Supplementary Material

Rearrangement and cyclisation reactions on the 1-arylpyrrol-2-iminyl – 2aryliminopyrrol-1-yl radical energy surface

Scott Borthwick^a, Jonathan Foot^a, Maria Ieva^a, Hamish McNab^{a#}, Lilian McNab^{b*}, Emma J. Rozgowska,^a and Andrew Wright^a

^aSchool of Chemistry, The University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ UK ^b6 Torphin Road, Edinburgh EH13 0HW *Lilian.McNab@gmail.com*

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Experimental

1-(p-Tolyl)pyrrole 6.

A mixture of *p*-toluidine (4.53 g, 42.3 mmol), 2,5-dimethoxytetrahydrofuran (6.01 g, 45 mmol) and glacial acetic acid (20 cm³) was heated under reflux for 2 h. The volatiles were removed under reduced pressure, water (100 cm³) was added and the reaction mixture extracted with dichloromethane (3×80 cm³). The combined organic extracts were washed with water (80 cm³), dried (MgSO₄) and concentrated to give crude **6** (5.71 g, 86%), mp 77-78 °C (lit.,¹ 81-82 °C) \square_{H} 7.30-7.19 (4H, m), 7.06 (2H, t, ³J 2.2), 6.33 (2H, t, ³J 2.2) and 2.37 (3H, s); \square_{C} 138.32 (quat), 135.22 (quat), 129.89, 120.39, 119.24, 109.90 and 20.72; *m/z* 157 (M⁺, 100%), 115 (39) and 91 (30).

1-(p-Tolyl)pyrrole-2-carbaldehyde 7

A solution of 1-*p*-tolylpyrrole **6** (4.023 g, 25.6 mmol) in DMF (40 cm³) was added to a solution of phosphoryl chloride (5.19 g, 33.2 mmol) in DMF (85 cm³) and stirred for 1 h. A further portion of phosphoryl chloride (5.19 g, 33.2 mmol) in DMF (85 cm³) was added and stirring continued for another hour. The reaction mixture was poured onto crushed ice, hydrolysed with dilute aqueous sodium hydroxide (2 M, 200 cm³) and acidified to pH 6-7 with dilute hydrochloric acid (2 M, 20 cm³). The mixture was then extracted with ether (3 × 250 cm³) and the combined organic extracts were washed with water (200 cm³) and dried (MgSO₄). The solvent was removed under reduced pressure to give crude aldehyde as an orange oil. Distillation removed remaining traces of DMF and the aldehyde crystallised as an orange solid. TLC showed that formylation had occurred at both the 2- and 3-positions and so the mixture was recrystallised from light petroleum (bp 40-60 °C) to yield only the 2-isomer **7** as white crystals (3.30 g, 70%), mp 54-56 °C (lit.,² 55 °C); $\square_{\rm H}$ 9.55 (1H, s), 7.25-7.23 (4H, m), 7.15-7.13 (2H, m), 7.05-7.03 (2H, m), 6.38 (1H, m) and 2.41 (3H, s) (spectrum consistent with literature data³); $\square_{\rm C}$ 178.99, 138.11 (quat), 136.08 (quat), 132.46 (quat), 130.90, 129.55, 125.71, 121.54, 110.56 and 21.00; *m/z* 185 (M⁺, 100 %), 157 (55), 128 (36) and 92 (83).

N,N-(Dimethylamino)pyrrole 9

2,5-Dimethoxytetrahydrofuran (11 g, 83 mmol) was added to a stirred solution of *N*,*N*-dimethylhydrazine (5 g, 83mmol) in acetic acid (15 cm³) and heated at reflux for 2.5 h. The mixture was then quenched with sodium bicarbonate solution and extracted with dichloromethane (100 cm³); the organic layer was washed with water (2 × 50 cm³) and then brine (50 cm³). The organic layer was then dried (MgSO₄) filtered and concentrated under vacuum. The residue was purified by distillation, bp 100-105 °C (15 Torr) [lit.,⁴ 138-140 °C (767 Torr)], to give **9** as a pale yellow oil (4.9 g, 54%); $\square_{\rm H}$ 6.90 (2H, d, ³J 2.2), 6.08 (2H, ³J 2.2) and 2.87 (6H, s); $\delta_{\rm C}$ 116.20 (2CH), 105.67 (2CH) and 48.27 (2CH₃).

FVP reactions

General conditions are given in the main paper.

