Symmetry as a New Element to Control Molecular Switches

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Supporting Information

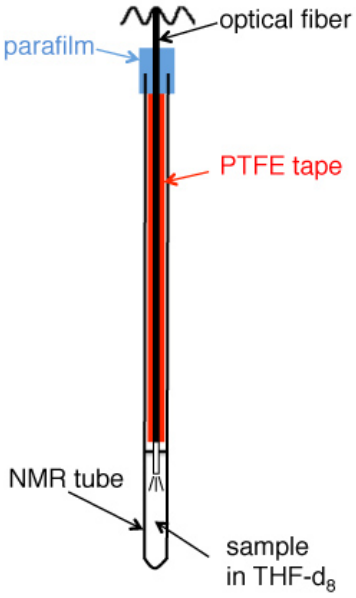
Crystal data

formula	$C_{96}H_{124}N_{12}$, 2 (C_6H_6)
formula weight	1602.35
Z, calculated density	2, 1.148 Mg · m^{-3}
F(000)	1736
description and size of crystal	colorless block, 0.060 · 0.130 · 0.270 mm^3
absorption coefficient	0.067 mm^{-1}
min/max transmission	0.99 / 1.00
temperature	123K
radiation(wavelength)	Mo K_α (λ = 0.71073 Å)
Crystal system, space group	monoclinic, P $2_1/n$
a	21.828(4) Å
b	9.4747(16) Å
c	22.495(4) Å
α	90°
β	95.114(10)°
γ	90°
V	4633.8(13) $Å^3$
min/max Θ	1.818° / 26.391°
number of collected reflections	53279
number of independent reflections	9461 (merging r = 0.148)
number of observed reflections	4724 ($I>2.0\sigma(I)$)
number of refined parameters	596
r	0.0633
rW	0.1986
goodness of fit	1.0530

NMR spectra

The NMR samples were irradiated with a monochromator via an optical fiber (length: 6 m) directly in a 700 MHz NMR Bruker spectrometer with a 5 mm cryogenic triple resonance (H/C/N/D) probe head. The insulation of the optical fiber was removed on the final centimeter of the fiber. This part was dipped into the solution to a depth of about 3mm and fixed by parafilm. The NMR tube was closed with a PTFE (polytetrafluoroethylene) tape and parafilm.

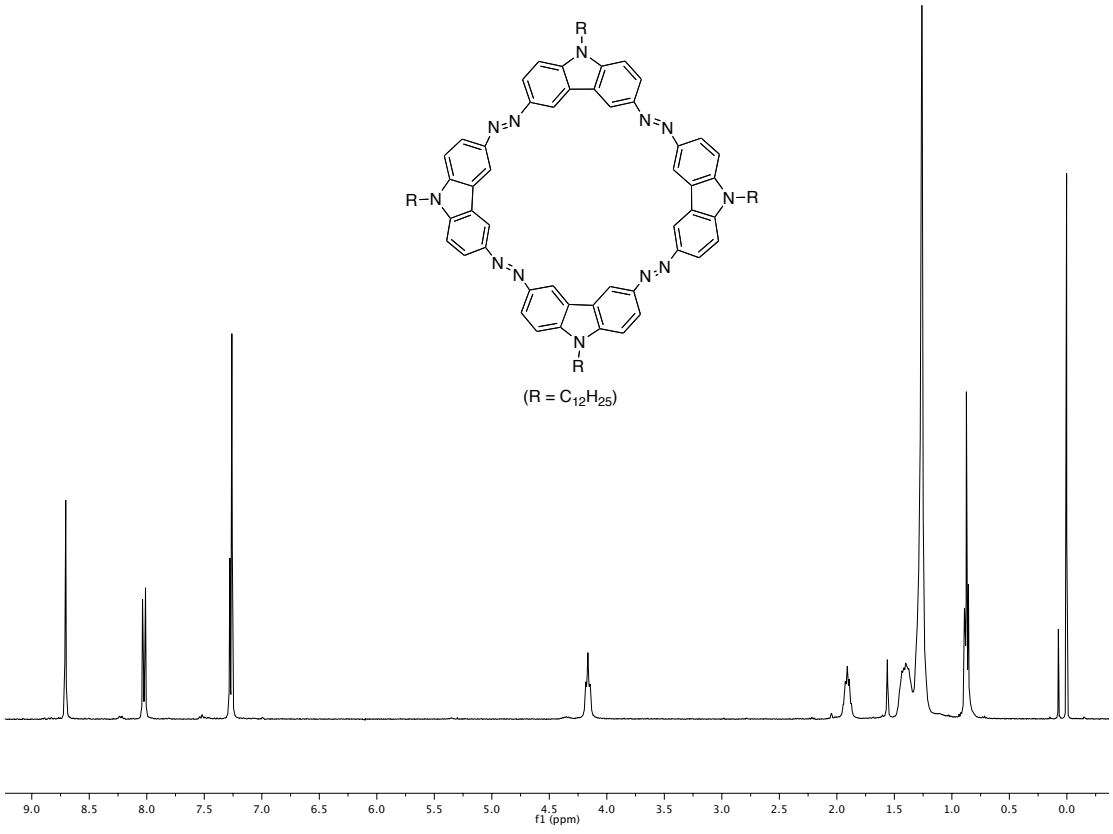
Monochromator: 150 W Xenon high stability lamp (output power > 10 mW at 470 nm) half-power bandwidth: 15 nm (Polychrome V - TILL Photonics)



