Electronic Supplementary Information

Computational study on the mechanism for the synthesis of the active pharmaceutical ingredients nitrofurantoin and dantrolene in both solution and mechanochemical conditions

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S1. Calculation of dielectric constant in ball-milling conditions

The solution of the wave equation for the electromagnetic wave in a dielectric medium yields a speed of propagation $v = \frac{1}{\sqrt{\varepsilon_0 \mu_0 \varepsilon \mu}}$. The speed of light in vacuum is $c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}$. Refractive index $n = \frac{c}{v} = \sqrt{\varepsilon \mu}$. Most materials with light in the optical range are characterized by $\mu \approx 1$. Thus, $\varepsilon = n^2$ [1].

The aldehyde and amine hydrochloride were mixed in a 1:1 proportion, the resulting dielectric constant was computed using the formula $\varepsilon_M = \sum_n \varphi_n \varepsilon_n$, where ε_M, φ_n, and ε_n stand for dielectric constant of mixture, molar fraction of each component, and dielectric constant of individual component, respectively [2].

Nitrofurantoin in ball-milling conditions: The refractive indices of 1-amino-hydantoin, hydrochloric acid, and 5-nitro-2-furaldehyde are 1.556 [3], 1.254 [4] and 1.579 [5]. Based on the molar masses, we have calculated the molar fractions of 1-amino-hydantoin hydrochloric acid, and 5-nitro-2-furaldehyde to be 0.393, 0.125, and 0.482, respectively. Based on these data, the dielectric constant of the mixture ε_M is 2.350.

Dantrolene in ball-milling conditions: The refractive indices of 1-amino-hydantoin, hydrochloric acid, and of 5-(4-nitrophenyl)-2-furaldehyde are 1.556 [3], 1.254 [4] and 1.618 [6]. Based on the molar masses, we have calculated the molar fractions of 1-amino-hydantoin, hydrochloric acid, and 5-(4-nitrophenyl)-2-furaldehyde to be 0.312, 0.099, and 0.589, respectively. Based on these data, the dielectric constant of the mixture ε_M is 2.453.

S2. Starting concentrations

Synthesis of nitrofurantoin in solvent. Based on the procedure described in [7], concentrations of acetic acid, 1-amino-hydantoin, and 5-nitro-2-furaldehyde are 0.35 M, 0.2 M, and 0.2 M, respectively.

Synthesis of nitrofurantoin in ball-milling conditions: We follow the published experimental data [8] and convert them to concentrations. The density of 1-amino-hydantoin is 1.50 g/cm^3, the molecular weight of 1-amino-hydantoin (A) is 151.55 g/mol [3]. (The data on density of 1-amino-hydantoin hydrochloride is unavailable, that is why the employed density value is taken for 1-amino-hydantoin) The density and molecular weight of 5-nitro-2-furaldehyde (B) are 1.47 g/cm^3 and 141.08 g/mol [5]. Since the initial ratio of reactants is 1:1, and assuming volumes of the mixture components A and B are exactly additive, we obtain:

$\rho_{AB} = \frac{m_A+m_B}{V_A+V_B} = \frac{n_A M_A+n_B M_B}{\frac{n_A M_A}{\rho_A}+\frac{n_B M_B}{\rho_B}}$.

Taking into account that the number of moles for A and B is the same,

$\rho_{AB} = \frac{M_A+M_B}{\frac{M_A}{\rho_A}+\frac{M_B}{\rho_B}} = 1.485\ \frac{g}{cm^3}$.

Thus, concentrations equal $C_A = C_B = \frac{n_A}{V_{AB}} = \frac{n_A}{\frac{m_A+m_B}{\rho_{AB}}} = \rho_{AB}\frac{1}{M_A+M_B} = 5.074$ M.

Synthesis of dantrolene in ball-milling conditions: We follow the published experimental data [8] and convert them to concentrations. Taking into account the density of 5-(4-nitrophenyl)-2-furaldehyde being 1.348 g/cm^3 [5] and molecular weight 217.18 g/mol, the concentrations of 1-amino-hydantoin hydrochloride (A) and 5-(4-mitrophenyl)-2-furaldehyde are 3.816 M.

S3. Benchmarking of the DFT functionals

The performance with another functional was evaluated. Transition state **TS2** (the highest, rate-determining barrier in solvent conditions) and product formation energies were calculated for nitrofurantoin in solvent conditions.

Table S1. Benchmarking of the DFT functionals via the calculation of the Gibbs free energy of the highest barrier (TS2) and reaction Gibbs free energy for the reaction of synthesis of nitrofurantoin in solution. (Reaction profile for this reaction is presented at Figure 1 of the article.) The energies are calculated with B3LYP-D3BJ/cc-pVTZ//B3LYP-D3BJ/cc-pVTZ. The effect of the dielectric environment (water) was introduced through implicit solvation *via* the PCM approach.

Method	Transition state TS2 (kcal/mol)	Products (kcal/mol)
B3LYP-GD3	22.2	-4.5
B3LYP-GD3BJ	21.4	-5.3
ωB97X-D	24.5	-3.2

S4. References

[1] P. O. Robitaille, H. Abou-Rachid and J. Brisson, *Defense Technology*, 2021, **17**, 1988-1994.
[2] B. S. Pladevall, A. de Aguirre, and F. Maseras, F., *ChemSusChem*, 2021, **14**, 2763-2768.
[3] https://www.chemspider.com/Chemical-Structure.65659.html (accessed on April 15, 2024); https://www.chemsrc.com/en/cas/2827-56-7_330251.html (accessed on April 15, 2024)
[4] https://pubchem.ncbi.nlm.nih.gov/compound/Hydrochloric-Acid (accessed on April 15, 2024)
[5] https://www.chembk.com/en/chem/698-63-5 (accessed on April 15, 2024)
[6] https://www.chembk.com/en/chem/5-(4-nitrophenyl)furan-2-carbaldehyde (accessed on April 15, 2024)
[7] C. Gallardo-Garrido, Y. Cho, J. Cortés-Ríos, D. Vasquez, C. D. Pessoa-Mahana, R. Araya-Maturana, H. Pessoa-Mahana, M. Faundez, *Tox. Appl. Pharm*., 2020, **401**, 115104.
[8] E. Colacino, A. Porcheddu, I. Halasz, C. Charnay, F. Delogu, R. Guerra and J. Fullenwarth, *Green Chemistry*, 2018, **20**, 2973-2977

S4. Cartesian coordinates, energies and low frequencies

NF-BM-Comp
Energy (POTENTIAL) = -1786.21073709 Eh
Gibbs energy= -1786.040523 Eh
Three lowest frequencies (cm^{-1}): 15.2765, 27.2072, 29.0340

