

Supporting Information

***Operando FT-IR spectroscopy as a useful tool for elucidating the fate of
phthalimide-N-oxyl catalytically active species***

Irina R. Subbotina^{1*}, Elena R. Lopat'eva¹, Igor B. Krylov^{1*} and Alexander O. Terent'ev¹

¹ N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 47 Leninsky Prospekt,
Moscow 119991, Russia.

E-mail: subbot@ioc.ac.ru, krylovigor@yandex.ru

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1. FTIR spectra of NHPI in acetonitrile solution

Figure S1 shows the IR spectrum of the NHPI solution in acetonitrile in the range of 700–2500 cm^{-1} . The assignment of the observed absorption bands based on the literature data^{1,2} is presented in Table S1.

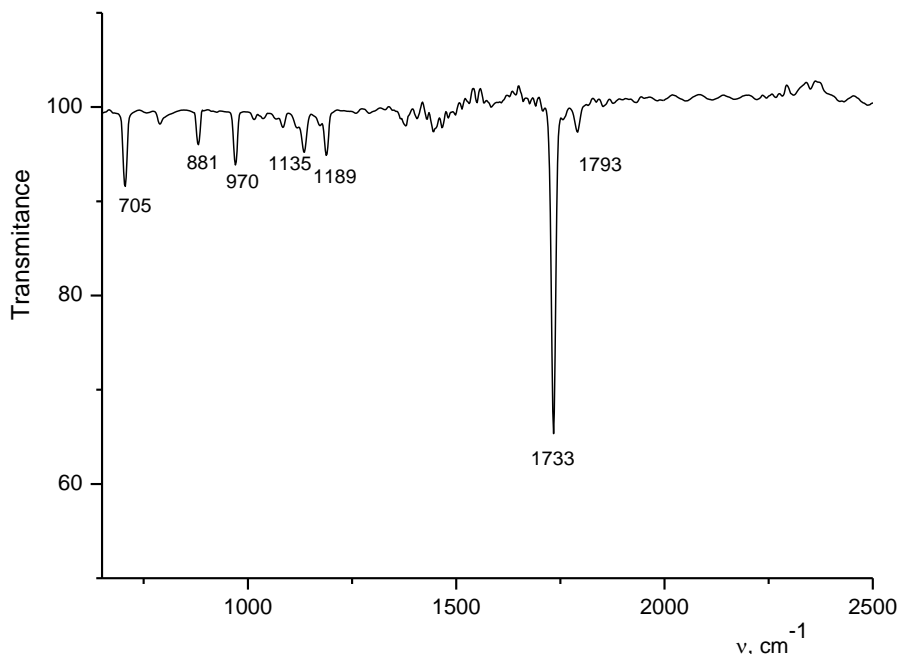


Fig. S1. IR spectra of NHPI in acetonitrile solution

As can be seen from the Fig. S1, the most intense absorption band in the area in question is 1733 cm^{-1} . This absorption band along with less intense peak at 1791 cm^{-1} is assigned to asymmetric and symmetric C=O stretching vibration in the NHPI carbonyl group, respectively.³ Typically, C=O vibrations exhibit strong intensities in IR spectra due to their significant dipole moments and are easily detectable. Additionally, minor noise observed in the spectrum around 1600 and 3700 cm^{-1} may be linked to residual water traces in the solvent.

Table S1. The assignment of the absorption bands of N-hydroxyphthalimide.

ν , cm^{-1}	Assignment
1793	ν (C=O) symmetric
1733	ν (C=O) asymmetric
1189	δ (C–H) , ν (C–C)
1135	δ -ring (in cyclic imide ring)
970	def(C–H)
881	Ring breathing δ (N–OH)
705	δ (O–H) out of plane bending

2. FTIR spectra of individual substances in the region of C=O band.

In Fig. S2, IR spectra of individual substances are presented: NHPI, PIDA, synthesized «trimer», phthalic anhydride, phthalic acid, and acetic acid in the region of C=O vibrations, 1600–1800 cm^{-1} . Iodobenzene have no signals in this region. The frequencies of the most intense band of C=O vibrations in the «trimer» and in PIDA are 1749 cm^{-1} and 1650 cm^{-1} , respectively.

