

Synthesis and characterization of bulky substituted hemihexaphyrazines bearing 2,6-diisopropylphenoxy groups

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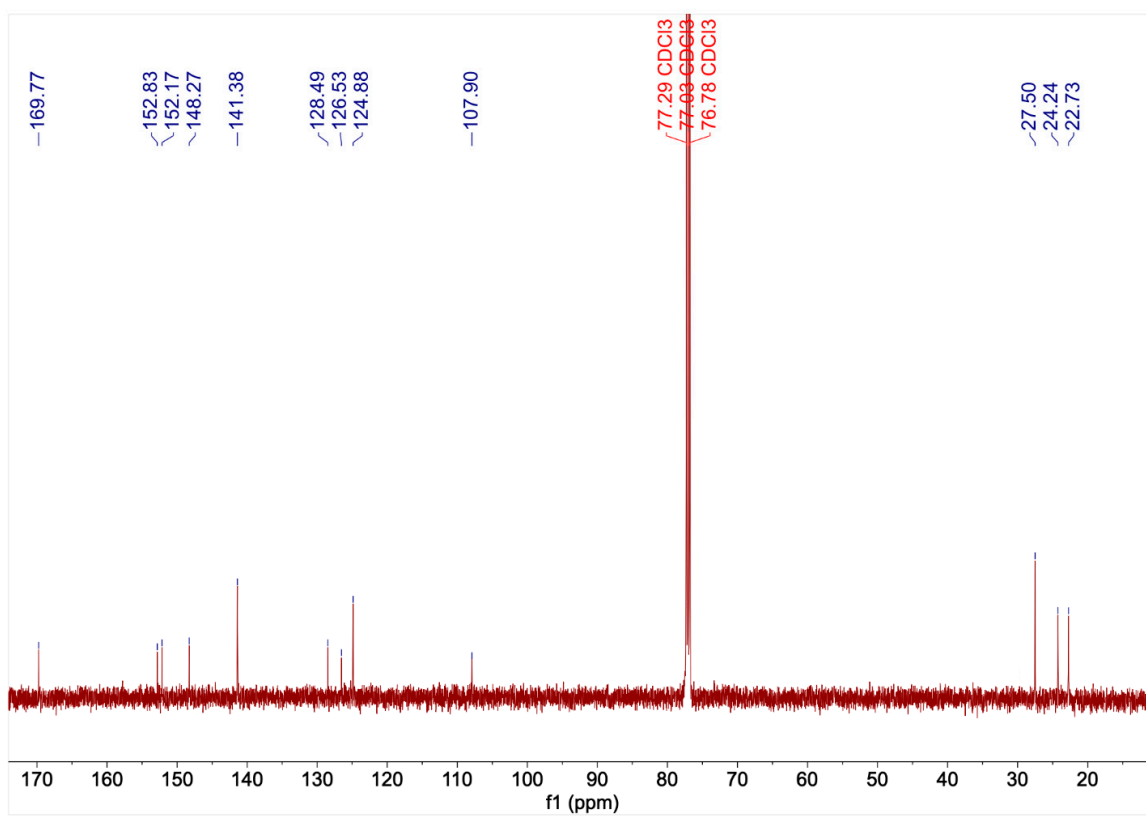


