): 0.101382			

TS.hydroxyphenylnitrite_cis.hydroxyphenyl+NO2

E(G3SX(MP3)) excl. ZPE (Hartree): -511.71578230
E(G3SX) excl. ZPE (Hartree): -511.72386061
E(G3X(MP2)) excl. ZPE (Hartree): -511.25528851
E(G3X(MP3)) excl. ZPE (Hartree): -511.67226465
E(G3X) excl. ZPE (Hartree): -511.64506315
E(MP2-Full/G3Xlarge) (Hartree): -511.26209054
E(MP2-Full/G3large) (Hartree): -511.26209054
E(MP2/6-31+G(d)) (Hartree): -510.30998407
E(MP2/6-31G(2df,p)) (Hartree): -510.61553603
E(MP2/6-31G(d)) (Hartree): -510.27415566
E(MP2/G3MP2large) (Hartree): -510.81822203
E(MP3/6-31+G(d)) (Hartree): -510.34370080
E(MP3/6-31G(2df,p)) (Hartree): -510.65877835
E(MP3/6-31G(d)) (Hartree): -510.31121293
E(MP4/6-31+G(d)) (Hartree): -510.44158760
E(MP4/6-31G(2df,p)) (Hartree): -510.76525061
E(MP4/6-31G(d)) (Hartree): -510.40350894
E(PMP2/6-31+G(d)) (Hartree): -510.57054299
E(PMP2/6-31G(2df,p)) (Hartree): -510.89330773
E(PMP2/6-31G(d)) (Hartree): -510.55749570
E(PMP2/G3MP2large) (Hartree): -511.08036541
E(PMP2/G3Xlarge) (Hartree): -511.52433005
E(PMP2/G3large) (Hartree): -511.52433005
E(PMP3/6-31+G(d)) (Hartree): -510.59677717
E(PMP3/6-31G(2df,p)) (Hartree): -510.92885545
E(PMP3/6-31G(d)) (Hartree): -510.58705807
E(PUHF/6-31+G(d)) (Hartree): -509.19089561
E(PUHF/6-31G(2df,p)) (Hartree): -509.24779381
E(PUHF/6-31G(d)) (Hartree): -509.19859023
E(PUHF/G3MP2large) (Hartree): -509.35428543
E(PUHF/G3Xlarge) (Hartree): -509.35577053
E(PUHF/G3large) (Hartree): -509.35577053
E(QCISD(T)/6-31G(d)) (Hartree): -510.45815872
E(QCISD/6-31G(d)) (Hartree): -510.38906531
E(UHF/6-31+G(d)) (Hartree): -508.92675272
E(UHF/6-31G(2df,p)) (Hartree): -508.96637517
E(UHF/6-31G(d)) (Hartree): -508.91162103
E(UHF/G3MP2large) (Hartree): -509.08855210
E(UHF/G3Xlarge) (Hartree): -509.08993552

E(UHF/G3large) (Hartree): -509.08993552
 E(RM062X/Aug-CC-pVTZ) (Hartree): -511.84353778
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	2.877097	0.243969	0.000438
C	2.569942	-1.111461	0.000209
C	1.228687	-1.525824	-0.000209
C	0.399176	-0.473151	-0.000451
C	0.536687	0.889519	-0.000177
C	1.897756	1.227910	0.000244
H	3.914449	0.546433	0.000790
H	3.345397	-1.863100	0.000381
H	0.903970	-2.554406	-0.000342
H	2.143909	2.281761	0.000410
O	-0.480398	1.742562	-0.000604
H	-1.251206	1.113121	0.000069
O	-1.833253	-1.043407	-0.000495
N	-2.548179	0.054016	0.000228
O	-3.720767	-0.125116	0.000696

 Rotational constants (GHz): 3.2215000 0.7795500 0.6276700
 Vibrational harmonic frequencies (cm-1):

i226.7940	72.2502	148.1116
162.1334	230.3959	267.9322
274.0921	417.7979	425.3203
490.5582	542.5182	601.8427
635.3437	718.1561	784.0201
830.1525	845.3934	866.6138
878.5542	934.7659	992.5897
1021.6133	1090.9438	1116.9456
1159.7842	1197.1972	1305.0066
1336.1312	1433.8374	1506.0268
1536.2795	1622.5976	1700.7855
1733.6302	3150.3051	3209.1118
3224.2178	3236.5064	3256.7525

 Zero-point correction (Hartree): 0.102418

TS.nitrophenol_cis.hydroxyphenyl+NO2

 E(UM062X/Aug-CC-pVTZ) (Hartree): -511.85113529
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-3.126940	-0.035174	0.000041
C	-2.662291	-1.351493	0.000073
C	-1.282245	-1.591895	0.000038
C	-0.450348	-0.497469	-0.000017
C	-0.861728	0.825200	-0.000081
C	-2.246152	1.044279	-0.000034
H	-4.200225	0.158170	0.000081
H	-3.362328	-2.187172	0.000147
H	-0.886939	-2.608954	0.000101
H	-2.603400	2.075226	-0.000065
O	-0.025584	1.889146	-0.000200
H	0.887846	1.564598	0.000073
N	2.946674	-0.355198	-0.000301
O	2.812719	0.829193	0.000517
O	3.877433	-1.077861	-0.000111

 Rotational constants (GHz): 2.7545900 0.6166800 0.5038700
 Vibrational harmonic frequencies (cm-1):

23.4246	80.6221	87.2488
96.5903	132.0198	175.4176
242.8389	414.7526	437.8390
527.2765	539.3857	572.0894
627.7484	696.4837	786.1435
807.6943	836.6833	898.0020
983.1926	984.5127	1023.9045
1047.4908	1119.2183	1166.1192
1209.0202	1283.7457	1306.9428
1374.8896	1435.8646	1488.7293
1491.8486	1601.1372	1645.2109
1735.1650	3114.7887	3121.3556
3131.9468	3142.2616	3759.6956

Zero-point correction (Hartree): 0.102858

TS.hydroxyphenylnitrite.hydroxyphenoxy+NO

E(G3SX(MP3)) excl. ZPE (Hartree): -511.79975918
E(G3SX) excl. ZPE (Hartree): -511.80871948
E(G3X(MP2)) excl. ZPE (Hartree): -511.34401122
E(G3X(MP3)) excl. ZPE (Hartree): -511.76125910
E(G3X) excl. ZPE (Hartree): -511.73414342
E(MP2-Full/G3Xlarge) (Hartree): -511.39108206
E(MP2-Full/G3large) (Hartree): -511.39108206
E(MP2/6-31+G(d)) (Hartree): -510.43638638
E(MP2/6-31G(2df,p)) (Hartree): -510.74334036
E(MP2/6-31G(d)) (Hartree): -510.40100823
E(MP2/G3MP2large) (Hartree): -510.94649742
E(MP3/6-31+G(d)) (Hartree): -510.46439469
E(MP3/6-31G(2df,p)) (Hartree): -510.78077592
E(MP3/6-31G(d)) (Hartree): -510.43271363
E(MP4/6-31+G(d)) (Hartree): -510.55799722
E(MP4/6-31G(2df,p)) (Hartree): -510.88266684
E(MP4/6-31G(d)) (Hartree): -510.52035565
E(PMP2/6-31+G(d)) (Hartree): -510.63710197
E(PMP2/6-31G(2df,p)) (Hartree): -510.95825418
E(PMP2/6-31G(d)) (Hartree): -510.61256250
E(PMP2/G3MP2large) (Hartree): -511.14989026
E(PMP2/G3Xlarge) (Hartree): -511.59478279
E(PMP2/G3large) (Hartree): -511.59478279
E(PMP3/6-31+G(d)) (Hartree): -510.65988268
E(PMP3/6-31G(2df,p)) (Hartree): -510.99024333
E(PMP3/6-31G(d)) (Hartree): -510.63900875
E(PUHF/6-31+G(d)) (Hartree): -509.24815154
E(PUHF/6-31G(2df,p)) (Hartree): -509.30285350
E(PUHF/6-31G(d)) (Hartree): -509.24553256
E(PUHF/G3MP2large) (Hartree): -509.41305215
E(PUHF/G3Xlarge) (Hartree): -509.41473899
E(PUHF/G3large) (Hartree): -509.41473899
E(QCISD(T)/6-31G(d)) (Hartree): -510.54546911
E(QCISD/6-31G(d)) (Hartree): -510.48723238
E(UHF/6-31+G(d)) (Hartree): -509.04450011
E(UHF/6-31G(2df,p)) (Hartree): -509.08490323
E(UHF/6-31G(d)) (Hartree): -509.03100110
E(UHF/G3MP2large) (Hartree): -509.20667006
E(UHF/G3Xlarge) (Hartree): -509.20804298
E(UHF/G3large) (Hartree): -509.20804298
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.93089521

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-2.204971	0.083194	0.523871
C	-1.887650	-1.095997	-0.190104
C	-0.695818	-1.225389	-0.847579
C	0.255482	-0.165014	-0.832794
C	-0.104476	1.024424	-0.109179
C	-1.328342	1.137152	0.563985
H	-3.152168	0.153385	1.039721
H	-2.603225	-1.906598	-0.209843
H	-0.437271	-2.124899	-1.389483
H	-1.556757	2.054114	1.088962
O	0.770933	2.029709	-0.140863
H	1.506468	1.710438	-0.697009
O	1.447919	-0.223896	-1.291975
N	1.572981	-0.324870	0.883301
O	1.659489	-1.326135	1.349756

Rotational constants (GHz): 1.8801200 1.3707500 1.1349000

Vibrational harmonic frequencies (cm-1):

1160.8596	105.5862	152.7077
226.7240	287.4492	308.3301
388.5092	413.6081	462.0803
524.5024	549.0138	581.4695
587.4224	693.0123	749.1046
780.5423	792.3760	871.7354
889.7816	984.5165	1015.7382

1031.7077	1139.3943	1166.8466
1205.5650	1274.5598	1348.2549
1394.6383	1424.3618	1498.8717
1524.8379	1612.9962	1665.6027
2045.0566	3203.0615	3214.2707
3221.9382	3230.2192	3640.7233

Zero-point correction (Hartree): 0.105268

TS.nitrophenol.nitrosophenol+O1D.tc

E(RM062X/Aug-CC-pVTZ) (Hartree): -511.79004783

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-2.401287	-0.821958	-0.000081
C	-1.411667	-1.802171	0.000198
C	-0.089503	-1.416818	0.000305
C	0.238394	-0.060570	0.000198
C	-0.755396	0.936518	-0.000069
C	-2.083841	0.525629	-0.000217
H	-3.443719	-1.110828	-0.000215
H	-1.677625	-2.848274	0.000307
H	0.747685	-2.104554	0.000526
H	-2.866241	1.274411	-0.000466
O	-0.399887	2.228381	-0.000206
H	-1.184662	2.786113	-0.000064
N	1.619707	0.217715	0.000182
O	2.067694	1.298444	0.000395
O	2.845495	-1.487407	-0.000612

Rotational constants (GHz): 2.0149700 1.2190300 0.7595300

Vibrational harmonic frequencies (cm-1):

i381.3363	112.2028	148.1845
234.3558	243.5580	285.2567
422.6407	423.0987	439.9060
448.6347	491.7803	560.8393
576.8774	676.3809	727.4589
783.0453	793.3014	883.4147
891.4981	1008.2423	1034.0316
1071.9787	1122.4864	1176.2850
1191.8944	1204.2233	1323.6895
1343.6349	1366.2521	1506.1901
1527.8500	1640.4588	1676.3547
1792.9212	3193.9626	3203.1684
3215.9216	3240.6031	3851.7268

Zero-point correction (Hartree): 0.104418

TS.nitrophenol_trans.nitrophenoxy+H

E(G3SX(MP3)) excl. ZPE (Hartree): -511.69367701

E(G3SX) excl. ZPE (Hartree): -511.69955135

E(G3X(MP2)) excl. ZPE (Hartree): -511.24049969

E(G3X(MP3)) excl. ZPE (Hartree): -511.65263039

E(G3X) excl. ZPE (Hartree): -511.62340907

E(MP2-Full/G3Xlarge) (Hartree): -511.30678118

E(MP2-Full/G3large) (Hartree): -511.30678118

E(MP2/6-31+G(d)) (Hartree): -510.35995361

E(MP2/6-31G(2df,p)) (Hartree): -510.65909200

E(MP2/6-31G(d)) (Hartree): -510.32212114

E(MP2/G3MP2large) (Hartree): -510.86290899

E(MP3/6-31+G(d)) (Hartree): -510.35871484

E(MP3/6-31G(2df,p)) (Hartree): -510.66574596

E(MP3/6-31G(d)) (Hartree): -510.32739793

E(MP4/6-31+G(d)) (Hartree): -510.48675418

E(MP4/6-31G(2df,p)) (Hartree): -510.80198045

E(MP4/6-31G(d)) (Hartree): -510.44907373

E(QCISD(T)/6-31G(d)) (Hartree): -510.44660719

E(QCISD/6-31G(d)) (Hartree): -510.35836525

E(RHF/6-31+G(d)) (Hartree): -508.81133543

E(RHF/6-31G(2df,p)) (Hartree): -508.84226609

E(RHF/6-31G(d)) (Hartree): -508.79425012

E(RHF/G3MP2large) (Hartree): -508.96589716

E(RHF/G3Xlarge) (Hartree): -508.96732180

E(RHF/G3large) (Hartree): -508.96732180
 E(UM062X/Aug-CC-pVTZ) (Hartree): -511.80256173
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	2.558882	-0.244973	-0.050661
C	1.846322	-1.454787	-0.061320
C	0.441832	-1.458514	-0.036569
C	-0.236716	-0.264170	-0.023893
C	0.440726	1.017057	0.007373
C	1.882289	0.955376	-0.006098
H	3.648798	-0.259596	-0.066491
H	2.382373	-2.403557	-0.086947
H	-0.126943	-2.387603	-0.027519
H	2.400464	1.914308	0.029525
O	-0.159748	2.117943	0.074174
N	-1.706384	-0.317659	-0.050253
O	-2.280651	0.543536	-0.670384
O	-2.226189	-1.247520	0.534743
H	-0.627299	2.748445	2.021958

 Rotational constants (GHz): 2.3225700 1.2269300 0.8455500
 Vibrational harmonic frequencies (cm-1):

i598.5477	71.8891	134.4700
185.5274	220.6387	241.4596
303.8834	359.0015	395.3419
462.8141	512.0688	556.3010
576.8743	653.2529	713.3710
800.9173	835.6736	843.5356
894.5936	940.1200	1018.7688
1039.6349	1041.9732	1096.4166
1136.8209	1163.1715	1256.4987
1317.5113	1360.2037	1435.2932
1449.7280	1464.7500	1560.2506
1598.1442	1672.1994	3128.4296
3138.6454	3147.7558	3154.3821

 Zero-point correction (Hartree): 0.095415

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Triplet surface

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aci-NP-1

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.76101511
E(G3SX) excl. ZPE (Hartree): -511.77042452
E(G3X(MP2)) excl. ZPE (Hartree): -511.30513555
E(G3X(MP3)) excl. ZPE (Hartree): -511.72291378
E(G3X) excl. ZPE (Hartree): -511.69552261
E(MP2-Full/G3Xlarge) (Hartree): -511.35472504
E(MP2-Full/G3large) (Hartree): -511.35472504
E(MP2/6-31+G(d)) (Hartree): -510.40090990
E(MP2/6-31G(2df,p)) (Hartree): -510.70626698
E(MP2/6-31G(d)) (Hartree): -510.36505764
E(MP2/G3MP2large) (Hartree): -510.91016787
E(MP3/6-31+G(d)) (Hartree): -510.43570283
E(MP3/6-31G(2df,p)) (Hartree): -510.75074310
E(MP3/6-31G(d)) (Hartree): -510.40326529
E(MP4/6-31+G(d)) (Hartree): -510.52241730
E(MP4/6-31G(2df,p)) (Hartree): -510.84602813
E(MP4/6-31G(d)) (Hartree): -510.48422726
E(PMP2/6-31+G(d)) (Hartree): -510.42803675
E(PMP2/6-31G(2df,p)) (Hartree): -510.73438588
E(PMP2/6-31G(d)) (Hartree): -510.39281017
E(PMP2/G3MP2large) (Hartree): -510.93759733
E(PMP2/G3Xlarge) (Hartree): -511.38220588
E(PMP2/G3large) (Hartree): -511.38220588
E(PMP3/6-31+G(d)) (Hartree): -510.45652294
E(PMP3/6-31G(2df,p)) (Hartree): -510.77232254
E(PMP3/6-31G(d)) (Hartree): -510.42470439
E(PUHF/6-31+G(d)) (Hartree): -509.04621117
E(PUHF/6-31G(2df,p)) (Hartree): -509.08560920
E(PUHF/6-31G(d)) (Hartree): -509.03227569
E(PUHF/G3MP2large) (Hartree): -509.20623203
E(PUHF/G3Xlarge) (Hartree): -509.20770265
E(PUHF/G3large) (Hartree): -509.20770265
E(QCISD(T)/6-31G(d)) (Hartree): -510.50718491
E(QCISD/6-31G(d)) (Hartree): -510.45100669
E(UHF/6-31+G(d)) (Hartree): -509.01523749
E(UHF/6-31G(2df,p)) (Hartree): -509.05356486
E(UHF/6-31G(d)) (Hartree): -509.00068445
E(UHF/G3MP2large) (Hartree): -509.17486414
E(UHF/G3Xlarge) (Hartree): -509.17627456
E(UHF/G3large) (Hartree): -509.17627456
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.89677927
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      2.597170      -0.164753      0.055622
  C      1.913388      -1.378557      0.079305
  C      0.503079      -1.432285      0.043549
  C     -0.217585      -0.277863     -0.017846
  C      0.451530      1.017485     -0.067968
  C      1.887921      1.008915     -0.015696
  H      3.676929     -0.151926      0.086260
  H      2.466678     -2.306117      0.123077
  H     -0.021127     -2.376044      0.054752
  H      2.370131      1.976080     -0.043033
  O     -0.187393      2.086998     -0.168071
  H     -1.809926      1.510287      0.147498
  N     -1.629289     -0.338410     -0.128471
  O     -2.354524      0.723051      0.370711
  O     -2.219418     -1.425183     -0.194022
Rotational constants (GHz):   2.4489200   1.2292800   0.8284500
Vibrational harmonic frequencies (cm-1):
    54.2971          124.2766          206.5663
   258.3009          317.0268          372.7133
   402.3524          456.2808          486.1424
   552.9174          575.2956          608.8392

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658.1252	709.6910	730.1799
802.9954	866.1376	899.0900
974.3480	996.2463	1028.8127
1062.8911	1120.3783	1159.1088
1208.4245	1270.2692	1364.0172
1409.1246	1435.0790	1477.1656
1519.6322	1565.7493	1610.7308
1627.9649	3213.5616	3223.8134
3235.7381	3244.6564	3445.4393

Zero-point correction (Hartree): 0.105421

aci-NP-3

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.75199336
E(G3SX) excl. ZPE (Hartree): -511.76130305
E(G3X(MP2)) excl. ZPE (Hartree): -511.29667160
E(G3X(MP3)) excl. ZPE (Hartree): -511.71454508
E(G3X) excl. ZPE (Hartree): -511.68708285
E(MP2-Full/G3Xlarge) (Hartree): -511.34390855
E(MP2-Full/G3large) (Hartree): -511.34390855
E(MP2/6-31+G(d)) (Hartree): -510.39305692
E(MP2/6-31G(2df,p)) (Hartree): -510.69551010
E(MP2/6-31G(d)) (Hartree): -510.35646395
E(MP2/G3MP2large) (Hartree): -510.89950516
E(MP3/6-31+G(d)) (Hartree): -510.42995902
E(MP3/6-31G(2df,p)) (Hartree): -510.74247918
E(MP3/6-31G(d)) (Hartree): -510.39692286
E(MP4/6-31+G(d)) (Hartree): -510.51613310
E(MP4/6-31G(2df,p)) (Hartree): -510.83665521
E(MP4/6-31G(d)) (Hartree): -510.47702462
E(PMP2/6-31+G(d)) (Hartree): -510.42444856
E(PMP2/6-31G(2df,p)) (Hartree): -510.72793814
E(PMP2/6-31G(d)) (Hartree): -510.38850889
E(PMP2/G3MP2large) (Hartree): -510.93122443
E(PMP2/G3Xlarge) (Hartree): -511.37568581
E(PMP2/G3large) (Hartree): -511.37568581
E(PMP3/6-31+G(d)) (Hartree): -510.45465093
E(PMP3/6-31G(2df,p)) (Hartree): -510.76799165
E(PMP3/6-31G(d)) (Hartree): -510.42227883
E(PUHF/6-31+G(d)) (Hartree): -509.05296794
E(PUHF/6-31G(2df,p)) (Hartree): -509.09125546
E(PUHF/6-31G(d)) (Hartree): -509.03918576
E(PUHF/G3MP2large) (Hartree): -509.21212625
E(PUHF/G3Xlarge) (Hartree): -509.21359647
E(PUHF/G3large) (Hartree): -509.21359647
E(QCISD(T)/6-31G(d)) (Hartree): -510.50079731
E(QCISD/6-31G(d)) (Hartree): -510.44624244
E(UHF/6-31+G(d)) (Hartree): -509.01745278
E(UHF/6-31G(2df,p)) (Hartree): -509.05463229
E(UHF/6-31G(d)) (Hartree): -509.00302466
E(UHF/G3MP2large) (Hartree): -509.17620264
E(UHF/G3Xlarge) (Hartree): -509.17760572
E(UHF/G3large) (Hartree): -509.17760572
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.88727214
Electronic state : 3-A

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Cartesian coordinates (Angs):

C	2.565125	-0.395855	0.095836
C	1.740824	-1.521757	0.125338
C	0.338331	-1.400875	0.065931
C	-0.225349	-0.165615	-0.032881
C	0.584221	1.045786	-0.121524
C	2.012433	0.853969	-0.015923
H	3.637918	-0.515785	0.151434
H	2.177474	-2.507867	0.195710
H	-0.289622	-2.278229	0.094571
H	2.615632	1.750090	-0.059520
O	0.087699	2.162122	-0.311115
H	-3.215127	-0.968920	-0.198515
N	-1.640256	0.011451	-0.078400
O	-2.307509	-1.150581	-0.481152
O	-2.222439	0.731789	0.750325

Rotational constants (GHz):	2.3990800	1.1966900	0.8381300
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Vibrational harmonic frequencies (cm-1):

