SUPPORTING INFORMATION

Impact of benzannulation on ESIPT in 2-(2’-hydroxyphenyl)-oxazoles: a unified perspective in terms of excited-state aromaticity and intramolecular charge transfer

Leandro D. Mena, D. M. A. Vera and María T. Baumgartner

a INFIQC, Departamento de Química Orgánica, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, Ciudad Universitaria, X5000HUA, Córdoba, Argentina.
b QUIAMM-INBIOTEC- Departamento de Química Facultad de Ciencias Exactas y Naturales, Universidad Nacional de Mar del Plata Mar del Plata, Argentina

* Corresponding authors: L. D. M.: lmena@fcq.unc.edu.ar, M. T. B.: tere@fcq.unc.edu.ar

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Contents

1. $^1$H and $^{13}$C NMR spectra of HNO 3
2. MOs involved in $S_0 \rightarrow S_1$ excitation 4
3. Emission energies for HNO (keto) computed with LR-PCM, cLR-PCM and SS-PCM models 5
4. Non-covalent interactions (NCI) analysis 5
5. QTAIM analysis 7
6. Energy levels 8
7. Relevant information about stationary points 9
8. Optimised coordinates for all compounds 10
1. $^1$H and $^{13}$C NMR spectra of HNO

Figure S1. $^1$H (top) and $^{13}$C NMR (bottom) of HNO in CDCl$_3$.
2. **MOs involved in $S_0 \rightarrow S_1$ excitation**

a) **HPO**

![HOMO and LUMO of HPO](image)

**Figure S2.** HOMO (left) and LUMO (right) of HPO in the $S_0$ state.

Excited State 1: Singlet-A 4.0217 eV
308.29 nm $f=0.5103$ $<S^2>=0.000$
42 $\rightarrow$ 43 0.69245

b) **HBO**

![HOMO and LUMO of HBO](image)

**Figure S3.** HOMO (left) and LUMO (right) of HBO in the $S_0$ state.

Excited State 1: Singlet-A 3.7671 eV
329.12 nm $f=0.8517$ $<S^2>=0.000$
55 $\rightarrow$ 56 0.69938

c) **HNO**

![HOMO and LUMO of HNO](image)

**Figure S4.** HOMO (left) and LUMO (right) of HNO in the $S_0$ state.

Excited State 1: Singlet-A 3.4113 eV
363.45 nm $f=0.6372$ $<S^2>=0.000$
68 $\rightarrow$ 69 0.69574
3. Emission energies for HNO (keto) computed with LR-PCM, cLR-PCM and SS-PCM models

|        | B3LYP  | CAM-B3LYP | M06-2X  | PBE0   | ωB97XD | MUE  |
|--------|--------|-----------|---------|--------|--------|------|
| **enol form** |        |           |         |        |        |      |
| LR-PCM | 2.86 (-0.13) | 3.23 (0.24) | 3.25 (0.26) | 3.00 (0.01) | 3.29 (0.30) | 0.19 |
| cLR-PCM | 3.69 (0.70)  | 3.49 (0.50) | 3.50 (0.51) | 3.09 (0.10) | 3.56 (0.57) | 0.48 |
| SS-PCM | 2.03 (-0.96) | 3.19 (0.20) | 3.1 (0.11)  | 2.23 (-0.76) | 3.45 (0.46) | 0.50 |
| **keto form** |        |           |         |        |        |      |
| LR-PCM | 2.57 (0.06)  | 2.88 (0.37) | 2.84 (0.33) | 2.68 (0.17) | 2.89 (0.38) | 0.26 |
| cLR-PCM | 2.65 (0.14)  | 3.07 (0.56) | 3.04 (0.53) | 2.78 (0.27) | 3.09 (0.58) | 0.42 |
| SS-PCM | 2.16 (-0.35) | 3.13 (0.62) | 3.04 (0.53) | 2.61 (-0.11) | 3.11 (0.60) | 0.44 |

Table S2. Emission energies of HNO (in eV) calculated using different functionals with continuum solvation models for cyclohexane. The error with respect to the experimental fluorescence energies are presented in parentheses. MUE: mean unsigned error (in eV).

|        | B3LYP  | CAM-B3LYP | M06-2X  | PBE0   | ωB97XD | MUE  |
|--------|--------|-----------|---------|--------|--------|------|
| **enol form** |        |           |         |        |        |      |
| LR-PCM | 2.96  | 3.43      | 3.44    | 3.12   | 3.49   | -    |
| cLR-PCM | 2.91  | 3.53      | 3.54    | 3.12   | 3.59   | -    |
| SS-PCM | 2.63  | 3.51      | 3.51    | 2.87   | 3.59   | -    |
| **keto form** |        |           |         |        |        |      |
| LR-PCM | 2.49 (-0.02) | 2.92 (0.41) | 2.89 (0.38) | 2.63 (0.12) | 2.95 (0.44) | 0.27 |
| cLR-PCM | 2.47 (-0.04) | 2.99 (0.48) | 2.96 (0.45) | 2.63 (0.12) | 3.02 (0.51) | 0.31 |
| SS-PCM | 2.29 (-0.22) | 2.99 (0.48) | 2.95 (0.44) | 2.51 (-0.00) | 3.03 (0.51) | 0.33 |

4. Non-covalent interactions (NCI) analysis

For the analysis of the OH--π interaction the RDG function has been used

\[
RDG (r) = \frac{1}{2(3\pi^2)^{1/3}} \frac{|\nabla \rho(r)|}{\rho(r)^{4/3}} \tag{1}
\]

where \( \rho(r) \) is the total electron density and the RDG \( (r) \) is the reduced density gradient of the exchange contribution. According to Atoms in Molecules (AIM) theory the nature of a weak interaction depends on both the \( \lambda_2 \) eigenvalue and the electron density:

\[
\Omega (r) = \text{Sign} (\lambda_2(r)) \rho(r) \tag{2}
\]

When \( \lambda_2>0 \) the interaction is bonding, and the opposite if \( \lambda_2<0 \). In Fig. S9-S11 the scatter plots of RDG function vs. \( \Omega(r) \) function are shown for HPO, HBO and HNO in the \( S_0 \) and \( S_1 \) states. It is important to note that the left spike (marked with red circle) shifts to
the left in $S_1$ in the case of HPO and HBO, indicating a strengthening in the OH–π interaction upon excitation, whereas remains almost unaltered in HNO.

a) HPO

![HPO RDG scatter plots](image)

Figure S5 RDG scatter plots (isovalue=0.6) in $S_0$ and $S_1$. The left spike correspond to the attractive OH-π interaction.

b) HBO

![HBO RDG scatter plots](image)

Figure S6 RDG scatter plots (isovalue=0.6) in $S_0$ and $S_1$. The left spike correspond to the attractive OH-π interaction.

c) HNO

![HNO RDG scatter plots](image)

Figure S7 RDG scatter plots (isovalue=0.6) in $S_0$ and $S_1$. The left spike correspond to the attractive OH-π interaction.
5. **QTAIM analysis**