Figure S1: ¹³C-NMR spectrum of **4** in CDCl₃

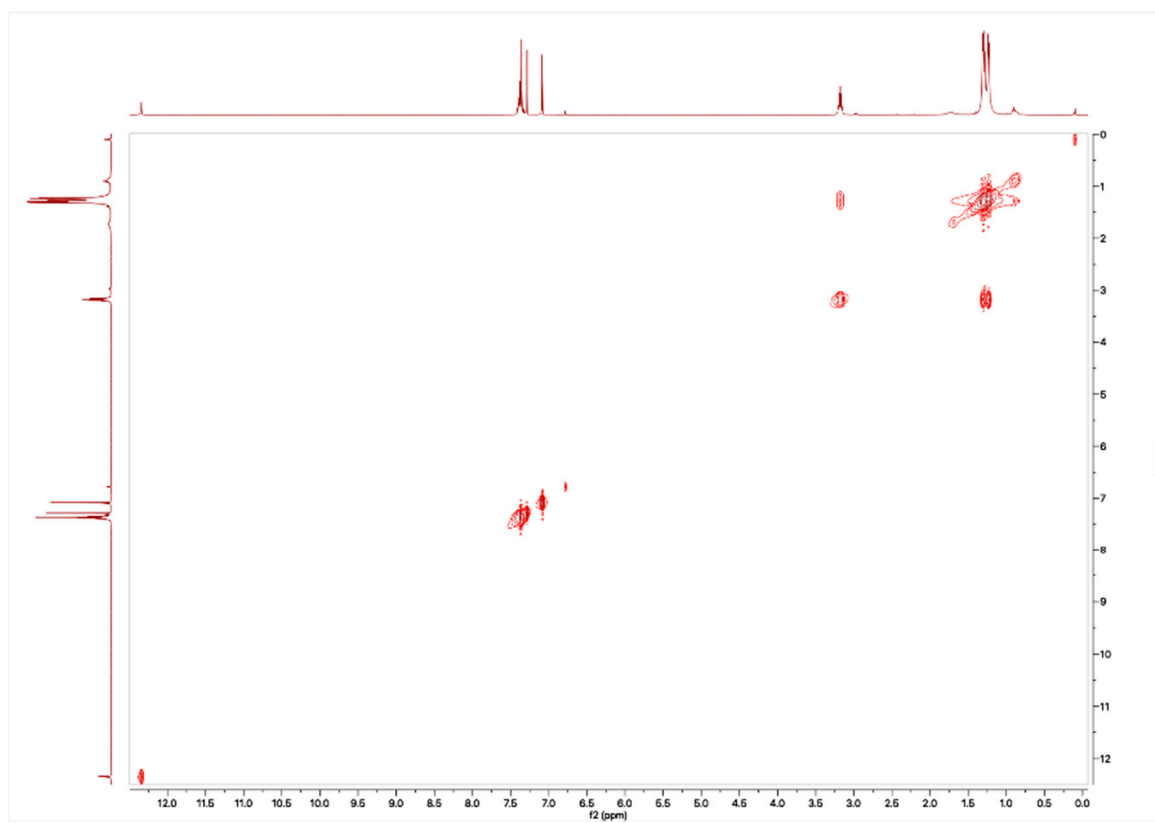


Figure S2: COSY ¹H-¹H NMR spectrum of **4** in CDCl₃

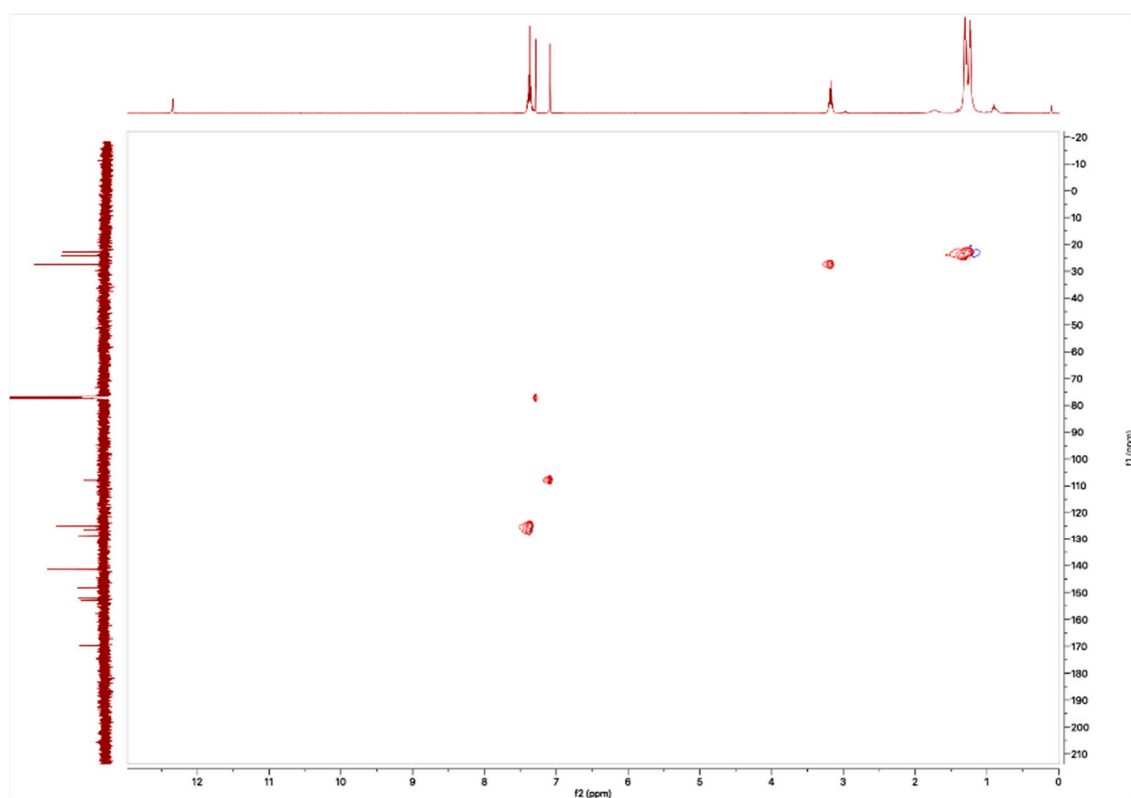


Figure S3: HSQC ^1H - ^{13}C NMR spectrum of **4** in CDCl_3

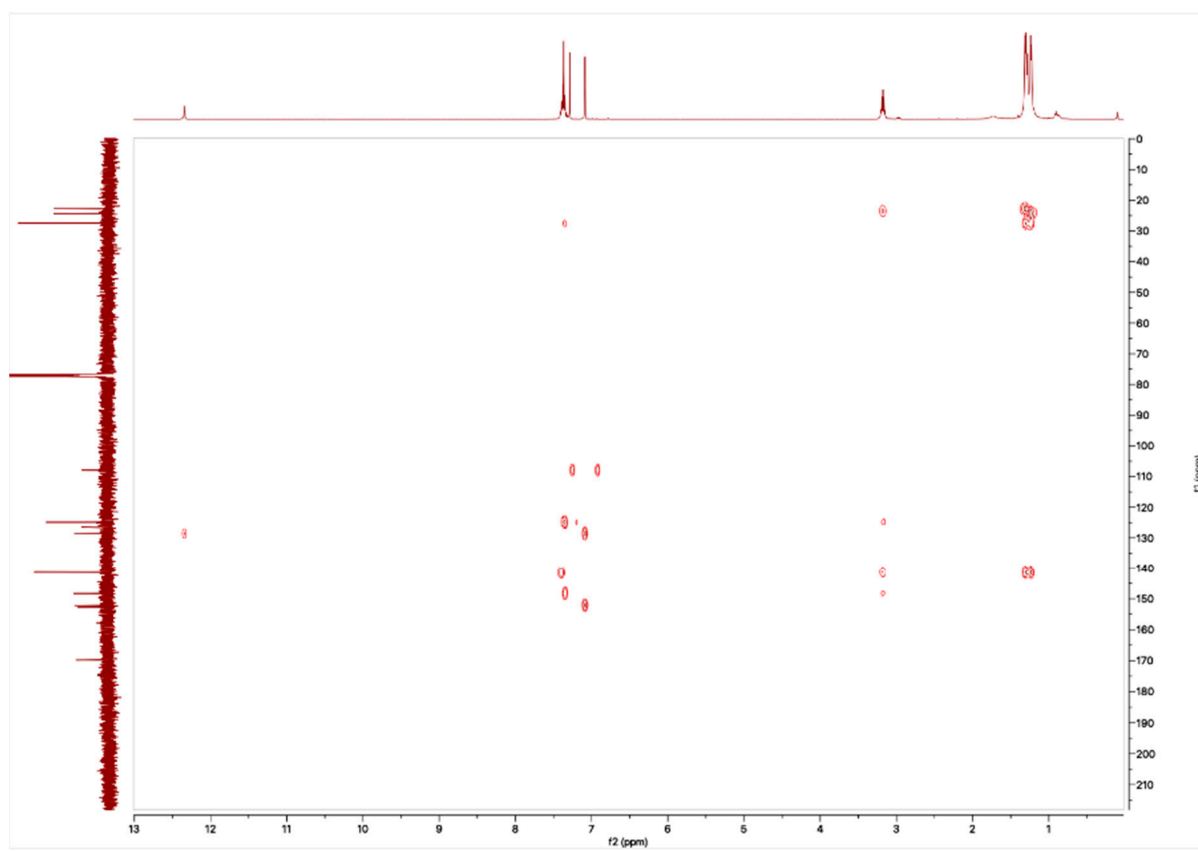


Figure S4: HMBC ^1H - ^{13}C NMR spectrum of **4** in CDCl_3

Table S1. Experimental (δ_{exp}) and computational (δ_{calc}) (GIAO) chemical shifts (**4**) ^{13}C и ^1H

| C | δ_{exp} | HSQC | HMBC | | | | δ_{calc} |
|---------|-----------------------|------------------------|-------|------|------|----------------|------------------------|
| 8,10 | 169.77 | | | | | | 171.35 |
| 111,114 | 152.82 | | 12.34 | | | | 151.84 |
| 12,13 | 128.49 | | 12.34 | 7.08 | | | 129.03 |
| 41 | 107.9 | 7.08 | | | | | 119.04 |
