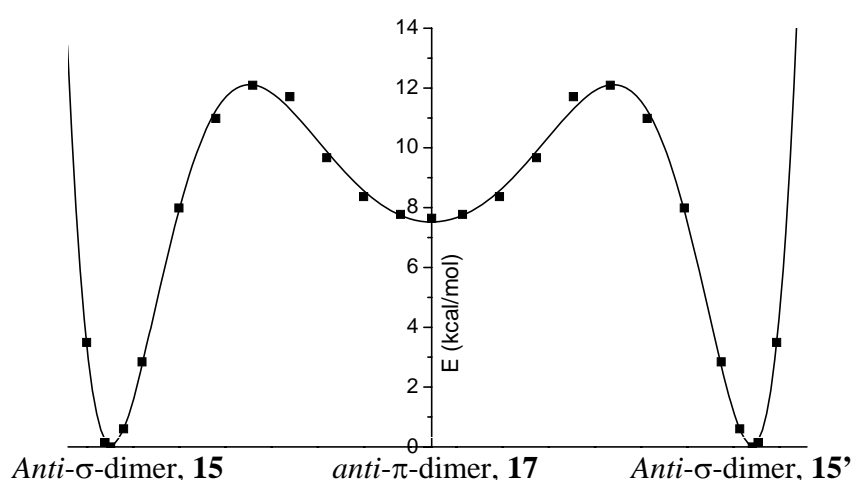


*Electronic Supplementary Information for*  
**Fluxional  $\sigma$ -bonds of 2,5,8-tri-*tert*-butyl-1,3-diazaphenalenyl dimers: stepwise [3,3], [5,5] and [7,7] sigmatropic rearrangement via  $\pi$ -dimer intermediates**

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20057-1227



**Figure S1.** Relaxed PES of the *anti*- $\sigma$ -1 dimer **15** calculated by UM05-2X/6-31G(d,p) along the C2-C18 distance (the left half) and the C7-C22 distance (the right half). See Figure 5 for the atom numbering.

**Table S1.** The  $\langle S^2 \rangle$  of  $\pi$ -dimer **4** for part of geometries on the potential surface calculated by UB3LYP/6-31+G(d,p). Note the sudden rise of  $\langle S^2 \rangle$  when the separation changes from 3.4 Å to 3.6 Å and compare it with the small discontinuity of the energy curve in Fig. 1 at 3.40 Å.

Separation (in Å)	3.00	3.20	3.40	3.60
$\langle S^2 \rangle$	0.0000	0.2466	0.3936	1.0135

**Table S2.** The lowest singlet-singlet excitation energies calculated by TD-M05-2X/6-31G(d,p). Note that the calculated numbers deviate from the experiment values, whereas the calculation and the experiment show the trend that **9** and **17** have smaller excitation energies than **4**.

$\pi$ -dimers	<b>4</b>	<b>9</b>	<b>17</b>
nm	681	758	816

**Table S3.** The total and relative energies (a. u.) of the dimers with cross and anti-parallel dipole arrangement.

Basis set	<i>cross</i> - $\sigma$ -1 ( <b>8</b> )	<i>anti</i> - $\sigma$ -1 ( <b>15</b> )	difference	<i>cross</i> - $\pi$ ( <b>9</b> )	<i>anti</i> - $\pi$ ( <b>17</b> )	difference
6-31G(d,p)	-2009.2134	-2009.2120	-0.0014	-2009.1993	-2009.1999	0.0006
6-311+G(2d,p)	-2009.6809	-2009.6780	-0.0029	-2009.6665	-2009.6671	0.0006

**Formula for the approximate spin projection (AP) procedure<sup>14</sup>**

$${}^{AP-LS}E = {}^{LS}E + J_{ab}(AP) \times [{}^{LS}\langle S^2 \rangle - S_{\min}(S_{\min} + 1)], \quad (\text{S1})$$

where  ${}^{LS}E$  and  ${}^{LS}\langle S^2 \rangle$  are the total energy and spin angular momentum of low spin state (LS), respectively;  $S_{\min}$  is the spin angular momentum of the pure LS state;

$J_{ab}(AP)$  is the effective exchange integral calculated by,

$$J_{ab} = \frac{{}^{LS}E - {}^{HS}E}{{}^{HS}\langle S^2 \rangle - {}^{LS}\langle S^2 \rangle}, \quad (\text{S2})$$

where  ${}^{HS}E$  and  ${}^{HS}\langle S^2 \rangle$  are the total energy and spin angular momentum of low spin state (LS), respectively.

**Estimation of the average CC distance for 8 and 15:**

Taking the occupation number (Ref. 7c) of  $\sigma$ -dimer **8** and  $\pi$ -dimer **9** at 273 that are 0.629 and 0.371, respectively. The bond distances of C7-C22 are taken from M05-2X/6-31G(d,p) optimized geometry (see Table 2), which are 1.633 Å and 3.274 Å for the  $\sigma$ -dimer **8** and  $\pi$ -dimer **9**, respectively.

The average distance is:

$$1.633 \times 0.629 + 3.274 \times 0.371 = 2.242 \text{ \AA}$$

**Optimized geometries and total energies of stationary structures reported in the paper:**

**4, UM05-2X/6-31G(d,p)**

Total Energy: -1945.03502425 a.u.

Optimized geometry:

C	0.108889000	0.091729000	1.598342000
C	0.825897000	-1.131219000	1.604446000
C	2.237153000	-1.093015000	1.586406000
C	2.946128000	0.112615000	1.609359000
C	2.224100000	1.301548000	1.561651000
C	0.810456000	1.319474000	1.562712000
C	0.079684000	2.530403000	1.590680000
C	-1.309523000	2.548521000	1.686227000
C	-1.990807000	1.326612000	1.683047000
C	-1.309967000	0.088087000	1.657430000
C	-1.978320000	-1.153423000	1.744658000
C	-1.286185000	-2.367783000	1.794223000
C	0.101866000	-2.346151000	1.686538000
C	-0.108889000	-0.091729000	-1.598342000
C	-0.825897000	1.131219000	-1.604446000
C	-2.237153000	1.093015000	-1.586406000
C	-2.946128000	-0.112615000	-1.609359000
C	-2.224100000	-1.301548000	-1.561651000
C	-0.810456000	-1.319474000	-1.562712000
C	-0.079684000	-2.530403000	-1.590680000
C	1.309523000	-2.548521000	-1.686227000
C	1.990807000	-1.326612000	-1.683047000
C	1.309967000	-0.088087000	-1.657430000
C	1.978320000	1.153423000	-1.744658000
C	1.286185000	2.367783000	-1.794223000
C	-0.101866000	2.346151000	-1.686538000
C	4.474496000	0.095356000	1.719881000
C	-2.094005000	3.855499000	1.845865000
C	-2.063610000	-3.666708000	2.030258000
C	-4.474496000	-0.095356000	-1.719881000
C	2.094005000	-3.855499000	-1.845865000
C	2.063610000	3.666708000	-2.030258000
C	-2.729348000	-3.594637000	3.415221000
C	-2.882846000	3.807697000	3.165487000
C	4.886933000	-0.728616000	2.951566000
C	2.882846000	-3.807697000	-3.165487000
C	2.729348000	3.594637000	-3.415221000
C	-4.886933000	0.728616000	-2.951566000
C	-1.157064000	-4.900607000	2.001909000

C	-3.074710000	4.038468000	0.679570000
C	5.062966000	1.500613000	1.881828000
C	1.178660000	-5.082870000	-1.891483000
C	3.149430000	3.853307000	-0.960868000
C	-5.084564000	0.539022000	-0.462300000
C	-5.062966000	-1.500613000	-1.881828000
C	1.157064000	4.900607000	-2.001909000
C	3.074710000	-4.038468000	-0.679570000
C	5.084564000	-0.539022000	0.462300000
C	-1.178660000	5.082870000	1.891483000
C	-3.149430000	-3.853307000	0.960868000
H	2.770446000	-2.035822000	1.609775000
H	2.736523000	2.252715000	1.575593000
H	0.643162000	3.454090000	1.585905000
H	-3.072305000	1.308341000	1.753318000
H	-3.058682000	-1.142016000	1.829943000
H	0.669316000	-3.266497000	1.713676000
H	-2.770446000	2.035822000	-1.609775000
H	-2.736523000	-2.252715000	-1.575593000
H	-0.643162000	-3.454090000	-1.585905000
H	3.072305000	-1.308341000	-1.753318000
H	3.058682000	1.142016000	-1.829943000
H	-0.669316000	3.266497000	-1.713676000
H	-3.430323000	4.743122000	3.308134000
H	4.564204000	-1.767290000	2.870646000
H	-3.438522000	-2.767356000	3.472659000
H	3.269349000	4.522596000	-3.621433000
H	-5.974984000	0.721913000	-3.056029000
H	3.604162000	-2.989503000	-3.172091000
H	3.438522000	2.767356000	-3.472659000
H	3.430323000	-4.743122000	-3.308134000
H	-4.564204000	1.767290000	-2.870646000
H	-3.604162000	2.989503000	3.172091000
H	-3.269349000	-4.522596000	3.621433000
H	5.974984000	-0.721913000	3.056029000
H	-2.205642000	3.669054000	4.010416000
H	4.448620000	-0.306683000	3.857893000
H	-1.977072000	-3.449518000	4.192828000
H	1.977072000	3.449518000	-4.192828000
H	-4.448620000	0.306683000	-3.857893000
H	2.205642000	-3.669054000	-4.010416000
H	-3.784734000	3.213254000	0.626884000
H	4.671351000	1.995021000	2.773244000
H	-0.410362000	-4.867778000	2.797774000
H	3.834856000	3.005237000	-0.932477000
H	-4.728119000	1.560475000	-0.327625000

H	0.478546000	-5.029365000	-2.727594000
H	0.410362000	4.867778000	-2.797774000
H	3.784734000	-3.213254000	-0.626884000
H	-4.671351000	-1.995021000	-2.773244000
H	-0.478546000	5.029365000	2.727594000
H	-3.834856000	-3.005237000	0.932477000
H	4.728119000	-1.560475000	0.327625000
H	-3.640836000	4.964660000	0.808381000
H	6.147599000	1.425577000	1.985803000
H	-1.763020000	-5.797450000	2.147442000
H	3.732102000	4.752588000	-1.176578000
H	-6.174393000	0.565421000	-0.543838000
H	1.787887000	-5.980228000	-2.019014000
H	1.763020000	5.797450000	-2.147442000
H	3.640836000	-4.964660000	-0.808381000
H	-6.147599000	-1.425577000	-1.985803000
H	-1.787887000	5.980228000	2.019014000
H	-3.732102000	-4.752588000	1.176578000
H	6.174393000	-0.565421000	0.543838000
H	-2.537902000	4.093158000	-0.269883000
H	4.854012000	2.129652000	1.014500000
H	-0.641872000	-4.991384000	1.042998000
H	2.699907000	3.964687000	0.027767000
H	-4.818816000	-0.038156000	0.426104000
H	0.609862000	-5.193634000	-0.965779000
H	0.641872000	4.991384000	-1.042998000
H	2.537902000	-4.093158000	0.269883000
H	-4.854012000	-2.129652000	-1.014500000
H	-0.609862000	5.193634000	0.965779000
H	-2.699907000	-3.964687000	-0.027767000
H	4.818816000	0.038156000	-0.426104000

**5, UM05-2X/6-31+G(d,p)**

Total Energy: -1001.59508944 a.u.