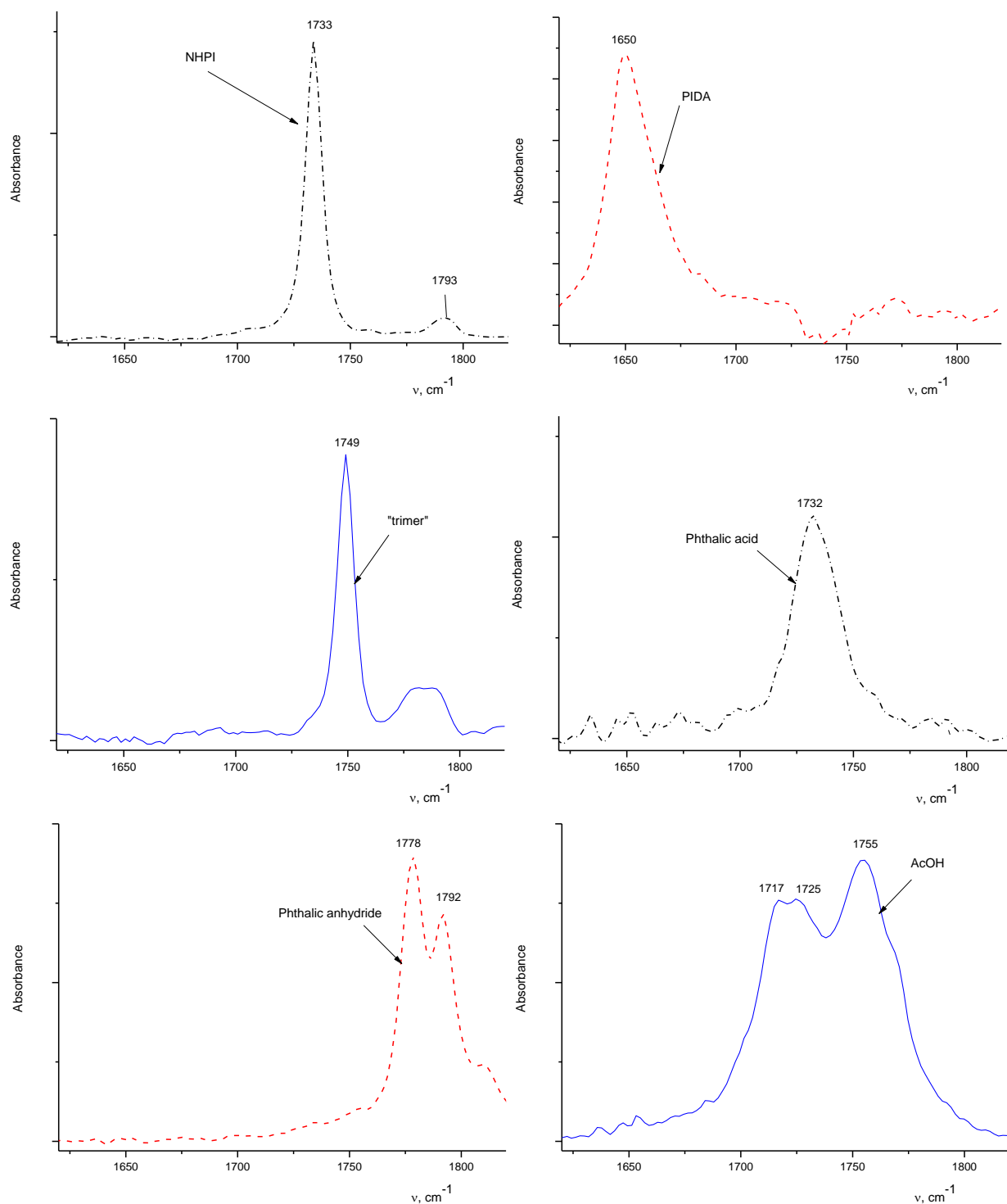


Fig. S2. IR spectra of NHPI, PIDA, «trimer», phthalic anhydride, phthalic acid and AcOH in the region of C=O band.

3. FTIR spectra of individual substances in the 1100–1350 cm^{-1} region.

In Fig. S3, IR spectra of individual substances in the range of 1100–1350 cm^{-1} are shown, characteristic of the C–O bond in $-(\text{C}=\text{O})-\text{O}-$ groups. Iodobenzene have no signals in this region.

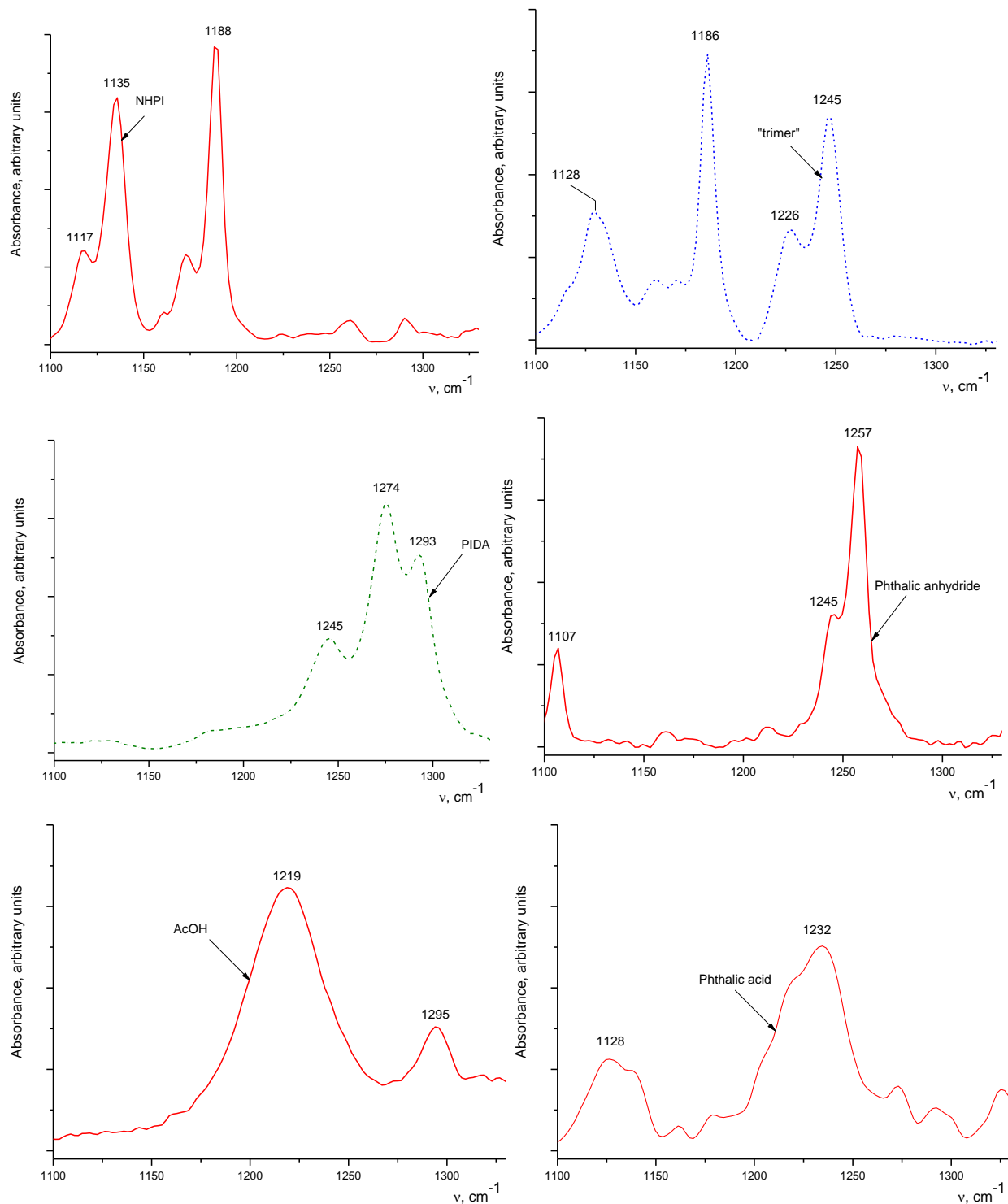


Fig. S3. IR spectra of NHPI, PIDA, "trimer", phthalic anhydride, phthalic acid and AcOH in the region of 1100–1350 cm^{-1} .

For the NHPI in this range two absorption bands are observed with maxima at 1135 and 1188 cm^{-1} . For the “trimer”, two bands of close frequency with maxima at 1128 and 1186 cm^{-1} are also observed, as well as two bands in the region above 1200 cm^{-1} – 1226 and 1245 cm^{-1} . The latter two bands are apparently associated with C–O vibrations in the O–(C=O) group in the “trimer”. For the PIDA the absorption bands at 1245, 1275 and 1293 cm^{-1} appear higher in frequency than for NHPI and the “trimer”, and, apparently, correspond to the bending vibration of the benzene ring and symmetric and antisymmetric C–O stretching vibrations in the carboxyl group.