| 42,43 | 152.17 | | | 7.08 | | | 152.20 |
| 44 | 107.9 | 7.08 | | | | | 119.04 |
| 57 | 148.27 | | 7.35 | | | | 151.37 |
| 71,75 | 141.38 | | 7.38 | 3.2 | 1.31 | 1.24 | 138.13 |
| 72 | 124.88 | 7.35 | 7.38 | | | | 129.78 |
| 73 | 126.63 | 7.38 | | | | | 122.53 |
| 109,112 | 27.5 | 3.18 | | | | | 39.20 |
| 110,113 | 24.24 | 1.31 | | 3.2 | 1.24 | | 24.72 |
| 111,114 | 22.73 | 1.24 | | | 1.31 | | 21.41 |
| | | | | | | MAE* | 1.696 |
| | | | | | | R ² | 0.992 |
| H | δ_{exp} | δ_{calc} | | | | | |
| 15 | 12.34 | 12.03 | | | | | |
| 41,44 | 7.08 | 8.02 | | | | | |
| 72,74 | 7.38 | 7.31 | | | | | |
| 73 | 7.35 | 7.32 | | | | | |
| 109,112 | 3.18 | 3.07 | | | | | |
| 110,113 | 1.31 | 1.13 | | | | | |
| 111,114 | 1.24 | 0.94 | | | | | |
| | MAE | 0.070 | | | | | |
| | R ² | 0.984 | | | | | |