According to the QTAIM approach, a bonding interaction is related to the existence of a path of maximum electron density \( \rho(r) \) (the bond path) connecting the corresponding atomic basins. A *bond critical point* (BCP) is a point along this bond path at the interatomic surface where \( \rho(r) \) reaches a minimum value. In the present case, we analysed the topology of \( \rho(r) \), looking for the presence of a BCP between the hydrogen atom and the N acceptor, and then we calculated \( \rho(r) \), its Laplacian, \( \nabla^2 \rho(r) \) and the potential energy density \( V(r) \) at that BCP. According to the equation proposed by Espinosa et al. [i], the H-bond energy can be estimated from \( V(r) \) as follows:

\[
E_{HB} = \frac{1}{2} V(r)
\]  

(1)

Topological analysis revealed the existence of strong hydrogen bonds in all compounds in both \( S_0 \) and \( S_1 \) states (Table 5 in main text). (Note: A H-bond is defined as “strong” when \( \rho(r) \geq 0.03 \) [ii].) Good correlations were found between the H-N distance and \( \rho(r) \), \( \nabla^2 \rho(r) \), total electron energy density \( H(r) \) and H-bond energy (Fig. S8). According to QTAIM analysis results, the H-bond in HPO results considerably strengthened by 2.05 kcal/mol in \( S_1 \), whereas in HBO the interaction increases its intensity in 1.17 kcal/mol. Unlike these cases, photoexcitation weakens the intramolecular H-bond of HNO by 0.18 kcal/mol, in agreement with the observed in IR calculations and NCI analysis.

**Table S3** Selected parameters related to H-bond for studied the *enol* forms of the studied compounds obtained from QTAIM analysis

| Dye/state | H-N distance (Å) | \( \rho(r) \), a.u. | \( \nabla^2 \rho(r) \), a.u. | H-bond energy\(^a\) | ΔE H-bond \( S_0 \rightarrow S_1 \) |
|-----------|------------------|------------------|------------------|-----------------|-----------------|
| HPO       |                  |                  |                  |                 |                 |
| \( S_0 \) | 1.8093           | 0.0399           | 0.1178           | 10.18           |                 |
| \( S_1 \) | 1.7317           | 0.0471           | 0.1341           | 12.23           | 2.05            |
| HBO       |                  |                  |                  |                 |                 |
| \( S_0 \) | 1.8003           | 0.0407           | 0.1201           | 10.50           |                 |
| \( S_1 \) | 1.7552           | 0.0451           | 0.1292           | 11.64           | 1.17            |
| HNO       |                  |                  |                  |                 |                 |
| \( S_0 \) | 1.8008           | 0.0407           | 0.1195           | 10.45           |                 |
| \( S_1 \) | 1.8046           | 0.0401           | 0.1184           | 10.26           | -0.18           |
Figure S8. Correlation between H-N bond length and $\rho(r)$, $\nabla^2 \rho(r)$, $H(r)$ and hydrogen bond energy estimated via potential energy density $V(r)$ BCP.

6. **Energy levels**

Figure S9. Jablonski diagram (in eV) related to the ESIPT process of HPO, HBO and HNO, calculated at B3LYP/6-31+G(d)/PCM in acetonitrile.
7. **Relevant information about stationary points**

![Image of stationary points](image1)

**Figure S10.** Structures of S₁ transition state for HPO, HBO and HNO showing the displacement vectors over the imaginary frequency mode.

![Image of density difference plots](image2)

**Figure S11.** Density difference plots (Δρ = ρS₁ − ρS₀, isovalue=0.0004) for the E* (left), TS* (middle) and K* (right) stationary points on the S₁ PES of HNO. The blue/red zones indicate a decrease/increase of electron density upon excitation, respectively.

![Image of density difference plots and electrostatic potential maps](image3)

**Figure S12.** (Left) Density difference plots (Δρ = ρS₁ − ρS₀, isovalue=0.0004) for the enol form of 1H2NBO (top), 2H1NBO (middle) and 2H3NBO (bottom). The blue/red zones indicate a decrease/increase of electron density upon excitation, respectively. (Right) Electrostatic potential maps and dipole moment vectors for the three compounds. It is apparent that the ICT character is larger for 2H3NBO than for its isomers.
8. **Optimised coordinates for all compounds**

### HPO (S₀), *enol* tautomer

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 3.1207120000 | 0.5437080000 | -0.0000780000 |
| C    | 3.1406930000 | -0.8119930000 | 0.0000240000 |
| O    | 1.8366470000 | -1.2535610000 | 0.0000720000 |
| N    | 1.7980640000 | 0.9691970000 | -0.0000950000 |
| C    | -0.3729240000 | -0.2200590000 | 0.0000200000 |
| C    | -1.0319890000 | -1.4654150000 | 0.0001220000 |
| C    | -1.1458050000 | 0.9699020000 | -0.0000590000 |
| C    | -2.4203710000 | -1.3891900000 | 0.0001450000 |
| H    | -0.4376110000 | -2.3739390000 | 0.0001830000 |
| C    | -2.5449130000 | 0.8863560000 | -0.0000350000 |
| C    | -3.1749180000 | -0.3552600000 | 0.0000660000 |
| H    | -2.9138030000 | -2.5069600000 | 0.0002240000 |
| H    | -3.1190660000 | 1.8083260000 | -0.0000970000 |
| H    | -4.2605830000 | -0.4028790000 | 0.0000830000 |
| O    | -0.5858580000 | 2.2067050000 | -0.0001590000 |
| H    | 0.4018020000 | 2.1164050000 | -0.0001660000 |
| H    | 3.9473010000 | 1.2390800000 | -0.0001390000 |
| H    | 3.9084120000 | -1.5689170000 | 0.0000720000 |

### HPO (S₁), *enol* tautomer

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 3.0931280000 | 0.5784970000 | -0.0000810000 |
| C    | 3.1418370000 | -0.8053470000 | 0.0000250000 |
| O    | 1.8591370000 | -1.2874470000 | 0.0000750000 |
| N    | 1.8063880000 | 0.9972030000 | -0.0000990000 |
| C    | 1.0539990000 | -0.1446030000 | -0.0000400000 |
| C    | -0.3371110000 | -0.2483390000 | 0.0000210000 |
| C    | -1.0387600000 | -1.4997380000 | 0.0001240000 |
| C    | -1.1544110000 | 0.9791500000 | -0.0000590000 |
| C    | -2.4272480000 | -1.5247730000 | 0.0001440000 |
| H    | -0.4688610000 | -2.4220980000 | 0.0001860000 |
| C    | -2.5495950000 | 0.9144220000 | -0.0000360000 |
| C    | -3.1958400000 | -0.3301000000 | 0.0000650000 |
| H    | -2.9392580000 | -2.4834430000 | 0.0002220000 |
| H    | -3.1078360000 | 1.8458000000 | -0.0000980000 |
| H    | -4.2802320000 | -0.3819060000 | 0.0000830000 |
| O    | -0.5677900000 | 2.1803660000 | -0.0001560000 |
| H    | 0.4328310000 | 2.0701700000 | -0.0001630000 |
| H    | 3.9289430000 | 1.2655770000 | -0.0001420000 |
| H    | 3.9429370000 | -1.5286290000 | 0.0000710000 |