	Atom	X	Y	Z
1	H	1.7885	-1.0062	1.3365
2	Cl	3.4639	0.0230	1.1299
3	C	-1.4120	-1.0319	0.9986
4	C	-1.4619	0.2235	-0.9439
5	C	0.0009	-0.0677	-0.6264
6	H	0.4049	-0.7674	-1.3618
7	H	0.5936	0.8434	-0.6114
8	N	-2.1979	-0.3886	0.0581
9	H	-3.2053	-0.3910	0.0981
10	O	-1.8973	0.8489	-1.8720
11	O	-1.7503	-1.7460	1.9108
12	N	-0.1049	-0.6775	0.6945
13	N	0.8986	-1.5584	1.1604
14	H	0.5430	-1.9869	2.0184
15	H	1.1157	-2.3024	0.4281
16	C	6.4538	-2.2419	-1.0844
17	C	6.5042	-3.4980	0.8577
18	C	5.0414	-3.2060	0.5411
19	H	4.4483	-4.1169	0.5261
20	H	4.6380	-2.5065	1.2770
21	N	7.2399	-2.8859	-0.1445
22	H	8.2473	-2.8839	-0.1852
23	O	6.9399	-4.1240	1.7853
24	O	6.7918	-1.5275	-1.9965
25	N	5.1467	-2.5958	-0.7797
26	N	4.1434	-1.7142	-1.2446
27	H	3.9270	-0.9704	-0.5118
28	H	4.4989	-1.2853	-2.1026
29	Cl	1.5782	-3.2961	-1.2139
30	H	3.2532	-2.2658	-1.4207

NF-BM-RA1

Energy (POTENTIAL) = -893.083212676 Eh

Gibbs energy= -893.011440 Eh

Three lowest frequencies (cm^{-1}): 33.2393, 67.5840, 139.3011

	Atom	X	Y	Z
1	C	-0.9733	-1.1961	-0.1875
2	C	-1.7174	0.9850	-0.0057
3	C	-0.4295	0.8715	0.8008
4	H	0.3738	1.4305	0.3160
5	H	-0.5751	1.2413	1.8135
6	N	-1.9394	-0.2723	-0.5442
7	H	-2.7009	-0.4951	-1.1658
8	O	-2.4056	1.9581	-0.1528
9	O	-0.8103	-2.3193	-0.6023
10	N	-0.1839	-0.5700	0.7668
11	N	1.1270	-1.0874	0.8991
12	H	1.3191	-1.3024	1.8752
13	H	1.1457	-1.9614	0.3647
14	H	1.9498	-0.3171	0.4353
15	Cl	2.9309	0.7847	-0.2411

NF-BM-RA2
Energy (POTENTIAL) = -1441.16962704 Eh
Gibbs energy= -1441.028797 Eh
Three lowest frequencies (cm^{-1}): 12.1653, 23.3720, 28.3361

	Atom	X	Y	Z
1	C	-2.7662	-1.1271	-0.5916
2	C	-4.9866	-0.4774	-0.6564
3	C	-4.4747	-0.2311	0.7559
4	H	-4.3759	0.8454	0.9173
5	H	-5.1397	-0.6711	1.4952
6	N	-3.9110	-0.9896	-1.3578
7	H	-3.9285	-1.2034	-2.3430
8	O	-6.0904	-0.2696	-1.0823
9	O	-1.6557	-1.4160	-0.9569
10	N	-3.1650	-0.8857	0.7270
11	N	-2.1509	-0.3776	1.5792
12	H	-2.3470	-0.6451	2.5412
13	H	-1.2100	-0.7550	1.3108
14	H	-2.0855	0.7202	1.4317
15	Cl	-2.0558	2.3597	0.6717
16	O	3.1984	-0.3541	0.3148
17	C	4.3032	0.1183	-0.2752
18	C	4.0509	1.1819	-1.0917
19	H	4.7740	1.7278	-1.6685
20	C	2.1753	0.4313	-0.1338
21	C	2.6547	1.3851	-0.9974
22	H	2.0661	2.1369	-1.4938
23	C	0.8282	0.1782	0.3235
24	H	0.0726	0.8591	-0.0925
25	O	0.5333	-0.7017	1.1180
26	N	5.5443	-0.5402	0.0273
27	O	5.5174	-1.4848	0.7981
28	O	6.5376	-0.0855	-0.5260

NF-BM-INT

Energy (POTENTIAL) = -1441.17150675 Eh

Gibbs energy= -1441.029809 Eh

Three lowest frequencies (cm^{-1}): 18.4424, 21.8952, 32.9804

	Atom	X	Y	Z
1	C	0.6085	-1.1522	1.1111
2	H	0.3728	-0.2737	1.7222
3	O	0.5319	-2.3452	1.8474
4	H	-0.4117	-2.5141	2.0227
5	C	-2.2171	0.4355	-0.4277
6	C	-2.4622	-1.3405	1.0812
7	C	-3.6323	0.4016	0.1205
8	H	-2.2214	0.2993	-1.5098
9	H	-1.7358	1.3872	-0.2021
10	N	-1.5940	-0.6795	0.2644
11	O	-2.2512	-2.3117	1.7806
12	O	-4.5513	1.1554	-0.1332
13	N	-3.6829	-0.6596	0.9782
14	H	-4.4968	-0.9235	1.5123
15	N	-0.3012	-1.0861	-0.0326
16	H	-0.3052	-1.9642	-0.5430
17	H	-4.1887	2.3795	-1.2896
18	Cl	-3.7589	3.2434	-2.1915
19	O	2.3796	0.1347	0.0620
20	C	3.6715	-0.0091	-0.3107
21	C	4.1458	-1.2490	-0.0101
22	H	5.1386	-1.6117	-0.2024
23	C	2.0146	-1.0494	0.6173
24	C	3.0572	-1.9282	0.6002
25	H	3.0385	-2.9303	0.9867
26	N	4.3034	1.1074	-0.9267
27	O	5.4756	0.9540	-1.2595
28	O	3.6486	2.1300	-1.0817

NF-BM-R1

Energy (POTENTIAL) = -432.226260871 Eh

Gibbs energy= -432.161485 Eh

Three lowest frequencies (cm^{-1}): 46.7582, 139.8312, 189.4267

	Atom	X	Y	Z
1	C	-0.6666	0.8014	-0.0196
2	C	1.4865	-0.0687	0.0072
3	C	0.5013	-1.2319	0.0127
4	H	0.6774	-1.8837	-0.8438
5	H	0.6160	-1.8188	0.9261
6	N	0.7139	1.0674	-0.0098
7	H	1.0823	2.0050	-0.0118
8	O	2.6923	-0.1269	0.0160
9	O	-1.5562	1.6220	0.0010
10	N	-1.9852	-1.2496	0.0556
11	H	-2.4933	-0.9101	0.8660
12	H	-2.5524	-1.0574	-0.7627
13	N	-0.7790	-0.5587	-0.0529

NF-BM-R3_P3
Energy (POTENTIAL) = -460.844959324 Eh
Gibbs energy= -460.856168 Eh
Vibrational frequency (cm^{-1}): 2931.0305