67.0736	116.1938	196.5415
211.5592	238.8581	328.1137
347.6524	451.6084	472.8755
515.6046	538.7275	570.4494
604.0735	713.5447	726.6809
803.2500	856.0351	899.1767
976.9892	1000.0833	1004.1443
1044.3075	1127.1217	1158.6410
1199.3446	1256.8102	1329.5503
1350.7653	1427.3599	1470.1971
1490.6733	1557.1070	1574.4276
1631.9871	3210.9410	3222.7004
3232.0832	3245.3549	3800.6270

Zero-point correction (Hartree): 0.104726

spiro-cis

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.71483601
E(G3SX) excl. ZPE (Hartree): -511.72498075
E(G3X(MP2)) excl. ZPE (Hartree): -511.26043337
E(G3X(MP3)) excl. ZPE (Hartree): -511.67697354
E(G3X) excl. ZPE (Hartree): -511.65091764
E(MP2-Full/G3Xlarge) (Hartree): -511.32051994
E(MP2-Full/G3large) (Hartree): -511.32051994
E(MP2/6-31+G(d)) (Hartree): -510.36679350
E(MP2/6-31G(2df,p)) (Hartree): -510.67396579
E(MP2/6-31G(d)) (Hartree): -510.33068381
E(MP2/G3MP2large) (Hartree): -510.87627896
E(MP3/6-31+G(d)) (Hartree): -510.39223654
E(MP3/6-31G(2df,p)) (Hartree): -510.70856747
E(MP3/6-31G(d)) (Hartree): -510.35992176
E(MP4/6-31+G(d)) (Hartree): -510.48541791
E(MP4/6-31G(2df,p)) (Hartree): -510.81040831
E(MP4/6-31G(d)) (Hartree): -510.44653736
E(PMP2/6-31+G(d)) (Hartree): -510.38986091
E(PMP2/6-31G(2df,p)) (Hartree): -510.69769979
E(PMP2/6-31G(d)) (Hartree): -510.35418818
E(PMP2/G3MP2large) (Hartree): -510.89953470
E(PMP2/G3Xlarge) (Hartree): -511.34382051
E(PMP2/G3large) (Hartree): -511.34382051
E(PMP3/6-31+G(d)) (Hartree): -510.41013586
E(PMP3/6-31G(2df,p)) (Hartree): -510.72695920
E(PMP3/6-31G(d)) (Hartree): -510.37825293
E(PUHF/6-31+G(d)) (Hartree): -508.97922305
E(PUHF/6-31G(2df,p)) (Hartree): -509.01988428
E(PUHF/6-31G(d)) (Hartree): -508.96497637
E(PUHF/G3MP2large) (Hartree): -509.13994624
E(PUHF/G3Xlarge) (Hartree): -509.14142643
E(PUHF/G3large) (Hartree): -509.14142643
E(QCISD(T)/6-31G(d)) (Hartree): -510.46198069
E(QCISD/6-31G(d)) (Hartree): -510.40591109
E(UHF/6-31+G(d)) (Hartree): -508.95278846
E(UHF/6-31G(2df,p)) (Hartree): -508.99271448
E(UHF/6-31G(d)) (Hartree): -508.93809791
E(UHF/G3MP2large) (Hartree): -509.11326039
E(UHF/G3Xlarge) (Hartree): -509.11468792
E(UHF/G3large) (Hartree): -509.11468792
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.85151016
Electronic state : 3-A

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Cartesian coordinates (Angs):

C	2.462211	0.260285	-0.155521
C	2.084835	-1.104949	-0.146153
C	0.785962	-1.471093	-0.029186
C	-0.250173	-0.458857	0.106277
C	0.172659	0.952119	0.065504
C	1.503652	1.264692	-0.046454
H	3.504279	0.526076	-0.249727
H	2.847771	-1.865151	-0.237310
H	0.463149	-2.501699	-0.018543

H	1.781254	2.309003	-0.048419
N	-1.590354	-0.775612	-0.300017
O	-2.456832	-0.079831	-0.836491
O	-1.351296	-0.742003	1.096851
O	-0.739440	1.915820	0.202012
H	-1.638312	1.555989	0.188345
Rotational constants (GHz):		2.5119400	1.2954300 0.9630000
Vibrational harmonic frequencies (cm-1):			
58.8701	190.4399	230.5013	
264.9641	336.1432	368.1277	
398.6282	434.1921	470.4873	
520.8281	537.1889	591.6469	
605.6410	716.8166	720.4449	
751.8516	832.2627	866.7971	
925.0968	946.4333	997.8625	
1022.8134	1122.1478	1148.8582	
1193.4280	1207.4031	1290.8296	
1338.0147	1382.7144	1449.4509	
1481.6253	1503.5515	1583.9047	
1636.4232	3212.6895	3224.8234	
3235.4373	3240.0831	3758.4241	
Zero-point correction (Hartree): 0.104335			

spiro_trans

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.70717894
E(G3SX) excl. ZPE (Hartree): -511.71729026
E(G3X(MP2)) excl. ZPE (Hartree): -511.25285809
E(G3X(MP3)) excl. ZPE (Hartree): -511.66939364
E(G3X) excl. ZPE (Hartree): -511.64330995
E(MP2-Full/G3Xlarge) (Hartree): -511.31162507
E(MP2-Full/G3large) (Hartree): -511.31162507
E(MP2/6-31+G(d)) (Hartree): -510.35780346
E(MP2/6-31G(2df,p)) (Hartree): -510.66460610
E(MP2/6-31G(d)) (Hartree): -510.32127767
E(MP2/G3MP2large) (Hartree): -510.86738376
E(MP3/6-31+G(d)) (Hartree): -510.38482911
E(MP3/6-31G(2df,p)) (Hartree): -510.70079535
E(MP3/6-31G(d)) (Hartree): -510.35210211
E(MP4/6-31+G(d)) (Hartree): -510.47721951
E(MP4/6-31G(2df,p)) (Hartree): -510.80163399
E(MP4/6-31G(d)) (Hartree): -510.43783308
E(PMP2/6-31+G(d)) (Hartree): -510.38027380
E(PMP2/6-31G(2df,p)) (Hartree): -510.68774565
E(PMP2/6-31G(d)) (Hartree): -510.34412593
E(PMP2/G3MP2large) (Hartree): -510.89005225
E(PMP2/G3Xlarge) (Hartree): -511.33433985
E(PMP2/G3large) (Hartree): -511.33433985
E(PMP3/6-31+G(d)) (Hartree): -510.40223586
E(PMP3/6-31G(2df,p)) (Hartree): -510.71869433
E(PMP3/6-31G(d)) (Hartree): -510.36988001
E(PUHF/6-31+G(d)) (Hartree): -508.97464936
E(PUHF/6-31G(2df,p)) (Hartree): -509.01492127
E(PUHF/6-31G(d)) (Hartree): -508.96004175
E(PUHF/G3MP2large) (Hartree): -509.13564056
E(PUHF/G3Xlarge) (Hartree): -509.13712852
E(PUHF/G3large) (Hartree): -509.13712852
E(QCISD(T)/6-31G(d)) (Hartree): -510.45388843
E(QCISD/6-31G(d)) (Hartree): -510.39852084
E(UHF/6-31+G(d)) (Hartree): -508.94886039
E(UHF/6-31G(2df,p)) (Hartree): -508.98839592
E(UHF/6-31G(d)) (Hartree): -508.93386993
E(UHF/G3MP2large) (Hartree): -509.10959471
E(UHF/G3Xlarge) (Hartree): -509.11102828
E(UHF/G3large) (Hartree): -509.11102828
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.84335521
Electronic state : 3-A
Cartesian coordinates (Angs):
C      2.455540      0.193290     -0.209280
C      2.044685     -1.156764     -0.136143
C      0.740621     -1.480572      0.041081

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C	-0.283355	-0.442876	0.156518
C	0.190292	0.953201	0.089951
C	1.518485	1.225919	-0.088190
H	3.498231	0.433815	-0.350515
H	2.784299	-1.940336	-0.221668
H	0.393254	-2.501422	0.105216
H	1.840646	2.259238	-0.128828
N	-1.602825	-0.759460	-0.320433
O	-2.455148	-0.100136	-0.902853
O	-1.385571	-0.701884	1.097481
O	-0.771114	1.871189	0.243509
H	-0.399600	2.758376	0.210100
Rotational constants (GHz):		2.4595800	1.2945300
Vibrational harmonic frequencies (cm ⁻¹):			0.9653400
75.2018	171.0267		225.7269
268.0468	337.7418		385.4539
390.4852	434.3702		506.3211
525.4319	550.0071		580.2417
616.9721	708.7045		718.1714
743.8653	819.9646		866.0482
894.1511	918.1425		994.3060
1027.6886	1117.2694		1145.9475
1160.9006	1202.4531		1271.2320
1329.7974	1358.6591		1446.3212
1494.2093	1505.3000		1574.6203
1625.6194	3193.3332		3213.1212
3232.8564	3238.9952		3859.3017
Zero-point correction (Hartree):		0.104176	

nitrophenol_cis

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.73141599
E(G3SX) excl. ZPE (Hartree): -511.74066891
E(G3X(MP2)) excl. ZPE (Hartree): -511.27690852
E(G3X(MP3)) excl. ZPE (Hartree): -511.69458290
E(G3X) excl. ZPE (Hartree): -511.66655895
E(MP2-Full/G3Xlarge) (Hartree): -511.32486842
E(MP2-Full/G3large) (Hartree): -511.32486842
E(MP2/6-31+G(d)) (Hartree): -510.37221487
E(MP2/6-31G(2df,p)) (Hartree): -510.67813568
E(MP2/6-31G(d)) (Hartree): -510.33833009
E(MP2/G3MP2large) (Hartree): -510.88033985
E(MP3/6-31+G(d)) (Hartree): -510.41151579
E(MP3/6-31G(2df,p)) (Hartree): -510.72657022
E(MP3/6-31G(d)) (Hartree): -510.38058249
E(MP4/6-31+G(d)) (Hartree): -510.49539736
E(MP4/6-31G(2df,p)) (Hartree): -510.81923906
E(MP4/6-31G(d)) (Hartree): -510.45936793
E(PMP2/6-31+G(d)) (Hartree): -510.39600463
E(PMP2/6-31G(2df,p)) (Hartree): -510.70334829
E(PMP2/6-31G(d)) (Hartree): -510.36281681
E(PMP2/G3MP2large) (Hartree): -510.90474638
E(PMP2/G3Xlarge) (Hartree): -511.34933579
E(PMP2/G3large) (Hartree): -511.34933579
E(PMP3/6-31+G(d)) (Hartree): -510.43017493
E(PMP3/6-31G(2df,p)) (Hartree): -510.74637387
E(PMP3/6-31G(d)) (Hartree): -510.39993126
E(PUHF/6-31+G(d)) (Hartree): -509.03002309
E(PUHF/6-31G(2df,p)) (Hartree): -509.07012651
E(PUHF/6-31G(d)) (Hartree): -509.01671588
E(PUHF/G3MP2large) (Hartree): -509.19018919
E(PUHF/G3Xlarge) (Hartree): -509.19165857
E(PUHF/G3large) (Hartree): -509.19165857
E(QCISD(T)/6-31G(d)) (Hartree): -510.48206943
E(QCISD/6-31G(d)) (Hartree): -510.42750572
E(UHF/6-31+G(d)) (Hartree): -509.00331090
E(UHF/6-31G(2df,p)) (Hartree): -509.04189093
E(UHF/6-31G(d)) (Hartree): -508.98931311
E(UHF/G3MP2large) (Hartree): -509.16275792
E(UHF/G3Xlarge) (Hartree): -509.16415726
E(UHF/G3large) (Hartree): -509.16415726

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E(UM062X/Aug-CC-pVTZ) (Hartree): -511.87080940
 Electronic state : 3-A
 Cartesian coordinates (Angs):

C	-2.558991	-0.192145	-0.039555
C	-1.899912	-1.418442	-0.008261
C	-0.522067	-1.447351	0.042868
C	0.196483	-0.254522	0.051565
C	-0.455809	0.986011	0.013862
C	-1.846227	0.991447	-0.029962
H	-3.638833	-0.160343	-0.076212
H	-2.457982	-2.342739	-0.022591
H	0.018947	-2.382498	0.071916
H	-2.341161	1.951591	-0.062741
N	1.601416	-0.316526	0.191029
O	2.393530	0.653432	-0.075980
O	2.249943	-1.433980	-0.112908
O	0.180790	2.171505	0.019475
H	1.134148	2.032036	-0.075372

Rotational constants (GHz): 2.3995000 1.2480000 0.8234600
 Vibrational harmonic frequencies (cm-1):

58.0438	135.9425	240.7202
241.8672	346.6948	363.0125
403.2987	457.4171	487.5579
544.2725	557.2281	576.6506
579.3913	719.3784	725.5506
777.3306	854.6960	883.6574
936.6241	970.7722	999.1753
1066.4385	1111.0772	1161.4918
1178.5129	1232.0733	1302.8039
1345.6513	1376.7298	1418.3022
1515.0939	1532.8059	1651.6036
1674.5288	3212.6589	3222.0480
3230.4321	3238.9310	3719.6952

Zero-point correction (Hartree): 0.104910

nitrophenol_trans

 E(G3SX(MP3)) excl. ZPE (Hartree): -511.72717934
 E(G3SX) excl. ZPE (Hartree): -511.73622515
 E(G3X(MP2)) excl. ZPE (Hartree): -511.27258089
 E(G3X(MP3)) excl. ZPE (Hartree): -511.69015302
 E(G3X) excl. ZPE (Hartree): -511.66206188
 E(MP2-Full/G3Xlarge) (Hartree): -511.31919178
 E(MP2-Full/G3large) (Hartree): -511.31919178
 E(MP2/6-31+G(d)) (Hartree): -510.36708555
 E(MP2/6-31G(2df,p)) (Hartree): -510.67143173
 E(MP2/6-31G(d)) (Hartree): -510.33169722
 E(MP2/G3MP2large) (Hartree): -510.87471081
 E(MP3/6-31+G(d)) (Hartree): -510.40675112
 E(MP3/6-31G(2df,p)) (Hartree): -510.72038120
 E(MP3/6-31G(d)) (Hartree): -510.37451988
 E(MP4/6-31+G(d)) (Hartree): -510.49042933
 E(MP4/6-31G(2df,p)) (Hartree): -510.81242390
 E(MP4/6-31G(d)) (Hartree): -510.45282136
 E(PMP2/6-31+G(d)) (Hartree): -510.38920245
 E(PMP2/6-31G(2df,p)) (Hartree): -510.69504309
 E(PMP2/6-31G(d)) (Hartree): -510.35459409
 E(PMP2/G3MP2large) (Hartree): -510.89738183
 E(PMP2/G3Xlarge) (Hartree): -511.34192063
 E(PMP2/G3large) (Hartree): -511.34192063
 E(PMP3/6-31+G(d)) (Hartree): -510.42401009
 E(PMP3/6-31G(2df,p)) (Hartree): -510.73883092
 E(PMP3/6-31G(d)) (Hartree): -510.39252245
 E(PUHF/6-31+G(d)) (Hartree): -509.02479071
 E(PUHF/6-31G(2df,p)) (Hartree): -509.06444444
 E(PUHF/6-31G(d)) (Hartree): -509.01101599
 E(PUHF/G3MP2large) (Hartree): -509.18510100
 E(PUHF/G3Xlarge) (Hartree): -509.18656643
 E(PUHF/G3large) (Hartree): -509.18656643
 E(QCISD(T)/6-31G(d)) (Hartree): -510.47673865
 E(QCISD/6-31G(d)) (Hartree): -510.42150918

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E(UHF/6-31+G(d)) (Hartree): -508.99993034
E(UHF/6-31G(2df,p)) (Hartree): -509.03797533
E(UHF/6-31G(d)) (Hartree): -508.98536831
E(UHF/G3MP2large) (Hartree): -509.15958943
E(UHF/G3Xlarge) (Hartree): -509.16098808
E(UHF/G3large) (Hartree): -509.16098808
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.86471022
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      2.542236      -0.257982      0.089594
  C      1.850984      -1.460795      0.084602
  C      0.467669      -1.457034      0.009356
  C     -0.212420     -0.251690     -0.053804
  C      0.475065      0.963220     -0.073959
  C      1.859274      0.946688      0.010554
  H      3.621367     -0.251816      0.150793
  H      2.383799     -2.398300      0.144028
  H     -0.104538     -2.372647      0.005104
  H      2.398753      1.885825      0.003275
  N     -1.630913     -0.237380     -0.182372
  O     -2.344213      0.607724      0.538924
  O     -2.296059     -1.327830     -0.245336
  O     -0.249040      2.100210     -0.194264
  H      0.334658      2.863314     -0.219245
Rotational constants (GHz):   2.4019000   1.2390400   0.8364500
Vibrational harmonic frequencies (cm-1):
  73.0945      132.6296      189.1442
 240.5248      333.2605      342.1390
 377.2188      412.0874      492.6906
 502.1778      557.0687      571.1572
 579.3480      728.0965      735.6704
 778.7165      854.5726      874.1012
 879.0887      971.6278      998.2023
1072.2210     1106.4243     1169.5655
1176.6936     1186.0148     1313.7720
1332.6601     1348.2435     1415.0577
1506.8466     1549.2820     1666.4552
1676.8671     3193.7899     3217.0033
3230.7980     3244.2828     3875.4157
Zero-point correction (Hartree): 0.104577

complex.hydroxyphenoxy+NO
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.81939707
E(G3SX) excl. ZPE (Hartree): -511.82819222
E(G3X(MP2)) excl. ZPE (Hartree): -511.36606492
E(G3X(MP3)) excl. ZPE (Hartree): -511.78375966
E(G3X) excl. ZPE (Hartree): -511.75503958
E(MP2-Full/G3Xlarge) (Hartree): -511.42115715
E(MP2-Full/G3large) (Hartree): -511.42115715
E(MP2/6-31+G(d)) (Hartree): -510.47052188
E(MP2/6-31G(2df,p)) (Hartree): -510.77407242
E(MP2/6-31G(d)) (Hartree): -510.43624551
E(MP2/G3MP2large) (Hartree): -510.97709108
E(MP3/6-31+G(d)) (Hartree): -510.50186404
E(MP3/6-31G(2df,p)) (Hartree): -510.81552922
E(MP3/6-31G(d)) (Hartree): -510.47107690
E(MP4/6-31+G(d)) (Hartree): -510.59171498
E(MP4/6-31G(2df,p)) (Hartree): -510.91320700
E(MP4/6-31G(d)) (Hartree): -510.55543069
E(PMP2/6-31+G(d)) (Hartree): -510.49759100
E(PMP2/6-31G(2df,p)) (Hartree): -510.80225519
E(PMP2/6-31G(d)) (Hartree): -510.46419910
E(PMP2/G3MP2large) (Hartree): -511.00439767
E(PMP2/G3Xlarge) (Hartree): -511.44851463
E(PMP2/G3large) (Hartree): -511.44851463
E(PMP3/6-31+G(d)) (Hartree): -510.52291104
E(PMP3/6-31G(2df,p)) (Hartree): -510.83743527
E(PMP3/6-31G(d)) (Hartree): -510.49294746
E(PUHF/6-31+G(d)) (Hartree): -509.12417684
E(PUHF/6-31G(2df,p)) (Hartree): -509.16455766

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E(PUHF/6-31G(d)) (Hartree): -509.11160203
E(PUHF/G3MP2large) (Hartree): -509.28517752
E(PUHF/G3Xlarge) (Hartree): -509.28659689
E(PUHF/G3large) (Hartree): -509.28659689
E(QCISD(T)/6-31G(d)) (Hartree): -510.57242961
E(QCISD/6-31G(d)) (Hartree): -510.51981114
E(UHF/6-31+G(d)) (Hartree): -509.09342083
E(UHF/6-31G(2df,p)) (Hartree): -509.13257214
E(UHF/6-31G(d)) (Hartree): -509.07991866
E(UHF/G3MP2large) (Hartree): -509.25410749
E(UHF/G3Xlarge) (Hartree): -509.25546724
E(UHF/G3large) (Hartree): -509.25546724
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.95241746
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      -2.389475      0.651023      0.612441
  C      -2.391179     -0.764116      0.515010
  C      -1.344289     -1.427685     -0.046615
  C      -0.214012     -0.696850     -0.553589
  C      -0.255905      0.759830     -0.431560
  C      -1.334635      1.410018      0.145185
  H      -3.237360      1.145659      1.065356
  H      -3.241097     -1.312781      0.896244
  H      -1.319293     -2.504802     -0.132578
  H      -1.331118      2.487903      0.219416
  N       2.395936     -0.236753      1.300844
  O       3.232348     -0.020625      0.562092
  O       0.790881     -1.205550     -1.081302
  O       0.793115      1.415341     -0.900357
  H       1.403517      0.734630     -1.243047
Rotational constants (GHz):   2.2653100   0.9135300   0.8139200
Vibrational harmonic frequencies (cm-1):
  24.6983      51.1965      65.3400
  68.3157      108.6130     174.8698
  275.4325     338.7675     449.2103
  465.1344     508.1100     570.7719
  579.2545     695.2064     748.5870
  771.9051     799.6853     881.3731
  887.4389     974.8897    1007.9206
 1021.8075    1138.6683    1165.9821
 1195.3864    1273.3757    1361.6647
 1388.2752    1447.1540    1511.7446
 1570.0866    1612.1029    1639.9728
 2064.0277    3206.1000    3217.8704
 3230.0046    3233.7477    3633.5143
Zero-point correction (Hartree): 0.103334

complex.hydroxyphenyl+NO2
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.71860269
E(G3SX) excl. ZPE (Hartree): -511.72755708
E(G3X(MP2)) excl. ZPE (Hartree): -511.26438160
E(G3X(MP3)) excl. ZPE (Hartree): -511.68209805
E(G3X) excl. ZPE (Hartree): -511.65363246
E(MP2-Full/G3Xlarge) (Hartree): -511.32930774
E(MP2-Full/G3large) (Hartree): -511.32930774
E(MP2/6-31+G(d)) (Hartree): -510.37661239
E(MP2/6-31G(2df,p)) (Hartree): -510.68037516
E(MP2/6-31G(d)) (Hartree): -510.34054536
E(MP2/G3MP2large) (Hartree): -510.88537460
E(MP3/6-31+G(d)) (Hartree): -510.38846384
E(MP3/6-31G(2df,p)) (Hartree): -510.70295059
E(MP3/6-31G(d)) (Hartree): -510.35629820
E(MP4/6-31+G(d)) (Hartree): -510.49312498
E(MP4/6-31G(2df,p)) (Hartree): -510.81532974
E(MP4/6-31G(d)) (Hartree): -510.45507444
E(PMP2/6-31+G(d)) (Hartree): -510.40242653
E(PMP2/6-31G(2df,p)) (Hartree): -510.70753338
E(PMP2/6-31G(d)) (Hartree): -510.36760316
E(PMP2/G3MP2large) (Hartree): -510.91119602
E(PMP2/G3Xlarge) (Hartree): -511.35517113