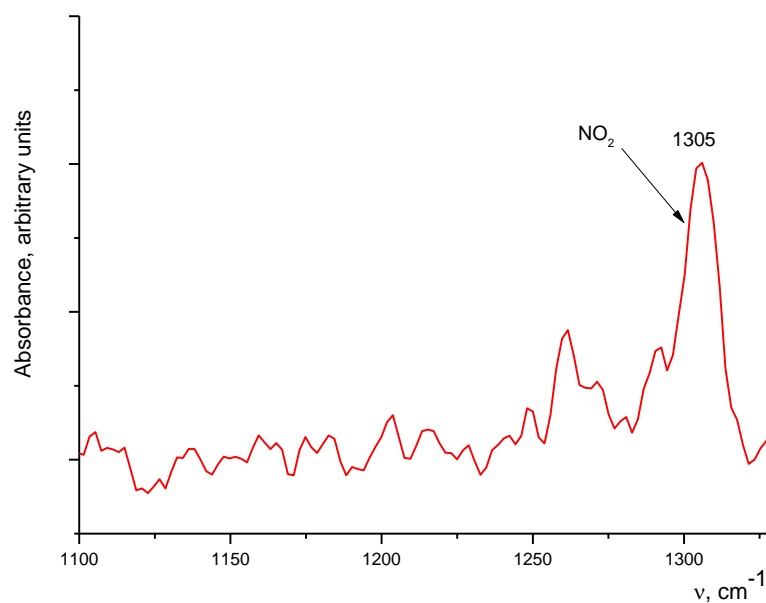


Fig. S4. IR spectrum of NO₂ in the region of 1100–1350 cm^{-1} .

4. The photographs of the reaction mixture

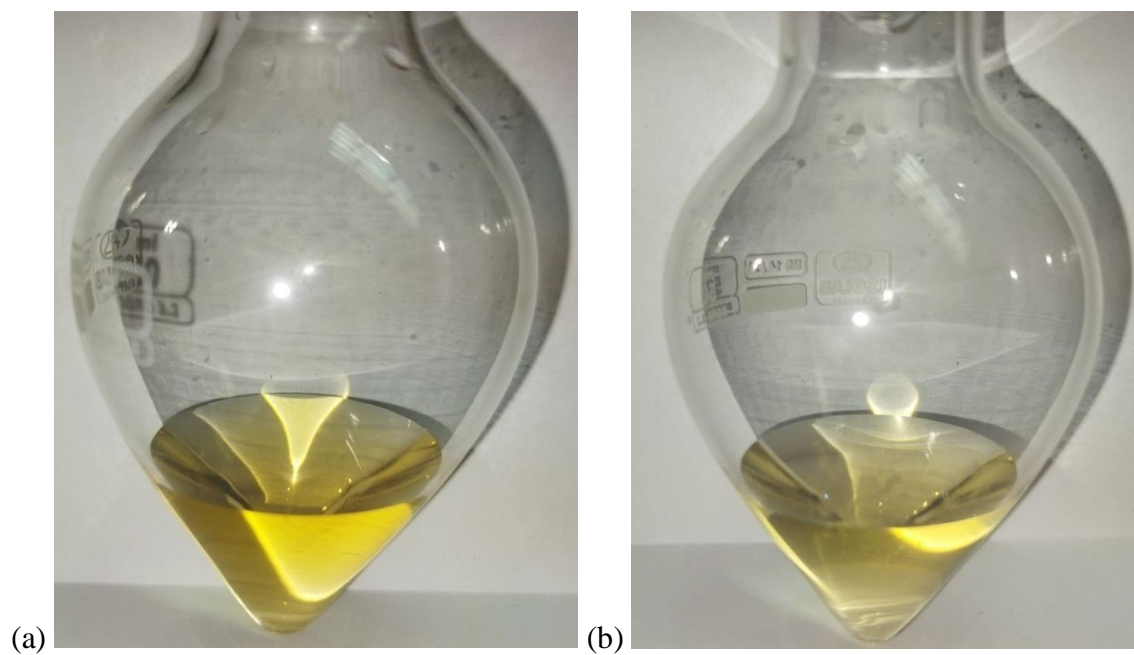


Fig. S5. Photographs of the reaction mixture (a) immediately after PINO decomposition (detected by EPR) and (b) day after PINO decomposition

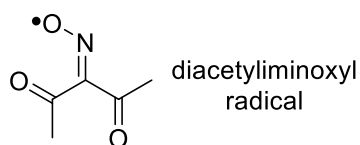
5. DFT calculations

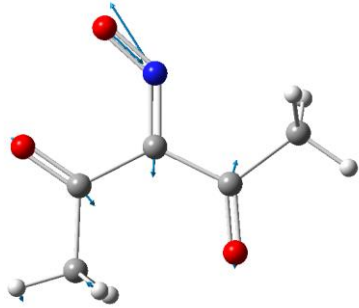
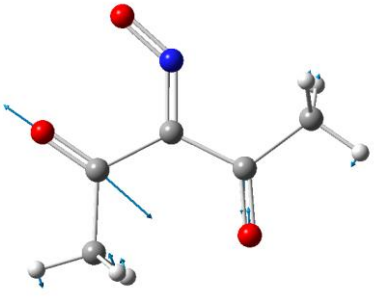
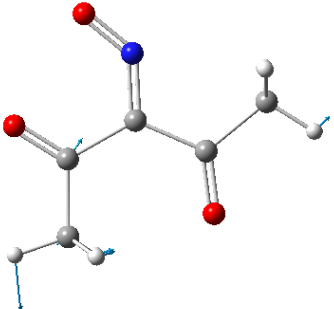
DFT calculations were performed in order to assign observed IR bands to PINO and NHPI vibration modes.

DFT calculations were performed in Gaussian 16 program package,⁴ results were visualized by GaussView6 program. B3LYP functional modified with D3 version of Grimme's dispersion with Becke-Johnson damping (keyword "EmpiricalDispersion=GD3BJ")⁵ and 6-311++g(d,p) basis set were used for geometry optimizations and anharmonic vibrational analysis (keyword "freq=anharmonic"). No scaling factor were applied and default Gaussian 16 settings were used unless otherwise noted. CPCM model (keyword "scrf=(cpcm,solvent=acetonitrile)")^{6,7} was used for modeling of MeCN solvent medium. Calculations were performed for temperature 298.150 K and 1 atm. pressure.