	Atom	X	Y	Z
1	Cl	0.9853	-0.8681	0.2351
2	H	-0.2583	-0.6479	-0.0011

NF-BM-R2

Energy (POTENTIAL) = -548.068467486 Eh

Gibbs energy= -548.020618 Eh

Three lowest frequencies (cm^{-1}): 62.7818, 134.5460, 137.7671

	Atom	X	Y	Z
1	O	-0.3553	-0.4914	0.0000
2	C	0.7544	0.2606	0.0000
3	C	0.4805	1.5965	0.0000
4	H	1.2004	2.3936	0.0000
5	C	-1.3997	0.3850	0.0000
6	C	-0.9324	1.6750	0.0000
7	H	-1.5370	2.5651	0.0000
8	C	-2.7623	-0.1329	0.0000
9	H	-3.5271	0.6639	0.0000
10	O	-3.0518	-1.3061	0.0000
11	N	2.0157	-0.4240	0.0000
12	O	2.0054	-1.6437	0.0000
13	O	3.0113	0.2905	0.0000

NF-BM-P1

Energy (POTENTIAL) = -76.4634843278 Eh

Gibbs energy= -76.459889 Eh

Three lowest frequencies (cm^{-1}): 1635.1854, 3797.0765, 3890.9317

	Atom	X	Y	Z
1	O	0.0000	0.0000	0.1116
2	H	0.0000	0.7596	-0.4783
3	H	0.0000	-0.7596	-0.4783

NF-BM-P2

Energy (POTENTIAL) = -903.841792117 Eh

Gibbs energy= -903.730593 Eh

Three lowest frequencies (cm^{-1}): 28.6187, 39.7805, 51.7576

	Atom	X	Y	Z
1	C	-7.7326	-0.3076	-0.3974
2	C	-9.2174	0.3678	1.2616
3	C	-7.9643	1.2179	1.3849
4	H	-8.1991	2.2734	1.2518
5	H	-7.4996	1.0799	2.3607
6	N	-8.9817	-0.4820	0.2025
7	H	-9.6377	-1.1733	-0.1270
8	O	-10.2119	0.4182	1.9388
9	O	-7.2995	-0.9307	-1.3383
10	N	-7.1205	0.7147	0.3112
11	N	-5.9048	1.2687	0.1414
12	O	-3.4492	2.4821	-0.0996
13	C	-2.2098	2.8504	-0.4859
14	C	-1.7704	2.1217	-1.5517
15	H	-0.8200	2.2255	-2.0414
16	C	-3.8275	1.4815	-0.9416
17	C	-2.8250	1.2289	-1.8494
18	H	-2.8536	0.4897	-2.6304
19	C	-5.1169	0.8668	-0.7905
20	H	-5.3609	0.0777	-1.4893
21	N	-1.5787	3.8964	0.2427
22	O	-2.1897	4.4038	1.1742
23	O	-0.4501	4.2125	-0.1282

NF-BM-TS2

Energy (POTENTIAL) = -1441.14870744 Eh

Gibbs energy= -1441.003953 Eh

Three lowest frequencies (cm^{-1}): -109.3199, 31.1593, 36.1089

	Atom	X	Y	Z
1	C	-7.5403	0.4353	1.4316
2	C	-9.4321	0.3351	0.0936
3	C	-8.3942	1.1615	-0.6541
4	H	-8.0844	0.6149	-1.5439
5	H	-8.7959	2.1369	-0.9230
6	N	-8.8406	-0.0289	1.2859
7	H	-9.2623	-0.6536	1.9545
8	O	-10.5449	0.0603	-0.2710
9	O	-6.7629	0.1892	2.3191
10	N	-7.3222	1.2578	0.3339
11	N	-6.0466	1.6572	0.0313
12	H	-5.8800	2.6508	-0.0109
13	H	-4.4918	0.0834	-2.4495
14	H	-5.9146	-0.5220	-1.9224
15	Cl	-6.8430	-1.8733	-1.3183
16	O	-3.5012	2.5897	-0.4265
17	C	-2.1696	2.7700	-0.3201
18	C	-1.5147	1.6028	-0.0773
19	H	-0.4552	1.4821	0.0522
20	C	-3.7126	1.2558	-0.2417
21	C	-2.5291	0.6098	-0.0270
22	H	-2.4046	-0.4431	0.1555
23	C	-5.0862	0.7822	-0.2924
24	H	-5.2538	-0.2317	0.0467
25	O	-5.3249	0.3661	-2.0462
26	N	-1.6798	4.1081	-0.4699
27	O	-2.4958	4.9940	-0.6708
28	O	-0.4673	4.2475	-0.3814

NF-BM-TS1

Energy (POTENTIAL) = -1441.15792398 Eh

Gibbs energy= 1411.017877 Eh

Three lowest frequencies (cm^{-1}): -522.2677, 27.8982, 40.3578

	Atom	X	Y	Z
1	C	1.2458	-0.5751	1.7685
2	C	3.2780	0.2931	1.0902
3	C	2.8451	-0.7561	0.0677
4	H	2.6259	-0.2712	-0.8855
5	H	3.6264	-1.4985	-0.0865
6	N	2.2872	0.3064	2.0474
7	H	2.2459	0.9636	2.8102
8	O	4.2740	0.9668	1.0641
9	O	0.1879	-0.6785	2.3507
10	N	1.6575	-1.3164	0.6872
11	N	0.6782	-1.9642	-0.0824
12	H	1.1023	-2.7164	-0.6263
13	H	-0.2754	-2.5207	-2.7549
14	H	-0.0056	-2.3524	0.5625
15	Cl	1.0393	-3.3004	-3.1207
16	O	-0.5748	0.9183	-0.1351
17	C	-1.4035	1.4749	0.7610
18	C	-2.6447	0.9097	0.7384
19	H	-3.4776	1.1819	1.3595
20	C	-1.2957	-0.0708	-0.7438
21	C	-2.5720	-0.1043	-0.2444
22	H	-3.3471	-0.7860	-0.5452
23	C	-0.5718	-0.8984	-1.6690
24	H	0.3854	-0.5334	-2.0307
25	O	-1.1341	-1.8708	-2.2347
26	N	-0.8621	2.5005	1.5991
27	O	0.3255	2.7680	1.4789
28	O	-1.6416	3.0241	2.3828

NF-BM-PA

Energy (POTENTIAL) = -1441.17255480 Eh

Gibbs energy= -1441.038165 Eh

Three lowest frequencies (cm^{-1}): 13.4102, 23.3723, 36.0540

	Atom	X	Y	Z
1	C	-7.7284	-0.2186	-0.4211
2	C	-9.2071	0.2852	1.2985
3	C	-7.9243	1.0574	1.5482
4	H	-8.1107	2.1307	1.5224
5	H	-7.4969	0.7963	2.5153
6	N	-8.9900	-0.4180	0.1305
7	H	-9.6719	-1.0186	-0.3066
8	O	-10.2067	0.2780	1.9673
9	O	-7.3287	-0.6996	-1.4602
10	N	-7.0688	0.6311	0.4472
11	N	-5.8660	1.2420	0.2843
12	H	-5.8557	2.9898	0.8929
13	H	-4.8459	-2.1706	-3.0772
14	H	-5.9072	-1.1029	-2.8288
15	Cl	-6.1356	4.2317	1.2380
16	O	-3.3759	2.4768	0.0128
17	C	-2.1668	2.8613	-0.4417
18	C	-1.7497	2.1023	-1.4955
19	H	-0.8244	2.2147	-2.0292
20	C	-3.7565	1.4315	-0.7741
21	C	-2.7877	1.1661	-1.7120
22	H	-2.8505	0.3983	-2.4634
23	C	-5.0181	0.7874	-0.5678
24	H	-5.1879	-0.0835	-1.1826
25	O	-4.9971	-1.2223	-3.1331
26	N	-1.5289	3.9477	0.2286
27	O	-2.1014	4.4526	1.1829
28	O	-0.4362	4.2885	-0.2165