$$*MAE = \frac{\sum_{i=1}^n |\delta_{\text{exp}} - \delta_{\text{calc}}|_i}{n}$$

R² - linear correlation coefficient

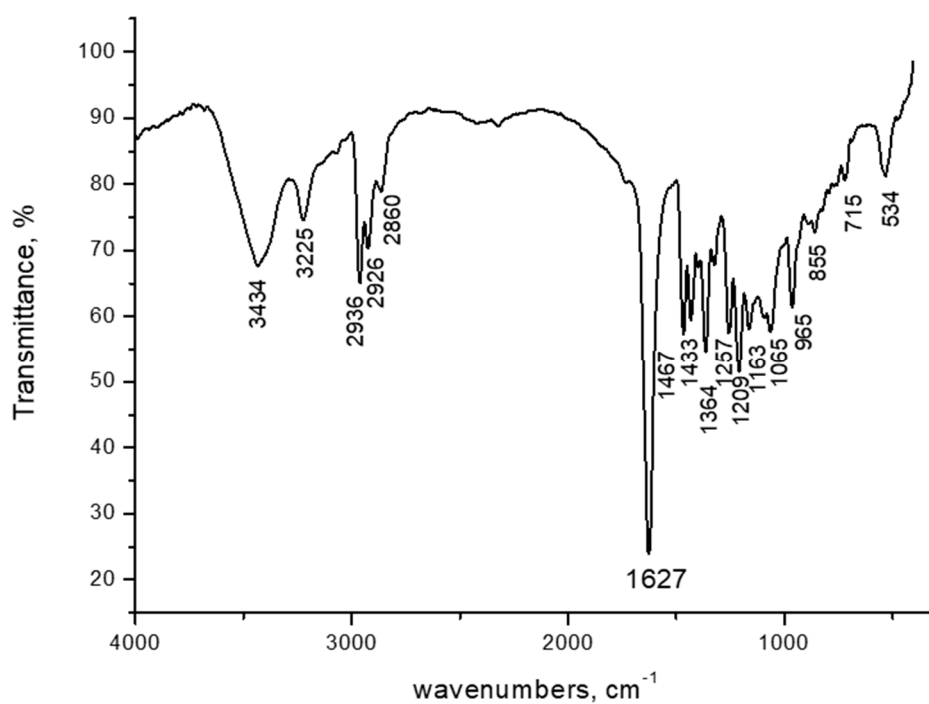


Figure S5: IR spectrum of **3** in palette with KBr

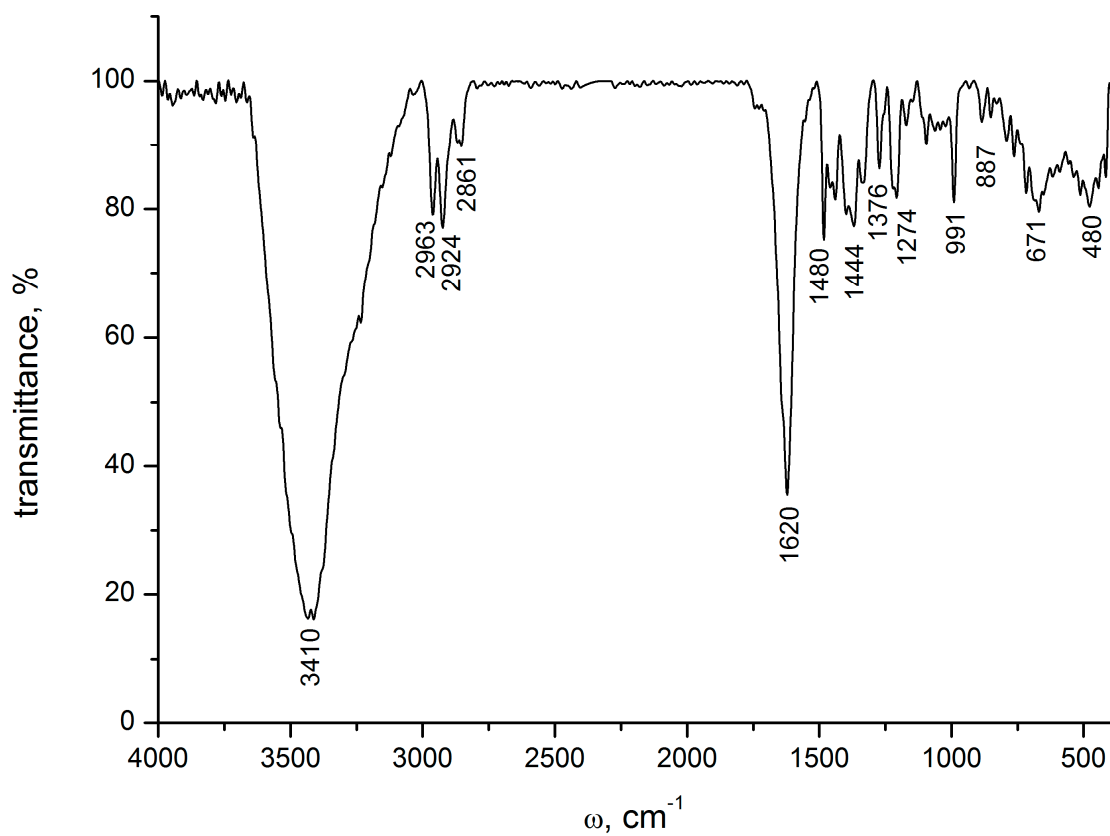


Figure S6: IR spectrum of **4** in palette with KBr

Table S2. a) Geometry parameters (Å) and E_{tot} (a.u.) of **4** optimized at DFT/CAM-B3LYP/6-31G(d,p) method

| | | | |
|---|--------------|--------------|--------------|
| N | 0.605448000 | -2.673510000 | -0.002625000 |
| C | -1.560122000 | -4.515174000 | -0.000713000 |
| C | -3.482671000 | -3.267893000 | 0.002053000 |
| N | -2.098696000 | -3.239990000 | 0.000266000 |
| C | -3.865660000 | -4.687591000 | -0.000951000 |
| C | -2.700530000 | -5.443600000 | 0.002808000 |
| N | -0.331588000 | -4.888084000 | -0.001851000 |
| N | -4.324003000 | -2.298088000 | 0.003052000 |
| C | -3.126561000 | 3.609806000 | 0.005296000 |
| C | -1.085203000 | 4.651364000 | 0.000148000 |
| N | -1.752902000 | 3.438811000 | 0.002962000 |
| C | -2.123373000 | 5.692824000 | -0.002850000 |
| C | -3.360524000 | 5.061538000 | 0.006341000 |
| N | 0.175319000 | 4.895101000 | -0.001833000 |
| N | -4.063621000 | 2.732153000 | 0.008185000 |
| C | 4.692525000 | 0.903613000 | 0.003210000 |
| C | 4.574211000 | -1.385062000 | -0.004776000 |
| N | 3.857768000 | -0.200616000 | -0.000378000 |
| C | 6.066816000 | 0.380532000 | 0.005047000 |
| C | 5.995160000 | -1.006481000 | -0.006090000 |