Optimized geometry:

C	-1.580325255	-0.000445102	-0.000000003
C	-1.574783692	0.711520821	1.233526213
C	-1.561224844	2.125943652	1.206913780
C	-1.577248504	2.814607070	-0.000000001
C	-1.561224881	2.125943652	-1.206913775
C	-1.574783745	0.711520816	-1.233526213
C	-1.562998725	-0.018518643	-2.445185219
C	-1.579531638	-1.408230365	-2.438401937
C	-1.561339453	-2.108654000	-1.238237524
C	-1.574373088	-1.424854312	0.000000003
C	-1.561339358	-2.108653995	1.238237540

C	-1.579531479	-1.408230354	2.438401948
C	-1.562998587	-0.018518630	2.445185225
C	1.580325255	0.000445102	-0.000000009
C	1.574783745	-0.711520816	-1.233526224
C	1.561224881	-2.125943652	-1.206913780
C	1.577248509	-2.814607070	-0.000000008
C	1.561224849	-2.125943652	1.206913775
C	1.574783692	-0.711520821	1.233526208
C	1.562998582	0.018518630	2.445185219
C	1.579531468	1.408230354	2.438401943
C	1.561339347	2.108653995	1.238237534
C	1.574373083	1.424854312	-0.000000004
C	1.561339458	2.108654000	-1.238237534
C	1.579531648	1.408230365	-2.438401943
C	1.562998730	0.018518643	-2.445185225
H	-1.560726163	2.666512166	2.146099856
H	-1.575911813	3.898090024	-0.000000003
H	-1.560726206	2.666512166	-2.146099851
H	-1.563115017	0.525161280	-3.382547899
H	-1.579725348	-1.950064776	-3.376562928
H	-1.560660323	-3.192363670	-1.236585735
H	-1.560660186	-3.192363659	1.236585751
H	-1.579725094	-1.950064760	3.376562944
H	-1.563114821	0.525161304	3.382547894
H	1.560726206	-2.666512166	-2.146099856
H	1.575911818	-3.898090024	-0.000000010
H	1.560726174	-2.666512166	2.146099851
H	1.563114810	-0.525161303	3.382547894
H	1.579725078	1.950064760	3.376562939
H	1.560660175	3.192363664	1.236585746
H	1.560660334	3.192363670	-1.236585746
H	1.579725369	1.950064770	-3.376562934
H	1.563115022	-0.525161281	-3.382547904

**8, UM05-2X/6-31G(d,p)**

Total Energy: -2009.21341992 a.u.

Optimized geometry:

N	-0.308848140	-2.215945732	-1.882945103
N	-2.319245009	-0.918473230	-1.837699898
C	-2.181378441	1.489018939	-1.693755583
C	-1.422190228	2.636179195	-1.544257508
C	-0.029548838	2.511200378	-1.306634837
C	0.590424666	1.280758235	-1.260398234
C	2.024214089	1.086869338	-0.844486380
C	2.653923183	-0.142827718	-1.483805418
C	1.870555709	-1.190718414	-1.797226869

C	0.415061517	-1.136171171	-1.688450277
C	-1.668642229	-2.057315327	-1.889252919
C	-1.575252876	0.215448537	-1.681027400
C	-0.185719117	0.136893594	-1.509216535
N	0.111621139	-2.565948448	1.727056602
N	2.126136167	-1.366849014	1.276802081
C	-1.944773233	1.038371012	1.906332022
C	-2.667370518	-0.190754404	1.995021426
C	-1.979661725	-1.381870481	1.946933646
C	-0.573328333	-1.396420896	1.757433949
C	1.414082300	-2.497098875	1.535138339
C	1.459745539	-0.230900554	1.267251119
C	2.130179693	1.023133455	0.784070157
C	1.544436926	2.269135847	1.418846311
C	0.240960120	2.274517895	1.754986675
C	-0.584677248	1.065763203	1.713425008
C	0.093320368	-0.173334005	1.586373690
C	-2.099366203	4.007407080	-1.631739748
C	4.154350971	-0.143132188	-1.780358908
C	-2.460183683	-3.346266614	-2.035372278
C	-2.695179499	4.183567204	-3.038356314
C	-3.223774844	4.098661156	-0.588220522
C	-1.123341169	5.159693496	-1.375091068
C	4.997592568	0.035556742	-0.505436799
C	4.471121647	1.004802124	-2.758445208
C	4.596596837	-1.449675851	-2.449844385
C	-2.184034073	-3.914609289	-3.436953407
C	-1.978209668	-4.351649287	-0.980141491
C	-3.957790291	-3.095866418	-1.867748642
C	-4.187752946	-0.135705434	2.130465237
C	2.177358278	-3.814233043	1.579292571
C	2.477628648	3.442761505	1.713916740
C	-4.581662849	0.727314077	3.340613834
C	-4.760809076	0.480904014	0.842534257
C	-4.803820947	-1.524644611	2.319644755
C	2.014839644	-4.419783831	2.981888116
C	1.559853016	-4.764681408	0.542710405
C	3.661249724	-3.614346534	1.274879465
C	3.442770983	3.009962708	2.835545741
C	1.712897233	4.676389569	2.202776189
C	3.312072593	3.859174093	0.492257099
H	-3.252338172	1.526624452	-1.848628387
H	0.565367098	3.397320446	-1.136272826
H	2.592268659	1.973428755	-1.115251958
H	2.265678215	-2.113456414	-2.197238161
H	-1.912099496	4.126121177	-3.796905407

H	-3.184533300	5.157715893	-3.117633479
H	-3.434334176	3.411178661	-3.255128644
H	-3.696085398	5.083078255	-0.635167454
H	-3.994983962	3.347489087	-0.761247896
H	-2.824121831	3.955634498	0.418636984
H	-0.318969963	5.180453236	-2.113358833
H	-1.661550734	6.107194979	-1.440923385
H	-0.682454086	5.092068829	-0.377550758
H	4.909558719	1.044090404	-0.096849234
H	6.051554505	-0.117293349	-0.749225286
H	4.701741513	-0.684683520	0.259737840
H	3.882104867	0.907935094	-3.672537366
H	4.274715899	1.986322222	-2.323435170
H	5.530221919	0.970979792	-3.024737525
H	5.662603377	-1.388558771	-2.676567773
H	4.442417843	-2.309240812	-1.795418253
H	4.062603983	-1.620404354	-3.386220393
H	-2.537040525	-3.226902539	-4.208708832
H	-1.115187181	-4.079441315	-3.575822575
H	-2.706552635	-4.866733891	-3.557902890
H	-2.086937936	-3.946190917	0.028434059
H	-0.927404722	-4.591353498	-1.132575863
H	-2.567869726	-5.268781731	-1.054993440
H	-4.327225710	-2.393281946	-2.613999265
H	-4.494440641	-4.041838241	-1.971573529
H	-4.173044773	-2.677685966	-0.882700204
H	-2.479455357	1.975232556	2.006131587
H	-0.230080149	3.165141805	2.151996052
H	3.190289476	0.938600023	1.001669417
H	-2.471277895	-2.337903219	2.052316033
H	-4.234883551	1.756684169	3.241268520
H	-4.165328579	0.313406900	4.261128534
H	-5.669954122	0.751171937	3.434077393
H	-4.402717529	1.502996842	0.705055612
H	-4.459327466	-0.105308897	-0.028948377
H	-5.852420172	0.505366786	0.896427791
H	-4.605417922	-2.172416595	1.463900436
H	-4.423985227	-2.009923378	3.221323272
H	-5.886595905	-1.425299932	2.419279825
H	0.958308310	-4.551789447	3.214718228
H	2.461476256	-3.771756058	3.739746861
H	2.512760900	-5.391502719	3.024383183
H	0.517452901	-4.963504547	0.788587111
H	2.112045220	-5.707781440	0.532447234
H	1.594480835	-4.324884657	-0.457182039
H	3.799751083	-3.192413857	0.278639543



H	4.125950661	-2.936669270	1.992096363
H	4.169981923	-4.580003556	1.322470167
H	4.072654917	2.172088516	2.530653634
H	2.884686218	2.712223624	3.724671323
H	4.099837787	3.842997179	3.098321101
H	0.987947138	5.016822500	1.459862794
H	1.188053150	4.477287432	3.138478205
H	2.418564981	5.489617744	2.383337774
H	2.679045967	4.202920408	-0.329303896
H	3.943595489	3.045806194	0.131862066
H	3.972640649	4.682657078	0.773158109

**9, UM05-2X/6-31G(d,p)**

Total Energy: -2009.19931019 a.u.