DT-BM-Comp
Energy (POTENTIAL) = -1786.21147316 Eh
Gibbs energy= -1786.041870 Eh
Three lowest frequencies (cm^{-1}): 14.2537, 22.7744, 24.1040

	Atom	X	Y	Z
1	H	1.7698	-1.0601	1.3533
2	Cl	3.4506	-0.0289	1.2036
3	C	-1.4278	-1.0861	0.9755
4	C	-1.4583	0.2433	-0.9174
5	C	0.0016	-0.0514	-0.5905
6	H	0.4201	-0.7199	-1.3464
7	H	0.5881	0.8619	-0.5322
8	N	-2.2044	-0.4118	0.0491
9	H	-3.2122	-0.4216	0.0746
10	O	-1.8846	0.9020	-1.8266
11	O	-1.7746	-1.8369	1.8544
12	N	-0.1186	-0.7125	0.7044
13	N	0.8831	-1.6071	1.1478
14	H	0.5206	-2.0685	1.9857
15	H	1.1098	-2.3221	0.3904
16	C	6.4699	-2.1875	-1.0608
17	C	6.5005	-3.5171	0.8319
18	C	5.0405	-3.2226	0.5051
19	H	4.4541	-4.1360	0.4466
20	H	4.6219	-2.5542	1.2611
21	N	7.2465	-2.8618	-0.1344
22	H	8.2543	-2.8519	-0.1599
23	O	6.9268	-4.1759	1.7410
24	O	6.8166	-1.4365	-1.9396
25	N	5.1607	-2.5613	-0.7898
26	N	4.1589	-1.6667	-1.2331
27	H	3.9322	-0.9518	-0.4756
28	H	4.5212	-1.2053	-2.0710
29	Cl	1.5914	-3.2449	-1.2888
30	H	3.2722	-2.2138	-1.4384

DT-BM-RA1

Energy (POTENTIAL) = -893.083780922 Eh

Gibbs energy= -893.011972 Eh

Three lowest frequencies (cm^{-1}): 33.1188, 67.2368, 139.3974

	Atom	X	Y	Z
1	C	-0.9729	-1.1958	-0.1883
2	C	-1.7175	0.9848	-0.0056
3	C	-0.4299	0.8715	0.8013
4	H	0.3731	1.4313	0.3171
5	H	-0.5759	1.2402	1.8142
6	N	-1.9392	-0.2721	-0.5445
7	H	-2.7010	-0.4950	-1.1659
8	O	-2.4060	1.9581	-0.1524
9	O	-0.8100	-2.3189	-0.6033
10	N	-0.1836	-0.5698	0.7659
11	N	1.1272	-1.0869	0.8994
12	H	1.3191	-1.3003	1.8759
13	H	1.1461	-1.9618	0.3664
14	H	1.9491	-0.3189	0.4354
15	Cl	2.9325	0.7835	-0.2434

DT-BM-RA2

Energy (POTENTIAL) = -1672.35041598 Eh

Gibbs energy= -1672.135411 Eh

Three lowest frequencies (cm^{-1}): 11.2986, 18.6346, 23.0312

	Atom	X	Y	Z
1	C	-2.7994	-1.1607	-0.6035
2	C	-5.0484	-0.6155	-0.5211
3	C	-4.4542	-0.3331	0.8510
4	H	-4.3971	0.7480	1.0017
5	H	-5.0439	-0.7994	1.6369
6	N	-4.0005	-1.0827	-1.2909
7	H	-4.0747	-1.3082	-2.2706
8	O	-6.1880	-0.4644	-0.8718
9	O	-1.7066	-1.4060	-1.0454
10	N	-3.1181	-0.9219	0.7354
11	N	-2.0774	-0.3669	1.5221
12	H	-2.1996	-0.6462	2.4926
13	H	-1.1259	-0.6951	1.2003
14	H	-2.0799	0.7313	1.3859
15	Cl	-2.1968	2.3986	0.6836
16	O	3.2135	-0.1574	0.2113
17	C	4.3365	0.3525	-0.3497
18	C	4.0079	1.4066	-1.1738
19	H	4.6905	2.0036	-1.7510
20	C	2.1543	0.5712	-0.2527
21	C	2.6076	1.5451	-1.1095
22	H	1.9940	2.2676	-1.6192
23	C	0.8273	0.2603	0.1827
24	H	0.0471	0.9070	-0.2412
25	O	0.5496	-0.6371	0.9757
26	C	5.5977	-0.2675	0.0007
27	C	5.6331	-1.3657	0.8707
28	C	6.7974	0.2282	-0.5281
29	C	6.8377	-1.9558	1.2048
30	H	4.7127	-1.7513	1.2807
31	C	8.0045	-0.3564	-0.1991
32	H	6.7857	1.0751	-1.1976
33	C	8.0086	-1.4433	0.6650
34	H	6.8813	-2.8010	1.8724
35	H	8.9348	0.0142	-0.5978
36	N	9.2906	-2.0674	1.0180

37	O	10.3082	-1.5975	0.5276
38	O	9.2697	-3.0220	1.7825

DT-BM-TS1

Energy (POTENTIAL) = -1672.33928354 Eh

Gibbs energy= -1672.121304 Eh

Three lowest frequencies (cm^{-1}): -47.9133, 19.1509, 24.0777

	Atom	X	Y	Z
1	C	1.0390	-0.9052	1.8641
2	C	2.7929	0.5229	1.3813
3	C	2.6293	-0.4461	0.2141
4	H	2.2925	0.0978	-0.6699
5	H	3.5703	-0.9431	-0.0158
6	N	1.8362	0.1565	2.2993
7	H	1.6757	0.6305	3.1737
8	O	3.5806	1.4293	1.4749
9	O	0.0314	-1.3252	2.3873
10	N	1.6173	-1.3650	0.7070
11	N	0.7944	-2.0594	-0.1983
12	H	1.3458	-2.6841	-0.7881
13	H	-0.3719	-2.4691	-2.8034
14	H	0.1375	-2.6057	0.3527
15	Cl	1.1202	-3.2081	-3.2667
16	O	-0.5168	0.8908	-0.1929
17	C	-1.2963	1.4665	0.7573
18	C	-2.5273	0.8487	0.7781
19	H	-3.3534	1.0995	1.4183
20	C	-1.2497	-0.1164	-0.7713
21	C	-2.4948	-0.1659	-0.1962
22	H	-3.2758	-0.8600	-0.4507
23	C	-0.5644	-0.9279	-1.7086
24	H	0.3867	-0.5871	-2.0998
25	O	-1.1408	-1.9151	-2.2681
26	C	0.3944	4.5620	3.0556
27	C	-0.8189	4.0128	3.4484
28	C	-1.3714	3.0025	2.6855
29	C	-0.7184	2.5435	1.5334
30	C	0.5010	3.1226	1.1588
31	C	1.0636	4.1297	1.9200
32	N	0.9879	5.6326	3.8704
33	H	-1.3059	4.3732	4.3399
34	H	-2.3043	2.5554	2.9940
35	H	1.0085	2.7824	0.2702
36	H	2.0066	4.5750	1.6485