### HPO (S₀), *keto* tautomer

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -3.1155610000 | 0.5421110000 | 0.0000490000 |
### HPO (S₁), keto tautomer

| Atoms | X     | Y     | Z     | Cartesian Coordinates |
|-------|-------|-------|-------|-----------------------|
| C     | -3.1328080000 | -0.8054370000 | 0.0000110000 |
| O     | -1.8236440000 | -1.2680450000 | -0.0000240000 |
| N     | -1.7751980000 | 0.9076510000 | 0.00000240000 |
| C     | -1.0166310000 | -0.1931280000 | 0.0000100000 |
| C     | 0.4001770000  | -0.2386260000 | 0.0000150000 |
| C     | 1.0987970000  | -1.4736930000 | -0.0001330000 |
| C     | 1.1047630000  | 1.0345640000  | 0.0000590000 |
| C     | 2.4785290000  | -1.4997280000 | 0.000001510000 |
| H     | 0.5319650000  | -2.4011530000 | -0.0001840000 |
| C     | 2.5390800000  | 0.9439260000  | 0.0000420000 |
| H     | 3.0132530000  | -2.4446750000 | -0.0002430000 |
| O     | 0.4887220000  | -2.4446750000 | -0.0002430000 |
| H     | 1.2783890000  | 1.8157670000  | 0.0001310000 |
| H     | 3.9170060000  | -1.5960210000 | -0.0008140000 |
| H     | 3.0969550000  | 1.8772200000  | 0.0001280000 |
| H     | 4.2796430000  | -0.2928250000 | -0.0001190000 |
| O     | -0.5736720000 | 2.1627850000  | 0.0000020000 |
| H     | 1.4832690000  | 1.8877380000  | 0.00006270000 |
| H     | 3.9087000000  | -1.5960210000 | -0.0008140000 |

### HPO (S₁), TS

-1264.5 cm⁻¹

| Atoms | X     | Y     | Z     | Cartesian Coordinates |
|-------|-------|-------|-------|-----------------------|
| C     | -3.0567700000 | 0.6067140000 | 0.0003850000 |
| C     | -3.1705260000 | -0.7585850000 | 0.0002180000 |
| O     | -1.8996070000 | -1.3157150000 | -0.0000280000 |
| N     | -1.7332260000 | 0.9353500000 | -0.0001780000 |
| C     | -1.0411050000 | -0.2368740000 | -0.0002200000 |
| C     | 0.3646780000  | -0.3167460000 | -0.0003250000 |
HPO K*$_{90}$ (S$_1$)

| C   | 3.1306990000 | 0.1341760000 | 0.5566760000 |
|-----|-------------|--------------|-------------|
| C   | 3.0347490000 | -0.1458710000 | -0.7542850000 |
| O   | 1.7499470000 | -0.5163750000 | -1.0789470000 |
| N   | 1.8838600000 | -0.1125580000 | 1.1453250000 |
| C   | 1.0375270000 | -0.5345580000 | 0.1135580000 |
| C   | -0.4529480000 | -0.3641820000 | 0.0704210000 |
| C   | -1.2902850000 | -1.4506440000 | 0.1433750000 |
| C   | -0.9926110000 | 0.9640410000 | -0.0585880000 |
| C   | -2.6983080000 | -1.2735400000 | 0.0810370000 |
| H   | -0.8751610000 | -2.4572430000 | 0.2418610000 |
| C   | -2.4305530000 | 1.1243050000 | -0.1207600000 |
| C   | -3.2532350000 | 0.0133400000 | -0.0514930000 |
| H   | -3.3501580000 | -2.1407330000 | 0.1334060000 |
| H   | -2.8306140000 | 2.1294660000 | -0.2211670000 |
| H   | -4.3338820000 | 0.1243370000 | -0.0993230000 |
| O   | -0.1972170000 | 1.9527860000 | -0.0943400000 |
| H   | 1.5332770000 | 0.5234120000 | 1.8559880000 |
| H   | 3.9831690000 | 0.4549370000 | 1.1356860000 |
| H   | 3.7543130000 | -0.1459640000 | -1.5570810000 |

HBO (S$_0$), enol tautomer

| C   | 4.3158560000 | -0.7382090000 | 0.0000130000 |
| C   | 4.2956690000 | 0.6708030000 | -0.0000760000 |
| H   | 3.1338780000 | -2.5746820000 | 0.0001360000 |
| C   | 3.1339300000 | -1.4897470000 | 0.0000680000 |
| C   | 3.0960490000 | 1.3879400000 | -0.0001130000 |
| C   | 1.9106180000 | 0.6462580000 | -0.0000590000 |
| C   | 1.9586450000 | -0.7545370000 | 0.0000300000 |
| H   | 3.0813840000 | 2.4734810000 | -0.0001830000 |
| O   | 0.6592230000 | -1.2169430000 | 0.0000700000 |
| N   | 0.5706680000 | 1.0331150000 | -0.0000770000 |
| C   | -0.1130860000 | -0.0848900000 | 0.0000070000 |
| C   | -1.5569080000 | -0.2107480000 | 0.0000290000 |
C  -2.1833890000  -1.4741750000  0.0001310000
C  -2.3601440000  0.9604260000 -0.0000510000
C  -3.5682020000 -1.5832800000  0.0001930000
C  -4.3526590000 -0.0000510000  0.0001310000
H  -1.5647680000 -2.3660750000  0.0001310000
C  -3.7567860000  0.8393100000 -0.0000780000
C  -4.3502280000 -1.7455360000 -0.0000510000
C  -5.4387000000 -0.4186110000  0.0000780000
O  -1.8344330000  2.0970600000 -0.0001600000
H  -0.8443580000  2.1460400000 -0.0001730000
H  -5.2374510000  1.2122940000 -0.0001800000
H  -5.2701450000 -1.2569970000 -0.0000380000

HBO (S\textsubscript{1}), enol tautomer

C  4.3185470000  -0.7250510000  0.0000180000
C  4.2874540000  0.6919560000 -0.0000790000
H  3.1508640000 -2.5759490000  0.0001360000
C  3.0938730000  1.4043990000 -0.0000520000
C  1.8875660000  0.6551940000 -0.0000960000
O  0.6757940000  1.2615250000  0.0000650000
N  0.5943060000  1.0367530000  0.0001080000
C  -0.1371540000 -0.1204910000  0.0001800000
C  -1.5267150000 -0.2388760000 -0.0001730000
C  -2.0562500000 -1.5014720000  0.0002500000
C  -2.3590180000  0.9723000000 -0.0000520000
C  -3.5904210000 -1.5570950000  0.0001800000
C  -1.6159010000 -2.4116050000  0.0001730000
C  -3.7511390000  0.8777800000  0.0001080000
C  -4.3750010000 -0.3760230000  0.0000950000
H  -4.0844190000 -2.5250310000  0.0002390000
H  -4.3280310000  1.7978810000  0.0000650000
H  -5.4587880000 -0.4426250000  0.0001250000
O  -1.7992920000  2.1899960000 -0.0001730000
H  -0.7998760000  2.0999710000 -0.0002300000
H  5.2297690000  1.2328110000 -0.0001050000
H  5.2774990000 -1.2347490000  0.0000460000