In order to check the performance of the chosen method, we first calculated unharmonic frequencies for the diacetyliminoxyl, an N-oxyl radical, for which experimental FT-IR data was reported previously. The problem of assignment of IR spectral lines for PINO radical arises from the fact that due to its limited stability, PINO cannot be isolated from oxidant and other components of the reaction mixture, in which PINO was generated. In contrast to PINO, diacetyliminoxyl was previously isolated from oxidant and IR spectrum of individual diacetyliminoxyl in CH₂Cl₂ is available.⁸ The computational procedure described above (except for changing "scrf=(cpcm,solvent=acetonitrile)" to "scrf=(cpcm,solvent=dichloromethane)") was applied to the prediction of anharmonic frequencies of diacetyliminoxyl (Table S2) and the corresponding parent NOH compound (Table S3). In summary, anharmonic frequency analysis provides significantly improved accuracy over unscaled harmonic frequency calculations, whereas scaling harmonic frequencies by a factor of 0.9679 (recommended for B3LYP functional for basis sets from 6-311G(d,p) to 6-311++G(3df,3pd)⁹) for the majority of bands in middle IR region gives frequency values very close to those predicted by anharmonic frequency analysis.

Table S2. Assignment of the most intensive IR bands in the FT-IR spectrum of diacetyliminoxyl radical in CH₂Cl₂,⁸ which do not overlap with CH₂Cl₂ solvent bands.^a

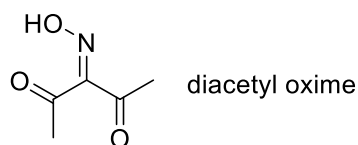


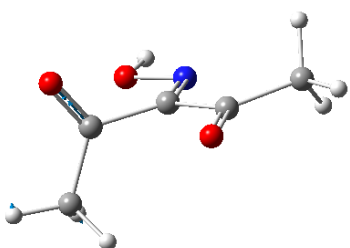
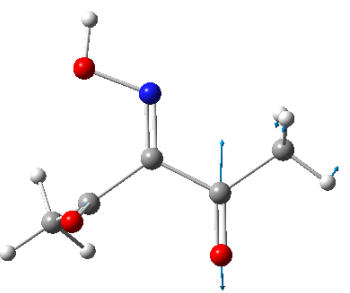
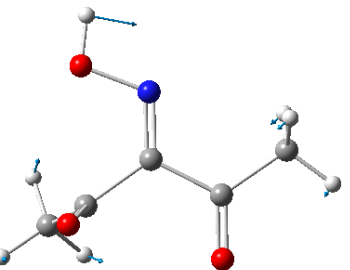
Experimental ⁸ IR freq., cm ⁻¹	Predicted harmonic IR freq., cm ⁻¹ , scaled by factor 0.9679⁹	Predicted anharmonic IR freq., cm ⁻¹ (predicted intensity, km/mol)	Displacement vectors/Assignment
1556 vs	1592 1541	1543 (494)	 v _{as} (C=N-O•)
1699 s	1725 1670	1695 (256)	 v(C=O)
1166 m	1188 1150	1152 (73)	
1685 sh	534, 1188	1671 (58)	Combined band

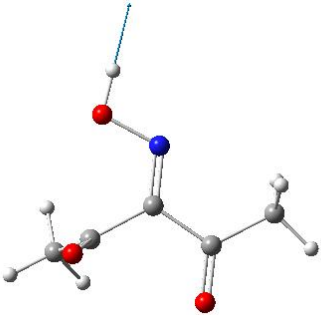
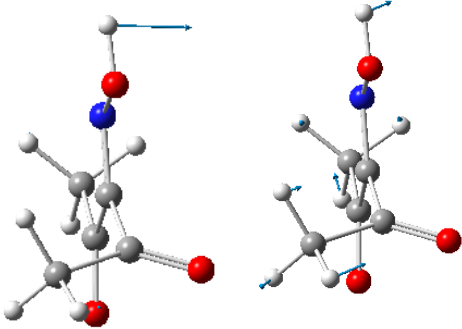
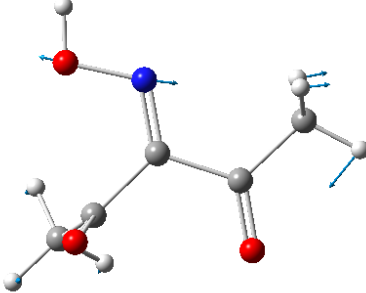
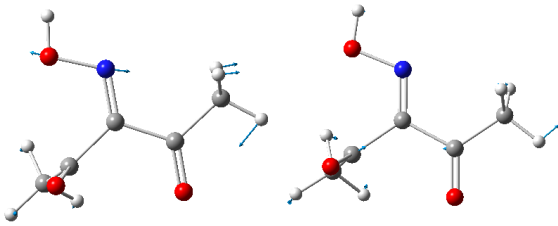
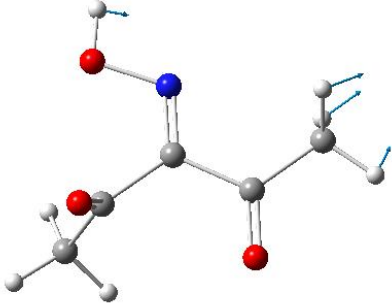
1362 m	1384 1339	1340 (58)	
613	621 601	614 (52)	

^a Lines are sorted according to predicted band intensity (given in parenthesis in column 3). Used abbreviations: vs – very strong, s – strong, sh – shoulder, m – medium, v - stretching

Table S3. Assignment of the most intensive IR bands in the FT-IR spectrum of diacetyl oxime in CH₂Cl₂,⁸ which do not overlap with CH₂Cl₂ solvent bands.^a



Experimental ⁸ IR freq., cm ⁻¹	Predicted harmonic IR freq., cm ⁻¹ (scaled by factor 0.9679) ⁹	Predicted anharmonic IR freq., cm ⁻¹ (predicted intensity, km/mol)	Displacement vectors/Assignment
1724 vs	1771 1714	1737.5 (204)	 v(C=O)
1690 vs	1726 1671	1691 (175)	 v(C=O)
1365 s	1379 1334	1340 (160)	

3526 s	3794 3672	3615 (151)	 <p>v(O-H)</p>
966 m	453, 538	938 (58)	<p>Combined band</p> 
976 m	994 963	961 (50)	
1700 sh	538, 1215	1694 (50)	<p>Combined band</p> 
1355 sh	1392 1347	1353 (26)	

^a Lines are sorted according to predicted band intensity (given in parenthesis in column 3). Used abbreviations: vs – very strong, s – strong, sh – shoulder, m – medium, v - stretching

According to results presented in Tables S2-S3, the mean error in IR frequency prediction was less than 15 cm^{-1} . Therefore, the same method was applied for prediction of IR spectra of PINO (Fig. S6, Table S4) and NHPI (Fig. S7, Table S5) in MeCN based on anharmonic vibrational analysis.