Optimized geometry:

N	-0.082338328	-2.407563206	-1.706437336
N	-2.105492728	-1.135759292	-1.645731209
C	-2.048029223	1.269946080	-1.649526493
C	-1.326433137	2.463788024	-1.690257062
C	0.071056754	2.410296003	-1.627101882
C	0.769622027	1.179865205	-1.604394040
C	2.174496711	1.075046264	-1.616091143
C	2.828850229	-0.169851606	-1.708269675
C	2.064438642	-1.326941411	-1.712201048
C	0.643135008	-1.274489159	-1.664711640
C	-1.415954576	-2.278510165	-1.694309171
C	-1.392789842	0.011787910	-1.624412192
C	0.014875780	-0.013665469	-1.619154025
C	-2.080096916	3.789951534	-1.841091287
C	4.357155278	-0.209611806	-1.789880247
C	-2.203765888	-3.576223257	-1.818967328
C	-2.915256186	3.744948708	-3.132297026
C	-3.015872392	4.009220544	-0.643410783
C	-1.134173158	4.990740821	-1.934934796
C	4.938712414	0.186693830	-0.423388670
C	4.856777827	0.768659348	-2.865709804
C	4.877070072	-1.603480114	-2.158054292
C	-1.990594437	-4.104548483	-3.247495869
C	-1.667377454	-4.605806110	-0.816775741
C	-3.695253712	-3.348601687	-1.579346495
N	0.082268311	-2.407522920	1.706468897
N	2.105460560	-1.135781337	1.645729288
C	-2.174464711	1.075150427	1.616063430
C	-2.828853975	-0.169727594	1.708257134
C	-2.064475219	-1.326838560	1.712214267

C	-0.643170510	-1.274427886	1.664728336
C	1.415888233	-2.278510430	1.694326608
C	1.392792483	0.011788458	1.624401736
C	2.048067991	1.269928738	1.649505273
C	1.326505115	2.463791268	1.690231444
C	-0.070985961	2.410339125	1.627070455
C	-0.769586630	1.179928500	1.604371143
C	-0.014874298	-0.013623377	1.619147632
C	-4.357160311	-0.209448664	1.789854978
C	2.203659650	-3.576244096	1.819022405
C	2.080205159	3.789933278	1.841070665
C	-4.856772303	0.768845952	2.865667374
C	-4.938690776	0.186851020	0.423349974
C	-4.877110559	-1.603300697	2.158038830
C	1.990444256	-4.104538318	3.247556254
C	1.667262951	-4.605828224	0.816837670
C	3.695158757	-3.348670591	1.579426575
C	2.915393777	3.744881117	3.132255433
C	1.134313818	4.990745579	1.934958762
C	3.015959474	4.009201551	0.643374032
H	-3.128846983	1.258270906	-1.693062181
H	0.653178755	3.321116858	-1.648728352
H	2.754823436	1.988632762	-1.600889915
H	2.510075528	-2.308782010	-1.780148597
H	-2.272374014	3.576604609	-3.998340432
H	-3.440118255	4.693789740	-3.268593844
H	-3.659375321	2.948254785	-3.102174621
H	-3.575443742	4.938713197	-0.773844621
H	-3.733786847	3.194078626	-0.542831037
H	-2.445246884	4.082354631	0.285072908
H	-0.471087824	4.912133340	-2.798974139
H	-1.722814243	5.903497448	-2.045663940
H	-0.524151208	5.094537133	-1.034957757
H	4.695852604	1.225077627	-0.187139832
H	6.027631312	0.091345806	-0.438257318
H	4.531871283	-0.449834001	0.365226269
H	4.440073520	0.516320754	-3.842888676
H	4.594249869	1.802545400	-2.638020604
H	5.945950302	0.713133922	-2.930453292
H	5.962031938	-1.559985993	-2.271801370
H	4.658176673	-2.339501407	-1.383894943
H	4.449899887	-1.950500743	-3.101383189
H	-2.377775848	-3.396299648	-3.983651542
H	-0.928338561	-4.261870451	-3.437613666
H	-2.516384963	-5.054382156	-3.372655882
H	-1.718298987	-4.223289822	0.205160807

H	-0.626764690	-4.840577730	-1.032696218
H	-2.260514083	-5.521477586	-0.882418036
H	-4.110017491	-2.641282748	-2.296864198
H	-4.223824143	-4.300332966	-1.670711481
H	-3.867033277	-2.948083326	-0.579432490
H	-2.754764803	1.988753959	1.600845787
H	-0.653082286	3.321176337	1.648686885
H	3.128885269	1.258224169	1.693046878
H	-2.510140701	-2.308665290	1.780173828
H	-4.594200174	1.802721129	2.637980376
H	-4.440102064	0.516496378	3.842857931
H	-5.945948609	0.713361145	2.930383726
H	-4.695807624	1.225227665	0.187092682
H	-4.531847285	-0.449694254	-0.365250286
H	-6.027611415	0.091523359	0.438203083
H	-4.658209402	-2.339337939	1.383896584
H	-4.449970860	-1.950313568	3.101384168
H	-5.962074590	-1.559785065	2.271756919
H	0.928179570	-4.261824386	3.437655492
H	2.377632293	-3.396288599	3.983707513
H	2.516202614	-5.054386204	3.372744149
H	0.626638036	-4.840564765	1.032737568
H	2.260371523	-5.521515899	0.882509626
H	1.718220674	-4.223329474	-0.205103642
H	3.866967807	-2.948176652	0.579507919
H	4.109929589	-2.641349757	2.296938526
H	4.223699675	-4.300415470	1.670820078
H	3.659491004	2.948167392	3.102095498
H	2.272528406	3.576532778	3.998310533
H	3.440283205	4.693705606	3.268561284
H	0.524261800	5.094562364	1.035004128
H	0.471257624	4.912148242	2.799021082
H	1.722980791	5.903486864	2.045675963
H	2.445315466	4.082379237	-0.285094781
H	3.733845464	3.194039578	0.542757211
H	3.575565162	4.938671911	0.773819803

**10, UM05-2X/6-31G(d,p)**

Total Energy: -2009.19436646 a.u.

Optimized geometry:

N	0.160971000	-2.354312000	1.712254000
N	2.181353000	-1.079488000	1.628868000
C	2.110007000	1.329639000	1.545462000
C	1.380964000	2.509047000	1.520790000
C	-0.018988000	2.437705000	1.355889000
C	-0.701111000	1.209619000	1.379497000

C	-2.108324000	1.081828000	1.227068000
C	-2.761738000	-0.160607000	1.522536000
C	-1.995684000	-1.290796000	1.648391000
C	-0.560974000	-1.235674000	1.607904000
C	1.500429000	-2.219470000	1.702480000
C	1.464294000	0.063411000	1.554892000
C	0.059839000	0.027498000	1.511309000
C	2.107801000	3.849708000	1.683843000
C	-4.280841000	-0.187023000	1.716259000
C	2.291369000	-3.511302000	1.853786000
C	2.901422000	3.829224000	3.001573000
C	3.078045000	4.078870000	0.516037000
C	1.139340000	5.034926000	1.740808000
C	-5.001988000	0.121843000	0.395346000
C	-4.677425000	0.861395000	2.770623000
C	-4.765408000	-1.550760000	2.220688000
C	2.082611000	-4.013202000	3.292224000
C	1.756114000	-4.560718000	0.871529000
C	3.781199000	-3.282405000	1.604026000
N	-0.090178000	-2.457855000	-1.669814000
N	-2.121328000	-1.224288000	-1.420780000
C	2.084318000	1.079888000	-1.567154000
C	2.766032000	-0.155559000	-1.721933000
C	2.034522000	-1.326227000	-1.736917000
C	0.618414000	-1.306695000	-1.633939000
C	-1.410492000	-2.359283000	-1.578270000
C	-1.435891000	-0.076603000	-1.400133000
C	-2.118755000	1.177525000	-1.239282000
C	-1.432745000	2.395462000	-1.454404000
C	-0.049019000	2.376290000	-1.465629000
C	0.695225000	1.147916000	-1.503973000
C	-0.031430000	-0.064821000	-1.516009000
C	4.289494000	-0.153002000	-1.865415000
C	-2.188163000	-3.663734000	-1.703977000
C	-2.237614000	3.678894000	-1.689383000
C	4.711524000	0.830411000	-2.969555000
C	4.917362000	0.271793000	-0.528486000
C	4.835434000	-1.534124000	-2.241820000
C	-1.976871000	-4.196762000	-3.130468000
C	-1.633472000	-4.682005000	-0.699258000
C	-3.681158000	-3.454423000	-1.457415000
C	-3.062752000	3.494106000	-2.975980000
C	-1.337338000	4.901801000	-1.884296000
C	-3.196322000	3.974434000	-0.526926000
H	3.187928000	1.329471000	1.640800000
H	-0.606180000	3.344412000	1.314535000

H	-2.695775000	1.988799000	1.221265000
H	-2.428867000	-2.263028000	1.835075000
H	2.234663000	3.654023000	3.847922000
H	3.402581000	4.789404000	3.147169000
H	3.661867000	3.047702000	3.001827000
H	3.616355000	5.019103000	0.659057000
H	3.813128000	3.276048000	0.445555000
H	2.537723000	4.137992000	-0.431481000
H	0.435483000	4.938507000	2.570143000
H	1.707575000	5.955624000	1.886721000
H	0.574619000	5.137524000	0.812310000
H	-4.836156000	1.156638000	0.088858000
H	-6.078818000	-0.011218000	0.526025000
H	-4.652230000	-0.541530000	-0.397934000
H	-4.167363000	0.671159000	3.717018000
H	-4.438878000	1.877059000	2.450945000
H	-5.755260000	0.814748000	2.943704000
H	-5.839467000	-1.498126000	2.408898000
H	-4.596898000	-2.339274000	1.486574000
H	-4.270501000	-1.828509000	3.153395000
H	2.472327000	-3.291615000	4.013856000
H	1.020924000	-4.167024000	3.488681000
H	2.608415000	-4.960835000	3.433124000
H	1.803706000	-4.195572000	-0.156921000
H	0.717118000	-4.795730000	1.094255000
H	2.353294000	-5.472643000	0.951400000
H	4.195544000	-2.559196000	2.305717000
H	4.314039000	-4.229997000	1.712195000
H	3.947006000	-2.900876000	0.595333000
H	2.648876000	2.003658000	-1.558152000
H	0.509997000	3.295622000	-1.580385000
H	-3.197101000	1.137311000	-1.286274000
H	2.500409000	-2.294456000	-1.852321000
H	4.422316000	1.856560000	-2.738903000
H	4.262196000	0.554633000	-3.925726000
H	5.798287000	0.810363000	-3.080562000
H	4.651766000	1.302580000	-0.286493000
H	4.567050000	-0.372766000	0.280571000
H	6.007033000	0.210837000	-0.592173000
H	4.658114000	-2.269745000	-1.456419000
H	4.390029000	-1.898888000	-3.169813000
H	5.914939000	-1.461959000	-2.388531000
H	-0.914221000	-4.342566000	-3.325134000
H	-2.375311000	-3.496961000	-3.868847000
H	-2.493922000	-5.152342000	-3.248073000
H	-0.587215000	-4.892523000	-0.913696000