HBO (S\textsubscript{0}), keto tautomer

C  -4.3069440000 -0.7366980000 -0.0001390000
C  -4.2875450000  0.6694390000  0.0000690000
H  -3.1238330000 -2.5719990000 -0.0002120000
C  -3.1230430000 -1.4874780000 -0.0000520000
C  -3.0883330000  1.3912160000  0.0002910000
C  -1.9141370000  0.6424270000  0.0001710000
C    -1.9501110000  -0.7544590000  0.0000100000
H    -3.0727280000  2.4757980000  0.0003860000
O    -0.6448130000  -1.2317060000  -0.0000380000
N    -0.5611520000  0.9721540000  0.0001040000
C     0.1690630000   -0.1518770000  0.0000580000
C     1.5775930000  -0.2277130000  -0.0000190000
C     2.2458640000  -1.4836410000  -0.0001190000
C     3.6216290000  -1.5451190000  -0.0000990000
H     1.6542690000   -2.3951750000  -0.0001680000
C     3.7527090000  0.8970290000  -0.0000240000
C     4.3693120000  -1.8147010000  -0.0000460000
H     4.1320620000  -2.5033100000  -0.0001260000
H     4.3355040000   1.8147010000  -0.0000460000
C     5.4562200000  -0.3872320000  -0.0001400000
O     1.7394700000  2.1706400000  -0.0000950000
H    -0.0378560000  1.8644850000  -0.0002800000
H     5.2280930000  1.2120040000  -0.0000470000
H     5.2601280000  -1.2563910000  -0.0002950000

HBO (S1), keto tautomer
C     -4.3288860000  -0.7699590000  0.0010860000
C     -4.3363720000   0.6345650000  0.0017920000
H     -3.1001310000  -2.5817250000  -0.0008200000
C     -3.1219060000  -1.4972660000  -0.0001950000
C     -3.1526190000  1.3854510000  0.0012920000
C     -1.9534320000   0.6630540000  0.0009990000
C     -1.9623530000  -0.7454660000  -0.0005780000
H     -3.1623940000  2.4701180000  0.0018090000
O     -0.6591510000  -1.2002580000  -0.0021110000
N     -0.6268530000   1.0212040000  -0.0009800000
C     0.1574320000  -0.0961190000  -0.0026740000
C     1.5798430000  -0.2088370000  -0.0009440000
C     2.2161220000  -1.4480780000  -0.0002910000
C     2.3992240000   1.0168870000  -0.0003380000
C     3.6399820000  -1.5495080000  0.0012620000
H     1.6244220000  -2.3584680000  -0.0010840000
C     3.8183870000   0.8624720000  0.0013620000
C     4.4303520000  -0.4056240000  0.0021510000
H     4.0931880000  -2.5363260000  0.0016700000
H     4.4131240000  1.7719660000  0.0020950000
H     5.5161360000  -0.4860760000  0.0033710000
O     1.8361920000  2.1670700000  -0.0013710000
H    -0.1843890000  1.9404610000  -0.0006870000
H    -5.2884160000  1.1577950000  0.0027550000
H    -5.2707520000  -1.3101010000  0.0014700000

HBO (S1), TS
-1346.5 cm⁻¹
C  4.3339950000  -0.6673360000  0.0001440000
C  4.2542450000   0.7403780000  -0.0000910000
H  3.2218800000  -2.5524340000   0.0004150000
C  4.2542450000  -1.4685130000  -0.0002790000
C  3.0314280000   1.4157100000   0.0002210000
C  1.8625070000   0.6275870000  -0.0002250000
C  1.9701930000  -0.7920640000   0.0000360000
H  2.9764210000   2.4994410000  -0.0004460000
O  0.7017580000  -1.3299060000   0.0000530000
N  0.5373590000  -0.9345210000  -0.0004410000
C  -0.1509290000  -0.2406220000   0.0001490000
C  -1.5557600000  -0.3163460000  -0.0000140000
C  -2.3135910000  -1.5015420000   0.0000120000
C  -2.2817030000   0.9746700000   0.0001060000
C  -3.7204400000  -1.4475460000   0.0001200000
H  -1.8080990000  -2.4618280000  -0.0000770000
C  -3.6948200000  -0.9819760000   0.0000780000
C  -4.1348400000 -0.2194140000   0.0001390000
H  -4.2802870000  -2.3784900000   0.0001310000
H  -4.1965560000  1.9451610000   0.0001100000
H  -5.4988490000  -0.2065980000   0.0001810000
O  -1.6018310000  2.0938830000  -0.002340000
H  -0.4287110000  1.8092310000  -0.0002730000
H  5.1749430000   1.3175560000  -0.0001190000
H  5.3081640000   2.3278490000   0.0001760000

HBO K*_{00} (S_1)

C  4.1882390000   0.2706800000   0.7900870000
C  4.2618530000   0.2094810000   0.6074000000
H  2.8981880000   0.1046770000   2.5458470000
C  2.9695510000   0.0660270000  -1.4637390000
C  3.1279740000  -0.0523100000  1.3940330000
C  1.9204690000  -0.2482220000   0.7246500000
C  1.8608390000  -0.1892870000  -0.6754500000
H  3.1888530000  -0.0988170000  2.4768100000
O  0.5715970000  -0.4287920000  -1.0967630000
N  0.6283110000   0.5022230000  1.1542620000
C  -0.1839340000  -0.7580570000   0.0395520000
C  -1.6293840000  -0.4102070000  0.0511800000
C  -2.5799590000 -1.4083380000  -0.0845670000
C  -2.0589420000   0.9849450000  0.0624290000
C  -3.9592350000  -1.1038840000  -0.1087280000
H  -2.2598500000  -2.4457780000  -0.1331570000
C  -3.4843410000  1.2590580000   0.0391130000
C  -4.4019310000   0.2335020000  -0.0436510000
H  -4.6829670000  -1.9096860000  -0.1766520000
H  -3.7948870000  2.2988880000   0.0900380000
H  -5.4667220000  0.4474080000  -0.0607820000
O  -1.2161020000  1.9253770000   0.1243710000
H  0.3856450000  -0.8168400000  2.0835250000
H  5.2176730000  0.3673700000  1.0989730000
H  5.0847260000  0.4753720000  -1.3677330000