37	O	2.0447	6.1165	3.4925
38	O	0.3893	5.9776	4.8798

DT-BM-INT
Energy (POTENTIAL) = -1672.34538350 Eh
Gibbs energy= -1672.130684 Eh
Three lowest frequencies (cm^{-1}): 11.1112, 15.1896, 21.8514

	Atom	X	Y	Z
1	C	0.6151	-1.1763	1.0979
2	H	0.3843	-0.3034	1.7199
3	O	0.5125	-2.3767	1.8226
4	H	-0.4343	-2.5430	1.9764
5	C	-2.1915	0.4726	-0.3869
6	C	-2.4707	-1.3602	1.0433
7	C	-3.6099	0.4382	0.1515
8	H	-2.1915	0.3871	-1.4742
9	H	-1.6972	1.4053	-0.1145
10	N	-1.5898	-0.6817	0.2560
11	O	-2.2798	-2.3602	1.7064
12	O	-4.5146	1.2192	-0.0750
13	N	-3.6825	-0.6571	0.9607
14	H	-4.5031	-0.9310	1.4793
15	N	-0.2954	-1.0828	-0.0463
16	H	-0.2995	-1.9486	-0.5771
17	H	-4.0865	2.5050	-1.1144
18	Cl	-3.5961	3.4339	-1.9198
19	O	2.4002	0.0883	0.0427
20	C	3.7114	-0.0388	-0.3397
21	C	4.1499	-1.2926	-0.0125
22	H	5.1340	-1.6894	-0.1876
23	C	2.0211	-1.0885	0.6072
24	C	3.0567	-1.9683	0.5999
25	H	3.0340	-2.9682	0.9922
26	C	5.5367	3.2756	-2.2038
27	C	4.2014	3.3596	-1.8329
28	C	3.6044	2.2738	-1.2217
29	C	4.3325	1.0998	-0.9764
30	C	5.6810	1.0463	-1.3631
31	C	6.2842	2.1261	-1.9743
32	N	6.1725	4.4225	-2.8512
33	H	3.6499	4.2655	-2.0263
34	H	2.5667	2.3262	-0.9313
35	H	6.2587	0.1523	-1.1810
36	H	7.3190	2.0940	-2.2741

37	0	7.3525	4.3231	-3.1666
38	0	5.4931	5.4234	-3.0449

DT-BM-TS2

Energy (POTENTIAL) = -1672.32716685 Eh

Gibbs energy= -1672.111424 Eh

Three lowest frequencies (cm^{-1}): -301.5212, 18.9733, 21.9891

	Atom	X	Y	Z
1	C	-7.5036	0.2793	1.4722
2	C	-9.4290	0.3558	0.1791
3	C	-8.3863	1.2279	-0.5064
4	H	-8.1235	0.7798	-1.4635
5	H	-8.7653	2.2386	-0.6520
6	N	-8.8203	-0.1414	1.3112
7	H	-9.2455	-0.8132	1.9300
8	O	-10.5582	0.1475	-0.1826
9	O	-6.7220	-0.0685	2.3221
10	N	-7.2821	1.1844	0.4480
11	N	-6.0103	1.6070	0.1694
12	H	-5.8372	2.5973	0.2192
13	H	-4.5963	0.2845	-2.4645
14	H	-6.0355	-0.3925	-1.9726
15	Cl	-6.9606	-1.7525	-1.6085
16	O	-3.4801	2.5757	-0.4420
17	C	-2.1310	2.7867	-0.3532
18	C	-1.5021	1.5898	-0.1362
19	H	-0.4442	1.4348	-0.0258
20	C	-3.6958	1.2381	-0.2759
21	C	-2.5119	0.5928	-0.0890
22	H	-2.3834	-0.4631	0.0726
23	C	-5.0694	0.7632	-0.3194
24	H	-5.2015	-0.2672	-0.0158
25	O	-5.4153	0.5222	-2.0059
26	C	-0.7290	6.7339	-0.8203
27	C	-2.0815	6.4771	-0.9903
28	C	-2.5415	5.1827	-0.8347
29	C	-1.6564	4.1461	-0.5097
30	C	-0.2953	4.4379	-0.3422
31	C	0.1720	5.7279	-0.4970
32	N	-0.2362	8.1067	-0.9868
33	H	-2.7513	7.2832	-1.2421
34	H	-3.5902	4.9692	-0.9709
35	H	0.3995	3.6528	-0.0845
36	H	1.2158	5.9651	-0.3700

37	O	0.9607	8.3062	-0.8305
38	O	-1.0494	8.9747	-1.2730

NF-BM-R1

Energy (POTENTIAL) = -432.226528694 Eh

Gibbs energy= -432.161728 Eh

Three lowest frequencies (cm^{-1}): 48.0439, 140.0751, 189.5314

	Atom	X	Y	Z
1	C	-0.6665	0.8014	-0.0196
2	C	1.4864	-0.0687	0.0072
3	C	0.5013	-1.2319	0.0128
4	H	0.6772	-1.8836	-0.8439
5	H	0.6159	-1.8187	0.9261
6	N	0.7140	1.0674	-0.0098
7	H	1.0824	2.0050	-0.0119
8	O	2.6923	-0.1270	0.0160
9	O	-1.5560	1.6222	0.0008
10	N	-1.9852	-1.2496	0.0556
11	H	-2.4933	-0.9105	0.8661
12	H	-2.5524	-1.0574	-0.7628
13	N	-0.7791	-0.5586	-0.0527

NF-BM-R3_P3
Energy (POTENTIAL) = -460.845013373 Eh
Gibbs energy= -460.856223 Eh
Vibrational frequency (cm^{-1}): 2930.5214

	Atom	X	Y	Z
1	Cl	0.9854	-0.8681	0.2351
2	H	-0.2584	-0.6479	-0.0011

NF-BM-P1

Energy (POTENTIAL) = -76.4636072122 Eh

Gibbs energy= -76.460014 Eh

Three lowest frequencies (cm^{-1}): 1634.9965, 3796.9517, 3890.5583

	Atom	X	Y	Z
1	O	0.0000	0.0000	0.1117
2	H	0.0000	0.7596	-0.4783
3	H	0.0000	-0.7596	-0.4783