H	-2.205955000	-5.610723000	-0.765530000
H	-1.696817000	-4.299428000	0.322151000
H	-3.855723000	-3.058966000	-0.456390000
H	-4.107536000	-2.750927000	-2.172646000
H	-4.198426000	-4.412167000	-1.551074000
H	-3.778717000	2.676326000	-2.881083000
H	-2.407375000	3.274976000	-3.820839000
H	-3.619542000	4.408677000	-3.195424000
H	-0.724783000	5.096041000	-1.001674000
H	-0.679377000	4.781748000	-2.747120000
H	-1.959914000	5.781760000	-2.057826000
H	-2.650482000	4.167973000	0.399509000
H	-3.892719000	3.151825000	-0.356479000
H	-3.787060000	4.863861000	-0.758386000

### 11, UM05-2X/6-31G(d,p)

Total Energy: -2009.19468042 a.u.

Optimized geometry:

N	0.123317895	-2.412950789	1.751972007
N	2.135742285	-1.133484497	1.598293217
C	2.086506604	1.272845165	1.493373303
C	1.376426589	2.451737801	1.446795901
C	-0.024596211	2.388323489	1.190525492
C	-0.738537212	1.157955774	1.384499131
C	-2.128227464	1.058292330	1.409179105
C	-2.784708987	-0.181273142	1.640855669
C	-2.027814800	-1.330209217	1.728373618
C	-0.607781729	-1.281388548	1.659819960
C	1.444589545	-2.285225432	1.703051837
C	1.426263971	-0.004896656	1.518958530
C	0.017134456	-0.029440350	1.517685319
C	2.106690166	3.785950316	1.661575753
C	-4.307791023	-0.197104872	1.781862363
C	2.243959881	-3.575180985	1.835167955
C	2.886421691	3.709852436	2.986628389
C	3.097763602	4.068695583	0.522458525
C	1.140327036	4.969415168	1.768009610
C	-4.946396635	0.192156183	0.439323694
C	-4.737066311	0.805357921	2.866323242
C	-4.834965511	-1.576126479	2.189956416
C	2.047012844	-4.100978205	3.266302630
C	1.703091472	-4.608696517	0.838355007
C	3.731680495	-3.340871358	1.578274805
N	-0.121726319	-2.413027784	-1.751901658
N	-2.134943196	-1.134802603	-1.598131532

C	2.127614005	1.059693739	-1.409326666
C	2.784868137	-0.179442301	-1.641064133
C	2.028721417	-1.328896175	-1.728429779
C	0.608676483	-1.281002873	-1.659728560
C	-1.443067198	-2.286105898	-1.702988759
C	-1.426167105	-0.005790072	-1.518843323
C	-2.087242065	1.271512359	-1.493174042
C	-1.377950380	2.450897939	-1.446731098
C	0.023131487	2.388382064	-1.190515876
C	0.737872158	1.158449650	-1.384502190
C	-0.017028727	-0.029447929	-1.517622813
C	4.307955872	-0.194325444	-1.782173196
C	-2.241702327	-3.576502472	-1.835125589
C	-2.109184537	3.784632464	-1.661432373
C	4.736645631	0.808434577	-2.866574590
C	4.946169618	0.195311623	-0.439574103
C	4.836001116	-1.573032259	-2.190246352
C	-2.044490590	-4.102141463	-3.266286701
C	-1.700188418	-4.609745452	-0.838384551
C	-3.729543413	-3.343044471	-1.578175108
C	-2.889662249	3.707803467	-2.986003325
C	-1.143616448	4.968651677	-1.768783600
C	-3.099774364	4.067108597	-0.521830970
H	3.159097153	1.259218783	1.635149924
H	-0.606509048	3.298907468	1.217367344
H	-2.713710177	1.964929627	1.334885348
H	-2.472990301	-2.303021548	1.882343963
H	2.212880120	3.486283133	3.815824591
H	3.373655032	4.668107081	3.182923993
H	3.657766443	2.939961380	2.959117614
H	3.646826005	4.990084028	0.731690567
H	3.823534694	3.260431305	0.419145643
H	2.582760021	4.197026593	-0.432397021
H	0.425480092	4.830547370	2.581796204
H	1.708957896	5.879011899	1.970742187
H	0.588040141	5.128560706	0.841258956
H	-4.707358431	1.225397192	0.180034534
H	-6.034151937	0.107170051	0.506330561
H	-4.582418852	-0.456674233	-0.359900282
H	-4.287838732	0.550207108	3.828219461
H	-4.450324483	1.827773453	2.615908499
H	-5.824004691	0.782664668	2.975950629
H	-5.916210819	-1.516742437	2.329194002
H	-4.640971663	-2.328482307	1.424656807
H	-4.389743702	-1.910039187	3.129492293
H	2.435646370	-3.388415493	3.997566484

H	0.987504328	-4.264014131	3.465495171
H	2.580648366	-5.046695098	3.389596859
H	1.754149835	-4.228641559	-0.184693242
H	0.662216019	-4.839440618	1.058169439
H	2.294333462	-5.525524732	0.905024504
H	4.151426496	-2.629377207	2.289032225
H	4.265626845	-4.289832581	1.667646572
H	3.890133234	-2.942946754	0.575154956
H	2.712521122	1.966711282	-1.335061003
H	0.604478903	3.299331387	-1.217404529
H	-3.159834038	1.257147881	-1.634862951
H	2.474529836	-2.301415740	-1.882397643
H	4.448219448	1.830513626	-2.616727337
H	4.288579707	0.552330425	-3.828760619
H	5.823705335	0.787266862	-2.975304985
H	4.706257081	1.228327102	-0.180200087
H	4.582397680	-0.453893247	0.359423270
H	6.033994507	0.111148891	-0.506410132
H	4.642916187	-2.325397978	-1.424726283
H	4.390652643	-1.907466302	-3.129534855
H	5.917143600	-1.512844175	-2.329954927
H	-0.984891654	-4.264494380	-3.465555873
H	-2.433629089	-3.389811636	-3.997508571
H	-2.577521084	-5.048199469	-3.389575216
H	-0.659284167	-4.840119711	-1.058446140
H	-2.291111002	-5.526794704	-0.904842980
H	-1.751122413	-4.229637454	0.184648096
H	-3.888227212	-2.945600873	-0.574896099
H	-4.149613742	-2.631468647	-2.288661817
H	-4.263024168	-4.292228912	-1.667938567
H	-3.660626618	2.937560981	-2.957833947
H	-2.216504892	3.484345297	-3.815539042
H	-3.377490343	4.665763319	-3.182262903
H	-0.591168530	5.128691201	-0.842282993
H	-0.428919970	4.829775746	-2.582698276
H	-1.712882696	5.877779287	-1.971851210
H	-2.584344879	4.195947818	0.432723193
H	-3.825042002	3.258462280	-0.417960368
H	-3.649465360	4.988145092	-0.730979485

**12**, UM05-2X/6-31G(d,p)

Total Energy: -2009.21113393 a.u.

Optimized geometry:

N	-0.564672000	-2.326893000	-1.959360000
N	-2.287486000	-0.684269000	-1.772977000
C	-1.776698000	1.668607000	-1.639128000



C	-0.914334000	2.662563000	-1.354493000
C	0.447952000	2.304632000	-0.775681000
C	0.950112000	0.976200000	-1.285283000
C	2.277113000	0.644965000	-1.407279000
C	2.700566000	-0.678865000	-1.733449000
C	1.753829000	-1.663540000	-1.901147000
C	0.373743000	-1.357312000	-1.804199000
C	-1.827778000	-1.960581000	-1.882892000
C	-1.383830000	0.261784000	-1.607144000
C	-0.004723000	-0.032210000	-1.538380000
C	-1.269175000	4.125329000	-1.634015000
C	4.199060000	-0.957823000	-1.834541000
C	-2.864463000	-3.071199000	-1.986303000
C	-2.664807000	4.260095000	-2.255019000
C	-1.245335000	4.995407000	-0.367345000
C	-0.254890000	4.693634000	-2.645611000
C	4.840730000	-0.719272000	-0.456926000
C	4.833344000	-0.014885000	-2.870515000
C	4.490821000	-2.397888000	-2.265710000
C	-2.826934000	-3.625712000	-3.418997000
C	-2.492650000	-4.186127000	-0.998557000
C	-4.268014000	-2.555155000	-1.670547000
N	-0.346947000	-2.424566000	1.930512000
N	1.856948000	-1.513671000	1.780705000
C	-1.914415000	1.386735000	1.439624000
C	-2.793017000	0.301635000	1.730980000
C	-2.268992000	-0.962992000	1.881326000
C	-0.869864000	-1.177447000	1.799625000
C	0.963747000	-2.538203000	1.860260000
C	1.359705000	-0.300221000	1.640085000
C	2.235049000	0.868350000	1.681264000
C	1.790206000	2.110651000	1.414229000
C	0.388686000	2.284060000	0.859866000
C	-0.557048000	1.213033000	1.331871000
C	-0.033206000	-0.075090000	1.567423000
C	-4.290404000	0.590747000	1.817754000
C	1.528301000	-3.950583000	1.931453000
C	2.716026000	3.312467000	1.672244000
C	-4.546407000	1.662749000	2.890329000
C	-4.776685000	1.100087000	0.449333000
C	-5.099861000	-0.653800000	2.192139000
C	1.322191000	-4.470989000	3.362648000
C	0.759277000	-4.842997000	0.947456000
C	3.016797000	-3.973863000	1.583211000
C	3.053316000	3.339376000	3.175222000
C	2.088468000	4.664868000	1.319849000