HNO (S\textsubscript{0}), enol tautomer

C  -5.5685237194  -0.7024964338  -0.0000727099
C  -4.3892456484  -1.415659367  -0.0000025150
C  -3.1281242101  -0.7529141363  -0.0000211004
C  -3.1045937952  0.6933514367  -0.0001158594
C  -4.3473681728  1.3937903343  -0.0001858579
C  -5.5473755227  0.7175605532  -0.0001651989
H  -1.9142606937  -2.5779412490  0.0001247579
H  -6.5205146285  -1.2266154753  -0.0000575201
H  -4.4050410801  -2.5030036814  0.0000674151
C  -1.9096937991  -1.4924076031  0.0000523833
C  -1.8675140628  1.3937048246  -0.0001371307
H  -4.3294447133  2.4811634161  -0.0002558271
H  -6.4833265418  1.2697960551  -0.0002198680
C  -0.7034048882  0.6541703889  -0.0000663503
C  -0.7534020112  -0.7628040350  0.0000270027
H  -1.8492661753  2.4797578368  -0.0002061717
O  0.5499442281  -1.2214459485  0.0000886198
N  0.6402416775  1.0340464922  -0.000035720
C  1.3197586969  -0.0845418768  0.0000137254
C  2.7619409799  -0.2112555776  0.0000691330
C  3.3873222078  -1.4757746585  0.0002331122
C  3.5656774170  0.9602842271  -0.0000204649
C  4.7716453025  -1.5853841285  0.0003156804
H  2.7676658147  -2.3668285577  0.0003041176
C  4.9623119148  0.8379289949  0.0000674159
C  5.5565439941  -0.4205988210  0.0002336988
H  5.5615424962  1.7435659596  -0.000071120
H  6.6405267275  -0.4971911406  0.0002963120
O  3.0404872573  2.2085342606  -0.0002286662
H  2.0503783646  2.1448774123  -0.0003234309
H  5.2408677121  -2.5643518354  0.0004465176

HBO (S\textsubscript{1}), enol tautomer

C  -5.5909410000  -0.6881030000  -0.0000830000
C  -4.3759370000  -1.4073100000  0.0000120000
C  -3.1407880000  -0.7531910000  -0.0000130000
C  -3.1132350000  0.6947090000  -0.0001410000
C  -4.3609260000  1.3924820000  -0.0002350000
C  -5.5761990000  0.7103530000  -0.0002060000
H  -1.9110150000  -2.5821080000  0.0001800000
H  -6.5327740000  -1.2282000000  -0.0000600000
H  -4.3995540000  -2.4938450000  0.0001060000
C  -1.9002770000  -1.4967190000  0.0000850000
C  -1.8904240000  1.3905320000  -0.0001710000
H  -4.3472770000  2.4792720000  -0.0003300000
H  -6.5082800000  1.2673830000  -0.0000740000
C  -0.6792680000  0.6453690000  -0.0000740000
C  -0.7409120000  -0.7788000000  0.0000520000
H  -1.8679020000  2.4762470000  -0.0002640000
O         0.5467940000  -1.2468770000  -0.0001270000
H  -1.8998230000  -2.5731940000  -0.0003200000
H  -6.5110780000  -1.2318900000  -0.0001770000
H  -4.3919450000  -2.5043260000  -0.0001610000
C         1.8998230000  -2.5731940000  -0.0001300000
O         5.5444000000  1.7785870000  -0.0000260000
O         4.3425610000  1.3927400000  -0.0000650000
O         5.5414070000  0.7126980000  -0.0001370000
H         4.3791730000  -1.4171950000  -0.0001280000
S          0.6939500000  -0.0000050000
C         3.1011030000  -0.0000900000
C         4.3425610000  1.3927400000  -0.0000650000
C         4.3425610000  1.3927400000  -0.0000650000
H         1.9002850000  -1.4880920000  -0.0000300000
C         1.8998230000  -2.5731940000  -0.0001300000
H         6.5110780000  -1.2318900000  -0.0002520000
H         4.3919450000  -2.5043260000  -0.0001610000
C         1.8637990000  1.3998660000  -0.0000910000
H         4.3273230000  2.4798790000  -0.0000200000
H         6.4781280000  1.2633740000  -0.0001780000
C         0.7101470000  0.6543450000  -0.0001110000
C         0.7468460000  -0.7596110000  -0.0000900000
H         1.8458890000  2.4850180000  -0.0001360000
O         -0.5622680000  -1.2319330000  -0.0001360000
N         -0.6455160000  0.9762890000  -0.0002790000
C         -1.3743850000  -0.1489930000  -0.0002030000
C         -2.7796560000  -0.2269090000  -0.0001370000
C         -3.4446630000  -1.4863360000  -0.0001440000
C         -3.5276140000  1.0273950000  -0.0001000000
C         -4.8189550000  -1.5511990000  -0.0000450000
H         -2.8501310000  -2.3958150000  -0.0003200000
C         -4.9607250000  0.8912370000  -0.0003190000
C         -5.5714900000  -0.3433910000  -0.0003100000