FVP of *N*,*N*-(dimethylamino)pyrrole 9 – temperature profile

Due to its low boiling point (138-140 °C at atmospheric pressure) N,N-(dimethylamino)pyrrole **9** was frozen in the inlet system using an acetone/dry ice bath which remained in place around the inlet as the vacuum was applied. The cooling bath was then slowly removed allowing the N,N-(dimethylamino)pyrrole **9** to volatilise into the furnace tube in a controlled manner.

*T*_f **550** °C, (24.8 mg, *T*_i RT, *P* 2.3-2.4 × 10⁻² Torr, *t* 16 min) gave *N*,*N*-(dimethylamino)pyrrole **9** (*ca* 97%) *T*_f **600** °C, (21.5 mg, *T*_i RT, *P* 2.4-3.0 × 10⁻² Torr, *t* 17 min) gave *N*,*N*-(dimethylamino)pyrrole **9** (*ca* 92%) and pyrrole **10** (*ca* 8%) *T*_f **650** °C, (21.3 mg, *T*_i RT, *P* 2.6-3.5 × 10⁻² Torr, *t* 16 min) gave *N*,*N*-(dimethylamino)pyrrole **9** (*ca* 63%) and pyrrole **10** (*ca* 37%) *T*_f **700** °C, (21.6 mg, *T*_i RT, *P* 2.6-3.2 × 10⁻² Torr, *t* 15 min) gave *N*,*N*-(dimethylamino)pyrrole **9** (*ca* 21%) and pyrrole **10** (*ca* 79%) *T*_f **750** °C, (24.3 mg, *T*_i RT, *P* 2.8-5.0 × 10⁻² Torr, *t* 17 min) gave *N*,*N*-(dimethylamino)pyrrole **9** (*ca* 18%) and pyrrole **10** (*ca* 82%) *T*_f **800** °C, (24.6 mg, *T*_i RT, *P* 2.5-6.0 × 10⁻² Torr, *t* 16 min) gave *N*,*N*-(dimethylamino)pyrrole **9** (*ca* 3%) and pyrrole **10** (*ca* 97%) *T*_f **850** °C, (25.5 mg, *T*_i RT, *P* 3.2-7.3 × 10⁻² Torr, *t* 19 min) gave pyrrole **10** (*ca* 99%).

N-(Dimethylamino)-3-(2-*p*-tolylvinyl)pyrrole 15

Synthesised as described in the main paper for **13**, from *N*-(dimethylamino)pyrrole-3-carboxaldehyde **14** in 60% yield, *N*-(dimethylamino)-3-(2-*p*-tolylvinyl)pyrrole **15** had mp 70 °C; (Found: M⁺ 226.1469. C₁₅H₁₈N₂ requires *M* 226.1470); $\delta_{\rm H}$ 7.34 (2H, d, ³*J* 8.1), 7.13 (2H, d, ³*J* 8.1), 6.97 (1H, m), 6.94 (1H, d, ³*J* 16.5), 6.84 (1H, t, ³*J* 2.8), 6.75 (1H, d, ³*J* 16.5), 6.31 (1H, t, ³*J* 2.8), 2.85 (6H, s) and 2.65 (3H, s); $\delta_{\rm C}$ 135.98 (quat), 135.45 (quat), 129.10 (2CH), 125.51 (2CH), 124.17 (CH), 121.24 (CH), 120.52 (quat), 117.80 (CH), 115.62 (CH), 103.12 (CH), 48.20 (2CH₃) and 21.04 (CH₃); *m/z* 226 (M⁺, 100%) and 167 (66).