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E(PMP2/G3large) (Hartree): -511.35517113
E(PMP3/6-31+G(d)) (Hartree): -510.40935367
E(PMP3/6-31G(2df,p)) (Hartree): -510.72494253
E(PMP3/6-31G(d)) (Hartree): -510.37834698
E(PUHF/6-31+G(d)) (Hartree): -508.99250766
E(PUHF/6-31G(2df,p)) (Hartree): -509.03333082
E(PUHF/6-31G(d)) (Hartree): -508.97823287
E(PUHF/G3MP2large) (Hartree): -509.15510610
E(PUHF/G3Xlarge) (Hartree): -509.15655624
E(PUHF/G3large) (Hartree): -509.15655624
E(QCISD(T)/6-31G(d)) (Hartree): -510.46672008
E(QCISD/6-31G(d)) (Hartree): -510.40626503
E(UHF/6-31+G(d)) (Hartree): -508.96392760
E(UHF/6-31G(2df,p)) (Hartree): -509.00332080
E(UHF/6-31G(d)) (Hartree): -508.94834839
E(UHF/G3MP2large) (Hartree): -509.12649274
E(UHF/G3Xlarge) (Hartree): -509.12789502
E(UHF/G3large) (Hartree): -509.12789502
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.85076227
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      -2.902938      -0.234564      0.048160
  C      -2.255252      -1.463439      0.019295
  C      -0.861941      -1.501880     -0.033071
  C      -0.204335      -0.303637     -0.051739
  C      -0.800388       0.936041     -0.027144
  C      -2.192734       0.956971      0.025446
  H      -3.982891      -0.200851      0.088248
  H      -2.821658      -2.383752      0.036664
  H      -0.326375      -2.441704     -0.058584
  H      -2.694325       1.915282      0.046298
  N       2.929855      -0.278106      0.322892
  O       2.768802       0.832664     -0.057028
  O       2.827061      -1.343734     -0.163555
  O      -0.121104       2.109914     -0.049916
  H       0.823719       1.930055     -0.094562
Rotational constants (GHz):   2.4116400   0.7877400   0.5967300
Vibrational harmonic frequencies (cm-1):
  15.2097      22.2170      58.4560
  80.8640      93.0681      119.6921
  229.2383     404.2270     419.1864
  425.2116     524.9096     526.3481
  628.8432     685.5359     762.6897
  778.8152     840.5189     864.5690
  954.0958     993.7060     995.8691
  1051.4759    1119.3282    1163.7279
  1190.2232    1281.6606    1320.1948
  1352.7432    1464.8882    1490.4973
  1499.1897    1620.3643    1672.5561
  1775.0875    3199.8803    3206.7288
  3217.2580    3228.4065    3847.9201
Zero-point correction (Hartree): 0.102803

complex.nitrosophenol.O3P.cc
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.69863075
E(G3SX) excl. ZPE (Hartree): -511.70832942
E(G3X(MP2)) excl. ZPE (Hartree): -511.25174108
E(G3X(MP3)) excl. ZPE (Hartree): -511.66772848
E(G3X) excl. ZPE (Hartree): -511.63884343
E(MP2-Full/G3Xlarge) (Hartree): -511.33497924
E(MP2-Full/G3large) (Hartree): -511.33497924
E(MP2/6-31+G(d)) (Hartree): -510.39071590
E(MP2/6-31G(2df,p)) (Hartree): -510.69096950
E(MP2/6-31G(d)) (Hartree): -510.35804039
E(MP2/G3MP2large) (Hartree): -510.89139673
E(MP3/6-31+G(d)) (Hartree): -510.41624109
E(MP3/6-31G(2df,p)) (Hartree): -510.72441535
E(MP3/6-31G(d)) (Hartree): -510.38614152
E(MP4/6-31+G(d)) (Hartree): -510.50479753
E(MP4/6-31G(2df,p)) (Hartree): -510.82153760

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E(MP4/6-31G(d)) (Hartree): -510.47010942
E(PMP2/6-31+G(d)) (Hartree): -510.39247897
E(PMP2/6-31G(2df,p)) (Hartree): -510.69275350
E(PMP2/6-31G(d)) (Hartree): -510.35955952
E(PMP2/G3MP2large) (Hartree): -510.89340651
E(PMP2/G3Xlarge) (Hartree): -511.33701517
E(PMP2/G3large) (Hartree): -511.33701517
E(PMP3/6-31+G(d)) (Hartree): -510.41742229
E(PMP3/6-31G(2df,p)) (Hartree): -510.72541779
E(PMP3/6-31G(d)) (Hartree): -510.38702778
E(PUHF/6-31+G(d)) (Hartree): -509.00437322
E(PUHF/6-31G(2df,p)) (Hartree): -509.03788679
E(PUHF/6-31G(d)) (Hartree): -508.98926429
E(PUHF/G3MP2large) (Hartree): -509.16027625
E(PUHF/G3Xlarge) (Hartree): -509.16162518
E(PUHF/G3large) (Hartree): -509.16162518
E(QCISD(T)/6-31G(d)) (Hartree): -510.46565191
E(QCISD/6-31G(d)) (Hartree): -510.41050673
E(UHF/6-31+G(d)) (Hartree): -509.00162059
E(UHF/6-31G(2df,p)) (Hartree): -509.03484300
E(UHF/6-31G(d)) (Hartree): -508.98667516
E(UHF/G3MP2large) (Hartree): -509.15706768
E(UHF/G3Xlarge) (Hartree): -509.15837049
E(UHF/G3large) (Hartree): -509.15837049
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.83425357
Point group : CS
Electronic state : 3-A"
Cartesian coordinates (Angs):
  C      -1.189019      -2.284864      0.000000
  C      -1.996636      -1.141577      0.000000
  C      -1.397513       0.093819      0.000000
  C       0.000000       0.202530      0.000000
  C       0.811066      -0.953941      0.000000
  C       0.187978      -2.201745      0.000000
  H      -1.652603      -3.262441      0.000000
  H      -3.072296      -1.233599      0.000000
  H      -1.964681       1.015201      0.000000
  H       0.811089      -3.084521      0.000000
  O       2.140513      -0.900383      0.000000
  H       2.401576       0.040137      0.000000
  N       0.494949       1.512972      0.000000
  O       1.701834       1.653552      0.000000
  O      -1.152720       3.452966      0.000000
Rotational constants (GHz):   1.9224200   1.1217200   0.7083800
Vibrational harmonic frequencies (cm-1):
  20.3678 ( A'')   72.5408 ( A')   128.8971 ( A')
  145.8987 ( A'')   213.5249 ( A'')   289.9744 ( A')
  313.6418 ( A'')   422.8952 ( A')   446.3009 ( A'')
  447.4283 ( A')   535.9029 ( A'')   574.3801 ( A')
  695.7086 ( A')   728.5701 ( A'')   770.0820 ( A'')
  794.5024 ( A')   795.9583 ( A'')   900.2699 ( A'')
  904.4525 ( A')   1005.8442 ( A'')   1014.5430 ( A'')
  1058.8339 ( A')   1135.7990 ( A')   1162.6735 ( A')
  1213.2893 ( A')   1228.5771 ( A')   1337.4298 ( A')
  1355.0754 ( A')   1388.3274 ( A')   1498.1222 ( A')
  1518.8936 ( A')   1616.1826 ( A')   1657.5289 ( A')
  1688.0305 ( A')   3204.8673 ( A')   3215.1555 ( A')
  3229.2900 ( A')   3237.7236 ( A')   3541.2901 ( A')
Zero-point correction (Hartree): 0.103677

complex.nitrosophenoxy_cis+OH
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.73134398
E(G3SX) excl. ZPE (Hartree): -511.74055556
E(G3X(MP2)) excl. ZPE (Hartree): -511.27884974
E(G3X(MP3)) excl. ZPE (Hartree): -511.69610347
E(G3X) excl. ZPE (Hartree): -511.66761979
E(MP2-Full/G3Xlarge) (Hartree): -511.33746049
E(MP2-Full/G3large) (Hartree): -511.33746049
E(MP2/6-31+G(d)) (Hartree): -510.39012396
E(MP2/6-31G(2df,p)) (Hartree): -510.69089162

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E(MP2/6-31G(d)) (Hartree): -510.35479401
 E(MP2/G3MP2large) (Hartree): -510.89348996
 E(MP3/6-31+G(d)) (Hartree): -510.41861245
 E(MP3/6-31G(2df,p)) (Hartree): -510.72877592
 E(MP3/6-31G(d)) (Hartree): -510.38642887
 E(MP4/6-31+G(d)) (Hartree): -510.51252964
 E(MP4/6-31G(2df,p)) (Hartree): -510.83100261
 E(MP4/6-31G(d)) (Hartree): -510.47514347
 E(PMP2/6-31+G(d)) (Hartree): -510.40448113
 E(PMP2/6-31G(2df,p)) (Hartree): -510.70628469
 E(PMP2/6-31G(d)) (Hartree): -510.36969114
 E(PMP2/G3MP2large) (Hartree): -510.90816716
 E(PMP2/G3Xlarge) (Hartree): -511.35218812
 E(PMP2/G3large) (Hartree): -511.35218812
 E(PMP3/6-31+G(d)) (Hartree): -510.42989370
 E(PMP3/6-31G(2df,p)) (Hartree): -510.74085873
 E(PMP3/6-31G(d)) (Hartree): -510.39818455
 E(PUHF/6-31+G(d)) (Hartree): -509.01291395
 E(PUHF/6-31G(2df,p)) (Hartree): -509.05037012
 E(PUHF/6-31G(d)) (Hartree): -508.99864305
 E(PUHF/G3MP2large) (Hartree): -509.17223229
 E(PUHF/G3Xlarge) (Hartree): -509.17361937
 E(PUHF/G3large) (Hartree): -509.17361937
 E(QCISD(T)/6-31G(d)) (Hartree): -510.48739455
 E(QCISD/6-31G(d)) (Hartree): -510.42943921
 E(UHF/6-31+G(d)) (Hartree): -508.99685109
 E(UHF/6-31G(2df,p)) (Hartree): -509.03317378
 E(UHF/6-31G(d)) (Hartree): -508.98202586
 E(UHF/G3MP2large) (Hartree): -509.15577394
 E(UHF/G3Xlarge) (Hartree): -509.15710318
 E(UHF/G3large) (Hartree): -509.15710318
 E(UM062X/Aug-CC-pVTZ) (Hartree): -511.86106087
 Electronic state : 3-A
 Cartesian coordinates (Angs):

C	-2.465508	-0.641909	0.179325
C	-2.381016	0.778200	0.429780
C	-1.215599	1.426077	0.264410
C	-0.059307	0.687445	-0.160809
C	-0.097924	-0.780567	-0.400417
C	-1.410217	-1.381892	-0.212940
H	-3.423936	-1.125166	0.318756
H	-3.265462	1.309250	0.748069
H	-1.110019	2.487781	0.436125
H	-1.483436	-2.444941	-0.391265
O	0.901732	-1.401811	-0.721878
H	2.305589	-1.128710	0.681497
N	1.066239	1.314316	-0.364704
O	2.623349	-0.649592	1.472200
O	2.136297	0.948585	-0.729866

 Rotational constants (GHz): 2.2277600 1.0381400 0.8542200
 Vibrational harmonic frequencies (cm-1):

40.3905	71.7381	123.6935
157.6536	206.4928	225.8741
375.6281	379.6429	413.5999
446.2049	471.1334	486.4734
520.1068	559.5254	620.6995
730.1099	749.1763	785.5202
878.5188	890.6657	1000.1434
1000.4374	1030.1165	1158.6426
1171.1875	1219.0714	1313.7137
1371.1821	1432.4061	1491.2684
1571.6198	1669.1170	1722.7011
1765.3633	3201.0764	3222.6845
3233.7554	3240.0357	3665.4156

 Zero-point correction (Hartree): 0.101635
 complex.nitrosophenoxy_trans+OH

 E(G3SX(MP3)) excl. ZPE (Hartree): -511.72001494
 E(G3SX) excl. ZPE (Hartree): -511.72902657
 E(G3X(MP2)) excl. ZPE (Hartree): -511.26712445

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E(G3X(MP3)) excl. ZPE (Hartree): -511.68425291
E(G3X) excl. ZPE (Hartree): -511.65588292
E(MP2-Full/G3Xlarge) (Hartree): -511.32464202
E(MP2-Full/G3large) (Hartree): -511.32464202
E(MP2/6-31+G(d)) (Hartree): -510.37611383
E(MP2/6-31G(2df,p)) (Hartree): -510.67623689
E(MP2/6-31G(d)) (Hartree): -510.33980388
E(MP2/G3MP2large) (Hartree): -510.88064660
E(MP3/6-31+G(d)) (Hartree): -510.40504029
E(MP3/6-31G(2df,p)) (Hartree): -510.71478880
E(MP3/6-31G(d)) (Hartree): -510.37225580
E(MP4/6-31+G(d)) (Hartree): -510.49855218
E(MP4/6-31G(2df,p)) (Hartree): -510.81634442
E(MP4/6-31G(d)) (Hartree): -510.46018582
E(PMP2/6-31+G(d)) (Hartree): -510.39299859
E(PMP2/6-31G(2df,p)) (Hartree): -510.69410168
E(PMP2/6-31G(d)) (Hartree): -510.35710448
E(PMP2/G3MP2large) (Hartree): -510.89788883
E(PMP2/G3Xlarge) (Hartree): -511.34194244
E(PMP2/G3large) (Hartree): -511.34194244
E(PMP3/6-31+G(d)) (Hartree): -510.41857628
E(PMP3/6-31G(2df,p)) (Hartree): -510.72909297
E(PMP3/6-31G(d)) (Hartree): -510.38616482
E(PUHF/6-31+G(d)) (Hartree): -509.00100434
E(PUHF/6-31G(2df,p)) (Hartree): -509.03851825
E(PUHF/6-31G(d)) (Hartree): -508.98654549
E(PUHF/G3MP2large) (Hartree): -509.16112100
E(PUHF/G3Xlarge) (Hartree): -509.16251631
E(PUHF/G3large) (Hartree): -509.16251631
E(QCISD(T)/6-31G(d)) (Hartree): -510.47352179
E(QCISD/6-31G(d)) (Hartree): -510.41596485
E(UHF/6-31+G(d)) (Hartree): -508.98229621
E(UHF/6-31G(2df,p)) (Hartree): -509.01874064
E(UHF/6-31G(d)) (Hartree): -508.96740915
E(UHF/G3MP2large) (Hartree): -509.14198571
E(UHF/G3Xlarge) (Hartree): -509.14331564
E(UHF/G3large) (Hartree): -509.14331564
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.85128726
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      -2.219897      -0.489137      -0.224558
  C      -1.317669      -1.619168      -0.329468
  C       0.010789      -1.430975      -0.379722
  C       0.530450      -0.083530      -0.344595
  C      -0.359476       1.110749      -0.312711
  C      -1.787585       0.784521      -0.203306
  H      -3.281681      -0.692233      -0.165947
  H      -1.729542      -2.617751      -0.350456
  H       0.713782      -2.250521      -0.432589
  H      -2.465638       1.623928      -0.138351
  O       0.062135       2.244802      -0.375277
  H      -0.617525      -0.001274       2.205679
  N       1.814831       0.146302      -0.364949
  O       0.351426      -0.035567       2.295646
  O       2.778579      -0.549364      -0.395061
Rotational constants (GHz):   1.7742100   1.2082600   1.0160300
Vibrational harmonic frequencies (cm-1):
  35.8025      49.6135      76.6230
  93.9507      135.0116     197.9138
  203.9465      345.0286     355.8161
  378.0312      457.4080     491.1799
  526.4562      563.9641     593.1070
  757.5788      759.3785     782.1219
  874.3958      881.4667     994.4728
 1007.4959     1041.7737    1140.4725
 1170.6987     1206.1652    1299.2212
 1370.3701     1431.7441    1464.3973
 1594.0978     1690.7523    1729.7733
 1787.6560     3197.9367    3217.4568
 3227.6043     3233.4173    3739.1761
Zero-point correction (Hartree): 0.100475