HNO (S0), keto tautomer

C         5.5602760000  -0.7059750000  -0.0001780000
C         3.7391730000  -1.4171950000  -0.0001280000
C         3.1217530000  -0.7503740000  -0.0000320000
C         3.1011030000  0.6939500000  -0.0000050000
C         4.3425610000  1.3927400000  -0.0000650000
C         5.5414070000  0.7126980000  -0.0001370000
H         1.8998230000  -2.5731940000  -0.0001300000
H         6.5110780000  -1.2318900000  -0.0002520000
H         4.3919450000  -2.5043260000  -0.0001610000
C         1.9002850000  -1.4880920000  -0.0000300000
C         1.8637990000  1.3998660000  -0.0000910000
H         4.3273230000  2.4798790000  -0.0000200000
H         6.4781280000  1.2633740000  -0.0001780000
C         0.7101470000  0.6543450000  -0.0001110000
C         0.7468460000  -0.7596110000  -0.0000900000
H         1.8458890000  2.4850180000  -0.0001360000
O         -0.5622680000  -1.2319330000  -0.0001360000
N         -0.6455160000  0.9762890000  -0.0002790000
C         -1.3743850000  -0.1489930000  -0.0002030000
C         -2.7796560000  -0.2269090000  -0.0001370000
C         -3.4446630000  -1.4863360000  -0.0001440000
C         -3.5276140000  1.0273950000  -0.0001000000
C         -4.8189550000  -1.5511990000  -0.0000450000
H         -2.8501310000  -2.3958150000  -0.0003200000
C         -4.9607250000  0.8912370000  -0.0003190000
C         -5.5714900000  -0.3433910000  -0.0003100000
| Atom | X       | Y       | Z       | E       | Standard Error |
|------|---------|---------|---------|---------|---------------|
| H    | -5.3268420000 | -2.5107140000 | -0.0000060000 |
| H    | -5.5467020000 | 1.8067060000 | 0.0005300000 |
| H    | -6.6581360000 | -0.3992040000 | 0.0005070000 |
| O    | -2.9534240000 | 2.1710690000 | -0.0000490000 |
| H    | -1.1674090000 | 1.8681210000 | -0.0000990000 |
| HNO (S1), keto tautomer | |
| C    | -5.5859960000 | -0.7365140000 | -0.0003620000 |
| C    | -4.3861130000 | -1.4306940000 | -0.0004380000 |
| C    | -3.1414080000 | -0.7519940000 | -0.0002680000 |
| C    | -3.1371720000 | 0.6979700000 | -0.0000870000 |
| C    | -5.5853730000 | 0.6775660000 | -0.0001090000 |
| C    | -1.1674090000 | 1.8681210000 | -0.0000990000 |
| C    | -6.5277190000 | 1.2788780000 | -0.0000490000 |
| O    | 0.5487190000 | -1.1910160000 | -0.0002090000 |
| HNO (S1), TS | |
| H    | -1581.4 cm⁻¹ |
| C    | -5.5816090000 | -0.6186570000 | 0.0001000000 |
| C    | -4.4044790000 | -1.3687710000 | 0.0001370000 |
| C    | -3.1403570000 | -0.7501730000 | 0.0000130000 |
| C    | -3.0716770000 | 0.7012350000 | -0.0001930000 |
| H    | -5.6390930000 | 0.4171430000 | 0.0002460000 |
| H    | 2.8258310000 | -2.3626950000 | -0.0000980000 |
| C    | 0.8424360000 | -1.5618410000 | 0.0000790000 |
| C    | 5.0339480000 | 0.8488940000 | 0.0003330000 |
| C    | 5.6390930000 | -0.4171430000 | 0.0002460000 |
| H    | 5.6317700000 | 1.7560670000 | 0.0004660000 |
| H    | 6.7217450000 | -0.5028230000 | 0.0003110000 |
| O    | 3.0566390000 | 2.1598690000 | 0.0003450000 |
| H    | 1.0532380000 | 1.9341250000 | 0.0003190000 |
| H    | 5.2940720000 | -2.5490020000 | 0.0000990000 |
| Atom | X Position | Y Position | Z Position |
|------|------------|------------|------------|
| H    | -6.5434720000 | -1.1238490000 | 0.0002120000 |
| H    | -4.4560300000 | -2.4549050000 | 0.0002780000 |
| C    | -1.9290840000 | -1.5314140000 | 0.0000780000 |
| C    | -1.8267890000 | 1.3636920000 | -0.0003520000 |
| H    | -4.2529640000 | 2.5221950000 | -0.0003490000 |
| H    | -6.4435260000 | 1.3710260000 | -0.0000980000 |
| C    | -0.6584260000 | 0.5796580000 | -0.0003170000 |
| C    | -0.7510680000 | -0.8491330000 | -0.0000680000 |
| H    | -1.7718630000 | 2.4477950000 | -0.0004710000 |
| O    | 0.5306560000 | -1.3642670000 | -0.0000720000 |
| N    | 0.6577260000 | -0.8919730000 | -0.0005420000 |
| C    | 1.3671140000 | -0.2729100000 | -0.0003340000 |
| C    | 1.8267890000 | 0.8369200000 | -0.0002640000 |
| H    | 1.7710690000 | -2.4886280000 | 0.1527840000 |
| O    | 2.7588110000 | 2.1053790000 | -0.0002990000 |
| H    | 1.5514140000 | 1.7749740000 | -0.0006500000 |
| H    | 5.2588920000 | -2.3273710000 | 0.0004570000 |

**HNO₉₅(S₁)**

| Atom | X Position | Y Position | Z Position |
|------|------------|------------|------------|
| C    | -5.5274080000 | -0.7969840000 | 0.2628370000 |
| C    | -4.3040970000 | -1.4471070000 | 0.2338820000 |
| C    | -3.0935070000 | -0.7354520000 | 0.0485370000 |
| C    | -3.1495570000 | 0.6987270000 | -0.1133940000 |
| C    | -4.4204230000 | 1.3307130000 | -0.0783680000 |
| C    | -5.5839490000 | -0.6032860000 | 0.1052420000 |
| H    | -5.5274080000 | -0.7969840000 | 0.2628370000 |
| C    | -4.3040970000 | -1.4471070000 | 0.2338820000 |
| C    | -3.0935070000 | -0.7354520000 | 0.0485370000 |
| C    | -3.1495570000 | 0.6987270000 | -0.1133940000 |
| C    | -4.4204230000 | 1.3307130000 | -0.0783680000 |
| C    | -5.5839490000 | -0.6032860000 | 0.1052420000 |
| H    | -1.7710690000 | -2.4886280000 | 0.1527840000 |
| H    | -6.4421140000 | -1.3655360000 | 0.4081840000 |
| H    | -4.2573940000 | -2.5271560000 | 0.3559840000 |
| C    | -1.8301210000 | -1.4131750000 | 0.0234610000 |
| C    | -1.9509910000 | 1.4520310000 | -0.3065010000 |
| H    | -4.4665510000 | 2.4110910000 | -0.1986160000 |
| H    | -6.5434960000 | 1.1135280000 | 0.1292470000 |
| C    | -0.7521610000 | 0.7625080000 | -0.3231940000 |
| C    | -0.7108450000 | -0.6460840000 | -0.1557170000 |
| H    | -1.9974980000 | 2.5300170000 | -0.4284700000 |
| O    | 0.5981090000 | -1.0668140000 | -0.2282310000 |
| N    | 0.5644810000 | 1.1360240000 | -0.5117110000 |
| C    | 1.3769380000 | 0.0290420000 | -0.4828230000 |
| C    | 2.8593800000 | -0.0177770000 | -0.3093400000 |
| C    | 3.6939230000 | -0.2389470000 | -1.3782870000 |
| C    | 3.4079670000 | 0.1668440000 | 1.0152320000 |
| C    | 5.1012590000 | -0.3003440000 | -1.1943640000 |