| N | 4.401012000 | 2.153946000 | 0.006483000 |
| N | 4.155118000 | -2.598624000 | -0.008892000 |
| C | -3.911468000 | -0.993050000 | 0.004555000 |
| C | -3.788051000 | 1.391475000 | 0.006622000 |
| S | -5.116197000 | 0.264759000 | 0.007252000 |
| N | -2.684106000 | -0.539344000 | 0.003531000 |
| C | 1.099131000 | 3.885189000 | 0.000688000 |
| S | 2.790823000 | 4.299376000 | 0.002789000 |
| N | 2.014590000 | 1.858223000 | 0.002948000 |
| C | 3.102232000 | 2.585760000 | 0.004112000 |
| C | 0.691785000 | -3.979198000 | -0.003905000 |
| S | 2.331600000 | -4.566122000 | -0.007489000 |
| N | 1.812026000 | -2.057833000 | -0.004304000 |
| C | 2.818636000 | -2.893911000 | -0.006772000 |
| H | -1.542936000 | -2.383517000 | -0.000177000 |
| H | -1.288914000 | 2.529342000 | 0.003136000 |
| H | 2.838142000 | -0.147909000 | -0.000131000 |
| C | -2.757082000 | -6.818395000 | 0.049570000 |
| C | -3.998443000 | -7.464640000 | 0.088229000 |
| C | -5.182606000 | -6.696295000 | -0.084705000 |
| C | -5.098168000 | -5.299440000 | -0.046605000 |
| C | -2.037477000 | 7.065940000 | -0.053333000 |
| C | -3.205335000 | 7.837233000 | -0.090493000 |
| C | -4.462045000 | 7.196175000 | 0.088660000 |
| C | -4.522789000 | 5.797947000 | 0.054255000 |
| C | 7.141683000 | -1.767089000 | -0.055988000 |
| C | 8.393516000 | -1.141135000 | -0.090375000 |
| C | 8.466132000 | 0.267589000 | 0.090639000 |
| C | 7.285457000 | 1.019047000 | 0.055526000 |
| N | 0.878182000 | 2.595433000 | 0.001271000 |