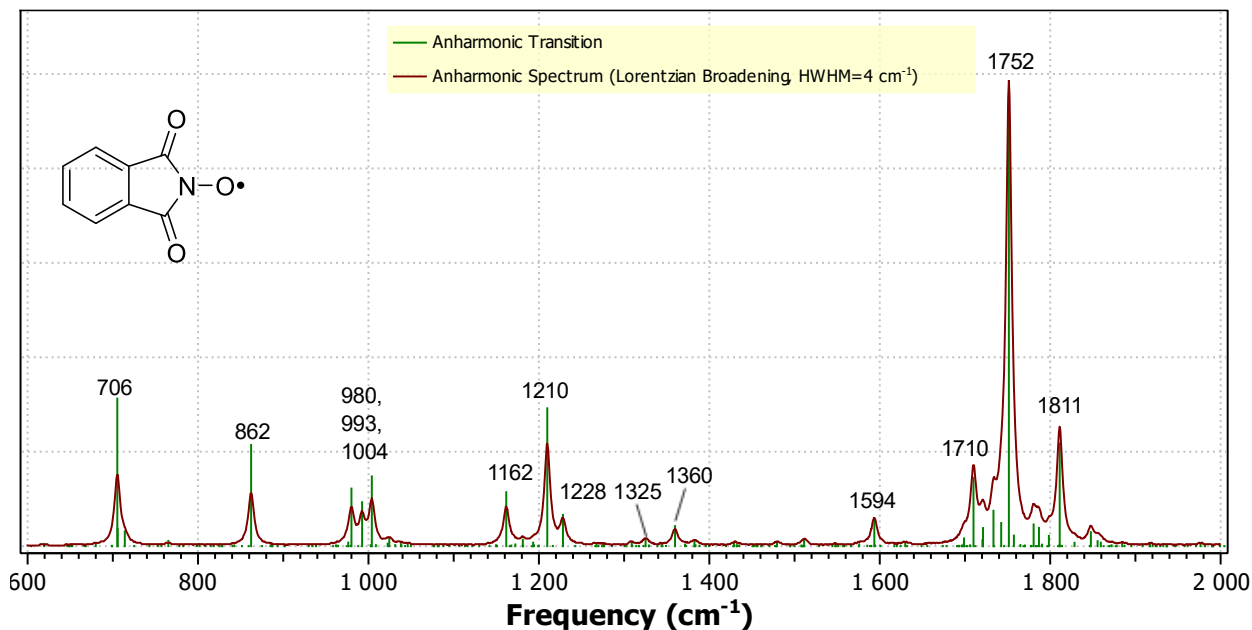


Fig. S6. Predicted PINO IR-spectrum

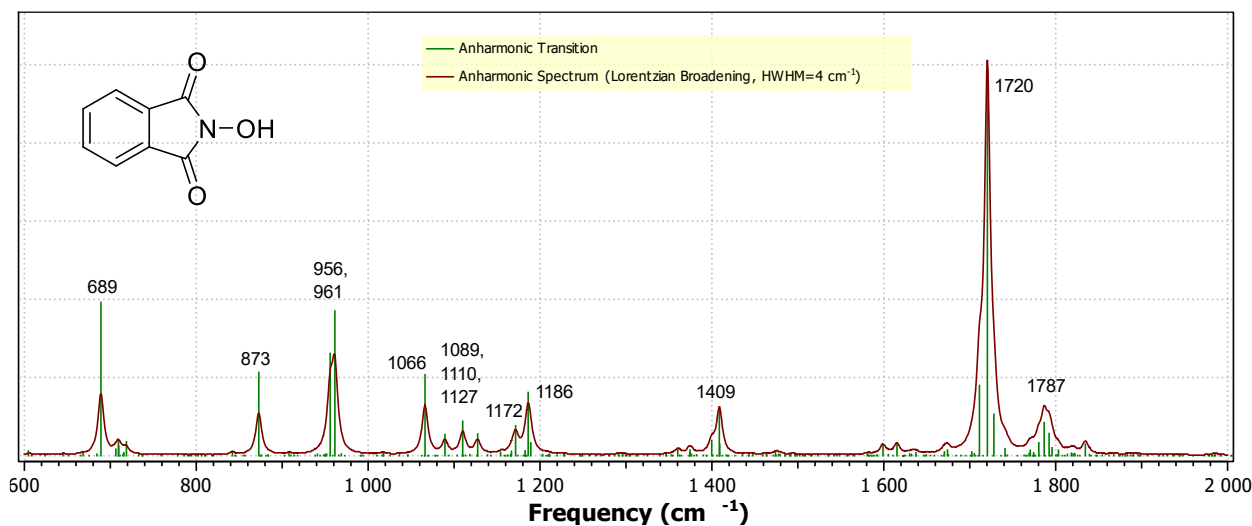
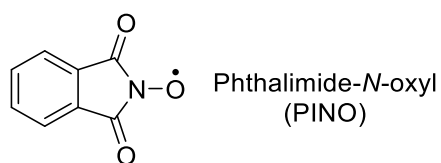
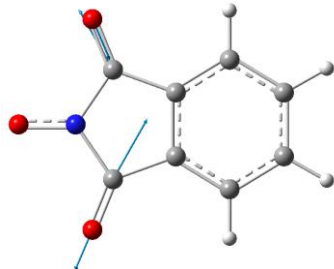
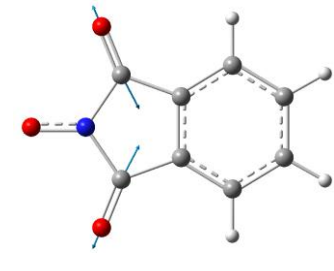
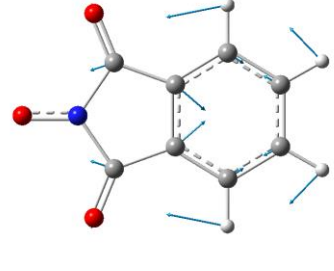
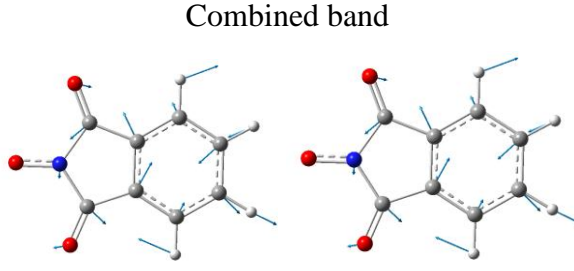
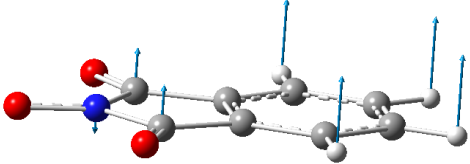
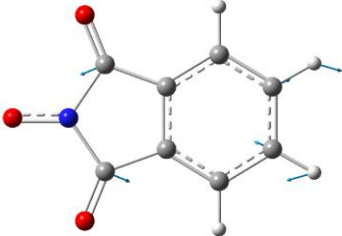
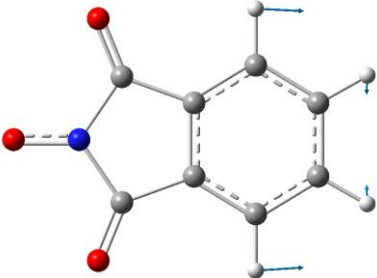
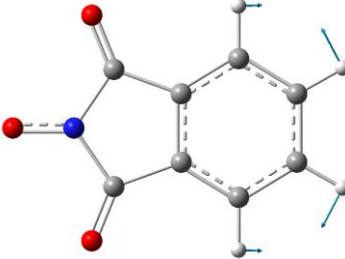
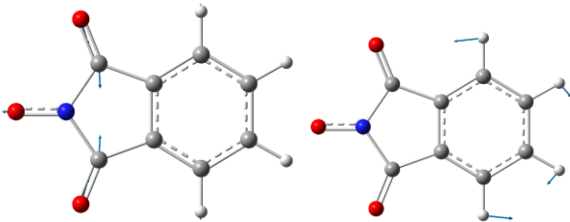
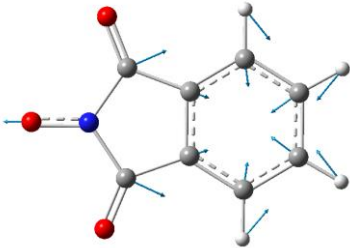