**HNO K90(S1)**
|    | 1H2NBO (S₀), enol tautomer | 1H2NBO (S₁), enol tautomer |
|----|-----------------------------|-----------------------------|
| O  | 1.9419620000  -0.8478170000 | 1.8212120000  -1.0077040000 |
| C  | 1.3882840000  0.3831020000 | 1.4275720000  4.0162650000 |
| C  | 0.0000000000  0.5919440000 | 4.5407640000  2.4091780000 |
| C  | -0.5131370000 1.9250990000 | -0.3422460000 3.7229020000 |
| O  | 2.2856910000  1.4984460000 | 4.0104740000  3.7229020000 |
| H  | 1.7443050000  2.8236430000 | 2.2351810000  4.9312520000 |
| C  | -0.8883370000  -0.5490910000 | -5.4173920000  4.6944760000 |
| C  | 3.6946920000  1.3172150000 | 2.6343790000  4.0967610000 |
| C  | -0.5355050000  -1.8139140000 | -1.1963360000  5.6173830000 |
| C  | -1.7326210000  -2.5291590000 | -4.1300110000  4.6844760000 |
| O  | -2.2437610000  -0.3422460000 | 1.5890310000  4.5407640000 |
| H  | -1.5890310000  2.0669400000 | 1.2134090000  1.5257740000 |
| C  | -2.7905790000  -1.6086750000 | 1.2134090000  1.5257740000 |
| C  | -1.9997740000  -3.9021390000 | 1.9419620000  -1.0077040000 |
| C  | -3.3426960000  -4.2898030000 | -0.7394620000  -1.5257740000 |
| H  | -3.5899080000  -5.3476890000 | 1.8212120000  -1.0077040000 |
| C  | -4.3872980000  -3.3432790000 | 1.0000000000  0.0000000000 |
| C  | -4.1300110000  -1.9663840000 | 1.0000000000  0.0000000000 |
| H  | -1.1963360000  -4.6325520000 | 1.0000000000  0.0000000000 |
| H  | -5.4173920000  -3.6877910000 | 1.0000000000  0.0000000000 |
| H  | -4.9265240000  -1.2293840000 | 1.0000000000  0.0000000000 |
| C  | 2.6434790000  3.9233620000 | 1.0000000000  0.0000000000 |
| H  | -0.0739460000  4.0162650000 | 1.0000000000  0.0000000000 |
| C  | 4.5407640000  2.4091780000 | 1.0000000000  0.0000000000 |
| C  | 4.0104740000  3.7229020000 | 1.0000000000  0.0000000000 |
| H  | 2.2351810000  4.9312520000 | 1.0000000000  0.0000000000 |
| H  | 4.0967610000  0.3095950000 | 1.0000000000  0.0000000000 |
| H  | 5.6173830000  2.2621190000 | 1.0000000000  0.0000000000 |
| H  | 4.6844760000  4.5755270000 | 1.0000000000  0.0000000000 |
| H  | 1.2134090000  -1.5257740000 | 1.0000000000  0.0000000000 |

The 1H2NBO (S₀), enol tautomer and 1H2NBO (S₁), enol tautomer coordinates are shown in the table.
2H1NBO (S\textsubscript{0}), enol tautomer

\begin{verbatim}
C  2.7607690000  0.5535820000  0.0000070000
C  2.4559720000 -0.8122350000  0.0000130000
C  3.4070980000 -1.8208520000  0.0000310000
C  4.7402050000 -1.3918030000  0.0000300000
C  5.0750110000 -0.2240500000  0.0000270000
C  4.0951240000  0.9737850000  0.0000210000
C  0.6048400000 -0.3547330000 -0.0001100000
H  3.1379690000 -2.8719340000  0.0000430000
H  5.5334760000 -2.1335790000  0.0000450000
H  6.1229150000  0.2638580000  0.0000460000
H  4.3544210000  2.0280580000  0.0000390000
C -0.8208450000  0.6411950000 -0.0000860000
C -1.8685400000 -0.3671940000 -0.0000490000
C -1.1896670000  2.0062070000 -0.0000310000
C -1.6376910000 -1.7728170000 -0.0000880000
C -3.2392800000  0.0632440000  0.0000350000
C -2.5533400000  2.3974450000  0.0000630000
C -2.6852720000 -2.6781730000 -0.0000550000
H -0.6288430000 -2.1560360000 -0.0001490000
C -4.2912520000 -0.8898950000  0.0000690000
C -3.5441840000  1.4547580000  0.0000920000
\end{verbatim}
H  -2.7756830000  3.4600160000  0.0001040000
C  -4.0278420000  -2.2440890000  0.0000240000
H  -2.4627080000  -2.2440890000  0.0000240000
H  -5.3161810000  -0.5261510000  0.0001330000
H  -4.5871310000  1.7612700000  0.0001640000
H  -4.8392780000  -2.9664380000  0.0000520000
O        1.0828360000  -0.9314990000  0.0000170000
N        1.5627760000  1.2592060000  0.0000410000
O        0.3063130000  3.0245700000  0.0000710000
H        0.6228040000  2.6511980000  0.0001950000

2H1NBO (S1), enol tautomer

C  2.7461950000  0.5582630000  -0.0000750000
C  2.4437360000  -0.8311020000  0.0000580000
C  3.3964200000  -1.8293990000  0.0000800000
C  4.7363120000  -1.3963210000  -0.0000370000
C  5.0708250000  -0.0218860000  0.0001710000
C  4.0980880000  0.9740450000  -0.0001930000
C  0.5791840000  0.3388920000  0.0000850000
H  3.1390100000  -2.8816170000  0.0001780000
H  5.5307810000  -2.1366920000  -0.0000260000
H  6.1200670000  0.2601310000  -0.0002600000
H  4.3567620000  2.0281870000  -0.0002970000
C  -0.7967310000  0.6245800000  0.0000890000
C  -1.8737060000  -0.3730970000  0.0000400000
C  -1.1916110000  2.0480670000  0.0000610000
C  -1.6504960000  -1.7662180000  0.0000360000
C  -3.2438770000  0.0802270000  -0.0000340000
C  -2.5266580000  2.4249660000  -0.0000110000
C  -2.0700700000  -2.6952530000  -0.0000220000
H  -0.6412480000  -2.1499650000  0.0000780000
C  -4.2875830000  -0.8763340000  -0.0000920000
C  -3.5445290000  1.4657900000  -0.0000610000
H  -2.7569560000  3.4859410000  -0.0000200000
C  -4.0287130000  -2.2496000000  -0.0000840000
H  -2.4799950000  -3.7572400000  -0.0000210000
H  -5.3148510000  -0.5193610000  -0.0001470000
H  -4.5845310000  1.7805950000  -0.0001210000
H  -4.8530520000  -2.9573710000  -0.0001310000
O  1.0804110000  -0.9616910000  0.0001370000
N  1.5854610000  1.2558850000  -0.0000590000
O  -0.2769020000  3.0329780000  0.0001970000
H  0.6457190000  2.6321910000  0.0004400000

2H1NBO (S0), keto tautomer

C  2.7580540000  0.5439800000  -0.0001200000
C  2.4403170000  -0.8070010000  0.0000920000
C  3.3846900000  -1.8074940000  0.0002290000

22
C  4.7147770000  -1.3895480000  0.0001420000
C  5.0506450000  -0.0343170000  -0.0000140000
C  4.0784810000   0.9625030000  -0.0002340000
H  0.5469480000   0.3051250000  -0.0000140000
H  3.1075200000  -2.8534870000   0.0003930000
H  5.5016990000  -2.1336720000  -0.0000890000
C  -1.8846880000  -0.3714540000  -0.0000380000
C  -1.1099120000  2.0418410000  -0.0000380000
C  -3.2234600000   0.0890350000  -0.0000380000
C  -2.5105690000  2.4233930000   0.0001400000
C  -2.7493860000  -2.6458610000  -0.0000380000
H  -0.6841000000  -2.1720850000  -0.0001440000
C  -4.2905250000  -0.8227510000   0.0000380000
C  -3.4916270000  1.5036640000   0.0000380000
H  -2.7150450000  3.4872990000  -0.0002610000
C  -4.0667820000  -2.1815310000  -0.0001810000
H  -2.5537650000  -3.7127110000  -0.0002560000
H  -5.3040450000  -0.4336930000  -0.0001010000
H  -4.5310340000  1.8197310000   0.0000610000
H  -4.8962350000  -2.8788490000  -0.0002370000
O  1.0709700000  -0.9383200000   0.0001100000
N  1.5439110000   1.2068740000   0.0000140000
O  -0.2324730000  2.9390820000   0.0004490000
H  1.2273160000  2.2009770000  -0.0004610000