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complex.nitrophenyl.OH

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.65821515
E(G3SX) excl. ZPE (Hartree): -511.66667676
E(G3X(MP2)) excl. ZPE (Hartree): -511.20260987
E(G3X(MP3)) excl. ZPE (Hartree): -511.62068348
E(G3X) excl. ZPE (Hartree): -511.59216512
E(MP2-Full/G3Xlarge) (Hartree): -511.23115795
E(MP2-Full/G3large) (Hartree): -511.23115795
E(MP2/6-31+G(d)) (Hartree): -510.28535799
E(MP2/6-31G(2df,p)) (Hartree): -510.58477961
E(MP2/6-31G(d)) (Hartree): -510.24963303
E(MP2/G3MP2large) (Hartree): -510.78722433
E(MP3/6-31+G(d)) (Hartree): -510.32427630
E(MP3/6-31G(2df,p)) (Hartree): -510.63398504
E(MP3/6-31G(d)) (Hartree): -510.29170999
E(MP4/6-31+G(d)) (Hartree): -510.41224608
E(MP4/6-31G(2df,p)) (Hartree): -510.73005249
E(MP4/6-31G(d)) (Hartree): -510.37438246
E(PMP2/6-31+G(d)) (Hartree): -510.32823017
E(PMP2/6-31G(2df,p)) (Hartree): -510.62977286
E(PMP2/6-31G(d)) (Hartree): -510.29403317
E(PMP2/G3MP2large) (Hartree): -510.83086145
E(PMP2/G3Xlarge) (Hartree): -511.27486795
E(PMP2/G3large) (Hartree): -511.27486795
E(PMP3/6-31+G(d)) (Hartree): -510.36119989
E(PMP3/6-31G(2df,p)) (Hartree): -510.67283231
E(PMP3/6-31G(d)) (Hartree): -510.33016496
E(PUHF/6-31+G(d)) (Hartree): -508.98542276
E(PUHF/6-31G(2df,p)) (Hartree): -509.02492335
E(PUHF/6-31G(d)) (Hartree): -508.97210501
E(PUHF/G3MP2large) (Hartree): -509.14553046
E(PUHF/G3Xlarge) (Hartree): -509.14696152
E(PUHF/G3large) (Hartree): -509.14696152
E(QCISD(T)/6-31G(d)) (Hartree): -510.41223709
E(QCISD/6-31G(d)) (Hartree): -510.35292745
E(UHF/6-31+G(d)) (Hartree): -508.93953667
E(UHF/6-31G(2df,p)) (Hartree): -508.97684079
E(UHF/6-31G(d)) (Hartree): -508.92467434
E(UHF/G3MP2large) (Hartree): -509.09882755
E(UHF/G3Xlarge) (Hartree): -509.10017903
E(UHF/G3large) (Hartree): -509.10017903
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.79177507
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      -2.518358      0.850643      0.000045
  C      -2.474426     -0.540721     -0.000037
  C      -1.262156     -1.212515     -0.000110
  C      -0.097245     -0.458461     -0.000110
  C      -0.168730      0.906676     -0.000016
  C      -1.344118      1.603505      0.000055
  H      -3.474650      1.356234      0.000102
  H      -3.394907     -1.106180     -0.000048
  H      -1.200116     -2.291070     -0.000182
  H      -1.361407      2.684314      0.000116
  N       1.213197     -1.120367     -0.000228
  O       2.200607     -0.408943      0.000184
  O       1.236312     -2.325682      0.000129
  O       2.286185      2.573086      0.000003
  H       2.344063      1.596816      0.000121
Rotational constants (GHz):   1.6630500   1.1773300   0.6893300
Vibrational harmonic frequencies (cm-1):
  23.2176      70.0750      71.7221
 129.8580     166.8627     239.8635
  330.7008     394.3274     415.9911
  453.2689     460.8702     539.9338
  616.8737     644.1327     696.6576
  751.2379     821.1025     887.5314
  894.7427     988.2580     995.8628
 1010.8158    1047.0659    1127.5463
```

1159.8743	1188.8189	1263.1279
1335.3184	1455.4790	1478.1292
1481.8509	1614.1266	1667.7898
1687.0725	3206.8222	3222.4936
3228.2672	3239.8896	3658.9693

Zero-point correction (Hartree): 0.101758

complex.phenyloxy.HONO_cis

E(G3SX(MP3)) excl. ZPE (Hartree): -511.71039008
 E(G3SX) excl. ZPE (Hartree): -511.71964520
 E(G3X(MP2)) excl. ZPE (Hartree): -511.25757853
 E(G3X(MP3)) excl. ZPE (Hartree): -511.67545027
 E(G3X) excl. ZPE (Hartree): -511.64715459
 E(MP2-Full/G3Xlarge) (Hartree): -511.30732742
 E(MP2-Full/G3large) (Hartree): -511.30732742
 E(MP2/6-31+G(d)) (Hartree): -510.36391301
 E(MP2/6-31G(2df,p)) (Hartree): -510.66290103
 E(MP2/6-31G(d)) (Hartree): -510.32971864
 E(MP2/G3MP2large) (Hartree): -510.86398424
 E(MP3/6-31+G(d)) (Hartree): -510.39556386
 E(MP3/6-31G(2df,p)) (Hartree): -510.70539566
 E(MP3/6-31G(d)) (Hartree): -510.36468177
 E(MP4/6-31+G(d)) (Hartree): -510.48782354
 E(MP4/6-31G(2df,p)) (Hartree): -510.80551063
 E(MP4/6-31G(d)) (Hartree): -510.45133480
 E(PMP2/6-31+G(d)) (Hartree): -510.39423306
 E(PMP2/6-31G(2df,p)) (Hartree): -510.69443933
 E(PMP2/6-31G(d)) (Hartree): -510.36101624
 E(PMP2/G3MP2large) (Hartree): -510.89464111
 E(PMP2/G3Xlarge) (Hartree): -511.33802188
 E(PMP2/G3large) (Hartree): -511.33802188
 E(PMP3/6-31+G(d)) (Hartree): -510.41994928
 E(PMP3/6-31G(2df,p)) (Hartree): -510.73077724
 E(PMP3/6-31G(d)) (Hartree): -510.38999966
 E(PUHF/6-31+G(d)) (Hartree): -509.02382149
 E(PUHF/6-31G(2df,p)) (Hartree): -509.06196558
 E(PUHF/6-31G(d)) (Hartree): -509.01101125
 E(PUHF/G3MP2large) (Hartree): -509.18143398
 E(PUHF/G3Xlarge) (Hartree): -509.18284350
 E(PUHF/G3large) (Hartree): -509.18284350
 E(QCISD(T)/6-31G(d)) (Hartree): -510.47051700
 E(QCISD/6-31G(d)) (Hartree): -510.41576379
 E(UHF/6-31+G(d)) (Hartree): -508.98988696
 E(UHF/6-31G(2df,p)) (Hartree): -509.02675101
 E(UHF/6-31G(d)) (Hartree): -508.97606862
 E(UHF/G3MP2large) (Hartree): -509.14712295
 E(UHF/G3Xlarge) (Hartree): -509.14848889
 E(UHF/G3large) (Hartree): -509.14848889
 E(UM062X/Aug-CC-pVTZ) (Hartree): -511.84644328

Electronic state : 3-A

Cartesian coordinates (Angs):

C	-2.872265	0.290576	0.222954
C	-2.617155	-1.069305	-0.078653
C	-1.323543	-1.510194	-0.371000
C	-0.333455	-0.579100	-0.351126
C	-0.499084	0.817913	-0.054381
C	-1.868947	1.209415	0.238829
H	-3.886161	0.593853	0.443968
H	-3.435614	-1.775957	-0.079375
H	-1.126320	-2.549252	-0.596689
H	-2.040130	2.252948	0.465205
O	0.435663	1.635123	-0.047840
H	1.975355	0.877320	-0.358810
N	3.067029	-0.629026	0.096612
O	2.816464	0.440560	-0.669751
O	2.264169	-0.819630	0.943802

Rotational constants (GHz): 2.8582100 0.7714600 0.6495900

Vibrational harmonic frequencies (cm-1):

35.3123	43.1026	71.6188
119.9663	174.0271	194.4935

209.1694	392.8103	461.8944
482.3826	520.8558	590.8883
684.8804	746.3640	789.1257
828.2290	866.6675	956.8873
962.8760	972.5500	1011.2109
1015.2264	1061.8720	1122.6815
1149.1330	1215.7618	1322.4882
1375.1004	1417.1974	1459.8058
1527.9445	1562.4416	1610.1010
1731.0577	3204.1089	3207.5319
3212.1807	3220.5763	3229.3326

Zero-point correction (Hartree): 0.101970

complex.phenyloxy.HONO_trans

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.71289027
E(G3SX) excl. ZPE (Hartree): -511.72186344
E(G3X(MP2)) excl. ZPE (Hartree): -511.25981472
E(G3X(MP3)) excl. ZPE (Hartree): -511.67762467
E(G3X) excl. ZPE (Hartree): -511.64919905
E(MP2-Full/G3Xlarge) (Hartree): -511.31005794
E(MP2-Full/G3large) (Hartree): -511.31005794
E(MP2/6-31+G(d)) (Hartree): -510.36550855
E(MP2/6-31G(2df,p)) (Hartree): -510.66308647
E(MP2/6-31G(d)) (Hartree): -510.32922403
E(MP2/G3MP2large) (Hartree): -510.86674081
E(MP3/6-31+G(d)) (Hartree): -510.39732698
E(MP3/6-31G(2df,p)) (Hartree): -510.70609716
E(MP3/6-31G(d)) (Hartree): -510.36473506
E(MP4/6-31+G(d)) (Hartree): -510.48898790
E(MP4/6-31G(2df,p)) (Hartree): -510.80524988
E(MP4/6-31G(d)) (Hartree): -510.45048239
E(PMP2/6-31+G(d)) (Hartree): -510.39548696
E(PMP2/6-31G(2df,p)) (Hartree): -510.69397782
E(PMP2/6-31G(d)) (Hartree): -510.36008308
E(PMP2/G3MP2large) (Hartree): -510.89664414
E(PMP2/G3Xlarge) (Hartree): -511.34000320
E(PMP2/G3large) (Hartree): -511.34000320
E(PMP3/6-31+G(d)) (Hartree): -510.42143069
E(PMP3/6-31G(2df,p)) (Hartree): -510.73094039
E(PMP3/6-31G(d)) (Hartree): -510.38968911
E(PUHF/6-31+G(d)) (Hartree): -509.02479796
E(PUHF/6-31G(2df,p)) (Hartree): -509.06161854
E(PUHF/6-31G(d)) (Hartree): -509.01032941
E(PUHF/G3MP2large) (Hartree): -509.18257891
E(PUHF/G3Xlarge) (Hartree): -509.18399693
E(PUHF/G3large) (Hartree): -509.18399693
E(QCISD(T)/6-31G(d)) (Hartree): -510.46949811
E(QCISD/6-31G(d)) (Hartree): -510.41499265
E(UHF/6-31+G(d)) (Hartree): -508.99122985
E(UHF/6-31G(2df,p)) (Hartree): -509.02709412
E(UHF/6-31G(d)) (Hartree): -508.97585660
E(UHF/G3MP2large) (Hartree): -509.14906935
E(UHF/G3Xlarge) (Hartree): -509.15043919
E(UHF/G3large) (Hartree): -509.15043919
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.84738174

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Electronic state : 3-A

Cartesian coordinates (Angs):

C	-3.008368	-0.117827	-0.209866
C	-2.631722	1.227702	0.021258
C	-1.298594	1.569346	0.264324
C	-0.390838	0.557213	0.266896
C	-0.682050	-0.831618	0.039784
C	-2.086587	-1.118546	-0.204785
H	-4.049609	-0.343244	-0.393641
H	-3.387523	2.000856	0.006705
H	-1.008892	2.596745	0.437430
H	-2.350513	-2.152911	-0.377913
O	0.180278	-1.726188	0.048864
H	1.805462	-1.167528	0.306293
N	2.591804	0.386867	-0.344509

O	2.679279	-0.724884	0.427192	
O	3.570118	1.031122	-0.305177	
Rotational constants (GHz):		2.8650900	0.6906300	0.5682800
Vibrational harmonic frequencies (cm ⁻¹):				
29.0764		48.8503		54.4321
107.4472		158.4914		177.2741
194.1876		390.7702		462.5216
479.3188		521.4775		591.0351
682.4284		757.8482		788.4555
829.1677		865.4810		919.3024
959.9636		970.7420		997.3891
1009.2606		1015.2126		1123.3033
1149.8956		1215.8349		1321.7583
1375.6941		1418.4739		1485.8705
1527.7945		1561.5906		1610.0613
1800.6537		3204.6805		3213.0202
3220.9913		3229.8812		3366.6573
Zero-point correction (Hartree): 0.102145				

complex.nitrophenoxy.H

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.67659325
E(G3SX) excl. ZPE (Hartree): -511.68613830
E(G3X(MP2)) excl. ZPE (Hartree): -511.22384796
E(G3X(MP3)) excl. ZPE (Hartree): -511.64160540
E(G3X) excl. ZPE (Hartree): -511.61421703
E(MP2-Full/G3Xlarge) (Hartree): -511.28635907
E(MP2-Full/G3large) (Hartree): -511.28635907
E(MP2/6-31+G(d)) (Hartree): -510.34594655
E(MP2/6-31G(2df,p)) (Hartree): -510.64182610
E(MP2/6-31G(d)) (Hartree): -510.31163710
E(MP2/G3MP2large) (Hartree): -510.84190700
E(MP3/6-31+G(d)) (Hartree): -510.36067085
E(MP3/6-31G(2df,p)) (Hartree): -510.66659340
E(MP3/6-31G(d)) (Hartree): -510.33003547
E(MP4/6-31+G(d)) (Hartree): -510.46323770
E(MP4/6-31G(2df,p)) (Hartree): -510.77707517
E(MP4/6-31G(d)) (Hartree): -510.42639093
E(PMP2/6-31+G(d)) (Hartree): -510.37475355
E(PMP2/6-31G(2df,p)) (Hartree): -510.67134955
E(PMP2/6-31G(d)) (Hartree): -510.34104898
E(PMP2/G3MP2large) (Hartree): -510.87075743
E(PMP2/G3Xlarge) (Hartree): -511.31524351
E(PMP2/G3large) (Hartree): -511.31524351
E(PMP3/6-31+G(d)) (Hartree): -510.38363369
E(PMP3/6-31G(2df,p)) (Hartree): -510.69013034
E(PMP3/6-31G(d)) (Hartree): -510.35359208
E(PUHF/6-31+G(d)) (Hartree): -508.97022785
E(PUHF/6-31G(2df,p)) (Hartree): -509.00635030
E(PUHF/6-31G(d)) (Hartree): -508.95745892
E(PUHF/G3MP2large) (Hartree): -509.12617460
E(PUHF/G3Xlarge) (Hartree): -509.12764029
E(PUHF/G3large) (Hartree): -509.12764029
E(QCISD(T)/6-31G(d)) (Hartree): -510.44072150
E(QCISD/6-31G(d)) (Hartree): -510.38050406
E(UHF/6-31+G(d)) (Hartree): -508.93797437
E(UHF/6-31G(2df,p)) (Hartree): -508.97334390
E(UHF/6-31G(d)) (Hartree): -508.92458163
E(UHF/G3MP2large) (Hartree): -509.09386250
E(UHF/G3Xlarge) (Hartree): -509.09528906
E(UHF/G3large) (Hartree): -509.09528906
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.80361644

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Electronic state : 3-A

Cartesian coordinates (Angs):

C	2.562608	-0.233294	-0.046509
C	1.841143	-1.433889	-0.091251
C	0.437566	-1.430272	-0.076718
C	-0.228312	-0.244294	-0.037900
C	0.456288	1.040311	0.049927
C	1.905291	0.963371	0.022025
H	3.643136	-0.261008	-0.058113

H	2.365178	-2.377425	-0.139736
H	-0.124117	-2.353091	-0.104036
H	2.428268	1.907514	0.082575
O	-0.127754	2.116677	0.190824
N	-1.694017	-0.276766	-0.092612
O	-2.236959	0.555082	-0.773624
O	-2.244119	-1.159004	0.533705
H	-1.431191	0.947736	2.342927
Rotational constants (GHz):	2.4032300	1.2124700	0.8623700
Vibrational harmonic frequencies (cm-1):			
52.1888	98.1777		114.0418
213.4325	215.8280		237.6775
333.2553	348.8778		369.5325
467.3503	482.6300		554.5948
563.7712	641.3337		695.7166
784.8992	802.9042		841.8854
896.2133	907.0150		989.1648
1015.5171	1039.9520		1095.5133
1139.8298	1157.8786		1253.7405
1335.5674	1424.4430		1448.1949
1456.5589	1521.0372		1565.9892
1627.6678	1684.5774		3212.8719
3224.3014	3231.2422		3236.6437
Zero-point correction (Hartree):	0.096326		

TS.aci-NP-2.aci-NP-1

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-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.74580520
E(G3SX) excl. ZPE (Hartree): -511.75513910
E(G3X(MP2)) excl. ZPE (Hartree): -511.29031163
E(G3X(MP3)) excl. ZPE (Hartree): -511.70814458
E(G3X) excl. ZPE (Hartree): -511.68055930
E(MP2-Full/G3Xlarge) (Hartree): -511.33626893
E(MP2-Full/G3large) (Hartree): -511.33626893
E(MP2/6-31+G(d)) (Hartree): -510.38313644
E(MP2/6-31G(2df,p)) (Hartree): -510.68806846
E(MP2/6-31G(d)) (Hartree): -510.34718738
E(MP2/G3MP2large) (Hartree): -510.89182604
E(MP3/6-31+G(d)) (Hartree): -510.42161195
E(MP3/6-31G(2df,p)) (Hartree): -510.73629516
E(MP3/6-31G(d)) (Hartree): -510.38898403
E(MP4/6-31+G(d)) (Hartree): -510.50698161
E(MP4/6-31G(2df,p)) (Hartree): -510.82993135
E(MP4/6-31G(d)) (Hartree): -510.46859303
E(PMP2/6-31+G(d)) (Hartree): -510.41316588
E(PMP2/6-31G(2df,p)) (Hartree): -510.71920157
E(PMP2/6-31G(d)) (Hartree): -510.37791289
E(PMP2/G3MP2large) (Hartree): -510.92219000
E(PMP2/G3Xlarge) (Hartree): -511.36668983
E(PMP2/G3large) (Hartree): -511.36668983
E(PMP3/6-31+G(d)) (Hartree): -510.44503078
E(PMP3/6-31G(2df,p)) (Hartree): -510.76059319
E(PMP3/6-31G(d)) (Hartree): -510.41310729
E(PUHF/6-31+G(d)) (Hartree): -509.04453722
E(PUHF/6-31G(2df,p)) (Hartree): -509.08417988
E(PUHF/6-31G(d)) (Hartree): -509.03087490
E(PUHF/G3MP2large) (Hartree): -509.20485148
E(PUHF/G3Xlarge) (Hartree): -509.20632062
E(PUHF/G3large) (Hartree): -509.20632062
E(QCISD(T)/6-31G(d)) (Hartree): -510.49283998
E(QCISD/6-31G(d)) (Hartree): -510.43804243
E(UHF/6-31+G(d)) (Hartree): -509.01047243
E(UHF/6-31G(2df,p)) (Hartree): -509.04893709
E(UHF/6-31G(d)) (Hartree): -508.99612495
E(UHF/G3MP2large) (Hartree): -509.17036396
E(UHF/G3Xlarge) (Hartree): -509.17176695
E(UHF/G3large) (Hartree): -509.17176695
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.88216311
Electronic state : 3-A
Cartesian coordinates (Angs):
C      2.590816      -0.234096      0.093331

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C	1.864381	-1.420654	0.125270
C	0.455056	-1.413798	0.059610
C	-0.223005	-0.236202	-0.047687
C	0.488043	1.039061	-0.116353
C	1.926905	0.962957	-0.020600
H	3.669833	-0.259022	0.147879
H	2.378039	-2.368689	0.198848
H	-0.103630	-2.337941	0.078394
H	2.448472	1.909091	-0.062760
N	-1.643963	-0.278001	-0.158719
O	-2.359606	0.732531	0.459547
O	-2.235239	-1.354241	-0.344494
O	-0.084739	2.128338	-0.264131
H	-2.061478	0.765948	1.379868
Rotational constants (GHz): 2.4098900 1.2081500 0.8291100			
Vibrational harmonic frequencies (cm-1):			
i272.1763	45.3417	114.9721	
202.9016	228.7056	317.5602	
359.8152	393.3975	467.5462	
502.9406	558.7073	565.7136	
614.2736	714.9766	727.9840	
802.5327	866.9413	904.0294	
981.0905	1005.3575	1021.3957	
1059.1377	1116.5356	1159.9387	
1191.3214	1254.8504	1351.6498	
1358.2355	1420.6825	1468.2573	
1491.1887	1508.7959	1566.3101	
1625.3816	3211.8239	3222.2033	
3232.0598	3238.7800	3765.6879	
Zero-point correction (Hartree): 0.103973			
TS.aci-NP-2.aci-NP-3.H-shift			

E(G3SX(MP3)) excl. ZPE (Hartree): -511.70345269			
E(G3SX) excl. ZPE (Hartree): -511.71323901			
E(G3X(MP2)) excl. ZPE (Hartree): -511.24787195			
E(G3X(MP3)) excl. ZPE (Hartree): -511.66521603			
E(G3X) excl. ZPE (Hartree): -511.63858759			
E(MP2-Full/G3Xlarge) (Hartree): -511.30067865			
E(MP2-Full/G3large) (Hartree): -511.30067865			
E(MP2/6-31+G(d)) (Hartree): -510.34713946			
E(MP2/6-31G(2df,p)) (Hartree): -510.65342447			
E(MP2/6-31G(d)) (Hartree): -510.31197345			
E(MP2/G3MP2large) (Hartree): -510.85634664			
E(MP3/6-31+G(d)) (Hartree): -510.37348983			
E(MP3/6-31G(2df,p)) (Hartree): -510.68959048			
E(MP3/6-31G(d)) (Hartree): -510.34203925			
E(MP4/6-31+G(d)) (Hartree): -510.46816012			
E(MP4/6-31G(2df,p)) (Hartree): -510.79257559			
E(MP4/6-31G(d)) (Hartree): -510.43029746			
E(PMP2/6-31+G(d)) (Hartree): -510.37509157			
E(PMP2/6-31G(2df,p)) (Hartree): -510.68242991			
E(PMP2/6-31G(d)) (Hartree): -510.34076213			
E(PMP2/G3MP2large) (Hartree): -510.88443532			
E(PMP2/G3Xlarge) (Hartree): -511.32882036			
E(PMP2/G3large) (Hartree): -511.32882036			
E(PMP3/6-31+G(d)) (Hartree): -510.39517861			
E(PMP3/6-31G(2df,p)) (Hartree): -510.71210587			
E(PMP3/6-31G(d)) (Hartree): -510.36452481			
E(PUHF/6-31+G(d)) (Hartree): -508.97443289			
E(PUHF/6-31G(2df,p)) (Hartree): -509.01514803			
E(PUHF/6-31G(d)) (Hartree): -508.96097552			
E(PUHF/G3MP2large) (Hartree): -509.13529524			
E(PUHF/G3Xlarge) (Hartree): -509.13680816			
E(PUHF/G3large) (Hartree): -509.13680816			
E(QCISD(T)/6-31G(d)) (Hartree): -510.45061763			
E(QCISD/6-31G(d)) (Hartree): -510.39321445			
E(UHF/6-31+G(d)) (Hartree): -508.94265440			
E(UHF/6-31G(2df,p)) (Hartree): -508.98223481			
E(UHF/6-31G(d)) (Hartree): -508.92833387			
E(UHF/G3MP2large) (Hartree): -509.10332252			

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E(UHF/G3Xlarge) (Hartree): -509.10477365
E(UHF/G3large) (Hartree): -509.10477365
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.83721715
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      2.598135      -0.336225      0.107857
  C      1.817756      -1.485454      0.093299
  C      0.406249      -1.407718      0.015501
  C     -0.192665     -0.191022     -0.060078
  C      0.570628      1.049786     -0.096302
  C      2.000480      0.901635      0.021864
  H      3.673667     -0.417636      0.175460
  H      2.284670     -2.458854      0.139011
  H     -0.202523     -2.300115      0.011654
  H      2.574070      1.817977      0.014594
  O      0.035114      2.155331     -0.245361