FVP of *N*,*N*-dimethylamino-3-(2-*p*-tolylvinyl)pyrrole 15

FVP of *N*,*N*-dimethylamino-3-(2-*p*-tolylvinyl)pyrrole **15** [116 mg (0.51 mmol) T_f 750 °C, T_i 140 °C, *P* 2.1-10 × 10⁻² Torr, t 1 h) gave a mixture of products: 8-methylpyrrolo[1,2-*a*]quinoline **19** (4.6 mg, 5%); $\delta_{\rm H}$ 7.71 (1H, s), 7.54 (1H, d, ³*J* 7.9), 7.34 (1H, m), 7.27 (1H, d, ³*J* 9.3), 7.15 (1H, d, ³*J* 7.9), 6.97 (1H, d, ³*J* 9.3), 6.80 (1H, t, ³*J* 3.2), 6.52 (1H, m) and 2.56 (3H, s): 3-(2-*p*-tolylvinyl)pyrrole **20** (10.3 mg, 11%) (Found: M⁺ 183.1047. C₁₃H₁₃N requires *M* 183.1048); $\delta_{\rm H}$ 8.16 (1H, br. s), 7.37 (2H, d, ³*J* 8.1), 7.15 (2H, d, ³*J* 8.1), 7.04 (1H, d, ³*J* 16.2), 6.90 (1H, dd, ³*J* 4.2), 6.81 (1H, d, ³*J* 16.2), 6.80 (1H, dd, ⁴*J* 2.6), 6.51 (1H, dd, ³*J* 4.2, ⁴*J* 2.6) and 2.36 (3H, s); $\delta_{\rm C}$ 136.04 (quat), 135.40 (quat), 129.12 (2CH), 125.56 (2CH), 124.60 (CH), 123.10 (quat), 121.20 (CH), 119.01 (CH), 117.12 (CH), 105.45 (CH) and 20.82 (CH₃) (spectra consistent with literature data⁵); *m/z* 183 (M⁺, 100%): a fraction which was tentatively identified as impure 8-methylbenzo[*g*]indole **S1** (trace) (Found: M⁺ 181.0891. C₁₃H₁₁N requires *M* 181.0892); $\delta_{\rm H}$ 9.01 (1H, br. s), 7.85-7.80 (2H, m), 7.67 (1H, d, ³*J* 8.5), 7.49 (1H, d, ³*J* 8.5), 7.36-7.13 (2H, m), 6.12 (1H, m) and 2.39 (3H, s); *m/z* 181 (M⁺, 100%) and 84 (92).

Formation of products from FVP of N,N-dimethylamino-3-(2-p-tolylvinyl)pyrrole 15



Scheme 9 (from main paper) Reagents and conditions: (i) FVP, 750 °C

Three products were isolated, in low yield, from FVP of **15**. The product of hydrogen-capture by the pyrrol-1-yl radical, **20**, retains the carbon skeleton of the precursor. Similarly, the formation of 8-methylbenzo[g]indole **S1**, tentatively identified in trace amounts from an impure fraction, is consistent with delocalisation of the pyrrol-1-yl radical to the 2-position, followed by cyclisation. Clearly this is not a favourable process for the initial radical. Finally the formation of 8-methylpyrrolo[1,2-a]quinoline **19** requires rearrangement of the vinyl group from the 3-position to the 2-position of the pyrrole, followed by cyclisation. Such 1,5-shifts are well-known in the thermal chemistry of pyrroles,⁶ and although the rearrangement is not normally quantitative at temperatures as low as 750 °C in our apparatus, they may well account for the formation of such a minor product (5%).

References

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- 2. C. F. Candy, R. A. Jones and P. H. Wright, J. Chem. Soc. (C), 1970, 2563-2567.
- 3. B. R. D'Arcy, K. G. Lewis and C. E. Mulquiney, Aust. J. Chem., 1985, **38**, 953-965.
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DFT calculations of energy surfaces¹

1. The iminyl $\mathbf{1}$ (X = N) – pyrrol-1-yl $\mathbf{3}$ (X = N) energy surface





mi27-02



Energy = -534.049795 Ha

С	-3.041371	-0.098898	0.017981
С	-1.798626	0.516948	-0.101642
Ν	-0.824730	-0.456447	0.108077
С	-1.454297	-1.657409	0.351084
С	-2.823808	-1.468448	0.306345
С	-1.555645	1.912875	-0.449369
С	1.237008	0.605989	0.922772
С	2.628621	0.713203	0.895519
С	3.384003	-0.091995	0.037568
С	0.597369	-0.304639	0.073369
С	1.348210	-1.109017	-0.792774
С	2.741198	-1.004674	-0.803380
Ν	-0.467255	2.542078	-0.577728
Η	-3.997836	0.405034	-0.103670
Н	-0.865528	-2.544983	0.564929
Н	-3.576884	-2.234936	0.470313
Н	-2.494089	2.482683	-0.623993
Н	0.645838	1.222527	1.599479
Η	3.124433	1.427805	1.555599
Н	4.472598	-0.006488	0.023278
Η	0.835689	-1.802085	-1.462286
Η	3.323703	-1.632576	-1.480926