| | | | |
|---|--------------|--------------|--------------|
| N | -2.614096000 | 0.813439000 | 0.004548000 |
| H | -1.857481000 | -7.419748000 | 0.086790000 |
| H | -6.013856000 | -4.722824000 | -0.082889000 |
| H | -1.080605000 | 7.570892000 | -0.094903000 |
| H | -5.493201000 | 5.319468000 | 0.094800000 |
| H | 7.100768000 | -2.848200000 | -0.098677000 |
| H | 7.356015000 | 2.098631000 | 0.098306000 |
| O | 9.588851000 | 1.039242000 | 0.189961000 |
| C | 10.673171000 | 0.835304000 | 1.037623000 |
| C | 11.931544000 | 1.035754000 | 0.447719000 |
| C | 10.530892000 | 0.609177000 | 2.424789000 |
| C | 13.056945000 | 0.744510000 | 1.221692000 |
| C | 11.701772000 | 0.342779000 | 3.138740000 |
| H | 14.036845000 | 0.841785000 | 0.763955000 |
| H | 11.619825000 | 0.141786000 | 4.202425000 |
| C | 12.953047000 | 0.359264000 | 2.545076000 |
| H | 13.840433000 | 0.131647000 | 3.126240000 |
| C | 9.272191000 | 0.800819000 | 3.280400000 |
| H | 9.669923000 | 0.819203000 | 4.300385000 |
| C | 8.226533000 | -0.322004000 | 3.294039000 |
| C | 8.639082000 | 2.180695000 | 3.069313000 |
| H | 9.381170000 | 2.971632000 | 3.205629000 |
| H | 8.211493000 | 2.292739000 | 2.074141000 |
| H | 7.836209000 | 2.339250000 | 3.795197000 |
| H | 7.621606000 | -0.359666000 | 2.390602000 |
| H | 7.544233000 | -0.158598000 | 4.133765000 |
| H | 8.693513000 | -1.299967000 | 3.432645000 |
| C | 12.224753000 | 1.661542000 | -0.921021000 |
| H | 12.976756000 | 1.013288000 | -1.386180000 |
| C | 12.873474000 | 3.040245000 | -0.695706000 |
| C | 11.092749000 | 1.828661000 | -1.934463000 |
| H | 10.581952000 | 0.892947000 | -2.140985000 |
| H | 10.353263000 | 2.557814000 | -1.598264000 |
| H | 11.522088000 | 2.193114000 | -2.873282000 |
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| H | 13.170693000 | 3.479074000 | -1.652828000 |
| H | 13.758615000 | 2.986858000 | -0.058656000 |
| O | 9.431364000 | -2.023822000 | -0.188946000 |
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| C | 12.910643000 | -2.089461000 | -1.222514000 |
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| H | 13.875416000 | -2.287848000 | -0.765298000 |
| H | 11.542332000 | -1.341003000 | -4.202534000 |
| C | 12.846628000 | -1.695205000 | -2.545793000 |
| H | 13.752549000 | -1.560507000 | -3.127324000 |
| C | 9.139791000 | -1.755314000 | -3.279953000 |
| H | 9.533488000 | -1.815138000 | -4.299909000 |
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| C | 8.368345000 | -3.062710000 | -3.067986000 |
| H | 9.025515000 | -3.925774000 | -3.202550000 |
| H | 7.930485000 | -3.129083000 | -2.073191000 |

| | | | |
|---|--------------|---------------|--------------|
| H | 7.554159000 | -3.139030000 | -3.794585000 |
| H | 7.617110000 | -0.430832000 | -2.391056000 |
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| H | 12.804127000 | -2.348893000 | 1.385425000 |
| C | 12.492449000 | -4.354077000 | 0.694133000 |
| C | 10.846502000 | -2.966291000 | 1.934330000 |
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| H | 11.236332000 | -3.374279000 | 2.872476000 |
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| H | 12.744028000 | -4.821370000 | 1.650863000 |
| H | 13.377684000 | -4.391882000 | 0.056093000 |
| O | -3.892206000 | -8.822981000 | 0.183626000 |
| C | -4.610160000 | -9.661704000 | 1.030476000 |
| C | -5.072631000 | -10.847497000 | 0.437558000 |
| C | -4.727208000 | -9.430960000 | 2.419221000 |
| C | -5.886171000 | -11.677284000 | 1.212268000 |
| C | -5.541980000 | -10.312463000 | 3.133729000 |
| H | -6.297559000 | -12.571020000 | 0.752741000 |
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| H | -6.799522000 | -12.055189000 | 3.120010000 |
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| C | -4.373100000 | -6.974086000 | 3.295164000 |
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| H | -1.871648000 | -7.971133000 | 3.778839000 |
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| H | -5.452951000 | -6.888861000 | 3.438068000 |
| C | -4.687927000 | -11.408620000 | -0.936552000 |
| H | -5.629724000 | -11.726947000 | -1.398948000 |
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| O | -6.466338000 | -7.153895000 | -0.176445000 |
| C | -6.944571000 | -8.143741000 | -1.029182000 |
| C | -7.846317000 | -9.045163000 | -0.440705000 |
| C | -6.683711000 | -8.154599000 | -2.417573000 |
| C | -8.277893000 | -10.121478000 | -1.218836000 |
| C | -7.161567000 | -9.253796000 | -3.135362000 |
| H | -8.932950000 | -10.857667000 | -0.762608000 |
| H | -6.955139000 | -9.300320000 | -4.200142000 |
| C | -7.910381000 | -10.257888000 | -2.544332000 |