  H     -3.048411     -0.341421      0.326324
  N     -1.603562     -0.111647     -0.159258
  O     -2.340796      0.688322      0.568091
  O     -2.351824     -1.181707     -0.328366
Rotational constants (GHz):   2.4878300   1.1734700   0.8200500
Vibrational harmonic frequencies (cm-1):
 12110.6225      59.4018      115.3153
  192.7037      206.7801      319.2191
  344.7742      426.7267      459.3696
  504.8154      554.0547      563.5405
  663.9989      709.5917      799.2022
  850.6501      902.8148      935.3913
  976.4592     1000.5477     1039.9962
 1067.2294     1082.1685     1120.7696
 1160.9488     1243.0494     1309.5950
 1326.4664     1377.1287     1432.3726
 1481.1320     1496.4895     1565.4421
 1634.6431     2279.0313     3213.2699
 3224.2866     3232.5547     3239.0597
Zero-point correction (Hartree): 0.100492

TS.aci-NP-2.aci-NP-3.introt
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E(G3SX(MP3)) excl. ZPE (Hartree): -511.75064175
E(G3SX) excl. ZPE (Hartree): -511.75992659
E(G3X(MP2)) excl. ZPE (Hartree): -511.29547733
E(G3X(MP3)) excl. ZPE (Hartree): -511.71350445
E(G3X) excl. ZPE (Hartree): -511.68604403
E(MP2-Full/G3Xlarge) (Hartree): -511.34384011
E(MP2-Full/G3large) (Hartree): -511.34384011
E(MP2/6-31+G(d)) (Hartree): -510.39456097
E(MP2/6-31G(2df,p)) (Hartree): -510.69415358
E(MP2/6-31G(d)) (Hartree): -510.35646976
E(MP2/G3MP2large) (Hartree): -510.89950613
E(MP3/6-31+G(d)) (Hartree): -510.43134905
E(MP3/6-31G(2df,p)) (Hartree): -510.74142209
E(MP3/6-31G(d)) (Hartree): -510.39700812
E(MP4/6-31+G(d)) (Hartree): -510.51735870
E(MP4/6-31G(2df,p)) (Hartree): -510.83506190
E(MP4/6-31G(d)) (Hartree): -510.47666192
E(PMP2/6-31+G(d)) (Hartree): -510.42773179
E(PMP2/6-31G(2df,p)) (Hartree): -510.72837551
E(PMP2/6-31G(d)) (Hartree): -510.39023680
E(PMP2/G3MP2large) (Hartree): -510.93308952
E(PMP2/G3Xlarge) (Hartree): -511.37748376
E(PMP2/G3large) (Hartree): -511.37748376
E(PMP3/6-31+G(d)) (Hartree): -510.45776169
E(PMP3/6-31G(2df,p)) (Hartree): -510.76867683
E(PMP3/6-31G(d)) (Hartree): -510.42403680
E(PUHF/6-31+G(d)) (Hartree): -509.05732580
E(PUHF/6-31G(2df,p)) (Hartree): -509.09423992
E(PUHF/6-31G(d)) (Hartree): -509.04261652
E(PUHF/G3MP2large) (Hartree): -509.21606906
E(PUHF/G3Xlarge) (Hartree): -509.21753850
E(PUHF/G3large) (Hartree): -509.21753850

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E(QCISD(T)/6-31G(d)) (Hartree): -510.49961095
 E(QCISD/6-31G(d)) (Hartree): -510.44578137
 E(UHF/6-31+G(d)) (Hartree): -509.01995782
 E(UHF/6-31G(2df,p)) (Hartree): -509.05574807
 E(UHF/6-31G(d)) (Hartree): -509.00465896
 E(UHF/G3MP2large) (Hartree): -509.17820566
 E(UHF/G3Xlarge) (Hartree): -509.17960568
 E(UHF/G3large) (Hartree): -509.17960568
 E(UM062X/Aug-CC-pVTZ) (Hartree): -511.88509607
 Electronic state : 3-A
 Cartesian coordinates (Angs):

C	-0.598390	1.064171	-0.026211
C	0.223030	-0.132260	0.032744
C	-0.313097	-1.386285	0.058026
C	-1.705488	-1.538635	0.034539
C	-2.552561	-0.419138	-0.011667
C	-2.030558	0.842837	-0.039398
O	-0.106297	2.197673	-0.067414
N	1.647526	0.045880	0.086679
O	2.262099	-0.136797	1.150923
O	2.245069	-0.429864	-1.089041
H	3.189488	-0.334239	-0.898989
H	0.340866	-2.246676	0.094506
H	-2.130367	-2.532126	0.054129
H	-3.623580	-0.565840	-0.025568
H	-2.653675	1.725490	-0.074759

 Rotational constants (GHz): 2.3777200 1.1339800 0.8778000
 Vibrational harmonic frequencies (cm-1):

i58.5618	112.9052	161.3164
186.7250	224.7543	305.0502
337.9363	475.8336	485.6415
530.1719	537.2216	581.8833
606.0416	723.1469	737.7237
807.2487	859.9711	897.6130
980.7974	999.4312	1010.3299
1035.5382	1125.5951	1154.1268
1177.4462	1268.8467	1317.8310
1352.9223	1425.5323	1460.7097
1503.5478	1558.5376	1568.8612
1622.5987	3208.0748	3217.1978
3225.9319	3232.1908	3796.8091

 Zero-point correction (Hartree): 0.104372

TS.nitrophenol.acinitrophenol

 E(G3SX(MP3)) excl. ZPE (Hartree): -511.72330454
 E(G3SX) excl. ZPE (Hartree): -511.73293014
 E(G3X(MP2)) excl. ZPE (Hartree): -511.26836580
 E(G3X(MP3)) excl. ZPE (Hartree): -511.68610775
 E(G3X) excl. ZPE (Hartree): -511.65844999
 E(MP2-Full/G3Xlarge) (Hartree): -511.31783041
 E(MP2-Full/G3large) (Hartree): -511.31783041
 E(MP2/6-31+G(d)) (Hartree): -510.36222693
 E(MP2/6-31G(2df,p)) (Hartree): -510.67052048
 E(MP2/6-31G(d)) (Hartree): -510.32878249
 E(MP2/G3MP2large) (Hartree): -510.87312889
 E(MP3/6-31+G(d)) (Hartree): -510.40024582
 E(MP3/6-31G(2df,p)) (Hartree): -510.71738937
 E(MP3/6-31G(d)) (Hartree): -510.36956232
 E(MP4/6-31+G(d)) (Hartree): -510.48519554
 E(MP4/6-31G(2df,p)) (Hartree): -510.81163420
 E(MP4/6-31G(d)) (Hartree): -510.44958200
 E(PMP2/6-31+G(d)) (Hartree): -510.38841506
 E(PMP2/6-31G(2df,p)) (Hartree): -510.69811998
 E(PMP2/6-31G(d)) (Hartree): -510.35559560
 E(PMP2/G3MP2large) (Hartree): -510.90001978
 E(PMP2/G3Xlarge) (Hartree): -511.34478880
 E(PMP2/G3large) (Hartree): -511.34478880
 E(PMP3/6-31+G(d)) (Hartree): -510.42093516
 E(PMP3/6-31G(2df,p)) (Hartree): -510.73923321
 E(PMP3/6-31G(d)) (Hartree): -510.39090012

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E(PUHF/6-31+G(d)) (Hartree): -509.01894225
E(PUHF/6-31G(2df,p)) (Hartree): -509.05965014
E(PUHF/6-31G(d)) (Hartree): -509.00524557
E(PUHF/G3MP2large) (Hartree): -509.18011569
E(PUHF/G3Xlarge) (Hartree): -509.18160458
E(PUHF/G3large) (Hartree): -509.18160458
E(QCISD(T)/6-31G(d)) (Hartree): -510.47117776
E(QCISD/6-31G(d)) (Hartree): -510.41383467
E(UHF/6-31+G(d)) (Hartree): -508.98960929
E(UHF/6-31G(2df,p)) (Hartree): -509.02881911
E(UHF/6-31G(d)) (Hartree): -508.97530848
E(UHF/G3MP2large) (Hartree): -509.14997469
E(UHF/G3Xlarge) (Hartree): -509.15138632
E(UHF/G3large) (Hartree): -509.15138632
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.86472869
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      2.563512      -0.109390      0.000050
  C      1.928171      -1.364156      0.000071
  C      0.557146      -1.462716      0.000070
  C     -0.214909      -0.295302     -0.000002
  C      0.426227      0.985462     -0.000094
  C      1.823046      1.047515     -0.000025
  H      3.642751     -0.056534      0.000099
  H      2.524191     -2.265384      0.000072
  H      0.057597     -2.418176      0.000076
  H      2.282249      2.025425     -0.000008
  N     -1.593737     -0.330210      0.000187
  O     -2.347482      0.721275      0.000362
  O     -2.186127     -1.511031     -0.000376
  O     -0.289811      2.091174     -0.000239
  H     -1.262430      1.806311      0.000059
Rotational constants (GHz):   2.4210700   1.2708500   0.8333900
Vibrational harmonic frequencies (cm-1):
  i2414.7172      24.2511      126.4665
    145.2033      272.2659      302.7164
    445.8570      449.6753      450.8647
    513.1319      547.4106      595.0086
    717.1011      722.4459      778.3973
    794.5813      868.8038      874.7765
    959.5371      973.1547     1007.3698
   1050.5499     1111.4894     1157.2151
   1184.7330     1233.1270     1327.0005
   1359.7167     1405.6900     1421.6043
   1518.0107     1547.5289     1623.8632
   1640.8087     2405.1540     3215.1292
   3227.1754     3236.3620     3258.6075
Zero-point correction (Hartree): 0.101362

TS.nitrophenol_cis.nitrophenol_trans
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.69902375
E(G3SX) excl. ZPE (Hartree): -511.70797311
E(G3X(MP2)) excl. ZPE (Hartree): -511.24156914
E(G3X(MP3)) excl. ZPE (Hartree): -511.65894557
E(G3X) excl. ZPE (Hartree): -511.63184292
E(MP2-Full/G3Xlarge) (Hartree): -511.28104669
E(MP2-Full/G3large) (Hartree): -511.28104669
E(MP2/6-31+G(d)) (Hartree): -510.32683750
E(MP2/6-31G(2df,p)) (Hartree): -510.63137131
E(MP2/6-31G(d)) (Hartree): -510.28764958
E(MP2/G3MP2large) (Hartree): -510.83667005
E(MP3/6-31+G(d)) (Hartree): -510.35965605
E(MP3/6-31G(2df,p)) (Hartree): -510.67420356
E(MP3/6-31G(d)) (Hartree): -510.32442674
E(MP4/6-31+G(d)) (Hartree): -510.44986443
E(MP4/6-31G(2df,p)) (Hartree): -510.77238905
E(MP4/6-31G(d)) (Hartree): -510.40816969
E(PMP2/6-31+G(d)) (Hartree): -510.35646265
E(PMP2/6-31G(2df,p)) (Hartree): -510.66212839
E(PMP2/6-31G(d)) (Hartree): -510.31845140

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E(PMP2/G3MP2large) (Hartree): -510.86625599
E(PMP2/G3Xlarge) (Hartree): -511.31069057
E(PMP2/G3large) (Hartree): -511.31069057
E(PMP3/6-31+G(d)) (Hartree): -510.38372844
E(PMP3/6-31G(2df,p)) (Hartree): -510.69927155
E(PMP3/6-31G(d)) (Hartree): -510.34967381
E(PUHF/6-31+G(d)) (Hartree): -508.97231398
E(PUHF/6-31G(2df,p)) (Hartree): -509.01159069
E(PUHF/6-31G(d)) (Hartree): -508.95694834
E(PUHF/G3MP2large) (Hartree): -509.13358301
E(PUHF/G3Xlarge) (Hartree): -509.13506664
E(PUHF/G3large) (Hartree): -509.13506664
E(QCISD(T)/6-31G(d)) (Hartree): -510.43970037
E(QCISD/6-31G(d)) (Hartree): -510.38292805
E(UHF/6-31+G(d)) (Hartree): -508.93958498
E(UHF/6-31G(2df,p)) (Hartree): -508.97768237
E(UHF/6-31G(d)) (Hartree): -508.92304194
E(UHF/G3MP2large) (Hartree): -509.10086106
E(UHF/G3Xlarge) (Hartree): -509.10227936
E(UHF/G3large) (Hartree): -509.10227936
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.82645272
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      2.366684      -0.357264      -0.455216
  C      1.684004      -1.540108       0.051905
  C      0.410486      -1.490581       0.479287
  C     -0.291973      -0.240150       0.266654
  C      0.502124       1.016309       0.142691
  C      1.779770       0.907291      -0.323831
  H      3.374776      -0.451999      -0.827270
  H      2.230815      -2.472624       0.089998
  H     -0.130241      -2.347983       0.847613
  H      2.351156       1.808581      -0.500063
  N     -1.631856      -0.265285      -0.159416
  O     -2.280132      -1.284958       0.080711
  O     -2.071743       0.737704      -0.713635
  O     -0.051450       2.192882       0.518912
  H      0.116520       2.383004       1.448788
Rotational constants (GHz):   2.1250200   1.3282800   0.8870500
Vibrational harmonic frequencies (cm-1):
  i487.6173           54.6629           80.1467
    171.2314          210.9216          281.4369
    363.7695          391.3910          435.1224
    478.6835          545.8503          591.3997
    623.2984          681.7226          723.2146
    769.0287          808.5511          859.6849
    903.7687          947.5868          997.3771
   1034.6138         1126.8372        1157.7136
   1174.8456         1208.6893        1303.1924
   1318.7091         1361.8037        1397.2822
   1409.5010         1532.8009        1556.5814
   1649.9842         3210.7777        3214.6964
   3241.2455         3253.9576        3814.7240
Zero-point correction (Hartree): 0.102260

TS.nitrophenol_cis.spiro_cis
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.71554018
E(G3SX) excl. ZPE (Hartree): -511.72557671
E(G3X(MP2)) excl. ZPE (Hartree): -511.26084334
E(G3X(MP3)) excl. ZPE (Hartree): -511.67732013
E(G3X) excl. ZPE (Hartree): -511.65133449
E(MP2-Full/G3Xlarge) (Hartree): -511.31942108
E(MP2-Full/G3large) (Hartree): -511.31942108
E(MP2/6-31+G(d)) (Hartree): -510.36587389
E(MP2/6-31G(2df,p)) (Hartree): -510.67228904
E(MP2/6-31G(d)) (Hartree): -510.32904666
E(MP2/G3MP2large) (Hartree): -510.87515918
E(MP3/6-31+G(d)) (Hartree): -510.39064435
E(MP3/6-31G(2df,p)) (Hartree): -510.70630193
E(MP3/6-31G(d)) (Hartree): -510.35778362

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E(MP4/6-31+G(d)) (Hartree): -510.48492919
E(MP4/6-31G(2df,p)) (Hartree): -510.80920365
E(MP4/6-31G(d)) (Hartree): -510.44536047
E(PMP2/6-31+G(d)) (Hartree): -510.39174620
E(PMP2/6-31G(2df,p)) (Hartree): -510.69895263
E(PMP2/6-31G(d)) (Hartree): -510.35552437
E(PMP2/G3MP2large) (Hartree): -510.90125874
E(PMP2/G3Xlarge) (Hartree): -511.34556548
E(PMP2/G3large) (Hartree): -511.34556548
E(PMP3/6-31+G(d)) (Hartree): -510.41074918
E(PMP3/6-31G(2df,p)) (Hartree): -510.72700613
E(PMP3/6-31G(d)) (Hartree): -510.37846940
E(PUHF/6-31+G(d)) (Hartree): -508.98022417
E(PUHF/6-31G(2df,p)) (Hartree): -509.02070430
E(PUHF/6-31G(d)) (Hartree): -508.96593844
E(PUHF/G3MP2large) (Hartree): -509.14084953
E(PUHF/G3Xlarge) (Hartree): -509.14232627
E(PUHF/G3large) (Hartree): -509.14232627
E(QCISD(T)/6-31G(d)) (Hartree): -510.46187678
E(QCISD/6-31G(d)) (Hartree): -510.40486894
E(UHF/6-31+G(d)) (Hartree): -508.95063899
E(UHF/6-31G(2df,p)) (Hartree): -508.99025143
E(UHF/6-31G(d)) (Hartree): -508.93572638
E(UHF/G3MP2large) (Hartree): -509.11097169
E(UHF/G3Xlarge) (Hartree): -509.11239573
E(UHF/G3large) (Hartree): -509.11239573
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.85133932
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      2.469029      0.257747      -0.082328
  C      2.088335      -1.103313      -0.164111
  C      0.780760      -1.463133      -0.130924
  C     -0.237023     -0.453105       0.031452
  C      0.173385      0.948986       0.036077
  C      1.515329      1.261026       0.012605
  H      3.516204      0.520295      -0.108970
  H      2.851041     -1.862457      -0.262953
  H      0.451237     -2.489641      -0.194174
  H      1.795178      2.303754       0.055347
  N     -1.599639     -0.760185      -0.244044
  O     -2.485638     -0.062220      -0.756906
  O     -1.341121     -0.777846       1.127843
  O     -0.738142      1.914747       0.127089
  H     -1.635871      1.562646       0.018221
Rotational constants (GHz):   2.5388600   1.2912400   0.9576200
Vibrational harmonic frequencies (cm-1):
  i239.6281      114.3366      194.7840
   235.4093      258.0890      351.0041
   409.7154      439.8828      478.6022
   518.8734      538.4096      602.5614
   606.6299      717.5560      735.6667
   758.8388      847.9937      871.0384
   958.0635      971.9762     1001.6908
  1029.2225     1128.2340     1153.4712
  1194.2304     1211.0715     1300.4702
  1347.4977     1387.1019     1451.2336
  1492.6123     1518.4442     1582.9085
  1637.2125     3214.4046     3225.0219
   3235.1106     3239.8631     3711.6420
Zero-point correction (Hartree): 0.104046

TS.nitrophenol_trans.spiro_trans
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.70561938
E(G3SX) excl. ZPE (Hartree): -511.71532339
E(G3X(MP2)) excl. ZPE (Hartree): -511.25019885
E(G3X(MP3)) excl. ZPE (Hartree): -511.66675112
E(G3X) excl. ZPE (Hartree): -511.64057516
E(MP2-Full/G3Xlarge) (Hartree): -511.29832281
E(MP2-Full/G3large) (Hartree): -511.29832281
E(MP2/6-31+G(d)) (Hartree): -510.34508283

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E(MP2/6-31G(2df,p)) (Hartree): -510.65049622
E(MP2/6-31G(d)) (Hartree): -510.30729501
E(MP2/G3MP2large) (Hartree): -510.85399622
E(MP3/6-31+G(d)) (Hartree): -510.37518549
E(MP3/6-31G(2df,p)) (Hartree): -510.68980543
E(MP3/6-31G(d)) (Hartree): -510.34132549
E(MP4/6-31+G(d)) (Hartree): -510.46804465
E(MP4/6-31G(2df,p)) (Hartree): -510.79106613
E(MP4/6-31G(d)) (Hartree): -510.42748349
E(PMP2/6-31+G(d)) (Hartree): -510.37665174
E(PMP2/6-31G(2df,p)) (Hartree): -510.68306189
E(PMP2/6-31G(d)) (Hartree): -510.33951908
E(PMP2/G3MP2large) (Hartree): -510.88599233
E(PMP2/G3Xlarge) (Hartree): -511.33037416
E(PMP2/G3large) (Hartree): -511.33037416
E(PMP3/6-31+G(d)) (Hartree): -510.40002582
E(PMP3/6-31G(2df,p)) (Hartree): -510.71542537
E(PMP3/6-31G(d)) (Hartree): -510.36681627
E(PUHF/6-31+G(d)) (Hartree): -508.98232296
E(PUHF/6-31G(2df,p)) (Hartree): -509.02235392
E(PUHF/6-31G(d)) (Hartree): -508.96779344
E(PUHF/G3MP2large) (Hartree): -509.14320795
E(PUHF/G3Xlarge) (Hartree): -509.14468833
E(PUHF/G3large) (Hartree): -509.14468833
E(QCISD(T)/6-31G(d)) (Hartree): -510.45065159
E(QCISD/6-31G(d)) (Hartree): -510.39308995
E(UHF/6-31+G(d)) (Hartree): -508.94655765
E(UHF/6-31G(2df,p)) (Hartree): -508.98551135
E(UHF/6-31G(d)) (Hartree): -508.93136345
E(UHF/G3MP2large) (Hartree): -509.10693609
E(UHF/G3Xlarge) (Hartree): -509.10835214
E(UHF/G3large) (Hartree): -509.10835214
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.84039775
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      2.477853      0.154756     -0.073704
  C      2.040260     -1.181224     -0.148687
  C      0.708568     -1.468689     -0.134925
  C     -0.254658     -0.418742     -0.011884
  C      0.209201      0.946625      0.017446
  C      1.566967      1.199246      0.005166
  H      3.535543      0.374459     -0.084886
  H      2.765353     -1.978208     -0.226331
  H      0.329207     -2.478219     -0.196139
  H      1.911909      2.224741      0.049777
  N     -1.629535     -0.715565     -0.204738
  O     -2.514866     -0.085459     -0.786084
  O     -1.415251     -0.715926      1.172666
  O     -0.731451      1.890315      0.089481
  H     -0.331872      2.762900      0.161786
Rotational constants (GHz):      2.5033600      1.2750300      0.9504400
Vibrational harmonic frequencies (cm-1):
  1435.7668      101.1331      170.6197
  215.3964      236.6592      352.4563
  385.5191      404.9882      432.9998
  522.7944      539.6997      595.7555
  606.1510      712.8001      749.2942
  763.4604      853.8068      869.5915
  952.3258      962.9987     1001.9188
 1045.5772     1124.4236     1149.5862
 1163.9163     1192.1448     1294.3715
 1347.2184     1349.7863     1456.1742
 1503.4437     1526.5404     1582.0272
 1628.7321     3196.4316     3218.1231
 3229.8050     3239.9357     3860.6669
Zero-point correction (Hartree): 0.103746

TS.nitrophenol_cis.introtNO2
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E(G3SX(MP3)) excl. ZPE (Hartree): -511.72742348
E(G3SX) excl. ZPE (Hartree): -511.73715303

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E(G3X(MP2)) excl. ZPE (Hartree): -511.27575427
E(G3X(MP3)) excl. ZPE (Hartree): -511.69217492
E(G3X) excl. ZPE (Hartree): -511.66434541
E(MP2-Full/G3Xlarge) (Hartree): -511.34602674