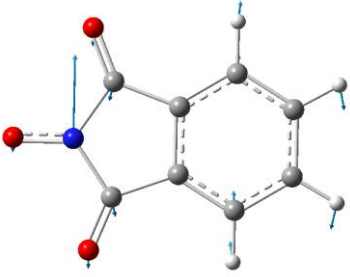
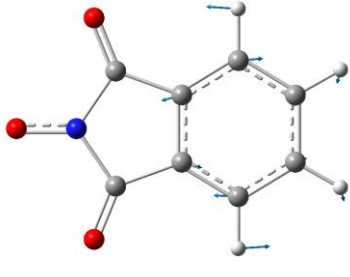
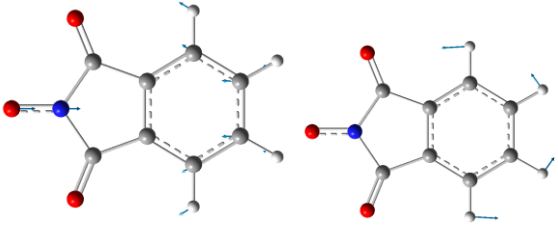
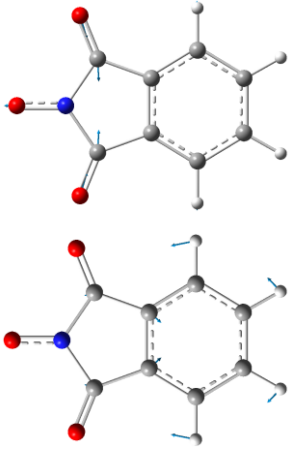
Fig. S7. Predicted NHPI IR-spectrum

Table S4. Assignment of the most intensive IR bands in the FT-IR spectrum of PINO in MeCN.^a



Experimental IR freq., cm ⁻¹	Predicted harmonic IR freq., cm ⁻¹ (scaled by factor 0.9679) ⁹	Predicted anharmonic IR freq., cm ⁻¹ (predicted intensity, km/mol)	Displacement vectors/Assignment
1749	1782 1724	1752 (696)	
Overlap	1840 1781	1811 (173)	
1214	1240 1200	1210 (155)	
1718	722, 1047	1710 (108)	Combined band 

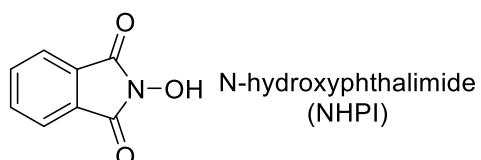
Overlap	708 685	705 (97)	
Overlap	879 850.5	862 (81)	
Overlap	1047 1014	1004 (65)	
Overlap	1184 1146	1162 (58)	
Overlap	583, 1201	1733 (57)	Combined band 
985	1009 976	980 (55)	

	1018 985	993 (40)	
Overlap	1633 1580	1594 (40)	
Overlap	482, 1315	1742 (38)	Combined band 
Overlap	583, 1240	1780 (36)	Combined band 
1233	519, 722	1228 (36)	Combined band

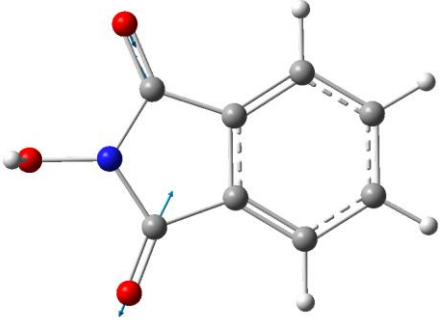
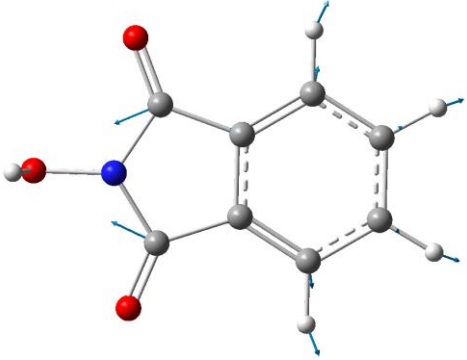
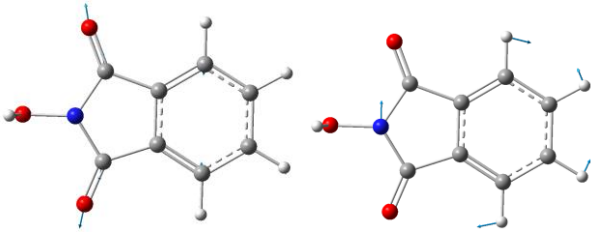
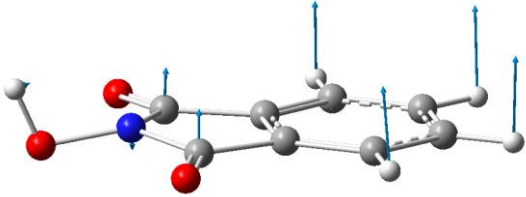
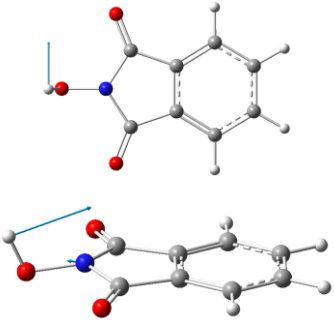
1324 weak	446, 754	1325 (10)	<p>Combined band</p>