| | | | |
|---|---------------|---------------|--------------|
| H | -8.251955000 | -11.105720000 | -3.128727000 |
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| H | -6.354997000 | -7.326543000 | -4.290825000 |
| C | -4.579625000 | -6.832667000 | -3.290103000 |
| C | -6.847107000 | -5.698092000 | -3.051176000 |
| H | -7.923344000 | -5.833870000 | -3.185875000 |
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| H | -6.505720000 | -4.951368000 | -3.774032000 |
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| H | -4.063083000 | -7.784428000 | -3.435220000 |
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| C | -10.016980000 | -8.630189000 | 0.711651000 |
| C | -7.984832000 | -7.913248000 | 1.948541000 |
| H | -6.927458000 | -8.053888000 | 2.151614000 |
| H | -8.138346000 | -6.884186000 | 1.618383000 |
| H | -8.530059000 | -8.050156000 | 2.887968000 |
| H | -10.149809000 | -7.650360000 | 0.242440000 |
| H | -10.543951000 | -8.617463000 | 1.670364000 |
| H | -10.497414000 | -9.372726000 | 0.071351000 |
| O | -2.959041000 | 9.177013000 | -0.190282000 |
| C | -3.589396000 | 10.083179000 | -1.037380000 |
| C | -3.923088000 | 11.312637000 | -0.446914000 |
| C | -3.736116000 | 9.861374000 | -2.424753000 |
| C | -4.649320000 | 12.220115000 | -1.221234000 |
| C | -4.458184000 | 10.820541000 | -3.138991000 |
| H | -4.962989000 | 13.153462000 | -0.763369000 |
| H | -4.606820000 | 10.663992000 | -4.202917000 |
| C | -4.956609000 | 11.968272000 | -2.545122000 |
| H | -5.527315000 | 12.684784000 | -3.126436000 |
| C | -3.044916000 | 8.791742000 | -3.279773000 |
| H | -3.189138000 | 9.162570000 | -4.299878000 |
| C | -3.642352000 | 7.378513000 | -3.294630000 |
| C | -1.527212000 | 8.778051000 | -3.066069000 |
| H | -1.108711000 | 9.778840000 | -3.200750000 |
| H | -1.251774000 | 8.432858000 | -2.070707000 |
| H | -1.052912000 | 8.110936000 | -3.791777000 |
| H | -3.430717000 | 6.810839000 | -2.391023000 |
| H | -3.213412000 | 6.822730000 | -4.133961000 |
| H | -4.725619000 | 7.405301000 | -3.434439000 |
| C | -3.474673000 | 11.835695000 | 0.922941000 |
| H | -4.375526000 | 12.253108000 | 1.388039000 |
| C | -2.485295000 | 12.994985000 | 0.700348000 |
| C | -2.856792000 | 10.871616000 | 1.935509000 |
| H | -3.499560000 | 10.021010000 | 2.141458000 |
| H | -1.888020000 | 10.497754000 | 1.598990000 |
| H | -2.701126000 | 11.412056000 | 2.874781000 |
| H | -1.569932000 | 12.628039000 | 0.225666000 |
| H | -2.209220000 | 13.445449000 | 1.658392000 |
| H | -2.897517000 | 13.780355000 | 0.063652000 |
| O | -5.691408000 | 7.784070000 | 0.183940000 |
| C | -6.060233000 | 8.821700000 | 1.034367000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -6.865258000 | 9.810317000 | 0.445704000 |
| C | -5.794123000 | 8.810049000 | 2.421724000 |
| C | -7.178647000 | 10.928708000 | 1.221086000 |
| C | -6.151302000 | 9.955815000 | 3.136908000 |
| H | -7.754904000 | 11.727783000 | 0.764349000 |
| H | -5.936799000 | 9.984292000 | 4.200734000 |
| C | -6.793304000 | 11.030653000 | 2.544624000 |
| H | -7.041838000 | 11.911655000 | 3.126921000 |
| C | -5.330907000 | 7.623650000 | 3.276970000 |
| H | -5.547466000 | 7.958100000 | 4.296835000 |
| C | -3.835486000 | 7.280610000 | 3.293097000 |
| C | -6.208557000 | 6.385249000 | 3.063963000 |
| H | -7.264933000 | 6.632292000 | 3.197692000 |
| H | -6.089394000 | 5.958677000 | 2.069215000 |
| H | -5.946126000 | 5.610745000 | 3.790570000 |
| H | -3.497454000 | 6.779182000 | 2.388803000 |
| H | -3.637426000 | 6.605293000 | 4.131013000 |
| H | -3.223303000 | 8.174133000 | 3.436515000 |
| C | -7.554100000 | 9.751342000 | -0.922954000 |
| H | -7.372058000 | 10.728080000 | -1.386593000 |
| C | -9.071918000 | 9.618617000 | -0.697008000 |
| C | -7.130048000 | 8.690561000 | -1.938489000 |
| H | -6.064593000 | 8.720110000 | -2.146018000 |
| H | -7.387969000 | 7.684144000 | -1.603629000 |
| H | -7.661956000 | 8.879803000 | -2.876471000 |
| H | -9.303491000 | 8.659646000 | -0.223079000 |
| H | -9.601284000 | 9.656726000 | -1.653726000 |
| H | -9.470320000 | 10.409399000 | -0.058184000 |