E(MP2-Full/G3large) (Hartree): -511.34602674
E(MP2/6-31+G(d)) (Hartree): -510.39389573
E(MP2/6-31G(2df,p)) (Hartree): -510.70066527
E(MP2/6-31G(d)) (Hartree): -510.35975969
E(MP2/G3MP2large) (Hartree): -510.90172659
E(MP3/6-31+G(d)) (Hartree): -510.42426997
E(MP3/6-31G(2df,p)) (Hartree): -510.73899078
E(MP3/6-31G(d)) (Hartree): -510.39293136
E(MP4/6-31+G(d)) (Hartree): -510.50824915
E(MP4/6-31G(2df,p)) (Hartree): -510.83133948
E(MP4/6-31G(d)) (Hartree): -510.47158534
E(PMP2/6-31+G(d)) (Hartree): -510.39819078
E(PMP2/6-31G(2df,p)) (Hartree): -510.70513089
E(PMP2/6-31G(d)) (Hartree): -510.36374819
E(PMP2/G3MP2large) (Hartree): -510.90654841
E(PMP2/G3Xlarge) (Hartree): -511.35088181
E(PMP2/G3large) (Hartree): -511.35088181
E(PMP3/6-31+G(d)) (Hartree): -510.42675762
E(PMP3/6-31G(2df,p)) (Hartree): -510.74139040
E(PMP3/6-31G(d)) (Hartree): -510.39509720
E(PUHF/6-31+G(d)) (Hartree): -509.00267143
E(PUHF/6-31G(2df,p)) (Hartree): -509.04093576
E(PUHF/6-31G(d)) (Hartree): -508.98765905
E(PUHF/G3MP2large) (Hartree): -509.16284671
E(PUHF/G3Xlarge) (Hartree): -509.16430020
E(PUHF/G3large) (Hartree): -509.16430020
E(QCISD(T)/6-31G(d)) (Hartree): -510.48096102
E(QCISD/6-31G(d)) (Hartree): -510.42686625
E(UHF/6-31+G(d)) (Hartree): -508.99580074
E(UHF/6-31G(2df,p)) (Hartree): -509.03349590
E(UHF/6-31G(d)) (Hartree): -508.98101333
E(UHF/G3MP2large) (Hartree): -509.15511925
E(UHF/G3Xlarge) (Hartree): -509.15651561
E(UHF/G3large) (Hartree): -509.15651561
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.86504538
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      -2.563459      0.109817      -0.000050
  C      -2.125557     -1.210237       0.000090
  C      -0.766721     -1.469423       0.000081
  C       0.127315     -0.413486     -0.000065
  C      -0.298763      0.916195     -0.000091
  C      -1.666880      1.163999     -0.000149
  H      -3.623570      0.322768     -0.000070
  H      -2.834692     -2.024384       0.000181
  H      -0.380367     -2.479184       0.000125
  H      -2.000392      2.191822     -0.000205
  N       1.542529     -0.692017     -0.000042
  O       2.249301     -0.321208       1.028305
  O       2.249573     -0.321506     -1.028227
  O       0.543669      1.964166       0.000103
  H       1.465366      1.680290     -0.000080
Rotational constants (GHz):   2.5835000   1.1596200   0.8964000
Vibrational harmonic frequencies (cm-1):
  194.1738      129.0160      190.3392
  208.7492      299.1503      350.5426
  377.2018      438.9059      509.0456
  517.9404      577.2928      589.3216
  626.3940      752.8565      754.8447
  783.8060      848.7686      865.9053
  897.1317      981.3819     1009.4309
 1062.6387     1103.7755     1159.9917
 1174.4507     1223.0392     1301.6687
 1341.9858     1368.8818     1385.4887
 1518.5788     1533.1201     1655.7833
 1684.7332     3209.5138     3219.8537
 3231.2611     3238.3345     3830.1064

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Zero-point correction (Hartree): 0.104685

TS.nitrophenol_trans.introtNO2

E(G3SX(MP3)) excl. ZPE (Hartree): -511.71979079
E(G3SX) excl. ZPE (Hartree): -511.72893924
E(G3X(MP2)) excl. ZPE (Hartree): -511.26580751
E(G3X(MP3)) excl. ZPE (Hartree): -511.68335535
E(G3X) excl. ZPE (Hartree): -511.65518977
E(MP2-Full/G3Xlarge) (Hartree): -511.31520616
E(MP2-Full/G3large) (Hartree): -511.31520616
E(MP2/6-31+G(d)) (Hartree): -510.36326120
E(MP2/6-31G(2df,p)) (Hartree): -510.66704795
E(MP2/6-31G(d)) (Hartree): -510.32742055
E(MP2/G3MP2large) (Hartree): -510.87078474
E(MP3/6-31+G(d)) (Hartree): -510.40361128
E(MP3/6-31G(2df,p)) (Hartree): -510.71665142
E(MP3/6-31G(d)) (Hartree): -510.37086473
E(MP4/6-31+G(d)) (Hartree): -510.48657877
E(MP4/6-31G(2df,p)) (Hartree): -510.80792684
E(MP4/6-31G(d)) (Hartree): -510.44849592
E(PMP2/6-31+G(d)) (Hartree): -510.38403758
E(PMP2/6-31G(2df,p)) (Hartree): -510.68941467
E(PMP2/6-31G(d)) (Hartree): -510.34899904
E(PMP2/G3MP2large) (Hartree): -510.89217707
E(PMP2/G3Xlarge) (Hartree): -511.33665602
E(PMP2/G3large) (Hartree): -511.33665602
E(PMP3/6-31+G(d)) (Hartree): -510.41978862
E(PMP3/6-31G(2df,p)) (Hartree): -510.73409299
E(PMP3/6-31G(d)) (Hartree): -510.38779573
E(PUHF/6-31+G(d)) (Hartree): -509.02145079
E(PUHF/6-31G(2df,p)) (Hartree): -509.06090629
E(PUHF/6-31G(d)) (Hartree): -509.00745562
E(PUHF/G3MP2large) (Hartree): -509.18173792
E(PUHF/G3Xlarge) (Hartree): -509.18320027
E(PUHF/G3large) (Hartree): -509.18320027
E(QCISD(T)/6-31G(d)) (Hartree): -510.46961745
E(QCISD/6-31G(d)) (Hartree): -510.41654955
E(UHF/6-31+G(d)) (Hartree): -508.99810704
E(UHF/6-31G(2df,p)) (Hartree): -509.03584467
E(UHF/6-31G(d)) (Hartree): -508.98329760
E(UHF/G3MP2large) (Hartree): -509.15767363
E(UHF/G3Xlarge) (Hartree): -509.15906949
E(UHF/G3large) (Hartree): -509.15906949
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.85855273

Electronic state : 3-A

Cartesian coordinates (Angs):

C	-2.560372	-0.133322	0.024901
C	-1.955774	-1.376368	-0.104349
C	-0.577132	-1.448545	-0.177561
C	0.195523	-0.298590	-0.106193
C	-0.402547	0.954162	0.045721
C	-1.792301	1.015605	0.097356
H	-3.637404	-0.054208	0.072466
H	-2.550804	-2.275710	-0.158775
H	-0.070272	-2.397110	-0.293024
H	-2.266110	1.983101	0.212527
N	1.613404	-0.483380	-0.193965
O	2.226006	-1.138909	0.756159
O	2.400313	0.461637	-0.602008
O	0.370278	2.055163	0.163960
H	-0.186397	2.826811	0.300429

Rotational constants (GHz): 2.4361500 1.2002500 0.8498200

Vibrational harmonic frequencies (cm-1):

164.0453	122.4644	220.6402
229.3453	327.8875	352.4941
371.9377	388.0673	441.8464
510.3583	571.1009	573.2358
577.3828	726.2824	744.3203
779.4517	809.3946	857.3795
876.9112	974.5910	1000.8369

1076.4860	1105.2411	1162.4816
1176.8657	1193.3724	1307.5136
1338.8584	1352.3384	1407.3359
1504.5444	1553.6342	1666.1409
1678.3825	3189.4819	3212.7333
3219.8494	3237.5879	3872.5701

Zero-point correction (Hartree): 0.104138

TS.aci-NP-2.phenyloxy+HONO_cis

E(G3SX(MP3)) excl. ZPE (Hartree): -511.69417800
 E(G3SX) excl. ZPE (Hartree): -511.70318611
 E(G3X(MP2)) excl. ZPE (Hartree): -511.23962141
 E(G3X(MP3)) excl. ZPE (Hartree): -511.65746364
 E(G3X) excl. ZPE (Hartree): -511.62934298
 E(MP2-Full/G3Xlarge) (Hartree): -511.27508832
 E(MP2-Full/G3large) (Hartree): -511.27508832
 E(MP2/6-31+G(d)) (Hartree): -510.32924617
 E(MP2/6-31G(2df,p)) (Hartree): -510.62923853
 E(MP2/6-31G(d)) (Hartree): -510.29464001
 E(MP2/G3MP2large) (Hartree): -510.83169352
 E(MP3/6-31+G(d)) (Hartree): -510.36552512
 E(MP3/6-31G(2df,p)) (Hartree): -510.67630647
 E(MP3/6-31G(d)) (Hartree): -510.33425287
 E(MP4/6-31+G(d)) (Hartree): -510.45821885
 E(MP4/6-31G(2df,p)) (Hartree): -510.77669266
 E(MP4/6-31G(d)) (Hartree): -510.42116021
 E(PMP2/6-31+G(d)) (Hartree): -510.37215427
 E(PMP2/6-31G(2df,p)) (Hartree): -510.67388517
 E(PMP2/6-31G(d)) (Hartree): -510.33866307
 E(PMP2/G3MP2large) (Hartree): -510.87530662
 E(PMP2/G3Xlarge) (Hartree): -511.31876056
 E(PMP2/G3large) (Hartree): -511.31876056
 E(PMP3/6-31+G(d)) (Hartree): -510.40120546
 E(PMP3/6-31G(2df,p)) (Hartree): -510.71349658
 E(PMP3/6-31G(d)) (Hartree): -510.37102819
 E(PUHF/6-31+G(d)) (Hartree): -509.01399528
 E(PUHF/6-31G(2df,p)) (Hartree): -509.05345824
 E(PUHF/6-31G(d)) (Hartree): -509.00152273
 E(PUHF/G3MP2large) (Hartree): -509.17367816
 E(PUHF/G3Xlarge) (Hartree): -509.17511513
 E(PUHF/G3large) (Hartree): -509.17511513
 E(QCISD(T)/6-31G(d)) (Hartree): -510.44976725
 E(QCISD/6-31G(d)) (Hartree): -510.39438224
 E(UHF/6-31+G(d)) (Hartree): -508.96678049
 E(UHF/6-31G(2df,p)) (Hartree): -509.00443651
 E(UHF/6-31G(d)) (Hartree): -508.95316791
 E(UHF/G3MP2large) (Hartree): -509.12570947
 E(UHF/G3Xlarge) (Hartree): -509.12708013
 E(UHF/G3large) (Hartree): -509.12708013
 E(UM062X/Aug-CC-pVTZ) (Hartree): -511.82717462

Electronic state : 3-A

Cartesian coordinates (Angs):

C	-2.730723	-0.454581	0.119378
C	-1.864558	-1.570628	0.124019
C	-0.479036	-1.398348	0.022352
C	-0.016664	-0.126911	-0.077836
C	-0.812579	1.072739	-0.101079
C	-2.245033	0.814478	0.012551
H	-3.796290	-0.619990	0.200163
H	-2.276830	-2.567316	0.201504
H	0.197330	-2.244674	0.015276
H	-2.891552	1.681863	0.007880
O	-0.351835	2.212858	-0.206193
H	3.237544	0.246707	1.125217
N	2.178451	-0.104267	-0.389346
O	2.651761	0.769294	0.547476
O	2.596599	-1.205554	-0.268899

Rotational constants (GHz): 2.3590600 0.9352400 0.6891700

Vibrational harmonic frequencies (cm-1):

i293.2773	35.7094	53.4881
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72.7425	160.0763	194.2594
244.6770	394.6028	440.9412
488.1475	516.8913	581.4199
633.1909	685.5903	693.0897
790.1945	816.2092	872.1214
944.4384	946.4447	968.8781
1008.3460	1017.8629	1115.6763
1143.8700	1202.3326	1312.1638
1364.9520	1377.2856	1418.2910
1501.4711	1553.5001	1609.0516
1674.8890	3188.1766	3204.5293
3215.1027	3225.4706	3683.0769

Zero-point correction (Hartree): 0.101035

TS.aci-NP-1.phenyloxy+HONO_trans

E(G3SX(MP3)) excl. ZPE (Hartree): -511.70764735
 E(G3SX) excl. ZPE (Hartree): -511.71667517
 E(G3X(MP2)) excl. ZPE (Hartree): -511.25274441
 E(G3X(MP3)) excl. ZPE (Hartree): -511.67040634
 E(G3X) excl. ZPE (Hartree): -511.64254787
 E(MP2-Full/G3Xlarge) (Hartree): -511.29045939
 E(MP2-Full/G3large) (Hartree): -511.29045939
 E(MP2/6-31+G(d)) (Hartree): -510.34431458
 E(MP2/6-31G(2df,p)) (Hartree): -510.64431011
 E(MP2/6-31G(d)) (Hartree): -510.30859809
 E(MP2/G3MP2large) (Hartree): -510.84697138
 E(MP3/6-31+G(d)) (Hartree): -510.37847633
 E(MP3/6-31G(2df,p)) (Hartree): -510.68918295
 E(MP3/6-31G(d)) (Hartree): -510.34629080
 E(MP4/6-31+G(d)) (Hartree): -510.47161522
 E(MP4/6-31G(2df,p)) (Hartree): -510.79022976
 E(MP4/6-31G(d)) (Hartree): -510.43352141
 E(PMP2/6-31+G(d)) (Hartree): -510.38543392
 E(PMP2/6-31G(2df,p)) (Hartree): -510.68701955
 E(PMP2/6-31G(d)) (Hartree): -510.35093774
 E(PMP2/G3MP2large) (Hartree): -510.88859440
 E(PMP2/G3Xlarge) (Hartree): -511.33213883
 E(PMP2/G3large) (Hartree): -511.33213883
 E(PMP3/6-31+G(d)) (Hartree): -510.41268142
 E(PMP3/6-31G(2df,p)) (Hartree): -510.72479157
 E(PMP3/6-31G(d)) (Hartree): -510.38169557
 E(PUHF/6-31+G(d)) (Hartree): -509.01794095
 E(PUHF/6-31G(2df,p)) (Hartree): -509.05644101
 E(PUHF/6-31G(d)) (Hartree): -509.00464765
 E(PUHF/G3MP2large) (Hartree): -509.17668195
 E(PUHF/G3Xlarge) (Hartree): -509.17811439
 E(PUHF/G3large) (Hartree): -509.17811439
 E(QCISD(T)/6-31G(d)) (Hartree): -510.46157191
 E(QCISD/6-31G(d)) (Hartree): -510.40497363
 E(UHF/6-31+G(d)) (Hartree): -508.97270135
 E(UHF/6-31G(2df,p)) (Hartree): -509.00956140
 E(UHF/6-31G(d)) (Hartree): -508.95816285
 E(UHF/G3MP2large) (Hartree): -509.13090310
 E(UHF/G3Xlarge) (Hartree): -509.13227232
 E(UHF/G3large) (Hartree): -509.13227232
 E(UM062X/Aug-CC-pVTZ) (Hartree): -511.83985618

Electronic state : 3-A

Cartesian coordinates (Angs):

C	2.773450	-0.091967	-0.055087
C	2.170771	-1.368196	0.064606
C	0.783186	-1.502845	0.155562
C	0.041687	-0.362353	0.117410
C	0.574266	0.967801	-0.010580
C	2.022193	1.042706	-0.092708
H	3.850935	-0.028745	-0.117981
H	2.797023	-2.249904	0.078447
H	0.318467	-2.476932	0.238826
H	2.461734	2.027355	-0.176175
O	-0.149106	1.981019	-0.051332
H	-1.837550	1.429810	0.175551

N	-2.080100	-0.328717	-0.338550	
O	-2.537437	0.755146	0.344452	
O	-2.716360	-1.300095	-0.156125	
Rotational constants (GHz):	2.5512000	0.9570900	0.7051500	
Vibrational harmonic frequencies (cm-1):				
i239.9884		58.8305		89.4366
145.4405		191.0330		216.4085
324.1856		393.4206		462.3066
483.3789		520.2240		584.8678
686.7609		722.6030		795.1117
825.7736		848.4477		867.7651
945.3418		967.8340		972.9197
1009.7277	1013.4765			1121.4445
1150.5667	1216.2262			1323.1356
1379.7099	1417.5094			1474.3523
1524.0235	1559.9188			1608.3992
1741.5179	3197.3704			3207.9969
3216.9092	3228.4173			3385.8083
Zero-point correction (Hartree):	0.102241			

TS.aci-NP-3.phenyloxy+HONO_cis

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.69411221
E(G3SX) excl. ZPE (Hartree): -511.70316244
E(G3X(MP2)) excl. ZPE (Hartree): -511.23951950
E(G3X(MP3)) excl. ZPE (Hartree): -511.65728236
E(G3X) excl. ZPE (Hartree): -511.62926425
E(MP2-Full/G3Xlarge) (Hartree): -511.27311446
E(MP2-Full/G3large) (Hartree): -511.27311446
E(MP2/6-31+G(d)) (Hartree): -510.32761808
E(MP2/6-31G(2df,p)) (Hartree): -510.62776266
E(MP2/6-31G(d)) (Hartree): -510.29323256
E(MP2/G3MP2large) (Hartree): -510.82974767
E(MP3/6-31+G(d)) (Hartree): -510.36452977
E(MP3/6-31G(2df,p)) (Hartree): -510.67535667
E(MP3/6-31G(d)) (Hartree): -510.33342598
E(MP4/6-31+G(d)) (Hartree): -510.45739697
E(MP4/6-31G(2df,p)) (Hartree): -510.77595874
E(MP4/6-31G(d)) (Hartree): -510.42050280
E(PMP2/6-31+G(d)) (Hartree): -510.37169736
E(PMP2/6-31G(2df,p)) (Hartree): -510.67349349
E(PMP2/6-31G(d)) (Hartree): -510.33837482
E(PMP2/G3MP2large) (Hartree): -510.87453099
E(PMP2/G3Xlarge) (Hartree): -511.31795820
E(PMP2/G3large) (Hartree): -511.31795820
E(PMP3/6-31+G(d)) (Hartree): -510.40119329
E(PMP3/6-31G(2df,p)) (Hartree): -510.71346257
E(PMP3/6-31G(d)) (Hartree): -510.37114858
E(PUHF/6-31+G(d)) (Hartree): -509.01456965
E(PUHF/6-31G(2df,p)) (Hartree): -509.05398792
E(PUHF/6-31G(d)) (Hartree): -509.00219448
E(PUHF/G3MP2large) (Hartree): -509.17414446
E(PUHF/G3Xlarge) (Hartree): -509.17557972
E(PUHF/G3large) (Hartree): -509.17557972
E(QCISD(T)/6-31G(d)) (Hartree): -510.45020687
E(QCISD/6-31G(d)) (Hartree): -510.39464851
E(UHF/6-31+G(d)) (Hartree): -508.96607664
E(UHF/6-31G(2df,p)) (Hartree): -509.00378468
E(UHF/6-31G(d)) (Hartree): -508.95262143
E(UHF/G3MP2large) (Hartree): -509.12489717
E(UHF/G3Xlarge) (Hartree): -509.12626469
E(UHF/G3large) (Hartree): -509.12626469
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.82680593
Electronic state : 3-A
Cartesian coordinates (Angs):
C      2.740283      -0.423880      0.087973
C      1.897988      -1.558006      0.094169
C      0.506899      -1.417287      0.022256
C      0.014020      -0.154262      -0.052809
C      0.786172      1.060651      -0.077284
C      2.225514      0.835430      0.006953

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H	3.810444	-0.567571	0.146624
H	2.333497	-2.546318	0.149958
H	-0.147693	-2.278831	0.017800
H	2.852392	1.717066	0.001906
O	0.295909	2.190717	-0.162026
H	-3.215713	-1.264565	0.462047
N	-2.155897	0.114447	-0.293469
O	-2.570682	-1.212370	-0.265269
O	-2.671091	0.782055	0.525845
Rotational constants (GHz):		2.3835300	0.9431200 0.6900100
Vibrational harmonic frequencies (cm-1):			
i297.1553	31.4276	51.2021	
77.9639	171.1221	189.7014	
257.1709	394.6172	443.4848	
487.0884	515.6160	576.4372	
607.1296	663.5488	686.5206	
791.2112	817.6301	872.3117	
884.3117	945.1982	970.0768	
1008.1228	1018.2777	1116.0697	
1145.2130	1203.1050	1312.0490	
1350.0595	1372.9402	1419.0828	
1499.9363	1553.0466	1608.0578	
1695.0137	3199.5604	3207.1125	
3215.7258	3225.7238	3700.6374	
Zero-point correction (Hartree): 0.100885			

TS.aci-NP-1.nitrosophenoxy_trans+OH

E(G3SX(MP3)) excl. ZPE (Hartree): -511.71149815
E(G3SX) excl. ZPE (Hartree): -511.72050312
E(G3X(MP2)) excl. ZPE (Hartree): -511.25511662
E(G3X(MP3)) excl. ZPE (Hartree): -511.67359411
E(G3X) excl. ZPE (Hartree): -511.64586005
E(MP2-Full/G3Xlarge) (Hartree): -511.27568175
E(MP2-Full/G3large) (Hartree): -511.27568175
E(MP2/6-31+G(d)) (Hartree): -510.32912925
E(MP2/6-31G(2df,p)) (Hartree): -510.62875888
E(MP2/6-31G(d)) (Hartree): -510.29311340
E(MP2/G3MP2large) (Hartree): -510.83146588
E(MP3/6-31+G(d)) (Hartree): -510.37641635
E(MP3/6-31G(2df,p)) (Hartree): -510.68630814
E(MP3/6-31G(d)) (Hartree): -510.34343909
E(MP4/6-31+G(d)) (Hartree): -510.46330563
E(MP4/6-31G(2df,p)) (Hartree): -510.78074551
E(MP4/6-31G(d)) (Hartree): -510.42442415
E(PMP2/6-31+G(d)) (Hartree): -510.37944211
E(PMP2/6-31G(2df,p)) (Hartree): -510.68111193
E(PMP2/6-31G(d)) (Hartree): -510.34427913
E(PMP2/G3MP2large) (Hartree): -510.88296746
E(PMP2/G3Xlarge) (Hartree): -511.32729439
E(PMP2/G3large) (Hartree): -511.32729439
E(PMP3/6-31+G(d)) (Hartree): -510.42111765
E(PMP3/6-31G(2df,p)) (Hartree): -510.73291793
E(PMP3/6-31G(d)) (Hartree): -510.38903360
E(PUHF/6-31+G(d)) (Hartree): -509.04993659
E(PUHF/6-31G(2df,p)) (Hartree): -509.08847641
E(PUHF/6-31G(d)) (Hartree): -509.03666987
E(PUHF/G3MP2large) (Hartree): -509.20943638
E(PUHF/G3Xlarge) (Hartree): -509.21088046
E(PUHF/G3large) (Hartree): -509.21088046
E(QCISD(T)/6-31G(d)) (Hartree): -510.46400919
E(QCISD/6-31G(d)) (Hartree): -510.40793317
E(UHF/6-31+G(d)) (Hartree): -508.99640625
E(UHF/6-31G(2df,p)) (Hartree): -509.03285902
E(UHF/6-31G(d)) (Hartree): -508.98228947
E(UHF/G3MP2large) (Hartree): -509.15467615
E(UHF/G3Xlarge) (Hartree): -509.15600110
E(UHF/G3large) (Hartree): -509.15600110
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.84316924
Electronic state : 3-A
Cartesian coordinates (Angs):

C	2.488870	-0.219885	0.153587
C	1.752604	-1.451057	0.271290
C	0.406721	-1.479384	0.101985
C	-0.261291	-0.273886	-0.221660
C	0.433256	1.025113	-0.290492
C	1.882068	0.950577	-0.126542
H	3.560434	-0.248488	0.299765
H	2.289688	-2.365150	0.480545
H	-0.166544	-2.392166	0.178654
H	2.423751	1.882668	-0.200921
O	-0.169073	2.076490	-0.450977
H	-1.763292	1.493953	1.013672
N	-1.593451	-0.252198	-0.461377
O	-1.941225	0.606429	1.371701
O	-2.315109	-1.172205	-0.654609
Rotational constants (GHz):		2.1142100	1.2166200
			0.9039400
Vibrational harmonic frequencies (cm-1):			
i875.9909	70.4714	105.0518	
155.2893	208.8695	223.3586	
257.6618	366.4085	399.5758	
427.6635	488.1191	519.5340	
566.4330	585.5876	722.4044	
751.8223	786.1644	794.2972	
866.8457	879.8638	998.5959	
1000.4575	1030.5323	1065.2383	
1154.0936	1193.2864	1207.9373	
1358.2421	1409.7265	1451.2606	
1539.1815	1650.1534	1673.6597	
1700.4604	3204.8643	3220.1673	
3231.1131	3235.1244	3726.4531	