C	4.023633000	3.186440000	0.873777000
H	-2.782140000	1.851522000	-1.989771000
H	1.176347000	3.080381000	-1.013663000
H	3.027474000	1.403780000	-1.229212000
H	2.015240000	-2.689645000	-2.117618000
H	-2.740625000	3.710711000	-3.194610000
H	-2.860660000	5.313717000	-2.462665000
H	-3.442992000	3.903067000	-1.576828000
H	-1.545277000	6.013410000	-0.626886000
H	-1.944894000	4.620962000	0.383910000
H	-0.252593000	5.052329000	0.073830000
H	-0.233199000	4.085157000	-3.551471000
H	-0.544543000	5.711127000	-2.918292000
H	0.756021000	4.738564000	-2.237035000
H	4.754209000	0.327808000	-0.160964000
H	5.903250000	-0.973106000	-0.493760000
H	4.352265000	-1.328273000	0.306849000
H	4.384350000	-0.165073000	-3.854262000
H	4.711640000	1.034248000	-2.596268000
H	5.904453000	-0.218020000	-2.944623000
H	5.570494000	-2.532776000	-2.357048000
H	4.126679000	-3.120193000	-1.533260000
H	4.038397000	-2.622916000	-3.233865000
H	-3.101078000	-2.852796000	-4.140865000
H	-1.826199000	-3.987508000	-3.656599000
H	-3.535040000	-4.452697000	-3.514237000
H	-2.440566000	-3.800232000	0.022645000
H	-1.519821000	-4.607470000	-1.247334000
H	-3.245669000	-4.977247000	-1.038281000
H	-4.573196000	-1.776045000	-2.368490000
H	-4.977393000	-3.383957000	-1.729637000
H	-4.304872000	-2.135329000	-0.663864000
H	-2.332085000	2.371800000	1.272948000
H	-0.010648000	3.255858000	1.138041000
H	3.248655000	0.677907000	2.013894000
H	-2.889291000	-1.827538000	2.071702000
H	-4.033110000	2.598331000	2.663076000
H	-4.207115000	1.317302000	3.868841000
H	-5.616665000	1.874516000	2.950343000
H	-4.301053000	2.048512000	0.189390000
H	-4.540193000	0.378570000	-0.335629000
H	-5.857443000	1.261211000	0.475783000
H	-5.010077000	-1.436531000	1.437322000
H	-4.781912000	-1.058988000	3.155114000
H	-6.155286000	-0.384965000	2.269389000
H	0.262924000	-4.450022000	3.621169000

H	1.870688000	-3.856970000	4.080742000
H	1.686000000	-5.498681000	3.439442000
H	-0.295624000	-4.886718000	1.213917000
H	1.175362000	-5.853386000	0.967482000
H	0.833623000	-4.451849000	-0.070372000
H	3.181098000	-3.583975000	0.576679000
H	3.598441000	-3.366795000	2.276189000
H	3.378519000	-5.004055000	1.621342000
H	3.580876000	2.435102000	3.479194000
H	2.142831000	3.416808000	3.772590000
H	3.688897000	4.200469000	3.397790000
H	1.847560000	4.741211000	0.257896000
H	1.188471000	4.865294000	1.904412000
H	2.807060000	5.455245000	1.546366000
H	3.834192000	3.223611000	-0.201595000
H	4.547643000	2.257926000	1.100943000
H	4.687848000	4.017158000	1.124768000

### 13, UM05-2X/6-31G(d,p)

Total Energy: -2009.19391849 a.u.

Optimized geometry:

N	-0.193552000	-2.398050000	-1.707180000
N	-1.950012000	-1.021770000	-0.826629000
C	-1.858765000	1.356884000	-1.443906000
C	-1.088308000	2.520546000	-1.736035000
C	0.277285000	2.405759000	-1.862444000
C	0.920550000	1.138433000	-1.801251000
C	2.315257000	0.945506000	-1.936871000
C	2.878120000	-0.319681000	-1.941216000
C	2.025176000	-1.447101000	-1.864926000
C	0.666687000	-1.295052000	-1.687310000
C	-1.400090000	-2.259482000	-1.301541000
C	-1.258765000	0.130844000	-1.318508000
C	0.118584000	0.000293000	-1.597063000
C	-1.825156000	3.852137000	-1.882055000
C	4.399508000	-0.484616000	-1.979698000
C	-2.319833000	-3.484123000	-1.408188000
C	-2.832790000	3.743603000	-3.038847000
C	-2.579037000	4.179070000	-0.583096000
C	-0.873085000	5.012304000	-2.184319000
C	4.941733000	-0.109581000	-0.589274000
C	5.030856000	0.428162000	-3.041417000
C	4.821389000	-1.925319000	-2.289900000
C	-1.990660000	-4.198027000	-2.731046000
C	-2.054325000	-4.475397000	-0.262649000

C	-3.800740000	-3.102787000	-1.435607000
N	-0.152212000	-2.312693000	1.387470000
N	1.943476000	-1.267841000	1.868444000
C	-2.176220000	1.253449000	1.625025000
C	-2.879647000	0.178117000	1.226928000
C	-2.121706000	-1.032399000	0.701917000
C	-0.732363000	-1.141023000	1.298958000
C	1.176261000	-2.323975000	1.725461000
C	1.341676000	-0.047814000	1.804538000
C	2.082325000	1.145169000	1.964935000
C	1.448026000	2.373721000	1.983049000
C	0.032078000	2.424027000	1.877752000
C	-0.714673000	1.284554000	1.672670000
C	-0.040621000	0.050020000	1.593628000
C	-4.405776000	0.125684000	1.309201000
C	1.801887000	-3.701432000	1.887311000
C	2.281954000	3.651047000	2.115548000
C	-4.975515000	1.325048000	2.075855000
C	-5.036195000	0.124565000	-0.095383000
C	-4.838546000	-1.142753000	2.069835000
C	0.821063000	-4.637778000	2.604683000
C	2.105331000	-4.247921000	0.482762000
C	3.102967000	-3.618128000	2.687651000
C	3.123544000	3.596716000	3.400484000
C	1.416417000	4.914399000	2.164119000
C	3.211819000	3.756596000	0.895257000
H	-2.921768000	1.437395000	-1.276330000
H	0.893268000	3.276515000	-2.046546000
H	2.940916000	1.823713000	-2.043807000
H	2.408224000	-2.452067000	-1.960721000
H	-2.318851000	3.508277000	-3.972554000
H	-3.362345000	4.691819000	-3.162313000
H	-3.573954000	2.963876000	-2.854777000
H	-3.125146000	5.119158000	-0.694589000
H	-3.297280000	3.397946000	-0.326440000
H	-1.877873000	4.282997000	0.247781000
H	-0.335365000	4.852228000	-3.120946000
H	-1.447152000	5.936380000	-2.278692000
H	-0.143259000	5.150447000	-1.382882000
H	4.731792000	0.939024000	-0.367864000
H	6.023804000	-0.262452000	-0.548577000
H	4.466443000	-0.720278000	0.182648000
H	4.628411000	0.206322000	-4.031708000
H	4.859377000	1.484023000	-2.830388000
H	6.111757000	0.269767000	-3.063752000
H	5.910172000	-1.971925000	-2.358906000

H	4.513228000	-2.615520000	-1.502621000
H	4.404927000	-2.268943000	-3.239280000
H	-2.165256000	-3.536618000	-3.581868000
H	-0.948934000	-4.509693000	-2.750087000
H	-2.634462000	-5.075006000	-2.832752000
H	-2.292843000	-4.060133000	0.716786000
H	-1.003619000	-4.763799000	-0.253334000
H	-2.664068000	-5.368873000	-0.420068000
H	-4.007565000	-2.383023000	-2.229439000
H	-4.392458000	-4.001758000	-1.622088000
H	-4.138212000	-2.676898000	-0.492182000
H	-2.682035000	2.143481000	1.975702000
H	-0.481450000	3.371705000	1.962299000
H	3.154614000	1.051524000	2.082281000
H	-2.657886000	-1.952483000	0.914476000
H	-4.752053000	2.269461000	1.575290000
H	-4.590020000	1.368294000	3.096656000
H	-6.062197000	1.230035000	2.124246000
H	-4.960407000	1.116921000	-0.547001000
H	-4.550878000	-0.587588000	-0.759225000
H	-6.097825000	-0.125892000	-0.022275000
H	-4.631117000	-2.058621000	1.516285000
H	-4.335443000	-1.203714000	3.037322000
H	-5.916069000	-1.109048000	2.244401000
H	-0.099181000	-4.754866000	2.035379000
H	0.566305000	-4.249227000	3.593553000
H	1.287367000	-5.617363000	2.732305000
H	1.223312000	-4.205546000	-0.158413000
H	2.448437000	-5.283130000	0.555287000
H	2.894170000	-3.653949000	0.017012000
H	3.827460000	-2.973202000	2.192740000
H	2.921677000	-3.215077000	3.685894000
H	3.527312000	-4.619898000	2.787850000
H	3.807772000	2.747706000	3.397324000
H	2.480594000	3.512346000	4.278769000
H	3.717737000	4.509262000	3.492815000
H	0.819581000	5.027327000	1.255642000
H	0.745975000	4.911181000	3.026397000
H	2.065005000	5.788448000	2.248761000
H	2.626947000	3.772391000	-0.027152000
H	3.898651000	2.910661000	0.846750000
H	3.801787000	4.674865000	0.952093000

**14, UM05-2X/6-31G(d,p)**

Total Energy: -2009.15418766 a.u.