mi31-02



Energy = -534.0185255 Ha

Cartesian Coordinates

С	-3.123748	0.108241	0.000721
С	-1.852220	0.665420	-0.001048
Ν	-0.926150	-0.354882	-0.001769
С	-1.573990	-1.561884	-0.000418
С	-2.940701	-1.303851	0.000855
С	-1.143705	1.930683	-0.000201
С	1.201830	-0.181473	1.234362
С	2.578529	-0.285502	1.220211
С	3.285336	-0.313530	0.001086
С	0.472952	0.016423	-0.000762
С	1.203402	-0.181790	-1.234886
С	2.580069	-0.285847	-1.218969
Ν	0.135402	1.911171	0.000128
Η	-4.067437	0.647879	0.001437
Η	-1.024939	-2.499258	-0.000733
Η	-3.723364	-2.059262	0.001781
Η	-1.677148	2.894766	0.000744
Η	0.638916	-0.183402	2.169073
Η	3.122484	-0.374880	2.163434
Η	4.373316	-0.402248	0.001767
Η	0.641586	-0.183850	-2.170263
Η	3.125298	-0.375119	-2.161466

Calculated Negative Frequency = -586.6398 cm⁻¹



Energy = -534.0339942 Ha

С	-3.093562	-0.160440	0.000084
С	-1.912580	0.574629	-0.000265
Ν	-0.853460	-0.306091	-0.000984
С	-1.310808	-1.591039	-0.001181
С	-2.705023	-1.529678	-0.000581
С	-1.298663	1.886410	0.001112
С	1.219619	0.152598	1.258521
С	2.497840	-0.330833	1.228591
С	3.165334	-0.581955	0.000006
С	0.439742	0.442051	0.000207
С	1.220493	0.155141	-1.258327
С	2.498662	-0.328383	-1.228530
Ν	-0.003824	1.868341	0.001276
Η	-4.106755	0.233508	-0.000021
Η	-0.637061	-2.443267	-0.001801
Η	-3.370015	-2.391059	-0.000258
Η	-1.843777	2.834995	0.001857
Η	0.703503	0.356114	2.198617
Η	3.018221	-0.527247	2.169504
Η	4.185790	-0.968163	-0.000013
Η	0.705061	0.361162	-2.198247
Η	3.019689	-0.522807	-2.169500



Energy = -534.0172811 Ha

Cartesian Coordinates

С	3.095544	-0.149778	0.032477
С	1.851619	0.504613	-0.007693
Ν	0.859734	-0.433898	-0.114958
С	1.408297	-1.664957	-0.113207
С	2.810847	-1.529321	-0.030942
С	1.322842	1.833420	0.056510
С	-1.434649	0.463876	-1.222035
С	-2.522047	-0.379184	-1.188237
С	-2.998485	-0.892030	0.039860
С	-0.709648	0.790751	0.001045
С	-1.286253	0.317151	1.255461
С	-2.379235	-0.521580	1.253274
Ν	0.032166	1.973188	0.028281
Η	4.074071	0.321186	0.105909
Η	0.805170	-2.567335	-0.195924
Η	3.528902	-2.348418	-0.038203
Η	1.955760	2.724855	0.112874
Η	-1.067369	0.897235	-2.152803
Η	-3.035463	-0.638997	-2.116656
Η	-3.867408	-1.552929	0.052181
Η	-0.808468	0.641119	2.180554
Η	-2.781488	-0.889516	2.199725

Calculated Negative Frequency = $-289.7431 \text{ cm}^{-1}$

mi30-01



Energy = -534.0465458 Ha

С	3.390535	-0.766795	-0.000228
С	1.962627	-0.438826	-0.000178
Ν	1.788536	0.934910	0.000568
С	3.008870	1.444683	0.000863
С	4.054308	0.424395	0.000422
С	-1.332129	-0.607345	-0.000205
С	-2.640224	-1.168709	0.000715
С	-3.772804	-0.365143	0.000897
С	-1.209316	0.808512	-0.001019
С	-2.352770	1.602481	-0.000890
С	-3.632578	1.029703	0.000071
С	0.979562	-1.468742	-0.000671
Ν	-0.336112	-1.562987	-0.000395
Η	3.808012	-1.772154	-0.000705
Η	3.163460	2.526628	0.001413
Η	5.128506	0.600659	0.000589
Η	-2.711683	-2.257575	0.001259
Η	-4.766454	-0.818317	0.001639
Η	-0.214245	1.254468	-0.001552
Η	-2.247310	2.690061	-0.001515
Η	-4.518371	1.669439	0.000168
Η	1.454629	-2.461952	-0.001167