Zero-point correction (Hartree): 0.100754			

TS.aci-NP-3.nitrosophenoxy_cis+OH

E(G3SX(MP3)) excl. ZPE (Hartree): -511.70990796
E(G3SX) excl. ZPE (Hartree): -511.71891491
E(G3X(MP2)) excl. ZPE (Hartree): -511.25356564
E(G3X(MP3)) excl. ZPE (Hartree): -511.67223782
E(G3X) excl. ZPE (Hartree): -511.64444675
E(MP2-Full/G3Xlarge) (Hartree): -511.27097000
E(MP2-Full/G3large) (Hartree): -511.27097000
E(MP2/6-31+G(d)) (Hartree): -510.32608447
E(MP2/6-31G(2df,p)) (Hartree): -510.62404937
E(MP2/6-31G(d)) (Hartree): -510.28944968
E(MP2/G3MP2large) (Hartree): -510.82683533
E(MP3/6-31+G(d)) (Hartree): -510.37535698
E(MP3/6-31G(2df,p)) (Hartree): -510.68379675
E(MP3/6-31G(d)) (Hartree): -510.34169975
E(MP4/6-31+G(d)) (Hartree): -510.46192450
E(MP4/6-31G(2df,p)) (Hartree): -510.77764200
E(MP4/6-31G(d)) (Hartree): -510.42228689
E(PMP2/6-31+G(d)) (Hartree): -510.37888932
E(PMP2/6-31G(2df,p)) (Hartree): -510.67895821
E(PMP2/6-31G(d)) (Hartree): -510.34310278
E(PMP2/G3MP2large) (Hartree): -510.88091929
E(PMP2/G3Xlarge) (Hartree): -511.32517172
E(PMP2/G3large) (Hartree): -511.32517172
E(PMP3/6-31+G(d)) (Hartree): -510.42239800
E(PMP3/6-31G(2df,p)) (Hartree): -510.73282623
E(PMP3/6-31G(d)) (Hartree): -510.38964916
E(PUHF/6-31+G(d)) (Hartree): -509.05713159
E(PUHF/6-31G(2df,p)) (Hartree): -509.09480710
E(PUHF/6-31G(d)) (Hartree): -509.04345063
E(PUHF/G3MP2large) (Hartree): -509.21626466
E(PUHF/G3Xlarge) (Hartree): -509.21771361
E(PUHF/G3large) (Hartree): -509.21771361
E(QCISD(T)/6-31G(d)) (Hartree): -510.46342718
E(QCISD/6-31G(d)) (Hartree): -510.40763117
E(UHF/6-31+G(d)) (Hartree): -509.00103303
E(UHF/6-31G(2df,p)) (Hartree): -509.03656492
E(UHF/6-31G(d)) (Hartree): -508.98651659

E(UHF/G3MP2large) (Hartree): -509.15884441
 E(UHF/G3Xlarge) (Hartree): -509.16016722
 E(UHF/G3large) (Hartree): -509.16016722
 E(UM062X/Aug-CC-pVTZ) (Hartree): -511.84192547
 Electronic state : 3-A
 Cartesian coordinates (Angs):

C	2.521464	-0.194692	0.130525
C	1.833846	-1.392374	-0.247036
C	0.485226	-1.390452	-0.450825
C	-0.221682	-0.187150	-0.316285
C	0.426613	1.067267	0.109022
C	1.870992	0.978473	0.290598
H	3.589474	-0.242973	0.295814
H	2.397142	-2.305640	-0.372642
H	-0.061031	-2.282648	-0.720087
H	2.371283	1.884040	0.602705
O	-0.210868	2.093187	0.294452
H	-2.976525	-1.269620	0.928651
N	-1.565597	-0.184868	-0.547152
O	-2.031558	-1.355038	1.126862
O	-2.240065	0.789912	-0.671361

 Rotational constants (GHz): 2.1150700 1.2046100 0.8759800
 Vibrational harmonic frequencies (cm-1):

i694.4592	59.5367	90.7263
113.7620	157.4160	190.6364
233.0433	278.3766	408.0312
447.2505	464.8383	493.3212
557.7725	589.4719	695.2094
737.5164	741.7801	795.9905
862.6553	883.8737	994.6191
1013.7549	1022.7475	1047.3271
1155.6707	1196.1854	1247.3574
1342.9350	1410.8380	1435.2807
1527.3069	1612.2154	1652.3076
1667.5000	3205.6565	3223.0157
3231.4127	3238.4451	3796.1973

 Zero-point correction (Hartree): 0.099834

TS.nitrophenol_cis.nitrophenyl+OH

 E(G3SX(MP3)) excl. ZPE (Hartree): -511.63271609
 E(G3SX) excl. ZPE (Hartree): -511.64365103
 E(G3X(MP2)) excl. ZPE (Hartree): -511.17732847
 E(G3X(MP3)) excl. ZPE (Hartree): -511.59352846
 E(G3X) excl. ZPE (Hartree): -511.56880797
 E(MP2-Full/G3Xlarge) (Hartree): -511.22582942
 E(MP2-Full/G3large) (Hartree): -511.22582942
 E(MP2/6-31+G(d)) (Hartree): -510.27797974
 E(MP2/6-31G(2df,p)) (Hartree): -510.58102183
 E(MP2/6-31G(d)) (Hartree): -510.24213424
 E(MP2/G3MP2large) (Hartree): -510.78205456
 E(MP3/6-31+G(d)) (Hartree): -510.29326145
 E(MP3/6-31G(2df,p)) (Hartree): -510.60545318
 E(MP3/6-31G(d)) (Hartree): -510.26113642
 E(MP4/6-31+G(d)) (Hartree): -510.40701335
 E(MP4/6-31G(2df,p)) (Hartree): -510.72695862
 E(MP4/6-31G(d)) (Hartree): -510.36723910
 E(PMP2/6-31+G(d)) (Hartree): -510.30597776
 E(PMP2/6-31G(2df,p)) (Hartree): -510.60965742
 E(PMP2/6-31G(d)) (Hartree): -510.27004150
 E(PMP2/G3MP2large) (Hartree): -510.81076381
 E(PMP2/G3Xlarge) (Hartree): -511.25459147
 E(PMP2/G3large) (Hartree): -511.25459147
 E(PMP3/6-31+G(d)) (Hartree): -510.31517569
 E(PMP3/6-31G(2df,p)) (Hartree): -510.62788714
 E(PMP3/6-31G(d)) (Hartree): -510.28302651
 E(PUHF/6-31+G(d)) (Hartree): -508.86167653
 E(PUHF/6-31G(2df,p)) (Hartree): -508.89848893
 E(PUHF/6-31G(d)) (Hartree): -508.84497339
 E(PUHF/G3MP2large) (Hartree): -509.02143064
 E(PUHF/G3Xlarge) (Hartree): -509.02285731

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E(PUHF/G3large) (Hartree): -509.02285731
E(QCISD(T)/6-31G(d)) (Hartree): -510.38461111
E(QCISD/6-31G(d)) (Hartree): -510.32183719
E(UHF/6-31+G(d)) (Hartree): -508.83052432
E(UHF/6-31G(2df,p)) (Hartree): -508.86664904
E(UHF/6-31G(d)) (Hartree): -508.81393363
E(UHF/G3MP2large) (Hartree): -508.98948704
E(UHF/G3Xlarge) (Hartree): -508.99085407
E(UHF/G3large) (Hartree): -508.99085407
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.75847682
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      -2.565477      0.116841     -0.012803
  C      -2.080201     -1.192419      0.168351
  C      -0.729248     -1.435210      0.133856
  C       0.120165     -0.353999     -0.117661
  C      -0.352143      0.928031     -0.362037
  C      -1.715862      1.183725     -0.221905
  H      -3.633974      0.289246      0.007997
  H      -2.771241     -2.000263      0.357810
  H      -0.308750     -2.414748      0.312088
  H      -2.108920      2.184515     -0.340697
  N       1.525642     -0.519530     -0.096385
  O       2.219004      0.529921     -0.098690
  O       2.040048     -1.611236     -0.027930
  O       0.849173      2.026259      0.507458
  H       1.214180      2.536602     -0.236015
Rotational constants (GHz):   2.3508300   1.2692300   0.8453600
Vibrational harmonic frequencies (cm-1):
  11693.8946      123.3534      142.6184
   173.2450      272.8557      316.6642
   407.6996      419.7397      451.1651
   560.0776      581.0700      599.1696
   677.5948      691.0936      727.6057
   747.6267      806.5647      859.8222
   869.1176      914.1314      983.4687
  1014.6717     1039.7769     1055.6620
  1154.0465     1174.0005     1190.7473
  1263.4289     1377.7688     1456.5337
  1461.6037     1574.5838     1622.5654
  1632.5313     3194.0602     3209.2174
  3223.4681     3237.2704     3743.1425
Zero-point correction (Hartree): 0.102403

TS.nitrophenol_trans.nitrophenyl+OH
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E(G3SX(MP3)) excl. ZPE (Hartree): -511.63271802
E(G3SX) excl. ZPE (Hartree): -511.64365208
E(G3X(MP2)) excl. ZPE (Hartree): -511.17733070
E(G3X(MP3)) excl. ZPE (Hartree): -511.59353002
E(G3X) excl. ZPE (Hartree): -511.56880900
E(MP2-Full/G3Xlarge) (Hartree): -511.22583951
E(MP2-Full/G3large) (Hartree): -511.22583951
E(MP2/6-31+G(d)) (Hartree): -510.27798900
E(MP2/6-31G(2df,p)) (Hartree): -510.58103049
E(MP2/6-31G(d)) (Hartree): -510.24214145
E(MP2/G3MP2large) (Hartree): -510.78206467
E(MP3/6-31+G(d)) (Hartree): -510.29326716
E(MP3/6-31G(2df,p)) (Hartree): -510.60545855
E(MP3/6-31G(d)) (Hartree): -510.26114099
E(MP4/6-31+G(d)) (Hartree): -510.40701723
E(MP4/6-31G(2df,p)) (Hartree): -510.72696232
E(MP4/6-31G(d)) (Hartree): -510.36724173
E(PMP2/6-31+G(d)) (Hartree): -510.30598350
E(PMP2/6-31G(2df,p)) (Hartree): -510.60966282
E(PMP2/6-31G(d)) (Hartree): -510.27004578
E(PMP2/G3MP2large) (Hartree): -510.81077011
E(PMP2/G3Xlarge) (Hartree): -511.25459776
E(PMP2/G3large) (Hartree): -511.25459776
E(PMP3/6-31+G(d)) (Hartree): -510.31517816
E(PMP3/6-31G(2df,p)) (Hartree): -510.62788953

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E(PMP3/6-31G(d)) (Hartree): -510.28302840
E(PUHF/6-31+G(d)) (Hartree): -508.86166970
E(PUHF/6-31G(2df,p)) (Hartree): -508.89848281
E(PUHF/6-31G(d)) (Hartree): -508.84496800
E(PUHF/G3MP2large) (Hartree): -509.02142311
E(PUHF/G3Xlarge) (Hartree): -509.02284979
E(PUHF/G3large) (Hartree): -509.02284979
E(QCISD(T)/6-31G(d)) (Hartree): -510.38461044
E(QCISD/6-31G(d)) (Hartree): -510.32183367
E(UHF/6-31+G(d)) (Hartree): -508.83052120
E(UHF/6-31G(2df,p)) (Hartree): -508.86664636
E(UHF/6-31G(d)) (Hartree): -508.81393132
E(UHF/G3MP2large) (Hartree): -508.98948352
E(UHF/G3Xlarge) (Hartree): -508.99085056
E(UHF/G3large) (Hartree): -508.99085056
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.75776258
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      -2.565474      0.116897      -0.012774
  C      -2.080232     -1.192380       0.168358
  C      -0.729286     -1.435205       0.133835
  C       0.120140     -0.354009     -0.117694
  C      -0.352126      0.928037     -0.362062
  C      -1.715839      1.183761     -0.221899
  H      -3.633966      0.289331      0.008057
  H      -2.771291     -2.000206      0.357822
  H      -0.308807     -2.414755      0.312049
  H      -2.108881      2.184557     -0.340691
  N       1.525615     -0.519546     -0.096392
  O       2.218969      0.529911     -0.098682
  O       2.040030     -1.611243     -0.027922
  O       0.849301      2.026159      0.507465
  H       1.214155      2.536683     -0.235966
Rotational constants (GHz):   2.3508900   1.2692300   0.8453700
Vibrational harmonic frequencies (cm-1):
  51.7742      135.9113      219.5541
  270.2838      369.9355      396.4009
  417.8046      426.8027      564.8210
  576.5478      609.7834      634.3592
  644.6482      672.0119      760.5636
  808.7750      816.8025      867.9593
  943.0092      967.8279      998.3026
 1010.9954     1044.1572     1118.0714
 1172.5834     1190.5200     1261.4968
 1387.7841     1455.9668     1467.4783
 1569.7918     1621.1904     1634.9005
 3019.5778     3198.4656     3222.7545
 3235.6834     3238.3136     3782.6884
Zero-point correction (Hartree): 0.108865

TS.spiro_cis.hydroxyphenoxy+NO
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.71693709
E(G3SX) excl. ZPE (Hartree): -511.72644506
E(G3X(MP2)) excl. ZPE (Hartree): -511.26052140
E(G3X(MP3)) excl. ZPE (Hartree): -511.67728516
E(G3X) excl. ZPE (Hartree): -511.65088738
E(MP2-Full/G3Xlarge) (Hartree): -511.29866466
E(MP2-Full/G3large) (Hartree): -511.29866466
E(MP2/6-31+G(d)) (Hartree): -510.34668243
E(MP2/6-31G(2df,p)) (Hartree): -510.65290817
E(MP2/6-31G(d)) (Hartree): -510.31095178
E(MP2/G3MP2large) (Hartree): -510.85460356
E(MP3/6-31+G(d)) (Hartree): -510.37711758
E(MP3/6-31G(2df,p)) (Hartree): -510.69280744
E(MP3/6-31G(d)) (Hartree): -510.34512130
E(MP4/6-31+G(d)) (Hartree): -510.47315309
E(MP4/6-31G(2df,p)) (Hartree): -510.79719537
E(MP4/6-31G(d)) (Hartree): -510.43463873
E(PMP2/6-31+G(d)) (Hartree): -510.38142020
E(PMP2/6-31G(2df,p)) (Hartree): -510.68854636

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E(PMP2/6-31G(d)) (Hartree): -510.34631683
E(PMP2/G3MP2large) (Hartree): -510.88975244
E(PMP2/G3Xlarge) (Hartree): -511.33386623
E(PMP2/G3large) (Hartree): -511.33386623
E(PMP3/6-31+G(d)) (Hartree): -510.40576939
E(PMP3/6-31G(2df,p)) (Hartree): -510.72218598
E(PMP3/6-31G(d)) (Hartree): -510.37441874
E(PUHF/6-31+G(d)) (Hartree): -508.98773930
E(PUHF/6-31G(2df,p)) (Hartree): -509.02857135
E(PUHF/6-31G(d)) (Hartree): -508.97431027
E(PUHF/G3MP2large) (Hartree): -509.14860502
E(PUHF/G3Xlarge) (Hartree): -509.15005540
E(PUHF/G3large) (Hartree): -509.15005540
E(QCISD(T)/6-31G(d)) (Hartree): -510.46404953
E(QCISD/6-31G(d)) (Hartree): -510.40527880
E(UHF/6-31+G(d)) (Hartree): -508.94950902
E(UHF/6-31G(2df,p)) (Hartree): -508.98936705
E(UHF/6-31G(d)) (Hartree): -508.93544570
E(UHF/G3MP2large) (Hartree): -509.10989824
E(UHF/G3Xlarge) (Hartree): -509.11128833
E(UHF/G3large) (Hartree): -509.11128833
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.84616530
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      -2.377996      0.267421      0.359060
  C      -2.048031     -1.086916      0.074002
  C      -0.793889     -1.454160     -0.271111
  C       0.286829     -0.458838     -0.300864
  C      -0.145907      0.965228     -0.143924
  C      -1.427606      1.279774      0.212336
  H      -3.388561      0.520201      0.641841
  H      -2.828466     -1.834014      0.120807
  H      -0.516766     -2.470904     -0.507950
  H      -1.692389      2.320655      0.331464
  N       1.494850     -0.855468      0.545523
  O       2.262680     -0.131722      1.106022
  O       1.398275     -0.645235     -1.091404
  O       0.768919      1.893008     -0.417570
  H       1.562840      1.448887     -0.758204
Rotational constants (GHz):   2.3306100   1.3241700   1.0189500
Vibrational harmonic frequencies (cm-1):
  i630.1230      85.2590      165.3432
    214.5355      270.8316      324.9642
    347.3981      417.1871      462.0630
    508.3799      528.9095      557.9081
    575.7650      622.5234      704.6450
    729.7250      792.1110      831.3228
    879.7151      933.0207      996.7469
   1006.4560     1116.7696     1143.5252
   1193.4498     1261.9201     1280.1495
   1329.2209     1387.4254     1443.6502
   1463.3881     1551.6606     1592.3738
   1641.3482     3208.8084     3222.4032
   3232.7224     3237.9119     3718.0042
Zero-point correction (Hartree): 0.102471

TS.spiro_trans.hydroxyphenoxy+NO
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.70829611
E(G3SX) excl. ZPE (Hartree): -511.71812747
E(G3X(MP2)) excl. ZPE (Hartree): -511.25378927
E(G3X(MP3)) excl. ZPE (Hartree): -511.66998102
E(G3X) excl. ZPE (Hartree): -511.64401648
E(MP2-Full/G3Xlarge) (Hartree): -511.30851320
E(MP2-Full/G3large) (Hartree): -511.30851320
E(MP2/6-31+G(d)) (Hartree): -510.35541066
E(MP2/6-31G(2df,p)) (Hartree): -510.66151009
E(MP2/6-31G(d)) (Hartree): -510.31839851
E(MP2/G3MP2large) (Hartree): -510.86463823
E(MP3/6-31+G(d)) (Hartree): -510.37678041
E(MP3/6-31G(2df,p)) (Hartree): -510.69266768

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E(MP3/6-31G(d)) (Hartree): -510.34419602
E(MP4/6-31+G(d)) (Hartree): -510.47888867
E(MP4/6-31G(2df,p)) (Hartree): -510.80250256
E(MP4/6-31G(d)) (Hartree): -510.43890998
E(PMP2/6-31+G(d)) (Hartree): -510.37685925
E(PMP2/6-31G(2df,p)) (Hartree): -510.68350194
E(PMP2/6-31G(d)) (Hartree): -510.34008272
E(PMP2/G3MP2large) (Hartree): -510.88623872
E(PMP2/G3Xlarge) (Hartree): -511.33016219
E(PMP2/G3large) (Hartree): -511.33016219
E(PMP3/6-31+G(d)) (Hartree): -510.39336919
E(PMP3/6-31G(2df,p)) (Hartree): -510.70963968
E(PMP3/6-31G(d)) (Hartree): -510.36103241
E(PUHF/6-31+G(d)) (Hartree): -508.96073319
E(PUHF/6-31G(2df,p)) (Hartree): -509.00093930
E(PUHF/6-31G(d)) (Hartree): -508.94581278
E(PUHF/G3MP2large) (Hartree): -509.12213882
E(PUHF/G3Xlarge) (Hartree): -509.12360170
E(PUHF/G3large) (Hartree): -509.12360170
E(QCISD(T)/6-31G(d)) (Hartree): -510.45471324
E(QCISD/6-31G(d)) (Hartree): -510.39641203
E(UHF/6-31+G(d)) (Hartree): -508.93622670
E(UHF/6-31G(2df,p)) (Hartree): -508.97581013
E(UHF/6-31G(d)) (Hartree): -508.92106487
E(UHF/G3MP2large) (Hartree): -509.09741444
E(UHF/G3Xlarge) (Hartree): -509.09882075
E(UHF/G3large) (Hartree): -509.09882075
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.83617735
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      2.415724      0.230583      -0.281199
  C      2.037176     -1.128407     -0.138111
  C      0.756333     -1.475164      0.115616
  C     -0.309542     -0.460204      0.273035
  C      0.155928      0.957640      0.122360
  C      1.464531      1.249206     -0.133347
  H      3.443692      0.485936     -0.488124
  H      2.793805     -1.896097     -0.223856
  H      0.439244     -2.498811      0.252826
  H      1.766458      2.286905     -0.209837
  N     -1.563150     -0.824981     -0.507621
  O     -2.399042     -0.101068     -0.943463
  O     -1.311174     -0.711644      1.158574
  O     -0.810850      1.862735      0.311880
  H     -0.453535      2.754816      0.256292
Rotational constants (GHz):   2.3552200   1.3124800   0.9875300
Vibrational harmonic frequencies (cm-1):
  i681.1253      66.4172      163.7926
  216.2696      272.3356      322.6804
  355.0343      390.5371      416.6924
  459.8231      513.8147      524.0099
  566.9117      615.3445      697.0812
  725.3650      789.3677      828.8234
  887.6835      911.7321      996.9885
 1017.5126     1111.2513     1134.7593
 1167.8893     1253.2016     1278.3357
 1326.4212     1359.9742     1437.4578
 1477.5134     1567.1390     1583.7927
 1636.6802     3187.4152     3208.1826
 3231.6002     3237.5511     3857.1558
Zero-point correction (Hartree): 0.102049

TS.nitrophenol_cis.hydroxyphenyl+NO2
-----
E(G3SX(MP3)) excl. ZPE (Hartree): -511.69570977
E(G3SX) excl. ZPE (Hartree): -511.70441152
E(G3X(MP2)) excl. ZPE (Hartree): -511.23797897
E(G3X(MP3)) excl. ZPE (Hartree): -511.65473859
E(G3X) excl. ZPE (Hartree): -511.62729447
E(MP2-Full/G3Xlarge) (Hartree): -511.27022453
E(MP2-Full/G3large) (Hartree): -511.27022453

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E(MP2/6-31+G(d)) (Hartree): -510.31711582
E(MP2/6-31G(2df,p)) (Hartree): -510.62358994
E(MP2/6-31G(d)) (Hartree): -510.28109275
E(MP2/G3MP2large) (Hartree): -510.82619815
E(MP3/6-31+G(d)) (Hartree): -510.34402623
E(MP3/6-31G(2df,p)) (Hartree): -510.65983464
E(MP3/6-31G(d)) (Hartree): -510.31157645
E(MP4/6-31+G(d)) (Hartree): -510.44323516
E(MP4/6-31G(2df,p)) (Hartree): -510.76755797
E(MP4/6-31G(d)) (Hartree): -510.40495200
E(PMP2/6-31+G(d)) (Hartree): -510.34922865
E(PMP2/6-31G(2df,p)) (Hartree): -510.65745713
E(PMP2/6-31G(d)) (Hartree): -510.31461825
E(PMP2/G3MP2large) (Hartree): -510.85881282
E(PMP2/G3Xlarge) (Hartree): -511.30289107
E(PMP2/G3large) (Hartree): -511.30289107
E(PMP3/6-31+G(d)) (Hartree): -510.36980229
E(PMP3/6-31G(2df,p)) (Hartree): -510.68705713
E(PMP3/6-31G(d)) (Hartree): -510.33867323
E(PUHF/6-31+G(d)) (Hartree): -508.95256271
E(PUHF/6-31G(2df,p)) (Hartree): -508.99416268
E(PUHF/6-31G(d)) (Hartree): -508.93919012
E(PUHF/G3MP2large) (Hartree): -509.11444670