Optimized geometry:

N	0.012476000	2.220729000	0.766883000
N	-2.043449000	1.303173000	1.609929000
C	-2.202923000	-1.100033000	1.862394000
C	-1.583939000	-2.370131000	2.028554000
C	-0.206924000	-2.440904000	2.070323000
C	0.599535000	-1.288733000	1.882721000
C	2.016478000	-1.290982000	1.964571000
C	2.749770000	-0.136904000	1.790042000
C	2.067859000	1.063289000	1.442625000
C	0.703256000	1.081353000	1.304419000
C	-1.358731000	2.307691000	1.211499000
C	-1.451557000	0.032087000	1.656791000
C	-0.045400000	-0.072205000	1.604882000
C	-2.474226000	-3.604958000	2.161650000
C	4.271286000	-0.092526000	1.930668000
C	-1.948287000	3.704184000	1.358889000
C	-3.428429000	-3.443018000	3.355641000
C	-3.290803000	-3.761833000	0.867468000
C	-1.662032000	-4.886253000	2.369273000
C	4.900603000	0.265836000	0.575223000
C	4.850536000	-1.433811000	2.388159000
C	4.654413000	0.973094000	2.971189000
C	-1.252356000	4.322588000	2.587860000
C	-1.713915000	4.613247000	0.147609000
C	-3.452706000	3.623695000	1.625433000
N	0.041670000	2.233941000	-0.737790000
N	2.070554000	1.285745000	-1.613366000
C	-2.045151000	-1.210341000	-1.991497000
C	-2.752615000	-0.043642000	-1.793005000
C	-2.043193000	1.133458000	-1.421918000
C	-0.677180000	1.120185000	-1.292251000
C	1.410840000	2.301291000	-1.201892000
C	1.452135000	0.028074000	-1.664874000
C	2.177915000	-1.118046000	-1.881324000
C	1.530447000	-2.372105000	-2.058091000
C	0.152336000	-2.411193000	-2.106106000
C	-0.628604000	-1.242551000	-1.909085000
C	0.043713000	-0.044914000	-1.614429000
C	-4.275416000	0.031138000	-1.908581000
C	2.027007000	3.687886000	-1.344240000
C	2.395606000	-3.623677000	-2.197316000
C	-4.871665000	-1.235518000	-2.529847000
C	-4.878759000	0.215137000	-0.506455000

C	-4.671267000	1.223884000	-2.795770000
C	1.145370000	4.464715000	-2.340982000
C	2.122042000	4.451045000	-0.012961000
C	3.435801000	3.581230000	-1.933590000
C	3.332121000	-3.485313000	-3.408262000
C	1.556893000	-4.891031000	-2.382033000
C	3.231759000	-3.785648000	-0.916236000
H	-3.278409000	-0.992379000	1.913979000
H	0.293470000	-3.382607000	2.253575000
H	2.508815000	-2.226904000	2.194281000
H	2.625618000	1.966567000	1.241498000
H	-2.864862000	-3.325152000	4.283160000
H	-4.062467000	-4.328668000	3.445803000
H	-4.079265000	-2.575239000	3.241159000
H	-3.928041000	-4.647712000	0.930694000
H	-3.929618000	-2.894612000	0.690865000
H	-2.623209000	-3.870383000	0.009324000
H	-1.072624000	-4.841620000	3.287504000
H	-2.343351000	-5.735828000	2.448155000
H	-0.988771000	-5.071480000	1.529270000
H	4.700149000	-0.520087000	-0.155109000
H	5.983300000	0.372699000	0.681973000
H	4.497641000	1.196167000	0.173788000
H	4.444309000	-1.735326000	3.356099000
H	4.649834000	-2.224834000	1.662307000
H	5.933866000	-1.341445000	2.489458000
H	5.740033000	0.996768000	3.094268000
H	4.330505000	1.970190000	2.669000000
H	4.200786000	0.746875000	3.938127000
H	-1.469899000	3.736377000	3.482650000
H	-0.171023000	4.356811000	2.448675000
H	-1.618433000	5.340609000	2.740709000
H	-2.161449000	4.207271000	-0.761017000
H	-0.656948000	4.773068000	-0.039147000
H	-2.176387000	5.582030000	0.351470000
H	-3.670057000	3.002246000	2.491573000
H	-3.835081000	4.632080000	1.799379000
H	-3.979283000	3.201901000	0.766630000
H	-2.558559000	-2.130410000	-2.238621000
H	-0.367853000	-3.340339000	-2.298227000
H	3.255623000	-1.034631000	-1.934048000
H	-2.583659000	2.040500000	-1.190385000
H	-4.688905000	-2.114239000	-1.907754000
H	-4.463590000	-1.420448000	-3.525976000
H	-5.953347000	-1.116003000	-2.620756000
H	-4.727174000	-0.688141000	0.087233000

H	-4.411291000	1.041846000	0.030345000
H	-5.953293000	0.402458000	-0.580848000
H	-4.377660000	2.177498000	-2.354470000
H	-4.206015000	1.144908000	-3.780264000
H	-5.756072000	1.240334000	-2.924844000
H	0.125599000	4.572585000	-1.978410000
H	1.114234000	3.943659000	-3.300457000
H	1.572679000	5.456939000	-2.503653000
H	1.194394000	4.423374000	0.550319000
H	2.386000000	5.490739000	-0.220355000
H	2.909800000	4.030634000	0.616444000
H	4.093284000	3.001922000	-1.284899000
H	3.419999000	3.096326000	-2.908807000
H	3.847933000	4.587565000	-2.040653000
H	3.997725000	-2.626604000	-3.310573000
H	2.754769000	-3.364757000	-4.326934000
H	3.950857000	-4.381310000	-3.502967000
H	0.887149000	-5.051759000	-1.534098000
H	0.960550000	-4.846342000	-3.295768000
H	2.220433000	-5.754976000	-2.456539000
H	2.577663000	-3.873448000	-0.045358000
H	3.890198000	-2.929332000	-0.758290000
H	3.850758000	-4.684075000	-0.982893000

**15, UM05-2X/6-31G(d,p)**

Total Energy: -2009.21203113 a.u.

Optimized geometry:

C	1.369003000	-2.078707000	1.665013000
C	2.326776000	0.049134000	0.863262000
N	1.012509000	2.019675000	1.454897000
C	-0.218428000	2.570521000	1.695380000
N	-1.357927000	1.924734000	1.769812000
C	-1.302518000	0.561367000	1.721768000
C	-2.473515000	-0.221773000	1.821050000
C	-2.401601000	-1.604569000	1.834999000
C	-1.130435000	-2.229818000	1.791424000
C	0.031062000	-1.498808000	1.649542000
C	2.473742000	-1.372531000	1.367502000
C	1.066170000	0.713150000	1.346182000
C	-0.069951000	-0.092391000	1.573387000
C	-0.212071000	4.078305000	1.898234000
C	-3.688546000	-2.433517000	1.861866000
C	3.856657000	-2.029432000	1.500690000
C	0.603876000	4.367817000	3.169177000
C	0.467382000	4.760459000	0.702808000



C	-1.630646000	4.620969000	2.060662000
C	-4.412044000	-2.227846000	0.519838000
C	-4.595324000	-1.980359000	3.015999000
C	-3.417720000	-3.932736000	2.028958000
C	4.030951000	-2.554792000	2.936875000
C	3.973358000	-3.209012000	0.520282000
C	5.016575000	-1.063968000	1.234076000
N	1.156604000	-1.957470000	-1.424423000
N	-1.207432000	-1.975512000	-1.803795000
C	1.304837000	2.151521000	-1.606664000
C	2.442988000	1.508012000	-1.291908000
C	2.356171000	0.080987000	-0.767410000
C	1.143777000	-0.651755000	-1.291296000
C	-0.037903000	-2.563224000	-1.723709000
C	-1.224099000	-0.614356000	-1.718697000
C	-2.432367000	0.108283000	-1.833812000
C	-2.432241000	1.492415000	-1.837737000
C	-1.194320000	2.179223000	-1.759866000
C	-0.001873000	1.505050000	-1.599214000
C	-0.029689000	0.096437000	-1.534319000
C	3.807416000	2.185989000	-1.450374000
C	0.039454000	-4.062546000	-1.972555000
C	-3.756662000	2.258397000	-1.889527000
C	3.676639000	3.552056000	-2.137661000
C	4.488573000	2.430305000	-0.090716000
C	4.723351000	1.318975000	-2.333010000
C	1.052048000	-4.307965000	-3.102290000
C	0.530288000	-4.762326000	-0.698618000
C	-1.323216000	-4.626947000	-2.370874000
C	-4.657417000	1.710843000	-3.006768000
C	-3.556887000	3.758121000	-2.136019000
C	-4.453759000	2.082573000	-0.529230000
H	-3.417986000	0.302018000	1.887476000
H	-1.055056000	-3.304980000	1.874298000
H	0.142354000	3.897173000	4.039984000
H	0.646140000	5.445914000	3.342276000
H	1.620369000	3.986939000	3.064286000
H	0.537117000	5.835480000	0.885581000
H	1.468239000	4.356759000	0.549481000
H	-0.113534000	4.606307000	-0.209404000
H	-2.131698000	4.163143000	2.913181000
H	-1.588255000	5.702352000	2.211281000
H	-2.230909000	4.412597000	1.173119000
H	-4.707887000	-1.184770000	0.394336000
H	-5.312445000	-2.846696000	0.481171000
H	-3.756406000	-2.500497000	-0.310741000