NF-BM-R2

Energy (POTENTIAL) = -779.247746017 Eh

Gibbs energy= -779.126090 Eh

Three lowest frequencies (cm^{-1}): 30.7386, 56.6186, 58.8878

	Atom	X	Y	Z
1	O	-0.5030	-0.8511	0.6343
2	C	-1.4977	-1.0394	-0.2701
3	C	-1.5339	0.0221	-1.1441
4	H	-2.2145	0.1512	-1.9661
5	C	0.1029	0.3355	0.3419
6	C	-0.5046	0.9040	-0.7484
7	H	-0.2362	1.8423	-1.2023
8	C	1.2100	0.7868	1.1559
9	H	1.6213	1.7584	0.8275
10	O	1.6669	0.1876	2.1077
11	C	-2.2848	-2.2491	-0.1509
12	C	-3.3268	-2.5060	-1.0529
13	C	-2.0149	-3.1759	0.8656
14	C	-4.0818	-3.6570	-0.9455
15	H	-3.5468	-1.8023	-1.8417
16	C	-2.7663	-4.3305	0.9792
17	H	-1.2143	-2.9840	1.5629
18	C	-3.7914	-4.5571	0.0717
19	H	-4.8856	-3.8670	-1.6321
20	H	-2.5701	-5.0519	1.7558
21	N	-4.5918	-5.7815	0.1883
22	O	-5.4916	-5.9555	-0.6231
23	O	-4.3160	-6.5617	1.0896

NF-BM-P2
Energy (POTENTIAL) = -1135.01737740 Eh
Gibbs energy= -1134.832228 Eh
Three lowest frequencies (cm^{-1}): 23.5288, 28.6176, 30.7268

	Atom	X	Y	Z
1	C	-7.5207	-0.6693	-0.0733
2	C	-9.1896	0.1935	1.2987
3	C	-8.0380	1.1843	1.2782
4	H	-8.3661	2.1461	0.8842
5	H	-7.6395	1.3319	2.2817
6	N	-8.7930	-0.8429	0.4859
7	H	-9.3489	-1.6623	0.2963
8	O	-10.2322	0.2876	1.8965
9	O	-6.9631	-1.4454	-0.8160
10	N	-7.0693	0.5457	0.4022
11	N	-5.8979	1.1886	0.1735
12	O	-3.5331	2.5599	-0.2434
13	C	-2.2945	2.9799	-0.6387
14	C	-1.7444	2.0427	-1.4765
15	H	-0.7784	2.0951	-1.9457
16	C	-3.7707	1.3541	-0.8308
17	C	-2.6914	0.9991	-1.5998
18	H	-2.5996	0.0967	-2.1786
19	C	-5.0066	0.6684	-0.5942
20	H	-5.1299	-0.2849	-1.0913
21	C	-1.8305	4.2492	-0.1301
22	C	-0.5715	4.7455	-0.5034
23	C	-2.6274	5.0054	0.7430
24	C	-0.1200	5.9570	-0.0220
25	H	0.0551	4.1779	-1.1752
26	C	-2.1817	6.2194	1.2291
27	H	-3.5965	4.6319	1.0353
28	C	-0.9317	6.6835	0.8417
29	H	0.8448	6.3473	-0.3024
30	H	-2.7851	6.8087	1.9004
31	N	-0.4564	7.9690	1.3542
32	O	-1.1883	8.5904	2.1149
33	O	0.6492	8.3567	0.9957

DT-BM-PA

Energy (POTENTIAL) = -1672.35262982 Eh

Gibbs energy= -1672.143735 Eh

Three lowest frequencies (cm^{-1}): 14.7358, 22.0651, 26.8770

	Atom	X	Y	Z
1	C	-7.7247	0.2560	-0.5662
2	C	-9.0929	0.4444	1.2984
3	C	-7.6940	0.8832	1.6965
4	H	-7.6884	1.9407	1.9630
5	H	-7.3321	0.3031	2.5439
6	N	-9.0035	0.1067	-0.0358
7	H	-9.7797	-0.2082	-0.5965
8	O	-10.0763	0.3948	1.9906
9	O	-7.4200	0.0965	-1.7302
10	N	-6.9186	0.6268	0.4898
11	N	-5.6727	1.2035	0.3676
12	H	-5.5306	2.6798	1.1117
13	H	-5.4661	-2.1214	-3.1539
14	H	-6.0470	-0.7477	-2.8124
15	Cl	-5.5983	3.8822	1.7422
16	O	-3.1310	2.3283	-0.0851
17	C	-1.8889	2.6242	-0.5591
18	C	-1.5336	1.7034	-1.5167
19	H	-0.6138	1.6851	-2.0727
20	C	-3.5676	1.2149	-0.7405
21	C	-2.6118	0.7994	-1.6342
22	H	-2.7096	-0.0416	-2.2984
23	C	-4.8516	0.6684	-0.4688
24	H	-5.0899	-0.2279	-1.0264
25	O	-5.2186	-1.2003	-3.0319
26	C	-1.2251	3.7827	-0.0032
27	C	-1.8728	4.5894	0.9435
28	C	0.0760	4.1124	-0.4108
29	C	-1.2357	5.6976	1.4698
30	H	-2.8765	4.3476	1.2585
31	C	0.7168	5.2182	0.1105
32	H	0.5881	3.4991	-1.1371
33	C	0.0515	5.9992	1.0475
34	H	-1.7223	6.3275	2.1968
35	H	1.7164	5.4828	-0.1935
36	N	0.7298	7.1745	1.6036

37	O	1.8629	7.4211	1.2102
38	O	0.1275	7.8457	2.4309

NF-SOL-R1
Energy (POTENTIAL) = -432.233833872 Eh
Gibbs energy= -432.169127 Eh
Three lowest frequencies (cm^{-1}): 43.9816, 148.1338, 194.0461

	Atom	X	Y	Z
1	C	-0.6643	0.8004	-0.0082
2	C	1.4835	-0.0680	0.0050
3	C	0.5008	-1.2294	0.0310
4	H	0.6451	-1.8681	-0.8415
5	H	0.6445	-1.8271	0.9324
6	N	0.7159	1.0666	-0.0161
7	H	1.0852	2.0043	-0.0353
8	O	2.6929	-0.1272	0.0034
9	O	-1.5518	1.6286	-0.0203
10	N	-1.9861	-1.2510	0.0416
11	H	-2.5181	-0.9706	0.8587
12	H	-2.5291	-1.0127	-0.7814
13	N	-0.7798	-0.5543	0.0153

NF-SOL-R3_P3
Energy (POTENTIAL) = -229.195108211 Eh
Gibbs energy= -229.160908 Eh
Three lowest frequencies (cm^{-1}): 74.6242, 430.0155, 544.9171

	Atom	X	Y	Z
1	C	-2.0479	0.9209	1.1825
2	H	-2.8202	1.4202	1.7578
3	H	-2.1143	-0.1574	1.3260
4	H	-2.1883	1.1179	0.1199
5	O	0.2951	0.8082	0.9216
6	C	-0.6969	1.4064	1.6130
7	O	-0.4813	2.2310	2.4701
8	H	1.1376	1.1631	1.2444