E(PUHF/G3Xlarge) (Hartree): -509.11589690
E(PUHF/G3large) (Hartree): -509.11589690
E(QCISD(T)/6-31G(d)) (Hartree): -510.44005281
E(QCISD/6-31G(d)) (Hartree): -510.37672857
E(UHF/6-31+G(d)) (Hartree): -508.91690288
E(UHF/6-31G(2df,p)) (Hartree): -508.95663768
E(UHF/6-31G(d)) (Hartree): -508.90205307
E(UHF/G3MP2large) (Hartree): -509.07821717
E(UHF/G3Xlarge) (Hartree): -509.07960793
E(UHF/G3large) (Hartree): -509.07960793
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.82584848
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      2.588420    -0.301508    -0.043530
  C      1.877075    -1.490440     0.113698
  C      0.490795    -1.449909     0.189210
  C     -0.087367    -0.217681     0.074385
  C      0.554302     1.000476    -0.033301
  C      1.949004     0.922042    -0.122366
  H      3.667686    -0.331620    -0.099776
  H      2.391942    -2.439214     0.159905
  H     -0.118118    -2.339715     0.281223
  H      2.500814     1.846689    -0.223905
  N     -1.989113    -0.247016    -0.291770
  O     -2.313828     0.712286     0.441025
  O     -2.360066    -1.392330    -0.273373
  O     -0.045844     2.197104    -0.072062
  H     -0.994015     2.078617     0.091640
Rotational constants (GHz):   2.3088200   1.1537400   0.7851200
Vibrational harmonic frequencies (cm-1):
i453.1669           69.3520           92.1614
173.7638           222.9085          259.5947
399.6683           426.7974          464.1852
533.3459           537.8618          603.0978
628.3522           679.6627          714.9981
762.4139           845.5846          863.9831
931.1888           967.7002         1006.0304
1049.9924          1101.8626         1150.6110
1164.7642          1204.4281         1299.9276
1334.7223          1363.9616         1468.5806
1498.3145          1512.6573         1599.2669
1671.3600          3205.8157         3211.1313
3220.6068          3231.5221         3716.0041
Zero-point correction (Hartree): 0.102946

TS.nitrophenol_trans.hydroxyphenyl+NO2
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E(G3SX(MP3)) excl. ZPE (Hartree): -511.68673813

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E(G3SX) excl. ZPE (Hartree): -511.69556549
E(G3X(MP2)) excl. ZPE (Hartree): -511.22955326
E(G3X(MP3)) excl. ZPE (Hartree): -511.64647410
E(G3X) excl. ZPE (Hartree): -511.61896917
E(MP2-Full/G3Xlarge) (Hartree): -511.26456824
E(MP2-Full/G3large) (Hartree): -511.26456824
E(MP2/6-31+G(d)) (Hartree): -510.31132898
E(MP2/6-31G(2df,p)) (Hartree): -510.61667860
E(MP2/6-31G(d)) (Hartree): -510.27444793
E(MP2/G3MP2large) (Hartree): -510.82057699
E(MP3/6-31+G(d)) (Hartree): -510.33890154
E(MP3/6-31G(2df,p)) (Hartree): -510.65376321
E(MP3/6-31G(d)) (Hartree): -510.30557512
E(MP4/6-31+G(d)) (Hartree): -510.43741662
E(MP4/6-31G(2df,p)) (Hartree): -510.76049089
E(MP4/6-31G(d)) (Hartree): -510.39814565
E(PMP2/6-31+G(d)) (Hartree): -510.34388828
E(PMP2/6-31G(2df,p)) (Hartree): -510.65096891
E(PMP2/6-31G(d)) (Hartree): -510.30841046
E(PMP2/G3MP2large) (Hartree): -510.85355155
E(PMP2/G3Xlarge) (Hartree): -511.29759665
E(PMP2/G3large) (Hartree): -511.29759665
E(PMP3/6-31+G(d)) (Hartree): -510.36521645
E(PMP3/6-31G(2df,p)) (Hartree): -510.68149698
E(PMP3/6-31G(d)) (Hartree): -510.33321280
E(PUHF/6-31+G(d)) (Hartree): -508.95244689
E(PUHF/6-31G(2df,p)) (Hartree): -508.99359774
E(PUHF/6-31G(d)) (Hartree): -508.93838058
E(PUHF/G3MP2large) (Hartree): -509.11467929
E(PUHF/G3Xlarge) (Hartree): -509.11613159
E(PUHF/G3large) (Hartree): -509.11613159
E(QCISD(T)/6-31G(d)) (Hartree): -510.43060337
E(QCISD/6-31G(d)) (Hartree): -510.36915433
E(UHF/6-31+G(d)) (Hartree): -508.91640228
E(UHF/6-31G(2df,p)) (Hartree): -508.95570681
E(UHF/6-31G(d)) (Hartree): -508.90087100
E(UHF/G3MP2large) (Hartree): -509.07815231
E(UHF/G3Xlarge) (Hartree): -509.07954314
E(UHF/G3large) (Hartree): -509.07954314
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.81688831
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      2.546990      -0.476295      0.011991
  C      1.734069      -1.594818      0.148766
  C      0.351456      -1.433130      0.168947
  C     -0.124972     -0.162999      0.036366
  C      0.625501      0.985940     -0.077739
  C      2.008561      0.796690     -0.105751
  H      3.621522     -0.593613     -0.004135
  H      2.165060     -2.582226      0.230340
  H     -0.332494     -2.269497      0.246262
  H      2.656764      1.659348     -0.209571
  N     -2.039706     -0.072271     -0.229146
  O     -2.257823      0.552918      0.822399
  O     -2.440570     -1.154720     -0.587432
  O      0.026757      2.191833     -0.170057
  H      0.690562      2.879305     -0.273633
Rotational constants (GHz):   2.2702100   1.1294300   0.7984800
Vibrational harmonic frequencies (cm-1):
  i607.5817      47.3747      88.5992
   131.7906      207.4710      261.3949
   348.5331      358.3617      436.3104
   458.8096      531.7670      540.4436
   620.4776      688.2282      712.5581
   764.0457      841.5642      851.2186
   926.0499      958.3700      998.5592
  1056.6608     1105.0927     1158.9482
  1169.5048     1178.1251     1304.7637
  1327.7392     1330.8428     1459.0418
  1487.9559     1522.7276     1605.2420
  1693.0453     3182.1684     3196.1902

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3215.9047          3231.0899          3873.7013
Zero-point correction (Hartree): 0.102223

TS.nitrophenol.nitrosophenol+O3P.cc
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E(G3SX(MP3)) excl. ZPE (Hartree): -511.69513848
E(G3SX) excl. ZPE (Hartree): -511.70495127
E(G3X(MP2)) excl. ZPE (Hartree): -511.24695700
E(G3X(MP3)) excl. ZPE (Hartree): -511.66312253
E(G3X) excl. ZPE (Hartree): -511.63477255
E(MP2-Full/G3Xlarge) (Hartree): -511.32363647
E(MP2-Full/G3large) (Hartree): -511.32363647
E(MP2/6-31+G(d)) (Hartree): -510.37934950
E(MP2/6-31G(2df,p)) (Hartree): -510.67968168
E(MP2/6-31G(d)) (Hartree): -510.34580815
E(MP2/G3MP2large) (Hartree): -510.87993947
E(MP3/6-31+G(d)) (Hartree): -510.40551868
E(MP3/6-31G(2df,p)) (Hartree): -510.71389922
E(MP3/6-31G(d)) (Hartree): -510.37461528
E(MP4/6-31+G(d)) (Hartree): -510.49448439
E(MP4/6-31G(2df,p)) (Hartree): -510.81122330
E(MP4/6-31G(d)) (Hartree): -510.45859019
E(PMP2/6-31+G(d)) (Hartree): -510.38776492
E(PMP2/6-31G(2df,p)) (Hartree): -510.68903252
E(PMP2/6-31G(d)) (Hartree): -510.35409235
E(PMP2/G3MP2large) (Hartree): -510.88948120
E(PMP2/G3Xlarge) (Hartree): -511.33324115
E(PMP2/G3large) (Hartree): -511.33324115
E(PMP3/6-31+G(d)) (Hartree): -510.41322732
E(PMP3/6-31G(2df,p)) (Hartree): -510.72247383
E(PMP3/6-31G(d)) (Hartree): -510.38221537
E(PUHF/6-31+G(d)) (Hartree): -509.00109007
E(PUHF/6-31G(2df,p)) (Hartree): -509.03610779
E(PUHF/6-31G(d)) (Hartree): -508.98616946
E(PUHF/G3MP2large) (Hartree): -509.15834190
E(PUHF/G3Xlarge) (Hartree): -509.15971329
E(PUHF/G3large) (Hartree): -509.15971329
E(QCISD(T)/6-31G(d)) (Hartree): -510.46009080
E(QCISD/6-31G(d)) (Hartree): -510.40457073
E(UHF/6-31+G(d)) (Hartree): -508.99223967
E(UHF/6-31G(2df,p)) (Hartree): -509.02629265
E(UHF/6-31G(d)) (Hartree): -508.97747148
E(UHF/G3MP2large) (Hartree): -509.14831562
E(UHF/G3Xlarge) (Hartree): -509.14962050
E(UHF/G3large) (Hartree): -509.14962050
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.83384122
Electronic state : 3-A
Cartesian coordinates (Angs):
  C      2.479412      -0.460764      0.104963
  C      1.682582      -1.575317     -0.179338
  C      0.329771      -1.402056     -0.337690
  C     -0.235636     -0.126660     -0.214393
  C      0.567625       0.996009       0.071979
  C      1.939884       0.802426       0.229551
  H      3.546217     -0.587988       0.231295
  H      2.126617     -2.554953     -0.271497
  H     -0.338091     -2.224858     -0.555276
  H      2.553854       1.663938       0.449453
  O      0.080434       2.229678       0.200472
  H     -0.881234       2.202290       0.059406
  N     -1.625619     -0.061153     -0.399564
  O     -2.176653       1.009415     -0.324300
  O     -2.430014     -1.673115       0.727970
Rotational constants (GHz):   2.0003900   1.2406500   0.8067600
Vibrational harmonic frequencies (cm-1):
  1137.5712          63.9185          106.0261
   158.2806          235.3908          288.6101
   382.6318          423.1808          445.2803
   458.7010          539.6553          574.0766
   687.4111          690.5842          742.4491
   789.6847          791.5383          896.7251

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898.3505	999.4810	1013.7838
1060.2768	1133.5967	1163.6574
1207.0634	1225.6453	1326.8632
1355.2337	1385.1903	1503.1504
1515.9195	1624.0389	1662.7146
1685.0465	3206.5471	3213.7612
3229.7030	3239.6133	3626.9219

Zero-point correction (Hartree): 0.103772

TS.acinitrophenol_cistrans.nitrophenoxy+H

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.66944936
E(G3SX) excl. ZPE (Hartree): -511.67846401
E(G3X(MP2)) excl. ZPE (Hartree): -511.21289585
E(G3X(MP3)) excl. ZPE (Hartree): -511.63117857
E(G3X) excl. ZPE (Hartree): -511.60372094
E(MP2-Full/G3Xlarge) (Hartree): -511.24126379
E(MP2-Full/G3large) (Hartree): -511.24126379
E(MP2/6-31+G(d)) (Hartree): -510.29951701
E(MP2/6-31G(2df,p)) (Hartree): -510.59599587
E(MP2/6-31G(d)) (Hartree): -510.26480672
E(MP2/G3MP2large) (Hartree): -510.79662025
E(MP3/6-31+G(d)) (Hartree): -510.33411179
E(MP3/6-31G(2df,p)) (Hartree): -510.64031114
E(MP3/6-31G(d)) (Hartree): -510.30243427
E(MP4/6-31+G(d)) (Hartree): -510.42587432
E(MP4/6-31G(2df,p)) (Hartree): -510.74025228
E(MP4/6-31G(d)) (Hartree): -510.38847253
E(PMP2/6-31+G(d)) (Hartree): -510.35180994
E(PMP2/6-31G(2df,p)) (Hartree): -510.64995846
E(PMP2/6-31G(d)) (Hartree): -510.31825434
E(PMP2/G3MP2large) (Hartree): -510.84961353
E(PMP2/G3Xlarge) (Hartree): -511.29432703
E(PMP2/G3large) (Hartree): -511.29432703
E(PMP3/6-31+G(d)) (Hartree): -510.37913109
E(PMP3/6-31G(2df,p)) (Hartree): -510.68684351
E(PMP3/6-31G(d)) (Hartree): -510.34865423
E(PUHF/6-31+G(d)) (Hartree): -508.99307885
E(PUHF/6-31G(2df,p)) (Hartree): -509.02962309
E(PUHF/6-31G(d)) (Hartree): -508.98080843
E(PUHF/G3MP2large) (Hartree): -509.14924212
E(PUHF/G3Xlarge) (Hartree): -509.15073014
E(PUHF/G3large) (Hartree): -509.15073014
E(QCISD(T)/6-31G(d)) (Hartree): -510.42824078
E(QCISD/6-31G(d)) (Hartree): -510.36840148
E(UHF/6-31+G(d)) (Hartree): -508.93678722
E(UHF/6-31G(2df,p)) (Hartree): -508.97160923
E(UHF/6-31G(d)) (Hartree): -508.92336143
E(UHF/G3MP2large) (Hartree): -509.09221003
E(UHF/G3Xlarge) (Hartree): -509.09362156
E(UHF/G3large) (Hartree): -509.09362156
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.79650562
Electronic state : 3-A

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Cartesian coordinates (Angs):

C	2.552830	-0.377982	0.083209
C	1.740414	-1.518666	0.107323
C	0.341303	-1.408150	0.044051
C	-0.227149	-0.173758	-0.022968
C	0.557527	1.052942	-0.099593
C	1.993235	0.866530	-0.015085
H	3.626933	-0.489041	0.132435
H	2.188486	-2.499382	0.175360
H	-0.290482	-2.285945	0.058249
H	2.590196	1.766559	-0.061450
O	0.057113	2.164957	-0.278389
N	-1.680244	-0.086896	0.003158
O	-2.304635	-0.963803	-0.593476
O	-2.183597	0.765775	0.699309
H	-2.653426	-2.264849	0.472124

Rotational constants (GHz): 2.4027600 1.2148800 0.8484200
Vibrational harmonic frequencies (cm-1):

i1014.6269	59.7176	115.9675
206.4703	211.0167	226.7560
339.4127	365.4490	389.7184
473.4446	491.7854	554.5364
562.4075	640.5450	703.9480
779.9764	803.0704	829.8230
892.2080	905.5128	987.9087
1010.7171	1041.3345	1098.7520
1138.7344	1157.7449	1254.0075
1335.2467	1383.8198	1426.3319
1452.0968	1517.0536	1563.3885
1627.3555	1636.5920	3212.3699
3218.7121	3228.5409	3235.0262

Zero-point correction (Hartree): 0.095860

TS.nitrophenol_trans.nitrophenoxy+H

E(G3SX(MP3)) excl. ZPE (Hartree): -511.65361140
E(G3SX) excl. ZPE (Hartree): -511.66217031
E(G3X(MP2)) excl. ZPE (Hartree): -511.19490357
E(G3X(MP3)) excl. ZPE (Hartree): -511.61255601
E(G3X) excl. ZPE (Hartree): -511.58520963
E(MP2-Full/G3Xlarge) (Hartree): -511.22254370
E(MP2-Full/G3large) (Hartree): -511.22254370
E(MP2/6-31+G(d)) (Hartree): -510.27607272
E(MP2/6-31G(2df,p)) (Hartree): -510.57069903
E(MP2/6-31G(d)) (Hartree): -510.23557122
E(MP2/G3MP2large) (Hartree): -510.77810391
E(MP3/6-31+G(d)) (Hartree): -510.30393375
E(MP3/6-31G(2df,p)) (Hartree): -510.60855641
E(MP3/6-31G(d)) (Hartree): -510.26714969
E(MP4/6-31+G(d)) (Hartree): -510.40064888
E(MP4/6-31G(2df,p)) (Hartree): -510.71342938
E(MP4/6-31G(d)) (Hartree): -510.35773221
E(PMP2/6-31+G(d)) (Hartree): -510.31997397
E(PMP2/6-31G(2df,p)) (Hartree): -510.61702072
E(PMP2/6-31G(d)) (Hartree): -510.28176090
E(PMP2/G3MP2large) (Hartree): -510.82223642
E(PMP2/G3Xlarge) (Hartree): -511.26672509
E(PMP2/G3large) (Hartree): -511.26672509
E(PMP3/6-31+G(d)) (Hartree): -510.34139949
E(PMP3/6-31G(2df,p)) (Hartree): -510.64819970
E(PMP3/6-31G(d)) (Hartree): -510.30679357
E(PUHF/6-31+G(d)) (Hartree): -508.93571672
E(PUHF/6-31G(2df,p)) (Hartree): -508.97200908
E(PUHF/6-31G(d)) (Hartree): -508.92127464
E(PUHF/G3MP2large) (Hartree): -509.09430173
E(PUHF/G3Xlarge) (Hartree): -509.09578486
E(PUHF/G3large) (Hartree): -509.09578486
E(QCISD(T)/6-31G(d)) (Hartree): -510.39951162
E(QCISD/6-31G(d)) (Hartree): -510.33743287
E(UHF/6-31+G(d)) (Hartree): -508.88838885
E(UHF/6-31G(2df,p)) (Hartree): -508.92215853
E(UHF/6-31G(d)) (Hartree): -508.87158727
E(UHF/G3MP2large) (Hartree): -509.04672804
E(UHF/G3Xlarge) (Hartree): -509.04815730
E(UHF/G3large) (Hartree): -509.04815730
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.77727602

Electronic state : 3-A

Cartesian coordinates (Angs):

C	2.524501	-0.358577	-0.123715
C	1.748577	-1.531282	-0.006314
C	0.335036	-1.466777	0.047834
C	-0.280622	-0.264039	-0.003892
C	0.475431	0.992853	-0.012588
C	1.929137	0.862669	-0.160944
H	3.600176	-0.441373	-0.189235
H	2.231450	-2.496728	0.018075
H	-0.261820	-2.365897	0.103809
H	2.492691	1.777864	-0.268169
O	-0.026993	2.077900	0.339205

N	-1.745278	-0.228574	-0.065669	
O	-2.246652	0.705004	-0.643038	
O	-2.342866	-1.159192	0.433576	
H	0.694178	2.727374	1.314981	
Rotational constants (GHz):			2.3723600	1.2259300 0.8457500
Vibrational harmonic frequencies (cm-1):				
i2066.0506		57.3426		103.4079
194.7930		214.8950		319.2365
355.5165		391.3854		433.9245
474.6870		541.3150		562.8917
600.1649		656.9959		690.1210
780.1947		813.0797		836.7953
883.4563		893.1041		979.5000
1007.7127		1016.0846		1087.9776
1119.5228		1150.8609		1254.3978
1343.8128		1396.7017		1414.7975
1439.7370		1564.6146		1606.8962
1631.6180		1688.5158		3217.1743
3228.5334		3235.9090		3240.7291
Zero-point correction (Hartree):			0.096659	

TS.acinitrophenol_transcis.oxime+O3P

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E(G3SX(MP3)) excl. ZPE (Hartree): -511.67061175
E(G3SX) excl. ZPE (Hartree): -511.67971154
E(G3X(MP2)) excl. ZPE (Hartree): -511.21741350
E(G3X(MP3)) excl. ZPE (Hartree): -511.63559179
E(G3X) excl. ZPE (Hartree): -511.60740188
E(MP2-Full/G3Xlarge) (Hartree): -511.24096395
E(MP2-Full/G3large) (Hartree): -511.24096395
E(MP2/6-31+G(d)) (Hartree): -510.30082354
E(MP2/6-31G(2df,p)) (Hartree): -510.59509495
E(MP2/6-31G(d)) (Hartree): -510.26574126
E(MP2/G3MP2large) (Hartree): -510.79728215
E(MP3/6-31+G(d)) (Hartree): -510.35418600
E(MP3/6-31G(2df,p)) (Hartree): -510.65856750
E(MP3/6-31G(d)) (Hartree): -510.32178963
E(MP4/6-31+G(d)) (Hartree): -510.43553888
E(MP4/6-31G(2df,p)) (Hartree): -510.74740133
E(MP4/6-31G(d)) (Hartree): -510.39760898
E(PMP2/6-31+G(d)) (Hartree): -510.35362538
E(PMP2/6-31G(2df,p)) (Hartree): -510.64949801
E(PMP2/6-31G(d)) (Hartree): -510.31940075
E(PMP2/G3MP2large) (Hartree): -510.85072073
E(PMP2/G3Xlarge) (Hartree): -511.29451213
E(PMP2/G3large) (Hartree): -511.29451213
E(PMP3/6-31+G(d)) (Hartree): -510.40148552
E(PMP3/6-31G(2df,p)) (Hartree): -510.70730658
E(PMP3/6-31G(d)) (Hartree): -510.36995588
E(PUHF/6-31+G(d)) (Hartree): -509.04819652
E(PUHF/6-31G(2df,p)) (Hartree): -509.08240518
E(PUHF/6-31G(d)) (Hartree): -509.03510267
E(PUHF/G3MP2large) (Hartree): -509.20331186
E(PUHF/G3Xlarge) (Hartree): -509.20472006
E(PUHF/G3large) (Hartree): -509.20472006
E(QCISD(T)/6-31G(d)) (Hartree): -510.43315192
E(QCISD/6-31G(d)) (Hartree): -510.37994955
E(UHF/6-31+G(d)) (Hartree): -508.99215532
E(UHF/6-31G(2df,p)) (Hartree): -509.02469777
E(UHF/6-31G(d)) (Hartree): -508.97819607
E(UHF/G3MP2large) (Hartree): -509.14658675
E(UHF/G3Xlarge) (Hartree): -509.14787744
E(UHF/G3large) (Hartree): -509.14787744
E(UM062X/Aug-CC-pVTZ) (Hartree): -511.80599367
Electronic state : 3-A
Cartesian coordinates (Angs):
C      2.518997      -0.310010      0.211846
C      1.719434      -1.513410      0.193950
C      0.380932      -1.471115      0.005489
C      -0.263537      -0.211928      -0.193606
C      0.532275      1.054753      -0.224758

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C	1.969912	0.901612	0.026919
H	3.583802	-0.403922	0.379297
H	2.211301	-2.464331	0.344495
H	-0.216754	-2.369339	-0.000194
H	2.551127	1.812827	0.034421
O	0.027395	2.132539	-0.460180
H	-3.148028	-0.978559	-0.534963
N	-1.560496	-0.060545	-0.387137
O	-2.235288	-1.236124	-0.360728
O	-2.192864	0.869551	1.116890
Rotational constants (GHz):	2.1621300	1.2046200	0.8520900
Vibrational harmonic frequencies (cm-1):			
i566.5685	59.9516		98.2084
147.1181	215.6571		250.7994
333.7330	370.1620		408.8614
458.7416	488.3316		530.7389
564.9890	585.9876		756.7936
778.1425	794.6034		862.9783
885.9052	1000.9342		1005.9742
1023.0407	1063.0935		1155.9455
1172.2384	1212.8920		1243.3214
1374.3097	1413.5556		1433.5703
1465.3496	1584.6901		1687.0903
1738.1589	3202.2323		3217.9245
3232.0199	3249.4995		3836.9261
Zero-point correction (Hartree):	0.102300		