H	-4.092138000	-2.108426000	3.976379000
H	-4.883778000	-0.933348000	2.919344000
H	-5.509195000	-2.579314000	3.021946000
H	-4.371011000	-4.463387000	2.066754000
H	-2.848904000	-4.334618000	1.187333000
H	-2.877550000	-4.145218000	2.954311000
H	3.963861000	-1.738295000	3.658562000
H	3.270206000	-3.293647000	3.189370000
H	5.010470000	-3.029099000	3.039781000
H	3.734093000	-2.902473000	-0.499444000
H	3.284242000	-4.007561000	0.797620000
H	4.987302000	-3.616911000	0.545695000
H	5.012556000	-0.221128000	1.928726000
H	5.958021000	-1.599176000	1.373125000
H	5.010406000	-0.680514000	0.212970000
H	1.320338000	3.183512000	-1.928115000
H	-1.170305000	3.257176000	-1.838768000
H	-3.346011000	-0.463094000	-1.928928000
H	3.237017000	-0.496105000	-1.042144000
H	3.116975000	4.260111000	-1.522819000
H	3.190030000	3.467419000	-3.111097000
H	4.674855000	3.965567000	-2.292163000
H	3.802131000	2.925560000	0.599413000
H	4.838629000	1.505560000	0.364778000
H	5.363970000	3.068532000	-0.235628000
H	4.943241000	0.350296000	-1.882331000
H	4.267442000	1.146583000	-3.310170000
H	5.676193000	1.831945000	-2.482834000
H	2.032248000	-3.916439000	-2.830119000
H	0.726833000	-3.823183000	-4.025514000
H	1.138884000	-5.380762000	-3.290232000
H	1.487708000	-4.349487000	-0.386315000
H	0.647701000	-5.832228000	-0.887463000
H	-0.190588000	-4.634381000	0.112376000
H	-2.058614000	-4.468013000	-1.581246000
H	-1.699587000	-4.146074000	-3.273963000
H	-1.227227000	-5.699825000	-2.554493000
H	-4.913363000	0.662949000	-2.848707000
H	-4.168251000	1.800625000	-3.978663000
H	-5.590296000	2.278819000	-3.035438000
H	-3.014610000	4.234267000	-1.316513000
H	-3.020345000	3.944541000	-3.069118000
H	-4.534146000	4.239592000	-2.206356000
H	-3.801386000	2.416468000	0.281310000
H	-4.699794000	1.032960000	-0.357594000
H	-5.380683000	2.661858000	-0.504953000

H	1.445251000	-3.118378000	1.964548000
H	3.163683000	0.665832000	1.174843000

**16, UM05-2X/6-31G(d,p)**

Total Energy: -2009.19256749 a.u.

Optimized geometry:

C	1.260270000	-2.210619000	1.511091000
C	2.410903000	-0.117570000	1.271208000
N	1.179015000	1.941276000	1.486065000
C	-0.027043000	2.537701000	1.624904000
N	-1.209716000	1.942562000	1.627587000
C	-1.220825000	0.582656000	1.577910000
C	-2.435517000	-0.137840000	1.604320000
C	-2.449188000	-1.531969000	1.634895000
C	-1.228970000	-2.221514000	1.588393000
C	-0.001669000	-1.548727000	1.534524000
C	2.455616000	-1.518074000	1.438909000
C	1.183233000	0.603056000	1.434075000
C	-0.014385000	-0.137009000	1.521003000
C	0.013343000	4.041428000	1.878712000
C	-3.785938000	-2.277860000	1.691555000
C	3.781837000	-2.279043000	1.550045000
C	0.668809000	4.239592000	3.256852000
C	0.864272000	4.753475000	0.820391000
C	-1.391103000	4.642816000	1.893252000
C	-4.502523000	-2.110481000	0.342061000
C	-4.664142000	-1.705876000	2.815497000
C	-3.604394000	-3.776433000	1.957325000
C	3.900382000	-2.836486000	2.978756000
C	3.821629000	-3.442876000	0.548637000
C	4.998333000	-1.385878000	1.287813000
N	1.088602000	-1.990459000	-1.471182000
N	-1.299241000	-1.884554000	-1.615564000
C	1.338768000	2.155419000	-1.514200000
C	2.507958000	1.423249000	-1.439022000
C	2.408878000	0.022954000	-1.237943000
C	1.153906000	-0.652084000	-1.405566000
C	-0.144141000	-2.530381000	-1.626826000
C	-1.251574000	-0.527653000	-1.553108000
C	-2.435827000	0.241486000	-1.579441000
C	-2.393991000	1.634201000	-1.615815000
C	-1.144808000	2.269721000	-1.576053000
C	0.051664000	1.544405000	-1.516184000
C	-0.014727000	0.137035000	-1.494494000
C	3.875437000	2.110146000	-1.556540000
C	-0.186694000	-4.026424000	-1.924288000

C	-3.698348000	2.435030000	-1.672712000
C	3.740881000	3.522957000	-2.141943000
C	4.545375000	2.238668000	-0.178347000
C	4.791343000	1.306434000	-2.493115000
C	0.479050000	-4.225837000	-3.297128000
C	0.599196000	-4.818204000	-0.875701000
C	-1.624324000	-4.542674000	-1.978164000
C	-4.613563000	1.883462000	-2.777125000
C	-3.454992000	3.919625000	-1.967498000
C	-4.405514000	2.320284000	-0.312607000
H	-3.349716000	0.437620000	1.649899000
H	-1.215239000	-3.302646000	1.614220000
H	0.088515000	3.736948000	4.033788000
H	0.714264000	5.305153000	3.495106000
H	1.680152000	3.831748000	3.258436000
H	0.987822000	5.803027000	1.097957000
H	1.847140000	4.289093000	0.741386000
H	0.376886000	4.720385000	-0.156927000
H	-2.004034000	4.194948000	2.674799000
H	-1.320744000	5.719076000	2.068467000
H	-1.895791000	4.473858000	0.940688000
H	-4.757058000	-1.063114000	0.166735000
H	-5.429506000	-2.689957000	0.336006000
H	-3.860547000	-2.450898000	-0.473567000
H	-4.164709000	-1.796628000	3.782117000
H	-4.902883000	-0.654484000	2.652272000
H	-5.606576000	-2.256909000	2.860049000
H	-4.587330000	-4.242837000	2.047225000
H	-3.079312000	-4.273816000	1.139799000
H	-3.058688000	-3.954854000	2.886619000
H	3.897685000	-2.026620000	3.711142000
H	3.068983000	-3.504957000	3.208806000
H	4.831813000	-3.398801000	3.084753000
H	3.598412000	-3.096973000	-0.462489000
H	3.096429000	-4.214738000	0.808344000
H	4.811646000	-3.905424000	0.560132000
H	5.061016000	-0.558251000	1.997389000
H	5.906460000	-1.982159000	1.395955000
H	4.988222000	-0.980178000	0.273904000
H	1.375116000	3.228664000	-1.628863000
H	-1.082576000	3.349024000	-1.612745000
H	-3.371372000	-0.298091000	-1.625033000
H	3.289253000	-0.604418000	-1.247200000
H	3.226285000	4.199407000	-1.456475000
H	3.206681000	3.512660000	-3.094355000
H	4.738442000	3.930992000	-2.315245000

H	3.854273000	2.673728000	0.546563000
H	4.878779000	1.269247000	0.193172000
H	5.428098000	2.878395000	-0.257322000
H	5.004164000	0.309540000	-2.104304000
H	4.340134000	1.199319000	-3.481549000
H	5.746579000	1.824991000	-2.603164000
H	1.510563000	-3.872902000	-3.273921000
H	-0.061267000	-3.674524000	-4.069882000
H	0.471726000	-5.286224000	-3.561347000
H	1.622028000	-4.454300000	-0.813297000
H	0.614263000	-5.875301000	-1.152221000
H	0.130395000	-4.734396000	0.107862000
H	-2.133458000	-4.375298000	-1.027548000
H	-2.198546000	-4.035809000	-2.752883000
H	-1.612845000	-5.615072000	-2.187575000
H	-4.899863000	0.847690000	-2.591935000
H	-4.120738000	1.933175000	-3.750117000
H	-5.529833000	2.476907000	-2.822732000
H	-2.903914000	4.409449000	-1.162913000
H	-2.908090000	4.057016000	-2.903112000
H	-4.417505000	4.426236000	-2.060423000
H	-3.739078000	2.641441000	0.491218000
H	-4.704829000	1.287751000	-0.119725000
H	-5.305406000	2.941005000	-0.304192000
H	1.266467000	-3.289968000	1.601506000
H	3.310872000	0.474551000	1.288571000

### 17, UM05-2X/6-31G(d,p)

Total Energy: -2009.19985743 a.u.

Optimized geometry:

C	-1.318853000	2.210259000	1.645117000
C	-2.439300000	0.079737000	1.682158000
N	-1.127656000	-1.937702000	1.756840000
C	0.093080000	-2.490953000	1.807755000
N	1.262295000	-1.854662000	1.730772000
C	1.222397000	-0.504870000	1.648999000
C	2.420805000	0.251537000	1.622745000
C	2.402396000	1.648125000	1.626444000
C	1.167169000	2.303195000	1.604129000
C	-0.055191000	1.591483000	1.613853000
C	-2.511592000	1.466858000	1.693905000
C	-1.185355000	-0.593075000	1.677420000
C	-0.007356000	0.179200000	1.635982000
C	0.126980000	-3.993490000	2.068375000
C	3.725422000	2.420019000	1.639452000