mi35-01



Energy = -534.0274203 Ha

Cartesian Coordinates

С	-3.092837	0.325229	-0.171449
С	-1.712262	0.601515	-0.019988
Ν	-1.008065	-0.584377	-0.142644
С	-1.887028	-1.585495	-0.273030
С	-3.205557	-1.061192	-0.326070
С	1.101996	0.930347	0.199588
С	2.313239	1.027315	-0.514940
С	3.136343	-0.079205	-0.669526
С	0.745762	-0.338404	0.817131
С	1.644969	-1.442307	0.683706
С	2.794237	-1.318513	-0.068946
С	-1.037050	1.827416	0.243363
Ν	0.262764	2.012776	0.248377
Η	-3.896317	1.059870	-0.168179
Η	-1.561268	-2.620477	-0.374192
Η	-4.113003	-1.634425	-0.508815
Η	2.556794	1.988939	-0.969878
Η	4.056055	0.002866	-1.252230
Η	0.131932	-0.292222	1.718884
Η	1.416584	-2.376066	1.201399
Η	3.472876	-2.168878	-0.169235
Η	-1.657430	2.721369	0.383089

Calculated Negative Frequency = $-318.7850 \text{ cm}^{-1}$



Energy = -534.0568049 Ha

С	-3.012740	0.308616	-0.234305
С	-1.683373	0.685839	-0.006164
Ν	-0.929725	-0.471882	0.103537
С	-1.750814	-1.557455	-0.017505
С	-3.048602	-1.103123	-0.245363
С	-1.011227	1.945320	0.070189
С	1.058935	0.947424	0.124832
С	2.423941	1.021641	-0.182699
С	3.209399	-0.119395	-0.308536
С	0.468052	-0.389608	0.566442
С	1.316028	-1.574749	0.191784
С	2.618470	-1.419160	-0.164084
Ν	0.299376	2.076976	0.076565
Η	-3.842588	0.991767	-0.399937
Η	-1.372167	-2.571918	0.057813
Η	-3.915890	-1.736456	-0.415491
Η	2.830025	2.015172	-0.383795
Η	4.262748	-0.033605	-0.579945
Η	0.888195	-2.571990	0.311315
Η	3.230849	-2.303241	-0.359238
Η	0.414560	-0.358350	1.683686
Η	-1.611708	2.860859	0.057317

mi32-07



Energy = -534.0267681 Ha

Cartesian Coordinates

С	3.010825	0.314594	-0.151556
С	1.665107	0.662901	-0.136472
Ν	0.937338	-0.476961	0.189577
С	1.804066	-1.529139	0.365073
С	3.096322	-1.065081	0.175089
С	0.968373	1.889474	-0.498931
С	-0.476313	-0.463210	0.165578
С	-1.219186	-1.455559	-0.464243
С	-2.612362	-1.329120	-0.549678
С	-1.086635	0.728305	0.684168
С	-2.517572	0.810063	0.594333
С	-3.249829	-0.184564	-0.026951
Ν	-0.264156	2.177273	-0.334730
Η	3.834159	0.988376	-0.377957
Η	1.433188	-2.512206	0.641286
Η	4.001527	-1.659733	0.269723
Η	1.594658	2.657410	-0.993015
Η	-0.710705	-2.313844	-0.907738
Η	-3.198156	-2.109394	-1.038696
Η	-0.611415	1.189758	1.554919
Η	-3.015888	1.680201	1.025339
Η	-4.336421	-0.094730	-0.096253

Calculated Negative Frequency = -552.9239 cm⁻¹

Page S13



Energy = -534.0494495 Ha

С	3.020963	0.362746	-0.142791
С	1.672684	0.691471	-0.086292
Ν	0.954726	-0.486981	0.121935
С	1.837200	-1.542163	0.186362
С	3.121116	-1.043190	0.038725
С	0.931069	1.918256	-0.283726
С	-0.445266	-0.469230	0.111625
С	-1.035956	0.880460	0.458853
С	-2.506874	0.945942	0.158304
С	-1.226247	-1.570765	-0.160910
С	-2.630057	-1.450749	-0.234761
С	-3.243292	-0.170297	-0.115863
Ν	-0.330831	2.062405	-0.085748
Η	3.836868	1.065713	-0.293471
Η	1.489274	-2.555673	0.359619
Η	4.033291	-1.634051	0.069674
Η	1.494710	2.791567	-0.640190
Η	-0.922010	0.997640	1.569331
Η	-2.958869	1.938150	0.211346
Η	-0.757214	-2.535102	-0.367519
Η	-3.235091	-2.330023	-0.459799
Η	-4.320263	-0.081062	-0.279463