NF-SOL-R2
Energy (POTENTIAL) = -548.076160296 Eh
Gibbs energy= -548.028210 Eh
Three lowest frequencies (cm^{-1}): 65.6273, 135.3598, 139.1407

	Atom	X	Y	Z
1	O	-0.3562	-0.4896	-0.0000
2	C	0.7538	0.2637	0.0000
3	C	0.4805	1.6002	0.0000
4	H	1.1965	2.4007	0.0001
5	C	-1.3995	0.3903	0.0000
6	C	-0.9315	1.6800	0.0000
7	H	-1.5340	2.5712	0.0001
8	C	-2.7574	-0.1324	-0.0000
9	H	-3.5290	0.6535	-0.0000
10	O	-3.0342	-1.3128	-0.0000
11	N	2.0070	-0.4237	0.0000
12	O	1.9940	-1.6467	-0.0000
13	O	3.0124	0.2780	0.0000

NF-SOL-P1
Energy (POTENTIAL) = -76.4670027177 Eh
Gibbs energy= -76.463456 Eh
Three lowest frequencies (cm^{-1}): 1631.3574, 3792.7827, 3879.0725

	Atom	X	Y	Z
1	O	0.0000	0.0000	0.1132
2	H	0.0000	0.7585	-0.4791
3	H	0.0000	-0.7585	-0.4791

NF-SOL-P2
Energy (POTENTIAL) = -903.852683385 Eh
Gibbs energy= -903.742330 Eh
Three lowest frequencies (cm^{-1}): 13.3671, 38.1957, 53.3690

	Atom	X	Y	Z
1	C	-7.7347	-0.3038	-0.3969
2	C	-9.2115	0.3715	1.2607
3	C	-7.9588	1.2178	1.3869
4	H	-8.1919	2.2734	1.2536
5	H	-7.4944	1.0731	2.3617
6	N	-8.9823	-0.4754	0.2032
7	H	-9.6408	-1.1649	-0.1265
8	O	-10.2069	0.4235	1.9422
9	O	-7.3045	-0.9275	-1.3405
10	N	-7.1168	0.7141	0.3116
11	N	-5.9024	1.2652	0.1388
12	O	-3.4531	2.4805	-0.1011
13	C	-2.2121	2.8513	-0.4861
14	C	-1.7701	2.1204	-1.5516
15	H	-0.8204	2.2213	-2.0432
16	C	-3.8267	1.4781	-0.9439
17	C	-2.8209	1.2266	-1.8497
18	H	-2.8461	0.4869	-2.6299
19	C	-5.1148	0.8621	-0.7939
20	H	-5.3562	0.0730	-1.4924
21	N	-1.5908	3.8931	0.2408
22	O	-2.2061	4.4028	1.1740
23	O	-0.4594	4.2216	-0.1179

NF-SOL-Comp
Energy (POTENTIAL) = -661.449801069 Eh
Gibbs energy= -661.331956 Eh
Three lowest frequencies (cm^{-1}): 27.8007, 57.3154, 60.2640

	Atom	X	Y	Z
1	N	-0.0575	0.3985	-1.6366
2	H	-0.9810	0.5077	-2.0415
3	H	-0.1358	0.5249	-0.6333
4	N	0.4146	-0.8848	-1.9043
5	C	1.6409	-1.1252	-2.6394
6	C	1.7079	-2.6470	-2.6672
7	N	0.5944	-3.0841	-1.9963
8	C	-0.1895	-2.0352	-1.5342
9	H	1.5988	-0.7250	-3.6528
10	O	2.5647	-3.3349	-3.1752
11	O	-1.2390	-2.1483	-0.9045
12	H	0.3157	-4.0555	-1.8213
13	H	2.5131	-0.7126	-2.1314
14	H	-1.8329	-3.6464	-0.5374
15	O	-2.2948	-4.4892	-0.2604
16	C	-2.3166	-6.8440	-0.2552
17	C	-1.6356	-5.5681	-0.6535
18	O	-0.5845	-5.5324	-1.2760
19	H	-2.4362	-6.8731	0.8276
20	H	-3.3139	-6.8772	-0.6937
21	H	-1.7370	-7.6986	-0.5880

NF-SOL-RA
Energy (POTENTIAL) = -1209.52964459 Eh
Gibbs energy= -1209.345055 Eh
Three lowest frequencies (cm^{-1}): 13.3445, 18.7923, 22.4999

	Atom	X	Y	Z
1	C	-0.7805	-0.7453	1.2603
2	H	-1.6655	-1.2151	0.8226
3	O	0.2415	-1.3874	1.4531
4	N	-0.1897	-0.0662	-1.4552
5	H	0.5892	0.3756	-0.9718
6	H	-0.4595	0.5068	-2.2480
7	C	-0.9083	0.6601	1.5952
8	O	-2.0943	1.2520	1.2598
9	C	-1.9892	2.5297	1.6482
10	C	-0.7838	2.7981	2.2319
11	C	-0.0800	1.5743	2.1972
12	N	-3.1109	3.3803	1.4047
13	O	-2.9965	4.5473	1.7632
14	O	-4.0953	2.8962	0.8636
15	H	0.9085	1.3838	2.5735
16	H	-0.4604	3.7429	2.6273
17	N	0.2385	-1.3133	-1.9021
18	C	1.4927	-1.5587	-2.5941
19	C	1.4895	-3.0690	-2.7606
20	N	0.3178	-3.4964	-2.1983
21	C	-0.4623	-2.4534	-1.6641
22	H	1.5275	-1.0694	-3.5693
23	O	2.3403	-3.7551	-3.2829
24	O	-1.5391	-2.5980	-1.1220
25	H	0.0205	-4.4585	-2.1614
26	H	2.3512	-1.2348	-2.0053
27	H	1.8083	-0.7694	1.6503
28	O	2.7455	-0.4730	1.7874
29	C	4.5634	0.7486	0.9133
30	C	3.1381	0.3032	0.7793
31	O	2.4079	0.6127	-0.1446
32	H	4.7017	1.2611	1.8650
33	H	5.2179	-0.1231	0.9150
34	H	4.8275	1.4074	0.0930