C	-3.840090000	2.219867000	1.788173000
C	-0.378986000	-4.208892000	3.505380000
C	-0.807669000	-4.723856000	1.099069000
C	1.542376000	-4.553722000	1.939658000
C	4.417131000	2.240181000	0.278505000
C	4.637577000	1.883512000	2.754325000
C	3.521266000	3.918344000	1.888767000
C	-3.877728000	3.002114000	3.111977000
C	-3.964118000	3.202734000	0.612927000
C	-5.043621000	1.274865000	1.761332000
N	-1.127760000	1.937619000	-1.756979000
N	1.262196000	1.854735000	-1.730922000
C	-1.318692000	-2.210347000	-1.645046000
C	-2.511479000	-1.467022000	-1.693878000
C	-2.439276000	-0.079897000	-1.682174000
C	-1.185374000	0.592995000	-1.677472000
C	0.092942000	2.490939000	-1.808003000
C	1.222384000	0.504944000	-1.649055000
C	2.420843000	-0.251383000	-1.622756000
C	2.402523000	-1.647973000	-1.626393000
C	1.167338000	-2.303121000	-1.604053000
C	-0.055069000	-1.591489000	-1.613803000
C	-0.007325000	-0.179203000	-1.636004000
C	-3.839931000	-2.220114000	-1.788139000
C	0.126724000	3.993513000	-2.068444000
C	3.725592000	-2.419793000	-1.639395000
C	-3.877516000	-3.002404000	-3.111919000
C	-3.963913000	-3.202951000	-0.612866000
C	-5.043519000	-1.275183000	-1.761345000
C	-0.379314000	4.209044000	-3.505402000
C	-0.807952000	4.723689000	-1.099017000
C	1.542073000	4.553859000	-1.939712000
C	4.637761000	-1.883170000	-2.754203000
C	3.521517000	-3.918113000	-1.888804000
C	4.417238000	-2.240004000	-0.278411000
H	3.348680000	-0.302271000	1.645861000
H	1.122399000	3.383803000	1.601799000
H	0.267528000	-3.696346000	4.221251000
H	-0.378690000	-5.275679000	3.742612000
H	-1.393003000	-3.822529000	3.612251000
H	-0.835835000	-5.787711000	1.346869000
H	-1.814438000	-4.314962000	1.163295000
H	-0.451870000	-4.624083000	0.070624000
H	2.219897000	-4.084800000	2.652315000
H	1.521721000	-5.630727000	2.122910000
H	1.938862000	-4.374835000	0.939080000

H	4.691265000	1.194623000	0.120795000
H	5.331422000	2.838243000	0.241406000
H	3.752690000	2.547354000	-0.532115000
H	4.157310000	1.982629000	3.729802000
H	4.893368000	0.834089000	2.604811000
H	5.570007000	2.452813000	2.768657000
H	4.496906000	4.404198000	1.950657000
H	2.969345000	4.396451000	1.078185000
H	2.993444000	4.098122000	2.828062000
H	-3.806029000	2.322190000	3.963170000
H	-3.056205000	3.717309000	3.177916000
H	-4.816461000	3.556545000	3.188495000
H	-3.825110000	2.691468000	-0.341640000
H	-3.218267000	3.995702000	0.676070000
H	-4.951217000	3.671486000	0.625633000
H	-5.027492000	0.578019000	2.601673000
H	-5.962027000	1.860954000	1.830010000
H	-5.078530000	0.702813000	0.832822000
H	-1.361143000	-3.291948000	-1.651498000
H	1.122637000	-3.383733000	-1.601686000
H	3.348678000	0.302488000	-1.645908000
H	-3.323438000	0.540105000	-1.719158000
H	-3.055986000	-3.717592000	-3.177819000
H	-3.805810000	-2.322504000	-3.963130000
H	-4.816240000	-3.556854000	-3.188443000
H	-3.217993000	-3.995858000	-0.675962000
H	-3.824973000	-2.691641000	0.341688000
H	-4.950975000	-3.671781000	-0.625582000
H	-5.078501000	-0.703131000	-0.832837000
H	-5.027395000	-0.578336000	-2.601686000
H	-5.961889000	-1.861325000	-1.830055000
H	-1.393319000	3.822647000	-3.612271000
H	0.267190000	3.696604000	-4.221357000
H	-0.379074000	5.275858000	-3.742516000
H	-1.814679000	4.314685000	-1.163218000
H	-0.836256000	5.787562000	-1.346718000
H	-0.452074000	4.623867000	-0.070604000
H	1.938611000	4.374901000	-0.939168000
H	2.219615000	4.085077000	-2.652442000
H	1.521314000	5.630881000	-2.122850000
H	4.893518000	-0.833752000	-2.604598000
H	4.157523000	-1.982224000	-3.729700000
H	5.570208000	-2.452443000	-2.768554000
H	2.969571000	-4.396287000	-1.078279000
H	2.993756000	-4.097864000	-2.828139000
H	4.497182000	-4.403920000	-1.950665000

H	3.752791000	-2.547286000	0.532163000
H	4.691285000	-1.194438000	-0.120613000
H	5.331572000	-2.838003000	-0.241324000
H	-1.361372000	3.291856000	1.651622000
H	-3.323422000	-0.540321000	1.719109000

**18, UM05-2X/6-31G(d,p)**

Total Energy: -2009.19256671 a.u.

Optimized geometry:

C	1.260268020	-2.210618936	1.511090366
C	2.410901900	-0.117571492	1.271207463
N	1.179015696	1.941274484	1.486064374
C	-0.027041447	2.537700017	1.624903321
N	-1.209714360	1.942562009	1.627586323
C	-1.220824224	0.582656548	1.577909340
C	-2.435516208	-0.137838392	1.604319331
C	-2.449188089	-1.531966833	1.634894321
C	-1.228971010	-2.221512341	1.588392336
C	-0.001670064	-1.548726387	1.534523356
C	2.455613991	-1.518074968	1.438908396
C	1.183232840	0.603055009	1.434074396
C	-0.014385158	-0.137008937	1.521002365
C	0.013345496	4.041426399	1.878711221
C	-3.785938039	-2.277856690	1.691554297
C	3.781833980	-2.279044517	1.550044350
C	0.668811364	4.239589903	3.256850682
C	0.864274615	4.753472576	0.820390639
C	-1.391099566	4.642815061	1.893251216
C	-4.502522650	-2.110477295	0.342060827
C	-4.664141328	-1.705872355	2.815495854
C	-3.604395069	-3.776429215	1.957324190
C	3.900378577	-2.836487369	2.978754791
C	3.821625223	-3.442877083	0.548636743
C	4.998330071	-1.385880643	1.287812455
N	1.088600223	-1.990458909	-1.471181462
N	-1.299241768	-1.884552430	-1.615563400
C	1.338768771	2.155417298	-1.514199440
C	2.507957846	1.423246841	-1.439021470
C	2.408876988	0.022952454	-1.237942550
C	1.153905051	-0.652084481	-1.405565487
C	-0.144142634	-2.530379912	-1.626825398
C	-1.251573922	-0.527651994	-1.553107428
C	-2.435825962	0.241487459	-1.579440418
C	-2.393989091	1.634201882	-1.615814405
C	-1.144806176	2.269720837	-1.576052415



C	0.051664888	1.544404360	-1.516183441
C	-0.014726983	0.137034956	-1.494493449
C	3.875436745	2.110142697	-1.556539426
C	-0.186696571	-4.026422294	-1.924287283
C	-3.698345069	2.435031403	-1.672711378
C	3.740881697	3.522953226	-2.141942197
C	4.545374562	2.238664222	-0.178346968
C	4.791341869	1.306430431	-2.493114055
C	0.479047039	-4.225835640	-3.297126740
C	0.599192615	-4.818202486	-0.875700695
C	-1.624326333	-4.542671177	-1.978163259
C	-4.613560061	1.883464199	-2.777123944
C	-3.454988214	3.919625660	-1.967497263
C	-4.405510864	2.320285895	-0.312606915
H	-3.349714477	0.437621965	1.649898314
H	-1.215240703	-3.302643924	1.614219328
H	0.088517273	3.736946473	4.033786374
H	0.714267028	5.305150452	3.495104588
H	1.680153708	3.831745421	3.258434678
H	0.987825237	5.803024093	1.097956527
H	1.847141934	4.289090135	0.741385671
H	0.376888786	4.720382900	-0.156926976
H	-2.004030611	4.194947626	2.674797908
H	-1.320739907	5.719074607	2.068466145
H	-1.895787477	4.473857450	0.940687594
H	-4.757056883	-1.063110545	0.166734896
H	-5.429505671	-2.689952479	0.336005829
H	-3.860547122	-2.450894573	-0.473566852
H	-4.164708584	-1.796624634	3.782115471
H	-4.902881564	-0.654480615	2.652270918
H	-5.606575334	-2.256904535	2.860047837
H	-4.587330975	-4.242832403	2.047224155
H	-3.079313592	-4.273812351	1.139798516
H	-3.058689395	-3.954850491	2.886617825
H	3.897682097	-2.026621691	3.711140500
H	3.068979480	-3.504957578	3.208804696
H	4.831808854	-3.398802745	3.084751748
H	3.598408532	-3.096974075	-0.462488856
H	3.096425017	-4.214738317	0.808343644
H	4.811641538	-3.905425534	0.560131743
H	5.061013574	-0.558254006	1.997388175
H	5.906456341	-1.982161985	1.395954411
H	4.988219335	-0.980180798	0.273903854
H	1.375117442	3.228661851	-1.628862396
H	-1.082573516	3.349023372	-1.612744405
H	-3.371370940	-0.298088732	-1.625032398

H	3.289251242	-0.604419863	-1.247199549
H	3.226286334	4.199403291	-1.456474463
H	3.206681903	3.512656574	-3.094353818
H	4.738442568	3.930987429	-2.315244129
H	3.854273110	2.673724489	0.546562745
H	4.878777811	1.269243391	0.193171885
H	5.428097637	2.878390403	-0.257321937
H	5.004162152	0.309536686	-2.104303207
H	4.340132982	1.199315762	-3.481547666
H	5.746577840	1.824986616	-2.603163011
H	1.510559856	-3.872901437	-3.273919751
H	-0.061269396	-3.674522515	-4.069880436
H	0.471722366	-5.286222219	-3.561345636
H	1.622024445	-4.454299279	-0.813296719
H	0.614258935	-5.875299087	-1.152220586
H	0.130391852	-4.734394221	0.107861919
H	-2.133460029	-4.375294915	-1.027547633
H	-2.198547784	-4.035806010	-2.752881954
H	-1.612848024	-5.615068783	-2.187574177
H	-4.899860609	0.847692790	-2.591934018
H	-4.120735219	1.933176870	-3.750115561
H	-5.529829322	2.476909550	-2.822730926
H	-2.903910123	4.409449116	-1.162912581
H	-2.908086346	4.057016260	-2.903110896
H	-4.417500512	4.426237076	-2.060422226
H	-3.739074918	2.641442347	0.491217769
H	-4.704826404	1.287753494	-0.119724991
H	-5.305402129	2.941007225	-0.304191918
H	1.266464328	-3.289967515	1.601505332
H	3.310870922	0.474548701	1.288570454

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