General Papers

2. The vinyl $\mathbf{1}$ (X = CH) – pyrrol-1-yl $\mathbf{3}$ (X = CH) energy surface







Energy = -557.3385771 Ha

С	3.971925	0.453164	0.000349
С	2.513530	0.363405	-0.000010
Ν	2.119050	-0.967791	0.000268
С	3.240614	-1.668171	0.000006
С	4.434319	-0.832510	0.000170
С	-0.874761	0.895467	-0.000093
С	-2.127978	1.565715	-0.000115
С	-3.326192	0.866772	-0.000122
С	-0.893752	-0.520237	-0.000082
С	-2.104251	-1.208481	-0.000099
С	-3.340306	-0.541193	-0.000113
С	1.684203	1.503833	-0.000062
С	0.308740	1.728285	-0.000088
С	-4.644952	-1.295808	-0.000064
Η	4.548418	1.377060	0.000541
Н	3.218393	-2.760870	0.000027
Н	5.466363	-1.179431	0.000227
Η	-2.143885	2.659030	-0.000129
Η	-4.271764	1.416031	-0.000144
Н	0.056050	-1.057638	-0.000108
Η	-2.090528	-2.301890	-0.000115
Η	2.264816	2.432748	-0.000029
Η	0.059853	2.795568	-0.000103
Η	-4.484037	-2.383592	-0.000701
Η	-5.252256	-1.041471	-0.885503
Н	-5.251600	-1.042445	0.886112



Energy = -557.2825262 Ha

Cartesian Coordinates

3.355660	-0.691058	0.167686
2.358208	0.269286	-0.010235
1.211791	-0.355979	-0.485523
1.412671	-1.691288	-0.484250
2.750135	-1.941006	-0.123497
2.148341	1.665632	0.261209
-1.107408	1.044235	-1.109915
-2.323955	0.403611	-1.062679
-2.755075	-0.296052	0.095921
-0.170018	0.964277	-0.004819
-0.674159	0.331494	1.198996
-1.906681	-0.294323	1.223361
0.851069	2.045510	0.173105
-4.083030	-1.002329	0.110907
4.376083	-0.515469	0.502615
0.660142	-2.387545	-0.850423
3.244734	-2.911485	-0.161698
2.968534	2.354963	0.468754
-0.804076	1.596708	-2.001281
-2.990244	0.452555	-1.928843
-0.035682	0.342043	2.083756
-2.239695	-0.785482	2.141583
0.511490	3.082106	0.213335
-4.880886	-0.368658	-0.311123
-4.377085	-1.294678	1.129677
-4.050402	-1.921136	-0.502419
	3.355660 2.358208 1.211791 1.412671 2.750135 2.148341 -1.107408 -2.323955 -2.755075 -0.170018 -0.674159 -1.906681 0.851069 -4.083030 4.376083 0.660142 3.244734 2.968534 -0.804076 -2.990244 -0.035682 -2.239695 0.511490 -4.880886 -4.377085 -4.050402	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$

Calculated Negative Frequency = $-448.8027 \text{ cm}^{-1}$



Energy =-557.3066668 Ha

С	3.483010	-0.416578	-0.000064
С	2.395625	0.445722	0.000009
Ν	1.242886	-0.316255	0.000128
С	1.559039	-1.649554	0.000144
С	2.946163	-1.740386	0.000033
С	1.988872	1.839889	-0.000104
С	-0.806854	0.274047	-1.252264
С	-2.137314	-0.036665	-1.220485
С	-2.858721	-0.193746	0.000007
С	0.004730	0.505734	0.000020
С	-0.806928	0.274282	1.252296
С	-2.137401	-0.036437	1.220495
С	0.639858	1.912277	-0.000100
С	-4.311177	-0.577248	-0.000058
Η	4.533608	-0.136768	-0.000160
Η	0.794025	-2.420687	0.000254
Η	3.514229	-2.668352	0.000037
Η	2.676267	2.685474	-0.000181
Η	-0.273605	0.382753	-2.199038
Η	-2.670036	-0.179117	-2.165726
Η	-0.273741	0.383166	2.199085
Η	-2.670179	-0.178709	2.165731
Η	0.018371	2.805689	-0.000154
Η	-4.438479	-1.677074	-0.001102
Η	-4.832213	-0.194465	-0.891901
Η	-4.831863	-0.196137	0.892689