2H1NBO (S1), keto tautomer

C  2.7618480000   0.5605500000  -0.0003100000
C  2.4494000000  -0.8008610000  -0.0000170000
C  3.4007700000  -1.7949800000  -0.0000550000
C  4.7312420000  -1.3679900000  -0.0000410000
C  5.0601720000  -0.0099650000   0.0000140000
C  4.0873900000  0.9853070000   0.0000550000
C  0.5483770000  0.3066050000   0.0000230000
H  3.1296920000  -2.8424970000  -0.0000900000
H  5.5225850000  -2.1074560000  -0.0000690000
H  6.1050930000  0.2772380000   0.0000280000
H  4.3448870000  2.0364620000   0.0001010000
C  -0.8343810000  0.6071860000   0.0000340000
C  -1.8787590000  -0.3629490000  -0.0000200000
C  -1.1812810000  2.0679810000   0.0000430000
C  -1.6524380000  -1.7693920000  -0.0000100000
C  -3.2552720000  0.0953100000   0.0000290000
C  -2.5536410000  2.4255090000  -0.0000270000
C  -2.6890000000  -2.6732450000   0.0000100000
H  -0.6414060000  -2.1451980000  -0.0000130000
|   |   |   |   |
|---|---|---|---|
| C | -4.2843140000 | -0.8607270000 | 0.00000270000 |
| C | -3.5528010000 | 1.4793400000 | -0.0000030000 |
| H | -2.7709820000 | 3.4864980000 | -0.0000940000 |
| C | -4.0190650000 | -2.2143910000 | 0.0000170000 |
| H | -2.4791420000 | -3.7359490000 | -0.0000160000 |
| H | -5.3113990000 | -0.5105310000 | 0.0000280000 |
| H | -4.5940670000 | 1.7827140000 | -0.0000310000 |
| H | -4.8372720000 | 3.4864980000 | -0.0000940000 |
| O | 1.0887870000 | -0.9414250000 | 0.0000140000 |
| N | 1.5591080000 | 1.2101260000 | 0.0000680000 |
| O | -0.2717790000 | 2.9377550000 | -0.0001600000 |
| H | 1.2527140000 | 2.2034170000 | 0.0001560000 |
| O | -2.1496200000 | 1.6911080000 | 0.0000000000 |
| C | -0.7914650000 | 0.5229380000 | 0.0000000000 |
| C | 0.0000000000 | 0.5229380000 | 0.0000000000 |
| C | 1.3863240000 | 0.6181340000 | 0.0000000000 |
| C | -0.1645820000 | 2.9565680000 | 0.0000000000 |
| O | 1.2481510000 | 3.0644080000 | 0.0000000000 |
| C | -0.6603500000 | -0.7696120000 | 0.0000000000 |
| C | 3.4651580000 | 1.9749580000 | 0.0000000000 |
| H | -0.7764590000 | 3.8546020000 | 0.0000000000 |
| C | 1.9133140000 | 4.3240290000 | 0.0000000000 |
| C | 1.9520860000 | -0.9845540000 | 0.0000000000 |
| C | -2.0955200000 | -2.3715460000 | 0.0000000000 |
| O | 0.1001480000 | -1.9089980000 | 0.0000000000 |
| H | 1.9804120000 | -0.2909380000 | 0.0000000000 |
| C | -0.8147200000 | -2.9405800000 | 0.0000000000 |
| C | -3.2274660000 | -3.1926260000 | 0.0000000000 |
| C | -3.0116940000 | -4.5728670000 | 0.0000000000 |
| H | -3.8656790000 | -5.2441080000 | 0.0000000000 |
| C | -1.7123430000 | -5.1194120000 | 0.0000000000 |
| C | -0.5730170000 | -4.3056630000 | 0.0000000000 |
| H | -4.2283050000 | -2.7720630000 | 0.0000000000 |
| H | -1.5899630000 | -6.1985550000 | 0.0000000000 |
| O | 0.4311660000 | -4.7163270000 | 0.0000000000 |
| H | 1.3169160000 | 5.2333150000 | 0.0000000000 |
| C | 3.2906520000 | 4.3931390000 | 0.0000000000 |
| C | 4.0770280000 | 3.2093040000 | 0.0000000000 |
| H | 4.0586020000 | 1.0636320000 | 0.0000000000 |
| H | 3.7832470000 | 5.3620180000 | 0.0000000000 |
| H | 5.1609700000 | 3.2831630000 | 0.0000000000 |
| H | -2.4520490000 | 0.7477330000 | 0.0000000000 |

2H3NBO \((\text{S}_0)\), \text{enol} tautomer

|   |   |   |   |
|---|---|---|---|
| O | -2.2824350000 | 1.2428860000 | 0.0000000000 |

2H3NBO \((\text{S}_1)\), \text{enol} tautomer
2H3NBO (S₀), keto tautomer
2H3NBO (S_1), keto tautomer

O  -0.3031250000  2.6649080000  -0.0000020000
C   -1.0482490000  1.6288200000  -0.0000060000
C   -0.4460180000  0.2755960000  -0.0000010000
C   -1.2809470000  0.8303090000  -0.0000030000
C   -2.7184130000  0.7261730000  -0.0000020000
C   -2.4644480000  1.7177110000  -0.0000060000
C   -3.3195320000  0.5788160000  -0.0000020000
C    0.9650550000  0.1462000000  -0.0000030000
C   -3.5434240000  1.8555270000  -0.0000050000
H   -2.8958410000  2.7156610000  -0.0000013000
C   -4.7274940000  0.6834900000  -0.0000020000
N    1.9267100000  0.1157040000  -0.0000180000
O    3.1779430000  1.0366300000  -0.0000100000
C    5.5205660000  0.9653200000  -0.0000020000
H    6.5471640000  0.4515330000  -0.0000040000
C    5.2731090000  1.2843960000  -0.0000070000
C    3.9600940000  1.7918840000  -0.0000080000
H    4.6746620000  2.1037890000  -0.0000180000
H    6.1077370000  1.9788150000  -0.0000120000
H    3.7527180000  2.8566840000  -0.0000160000
H    -5.1802950000  1.6709310000  -0.0000050000
C   -5.5358870000  0.4632000000  -0.0000100000
C   -4.9480570000  1.7285620000  -0.0000050000
H   -3.0930780000  2.8452630000  -0.0000080000
H   -6.6172540000  0.3608470000  -0.0000100000
H   -5.5669490000  2.6217400000  -0.0000070000
H    1.6523130000  2.0958520000  -0.0000100000

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[2] A. J. Stasyuk, M. K. Cyrański, D. T. Gryko, M. Solà, J. Chem. Theory Comput., 2015, 11, 1046-1054.

26