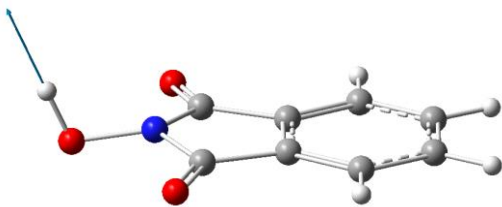
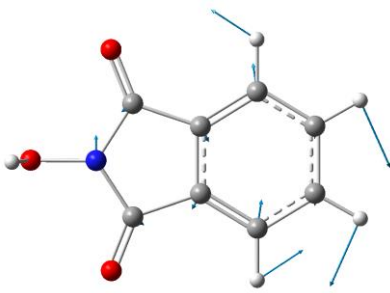
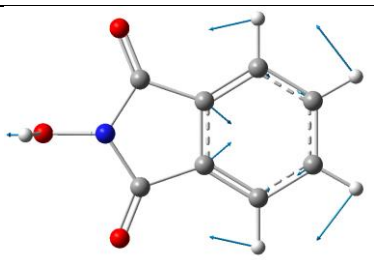
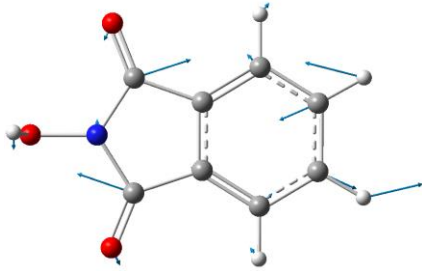
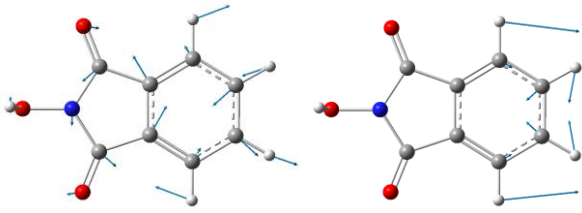
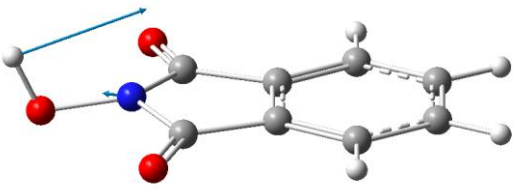
^a Lines are sorted according to predicted band intensity (given in parenthesis in column 3).

Table S5. Assignment of the most intensive IR bands in the FT-IR spectrum of NHPI in MeCN.^a



Experimental IR freq., cm ⁻¹	Predicted harmonic IR freq., cm ⁻¹ (scaled by factor 0.9679) ⁹	Predicted anharmonic IR freq., cm ⁻¹ (predicted intensity, km/mol)	Displacement vectors/Assignment

1733vs	1751 (1695)	1721 (694)	
970? m	979 (947)	961 (149)	
Overlap	610, 1136	1711 (128)	Combined band 
705 m	712 (689)	689 (113)	
970? m	282, 1459	956 (104)	Combined band 

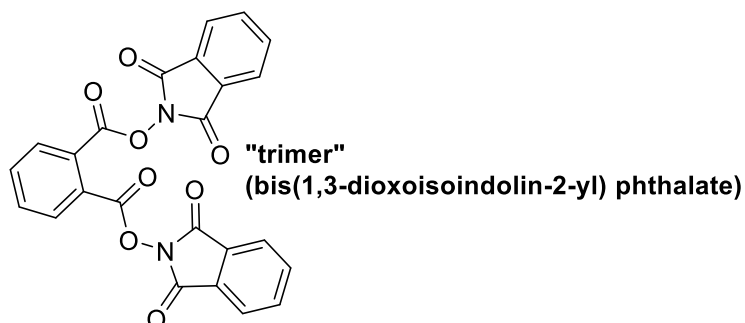
	3737 (3617)	3501 (97)	
1135? m	1090 (1055)	1066 (92)	
1189? m	1210 (1171)	1186 (80)	
881 m	887 (859)	873 (78)	
Overlap	718, 1038	1728 (76)	Combined band 
Overlap	1459 (1412)	1409 (69)	

Overlap	1819 (1760)	1787 (63)	
Overlap	610, 1210	1792 (42)	<p>Combined band</p>
1135? m	1136 (1100)	1110 (41)	
1189? m	1179 (1141)	1172 (37)	

^a Lines are sorted according to predicted band intensity (given in parenthesis in column 3). Used abbreviations: vs – very strong, s – strong, m – medium.

For “trimer” (bis(1,3-dioxoisindolin-2-yl) phthalate) anharmonic vibrational analysis was not performed due to its high computational cost. Predicted harmonic vibrations are given below in Table S6.

Table S6. Assignment of the most intensive IR bands in the FT-IR spectrum of “trimer” in MeCN.^a



Experimental IR freq., cm^{-1}	Predicted harmonic IR freq., cm^{-1} (scaled by factor 0.9679) ⁹	Predicted intensity	Displacement vectors/Assignment
1749	1760 (1703) $\nu(\text{C}=\text{O})$	2839	

1775-1785	1798 (1740) $\nu(\text{C}=\text{O})$	1148	
998	1044 (1011)	563	

^a Lines are sorted according to predicted band intensity (given in column 3).

Xyz coordinates of optimized structures on B3LYP-D3BJ/6-311++g(d,p)/CPCM(MeCN or CH₂Cl₂) level of theory are given below:

Diacetyliminoxyl radical (in CH₂Cl₂)

Charge = 0

Spin multiplicity = 2

Electronic Energy (EE) = -474.649575

EE + Thermal Enthalpy Correction = -474.532045

EE + Thermal Free Energy Correction = -474.578978

C -1.30203700 -1.99941500 -0.00002500

C -1.28295000 -0.49584800 -0.00000200

H -2.33858000 -2.33173100 -0.00008600

H -0.77366300 -2.38261100 -0.87456500
H -0.77376200 -2.38262900 0.87456800
C 0.04476400 0.22295500 0.00002000
C 1.39961300 -0.39734000 0.00003500
C 2.58701700 0.53466300 0.00002900
H 2.56565200 1.18154000 -0.88039600
H 3.49925900 -0.05877300 -0.00002900
H 2.56571300 1.18145200 0.88052100
N 0.00745800 1.52589700 0.00002500
O -0.91045200 2.30772800 0.00001900
O -2.30216800 0.16612900 -0.00007300
O 1.52821200 -1.60868500 -0.00001200

Diacetyl oxime (in CH₂Cl₂)