Energy = -557.2704077 Ha

Cartesian Coordinates

С	3.540535	-0.013799	-0.000046
С	2.302708	0.611522	-0.000001
Ν	1.326172	-0.369652	-0.000002
С	1.926297	-1.610655	-0.000046
С	3.297719	-1.419267	-0.000076
С	1.776755	1.964779	0.000064
С	-0.809122	-0.173533	-1.221496
С	-2.195501	-0.200168	-1.208144
С	-2.922829	-0.190729	0.000035
С	-0.079694	-0.051055	0.000035
С	-0.809100	-0.173739	1.221527
С	-2.195513	-0.200347	1.208175
С	0.451746	2.074149	0.000107
С	-4.430211	-0.185936	-0.000065
Η	4.506687	0.485178	-0.000053
Η	1.329790	-2.518523	-0.000057
Η	4.045057	-2.209515	-0.000113
Η	2.468663	2.817303	0.000080
Η	-0.253467	-0.208585	-2.159892
Η	-2.736890	-0.255451	-2.156607
Η	-0.253452	-0.208955	2.159920
Η	-2.736901	-0.255761	2.156627
Η	-0.275884	2.883495	0.000161
Η	-4.825606	0.846151	-0.003296
Η	-4.837018	-0.684849	0.893306
Η	-4.836915	-0.690257	-0.890475

Calculated Negative Frequency = $-449.1627 \text{ cm}^{-1}$



Energy = -557.2819893 Ha

С	-3.472610	-0.042161	0.081226
С	-2.221364	0.554226	-0.048936
Ν	-1.272326	-0.461539	0.039960
С	-1.922221	-1.667958	0.218778
С	-3.283784	-1.438908	0.248350
С	-1.956456	1.967316	-0.311244
С	0.804900	0.293012	1.108942
С	2.197355	0.393744	1.109104
С	2.967157	-0.131833	0.059530
С	0.151016	-0.330426	0.040382
С	0.901810	-0.863914	-1.013534
С	2.294243	-0.767650	-0.996064
С	-0.832841	2.604301	-0.607465
С	4.471632	-0.003972	0.052149
Η	-4.419250	0.491982	0.033834
Η	-1.346724	-2.581427	0.339862
Н	-4.053041	-2.196182	0.378533
Η	-2.876916	2.569267	-0.267289
Η	0.217403	0.695933	1.935322
Н	2.696712	0.882728	1.949543
Η	0.386576	-1.348098	-1.845151
Η	2.869046	-1.191215	-1.823992
Η	4.953310	-0.931937	-0.294476
Η	4.862272	0.229935	1.053678
Η	4.797782	0.803333	-0.626737
Η	0.226087	2.411788	-0.760151



Energy = -557.2758494 Ha

Cartesian Coordinates

3.456492	0.183482	-0.136936
2.140397	0.628418	-0.144210
1.333663	-0.461343	0.181544
2.130669	-1.571944	0.377365
3.449002	-1.199271	0.198914
1.582895	1.923136	-0.506648
-0.082666	-0.419296	0.159195
-0.827951	-1.347663	-0.564683
-2.221023	-1.232934	-0.626383
-0.728421	0.670226	0.802180
-2.142895	0.745989	0.744198
-2.896314	-0.176658	0.019110
0.308818	2.280455	-0.360538
-4.399994	-0.069353	-0.067155
4.325207	0.800585	-0.356056
1.687764	-2.522529	0.660719
4.312132	-1.851060	0.309843
2.305950	2.625815	-0.949606
-0.315588	-2.150724	-1.097819
-2.792645	-1.970915	-1.194771
-0.200951	1.196712	1.597951
-2.648462	1.546346	1.290278
-4.787209	0.722888	0.590339
-4.887731	-1.016387	0.216964
-4.722375	0.162787	-1.096803
-0.225786	3.198368	-0.608299
	3.456492 2.140397 1.333663 2.130669 3.449002 1.582895 -0.082666 -0.827951 -2.221023 -0.728421 -2.142895 -2.896314 0.308818 -4.399994 4.325207 1.687764 4.312132 2.305950 -0.315588 -2.792645 -0.200951 -2.648462 -4.787209 -4.887731 -4.722375 -0.225786	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$