$E_{\text{tot}} = -6418.125671$ a.u.

b) Geometry parameters (Å) and E_{tot} (a.u.) of **H₃Hhp** optimized at DFT/CAM-B3LYP/6-31G(d,p) method of D_{3h} symmetry.

| | | | |
|---|--------------|-------------|-------------|
| C | -1.194031000 | 3.855812000 | 0.000000000 |
| C | 1.194031000 | 3.855812000 | 0.000000000 |
| N | -0.677229000 | 2.653570000 | 0.000000000 |
| N | 0.677229000 | 2.653570000 | 0.000000000 |
| S | 0.000000000 | 5.123887000 | 0.000000000 |
| N | -2.518818000 | 4.199969000 | 0.000000000 |
| N | 2.518818000 | 4.199969000 | 0.000000000 |
| H | -2.457867000 | 1.419050000 | 0.000000000 |
| C | -6.961197000 | 2.380995000 | 0.000000000 |
| C | -7.633286000 | 3.600421000 | 0.000000000 |
| C | -5.577908000 | 2.417120000 | 0.000000000 |
| H | -8.718080000 | 3.613659000 | 0.000000000 |
| C | -6.934699000 | 4.810409000 | 0.000000000 |
| C | -4.882241000 | 3.622050000 | 0.000000000 |
| H | -7.488561000 | 5.743249000 | 0.000000000 |
| C | -5.542600000 | 4.838076000 | 0.000000000 |
| H | -4.987078000 | 5.768843000 | 0.000000000 |
| H | -7.489504000 | 1.434515000 | 0.000000000 |
| C | -3.443508000 | 3.308962000 | 0.000000000 |
| N | -3.342132000 | 1.929581000 | 0.000000000 |

| | | | |
|---|--------------|--------------|-------------|
| C | -4.587399000 | 1.327685000 | 0.000000000 |
| C | -2.742216000 | -2.961967000 | 0.000000000 |
| C | -3.936247000 | -0.893845000 | 0.000000000 |
| N | -1.959444000 | -1.913282000 | 0.000000000 |
| N | -2.636673000 | -0.740287000 | 0.000000000 |
| S | -4.437417000 | -2.561944000 | 0.000000000 |
| N | -2.377871000 | -4.281345000 | 0.000000000 |
| N | -4.896689000 | 0.081376000 | 0.000000000 |
| H | 0.000000000 | -2.838101000 | 0.000000000 |
| C | 1.418596000 | -7.219071000 | 0.000000000 |
| C | 0.698587000 | -8.410830000 | 0.000000000 |
| C | 0.695667000 | -6.039170000 | 0.000000000 |
| H | 1.229520000 | -9.356909000 | 0.000000000 |
| C | -0.698587000 | -8.410830000 | 0.000000000 |
| C | -0.695667000 | -6.039170000 | 0.000000000 |
| H | -1.229520000 | -9.356909000 | 0.000000000 |
| C | -1.418596000 | -7.219071000 | 0.000000000 |
| H | -2.502426000 | -7.203358000 | 0.000000000 |
| H | 2.502426000 | -7.203358000 | 0.000000000 |
| C | -1.143891000 | -4.636647000 | 0.000000000 |
| N | 0.000000000 | -3.859162000 | 0.000000000 |
| C | 1.143891000 | -4.636647000 | 0.000000000 |
| C | 3.936247000 | -0.893845000 | 0.000000000 |
| C | 2.742216000 | -2.961967000 | 0.000000000 |
| N | 2.636673000 | -0.740287000 | 0.000000000 |
| N | 1.959444000 | -1.913282000 | 0.000000000 |
| S | 4.437417000 | -2.561944000 | 0.000000000 |
| N | 4.896689000 | 0.081376000 | 0.000000000 |
| N | 2.377871000 | -4.281345000 | 0.000000000 |
| H | 2.457867000 | 1.419050000 | 0.000000000 |
| C | 5.542600000 | 4.838076000 | 0.000000000 |
| C | 6.934699000 | 4.810409000 | 0.000000000 |
| C | 4.882241000 | 3.622050000 | 0.000000000 |
| H | 7.488561000 | 5.743249000 | 0.000000000 |
| C | 7.633286000 | 3.600421000 | 0.000000000 |
| C | 5.577908000 | 2.417120000 | 0.000000000 |
| H | 8.718080000 | 3.613659000 | 0.000000000 |
| C | 6.961197000 | 2.380995000 | 0.000000000 |
| H | 7.489504000 | 1.434515000 | 0.000000000 |
| H | 4.987078000 | 5.768843000 | 0.000000000 |
| C | 4.587399000 | 1.327685000 | 0.000000000 |
| N | 3.342132000 | 1.929581000 | 0.000000000 |
| C | 3.443508000 | 3.308962000 | 0.000000000 |

E_{tot}= -3167.103429 a.u.