Charge = 0

Spin multiplicity = 1

Electronic Energy (EE) = -475.280150

EE + Thermal Enthalpy Correction = -475.150292

EE + Thermal Free Energy Correction = -475.198327

N 0.06882700 1.53835600 -0.02681200
C 0.10392300 0.26262700 0.04138800
C -1.12974000 -0.61916400 0.19692800
C 1.43823700 -0.41314900 -0.02930400
O -1.46058200 -0.97438300 1.30632000
O 1.46219500 -1.63149500 -0.05240300
O -1.22182300 2.03251200 0.02459900
H -1.11334600 2.98986300 -0.04961000
C -1.84225000 -0.98881500 -1.06702800
H -2.72265100 -1.59107800 -0.84670100
H -2.12638200 -0.07932800 -1.60415700
H -1.15703900 -1.54603300 -1.71353400
C 2.67557300 0.43796900 -0.07293600
H 2.63175500 1.12963700 -0.91688500
H 2.74333500 1.04358000 0.83418100
H 3.54975300 -0.20502000 -0.15802300

Phthalimide-N-oxyl radical (PINO) (in MeCN)

Charge = 0

Spin multiplicity = 2

Electronic Energy (EE) = -587.828296

EE + Thermal Enthalpy Correction = -587.711851

EE + Thermal Free Energy Correction = -587.756420

O -3.01428600 0.00002400 0.00007700

N -1.75651700 -0.00001900 0.00043400

C -0.93378900 1.20257400 0.00053800

C -0.93376100 -1.20263500 -0.00065000

C 0.45112200 0.70222400 -0.00095000

O -1.38870200 2.31357900 0.00014900

C 0.45112900 -0.70219900 -0.00100300

O -1.38857900 -2.31365800 0.00039700

C 1.63586400 1.42219400 -0.00036500

C 1.63588400 -1.42214800 -0.00007100

C 2.83133700 0.69991800 0.00035100

H 1.63134200 2.50437000 -0.00030900

C 2.83134200 -0.69985200 0.00052800

H 1.63140100 -2.50432400 -0.00005600

H 3.77531200 1.23020200 0.00091800

H 3.77532000 -1.23013300 0.00115900

N-hydroxyphthalimide (NHPI) (in MeCN)

Charge = 0

Spin multiplicity = 1

Electronic Energy (EE) = -588.464868

EE + Thermal Enthalpy Correction = -588.335741

EE + Thermal Free Energy Correction = -588.380490

N -1.67038100 0.00000100 0.09598000

C -0.90517500 1.17825000 0.00936400

C -0.90517500 -1.17825100 0.00939600

C 0.50343600 0.69934600 0.00445400

O -1.35279400 2.29893200 -0.04343400

C 0.50343600 -0.69934700 0.00445500
O -1.35279600 -2.29893100 -0.04343200
C 1.68353400 1.42142200 0.00380600
C 1.68353400 -1.42142300 0.00380000
C 2.88251400 0.69838000 -0.00111300
H 1.67931600 2.50391000 0.00511300
C 2.88251400 -0.69838100 -0.00111600
H 1.67931600 -2.50391000 0.00511100
H 3.82593200 1.23004200 -0.00543400
H 3.82593200 -1.23004200 -0.00543700
O -3.02600200 -0.00000100 -0.11694900
H -3.43680200 0.00000900 0.76103700

“trimer”, bis(1,3-dioxoisindolin-2-yl) phthalate (in MeCN)

Charge = 0

Spin multiplicity = 1

Electronic Energy (EE) = -1633.613672

EE + Thermal Enthalpy Correction = -1633.267850

EE + Thermal Free Energy Correction = -1633.356352

0 1

O -1.27403800 1.34017600 -0.21798800
O -0.37347600 -3.62753300 1.56748500
O -1.27410000 -1.34019600 0.21794900
O -2.03671700 -1.92938800 -1.84311600
O -0.37346000 3.62764400 -1.56735300
O -2.03654200 1.92933300 1.84312900
O 0.82456000 0.43779000 1.52160900
O 0.82441900 -0.43796400 -1.52181100
N -0.10774100 -2.00446600 -0.07365700
N -0.10764400 2.00439200 0.07359400
C 1.72848000 -3.28747100 0.34989600
C 2.08995700 -2.31705000 -0.59085000
C 0.31252600 -3.06968500 0.74715100
C 1.72853900 3.28748000 -0.34986300
C -2.19748100 -1.33638000 -0.81594200

C -3.40719500 -0.57462800 -0.40869900
C 2.09005100 2.31697500 0.59078200
C -2.19737700 1.33636300 0.81594500
C -3.40714800 0.57469000 0.40872700
C 0.92788200 1.42697600 0.83995500
C 0.92776400 -1.42710200 -0.84009200
C 0.31258400 3.06969800 -0.74711900
C 3.36117800 2.27528300 1.13527100
C 4.27777400 3.24228700 0.70578100
C 3.91685000 4.21205900 -0.23260900
C 2.62700800 4.24935800 -0.77588000
H 3.63585800 1.52143500 1.86189400
H 5.28394000 3.23821700 1.10611600
H 4.64822100 4.94655600 -0.54607400
H 2.34425200 4.99939900 -1.50331000
C -4.62399800 1.12133700 0.82161100
C -5.82988800 0.55850900 0.41509700
C -5.82993500 -0.55829500 -0.41500300
C -4.62409000 -1.12119900 -0.82154900
H -4.61474200 2.00703200 1.44311200
H -6.76416100 0.99859600 0.74007100
H -6.76424400 -0.99832300 -0.73995200
H -4.61490700 -2.00689600 -1.44304900
C 3.36107400 -2.27538400 -1.13536300
C 4.27769900 -3.24232500 -0.70579200
C 3.91681100 -4.21201200 0.23269900
C 2.62697900 -4.24928600 0.77599400
H 3.63572600 -1.52160100 -1.86206400
H 5.28385900 -3.23827100 -1.10614300
H 4.64820300 -4.94646200 0.54622600
H 2.34425100 -4.99926200 1.50350200

6. The summary: assignment of the absorption bands in the region 1100–1350 cm⁻¹

Table S7. The assignment of the absorption bands in Fig.5.

ν , cm ⁻¹	Assignment	Compound
1135	δ -ring (in cyclic imide ring)	NHPI
1189	δ (C–H), ν (C–C)	NHPI, “trimer”
1214	Asymmetric breathing mode of imide and benzene rings in plane	PINO
1219	ν (C–O)	AcOH (in acetonitrile)
1233	Combined band	PINO
1245	ν (C–O)	“trimer”
1259	ν (C–O)	NHPI, Phthalic anhydride
1305	ν (N–O)	HNO ₃ , NO ₂ (in acetonitrile)
1324	ν (N–O)• ^a	PINO

^a Combined band according to DFT

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