Calculated Negative Frequency = $-407.7119 \text{ cm}^{-1}$



Energy = -557.3249804 Ha

С	3.456488	0.288210	-0.211272
С	2.129001	0.678301	-0.123412
Ν	1.366191	-0.468599	0.126386
С	2.211766	-1.563014	0.184318
С	3.505137	-1.122055	-0.010868
С	1.455872	1.946690	-0.291624
С	-0.034777	-0.438422	0.151138
С	-0.645275	0.894448	0.525738
С	-2.123543	0.947853	0.241160
С	-0.821451	-1.539663	-0.109481
С	-2.225361	-1.433124	-0.156583
С	-2.873801	-0.161747	-0.029655
С	0.142532	2.070641	-0.025862
С	-4.368312	-0.079399	-0.230180
Н	4.296255	0.954526	-0.394005
Н	1.827300	-2.556007	0.393165
Н	4.393809	-1.748499	0.004916
Η	2.049652	2.793345	-0.642791
Η	-0.532562	0.975084	1.642236
Η	-2.602265	1.927698	0.327194
Η	-0.353807	-2.501055	-0.330672
Η	-2.821543	-2.322091	-0.371939
Η	-4.735464	0.952034	-0.125527
Η	-4.900223	-0.705837	0.506283
Η	-4.656857	-0.445515	-1.230114
Н	-0.377288	3.024194	-0.143952



Energy = -557.303685 Ha

Cartesian Coordinates

-3.498161	-0.232776	-0.156683
-2.219679	0.369463	-0.028958
-1.252793	-0.626373	-0.127706
-1.874679	-1.804745	-0.229914
-3.283345	-1.608371	-0.274915
0.573833	1.312919	0.198113
1.811709	1.653685	-0.392742
2.834278	0.729022	-0.508478
0.420114	-0.020700	0.758976
1.511745	-0.941574	0.644003
2.685253	-0.596070	0.002694
-1.859159	1.733535	0.138646
-0.553692	2.190860	0.163780
3.830401	-1.568781	-0.121677
-4.451790	0.292549	-0.160498
-1.316231	-2.736185	-0.324600
-4.030850	-2.383514	-0.436435
1.935200	2.659100	-0.804298
3.769375	1.008897	-0.999615
-0.189524	-0.092522	1.662677
1.415082	-1.925899	1.108694
-2.674938	2.461277	0.138920
4.750153	-1.163310	0.332883
4.060246	-1.767488	-1.182724
3.603562	-2.529958	0.361917
-0.372437	3.262865	0.039937
	$\begin{array}{r} -3.498161\\ -2.219679\\ -1.252793\\ -1.874679\\ -3.283345\\ 0.573833\\ 1.811709\\ 2.834278\\ 0.420114\\ 1.511745\\ 2.685253\\ -1.859159\\ -0.553692\\ 3.830401\\ -4.451790\\ -1.316231\\ -4.030850\\ 1.935200\\ 3.769375\\ -0.189524\\ 1.415082\\ -2.674938\\ 4.750153\\ 4.060246\\ 3.603562\\ -0.372437\end{array}$	-3.498161 -0.232776 -2.219679 0.369463 -1.252793 -0.626373 -1.874679 -1.804745 -3.283345 -1.608371 0.573833 1.312919 1.811709 1.653685 2.834278 0.729022 0.420114 -0.020700 1.511745 -0.941574 2.685253 -0.596070 -1.859159 1.733535 -0.553692 2.190860 3.830401 -1.568781 -4.451790 0.292549 -1.316231 -2.736185 -4.030850 -2.383514 1.935200 2.659100 3.769375 1.008897 -0.189524 -0.092522 1.415082 -1.925899 -2.674938 2.461277 4.750153 -1.163310 4.060246 -1.767488 3.603562 -2.529958 -0.372437 3.262865

Calculated Negative Frequency = -384.7188 cm⁻¹



Energy = -557.3344448 Ha

С	-3.362922	-0.350878	-0.235863
С	-2.187768	0.388804	-0.055270
Ν	-1.144286	-0.515476	0.110554
С	-1.646981	-1.790231	0.068966
С	-3.016848	-1.719138	-0.159878
С	-1.911849	1.788598	-0.074258
С	0.477450	1.350033	0.120914
С	1.819982	1.729655	-0.056894
С	2.847318	0.801608	-0.096197
С	0.193635	-0.080748	0.557186
С	1.299731	-1.042138	0.206538
С	2.568013	-0.616295	-0.035693
С	-0.608853	2.243798	-0.027709
С	3.700975	-1.583805	-0.271476
Η	-4.346612	0.072576	-0.425462
Η	-1.010530	-2.659071	0.200054
Η	-3.681100	-2.572361	-0.274728
Η	2.038289	2.787650	-0.228959
Η	3.875253	1.131818	-0.261607
Η	1.087084	-2.111163	0.262866
Η	0.135762	-0.049164	1.674731
Η	-2.747176	2.478853	-0.199796
Η	4.496827	-1.447290	0.481014
Η	4.164319	-1.417628	-1.258987
Η	3.362414	-2.629024	-0.223144
Η	-0.395823	3.307557	-0.162051

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