NF-SOL-TS1

Energy (POTENTIAL) = -1209.51823635 Eh

Gibbs energy= -1209.329374 Eh

Three lowest frequencies (cm^{-1}): -165.3947, 16.5512, 23.3328

	Atom	X	Y	Z
1	C	0.2941	-1.8635	-0.7759
2	H	-0.5877	-2.4738	-1.0080
3	O	1.3355	-2.4491	-0.3264
4	N	0.6286	-1.3610	-2.4973
5	H	1.5109	-0.8142	-2.4200
6	H	-0.1270	-0.7992	-2.8880
7	C	-0.0742	-0.5440	-0.1958
8	O	-1.2083	0.0477	-0.6689
9	C	-1.3274	1.2156	0.0006
10	C	-0.3106	1.3927	0.8904
11	C	0.5072	0.2419	0.7587
12	N	-2.4415	2.0353	-0.3155
13	O	-2.5424	3.0918	0.3044
14	O	-3.2239	1.6469	-1.1765
15	H	1.4088	0.0179	1.2988
16	H	-0.1757	2.2335	1.5454
17	N	0.8372	-2.4499	-3.3468
18	C	2.0196	-3.2962	-3.2928
19	C	1.5728	-4.4916	-4.1246
20	N	0.2509	-4.2688	-4.4353
21	C	-0.2382	-3.0669	-3.9273
22	H	2.8897	-2.8161	-3.7371
23	O	2.2398	-5.4450	-4.4444
24	O	-1.3692	-2.6363	-3.9908
25	H	-0.3183	-4.8959	-4.9825
26	H	2.2483	-3.6090	-2.2753
27	H	2.5960	-1.6626	-0.2076
28	O	3.5061	-1.1797	-0.0845
29	C	5.0996	0.3538	-0.8975
30	C	3.7877	-0.3557	-1.0659
31	O	3.0570	-0.1648	-2.0362
32	H	5.0721	0.9531	0.0127
33	H	5.9000	-0.3764	-0.7815
34	H	5.2974	0.9916	-1.7527

NF-SOL-INT
Energy (POTENTIAL) = -1209.53951883 Eh
Gibbs energy= -1209.348260 Eh
Three lowest frequencies (cm^{-1}): 14.2095, 25.1967, 28.4558

	Atom	X	Y	Z
1	C	-0.3757	-0.7939	0.6933
2	H	-1.2704	-1.4141	0.6090
3	O	0.5797	-1.5321	1.3724
4	N	0.1168	-0.4427	-0.6734
5	H	1.6501	0.4757	-0.5479
6	H	-0.5259	0.2066	-1.1205
7	C	-0.7150	0.4847	1.3945
8	O	-1.6559	1.2723	0.8050
9	C	-1.7921	2.3557	1.6066
10	C	-0.9702	2.2828	2.6900
11	C	-0.2666	1.0581	2.5477
12	N	-2.7221	3.3470	1.2061
13	O	-2.8419	4.3227	1.9444
14	O	-3.3421	3.1760	0.1613
15	H	0.4772	0.6543	3.2092
16	H	-0.8854	3.0100	3.4760
17	N	0.2418	-1.5662	-1.4866
18	C	1.5097	-2.2026	-1.7824
19	C	1.0786	-3.3728	-2.6564
20	N	-0.2894	-3.2915	-2.7480
21	C	-0.8265	-2.2104	-2.0410
22	H	2.1865	-1.5474	-2.3312
23	O	1.7904	-4.2053	-3.1668
24	O	-1.9967	-1.9046	-1.9530
25	H	-0.8636	-3.9334	-3.2721
26	H	2.0087	-2.5653	-0.8840
27	H	1.4104	-1.0046	1.4215
28	O	2.8304	-0.0183	1.4355
29	C	4.4505	1.5728	0.6587
30	C	3.1869	0.7737	0.5748
31	O	2.4902	1.0163	-0.5263
32	H	4.2063	2.6351	0.6671
33	H	4.9997	1.3123	1.5571
34	H	5.0623	1.3866	-0.2234

NF-SOL-PA
Energy (POTENTIAL) = -1209.54287775 Eh
Gibbs energy= -1209.357874 Eh
Three lowest frequencies (cm^{-1}): 14.7098, 25.7523, 38.6443

	Atom	X	Y	Z
1	C	-1.2354	-0.6912	0.3361
2	H	-1.9324	-1.4982	0.5066
3	O	1.9822	-2.4609	0.8110
4	N	-0.2754	-0.7618	-0.5176
5	H	1.0951	0.4395	-0.6144
6	C	-1.4132	0.4865	1.1333
7	O	-0.5710	1.5443	0.9748
8	C	-0.9674	2.4776	1.8651
9	C	-2.0440	2.0607	2.5941
10	C	-2.3353	0.7641	2.1165
11	N	-0.2300	3.6858	1.9089
12	O	-0.5968	4.5289	2.7255
13	O	0.7188	3.8178	1.1399
14	H	-3.1190	0.1075	2.4501
15	H	-2.5461	2.6159	3.3644
16	N	-0.0772	-1.8779	-1.2512
17	C	1.0498	-1.9003	-2.1740
18	C	1.1681	-3.3684	-2.5289
19	N	0.2179	-4.0112	-1.7743
20	C	-0.5162	-3.1616	-0.9532
21	H	0.8627	-1.2970	-3.0603
22	O	1.9358	-3.8764	-3.3102
23	O	-1.3598	-3.4936	-0.1532
24	H	0.0635	-5.0080	-1.7817
25	H	1.9632	-1.5704	-1.6824
26	H	2.0633	-1.5173	1.0379
27	O	2.4096	0.2841	1.3136
28	C	3.6349	2.1412	0.4074
29	C	2.5899	1.0682	0.3967
30	O	1.8589	1.0658	-0.7135
31	H	3.1455	3.0875	0.6417
32	H	4.3824	1.9277	1.1647
33	H	4.0978	2.2376	-0.5725
34	H	2.8901	-2.7681	0.7299

NF-SOL-TS2

Energy (POTENTIAL) = -1209.51169835 Eh

Gibbs energy= -1209.323125 Eh

Three lowest frequencies (cm^{-1}): -261.6497, 18.0121, 25.3706

	Atom	X	Y	Z
1	C	-0.3672	-1.1610	0.9650
2	H	-0.8315	-2.0561	1.3530
3	O	1.2816	-1.4658	1.8528
4	N	-0.1174	-1.1216	-0.3437
5	H	0.5311	-0.3349	-0.6943
6	C	-0.7234	0.0928	1.6118
7	O	-1.0438	0.0145	2.9320
8	C	-1.3338	1.2728	3.3145
9	C	-1.2160	2.1599	2.2862
10	C	-0.8176	1.3839	1.1708
11	N	-1.7107	1.4679	4.6736
12	O	-1.9660	2.6202	5.0098
13	O	-1.7547	0.4896	5.4087
14	H	-0.6121	1.7299	0.1743
15	H	-1.3931	3.2183	2.3299
16	N	-0.0650	-2.3207	-1.0342
17	C	-0.8316	-2.4952	-2.2601
18	C	-0.1783	-3.7216	-2.8770
19	N	0.8804	-4.0351	-2.0515
20	C	1.0021	-3.1814	-0.9663
21	H	-1.8869	-2.6737	-2.0619
22	O	-0.5092	-4.3087	-3.8765
23	O	1.8758	-3.2246	-0.1179
24	H	1.5005	-4.8182	-2.1926
25	H	-0.7291	-1.6383	-2.9271
26	H	1.8029	-0.6330	1.5065
27	O	2.5380	0.5534	1.0048
28	C	3.3869	2.1930	-0.4841
29	C	2.4258	1.0706	-0.1424
30	O	1.5643	0.7558	-1.0110
31	H	4.3765	1.9844	-0.0825
32	H	3.4398	2.3517	-1.5581
33	H	3.0268	3.1112	-0.0156
34	H	1.6171	-2.2040	1.2939