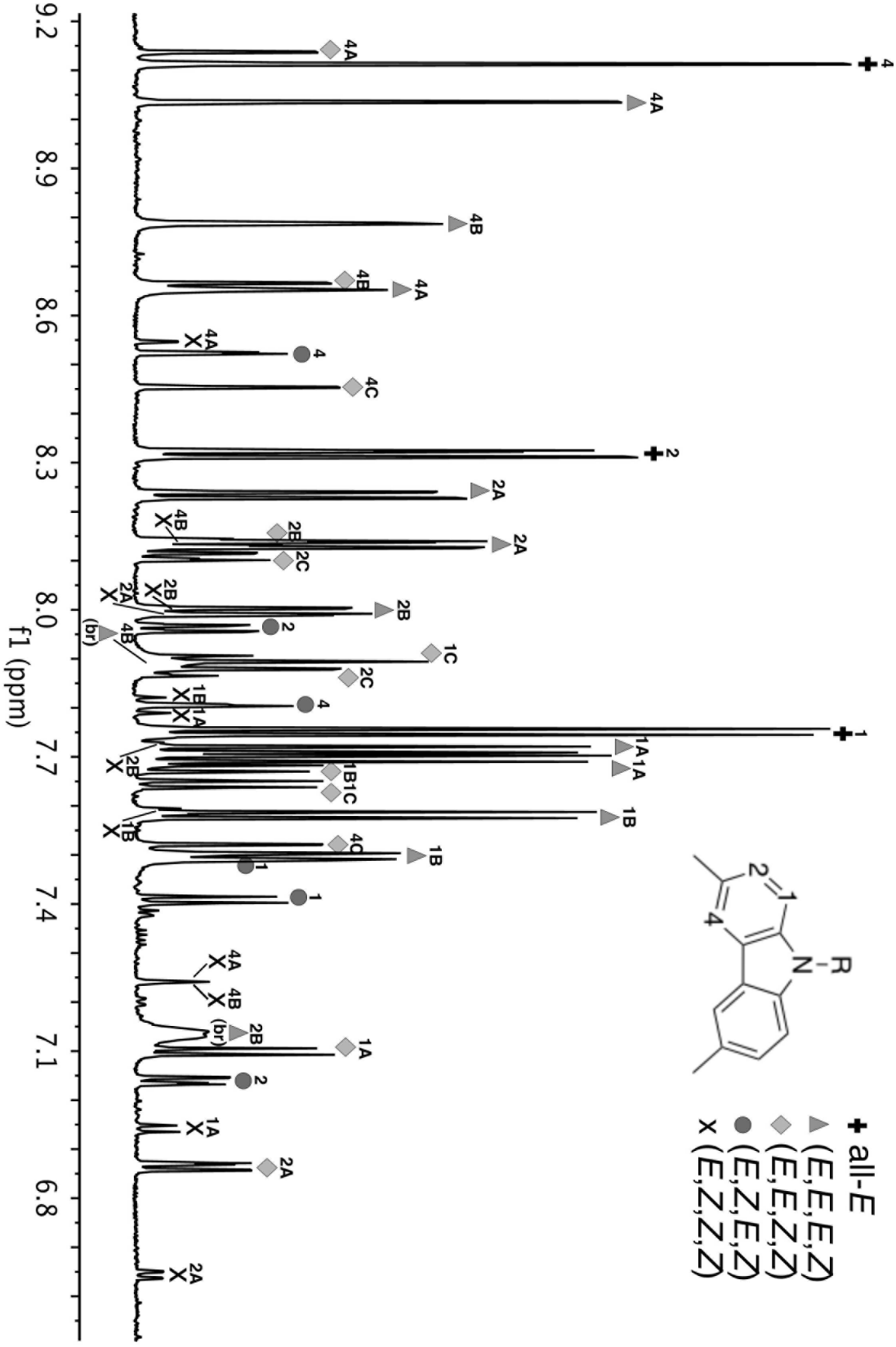
Macrocycle **7**

The synthesis and characterization of macrocycle **7** were already published earlier.[1]

^{1}H-NMR spectrum in $CDCl_3$ (400MHz)

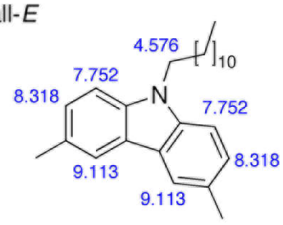


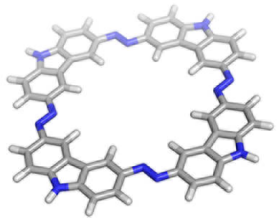
^{1}H-NMR spectrum in THF-d_8 (700MHz) ca. 125 μM, in the photostationary state (aromatic region with assignment)



Complete Assignment:

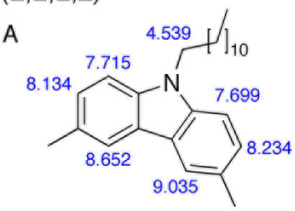
all-*E*



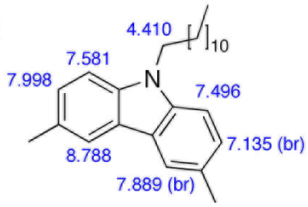


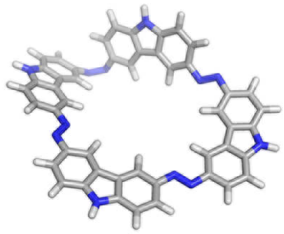
(*E*,*E*,*E*,*Z*)

A



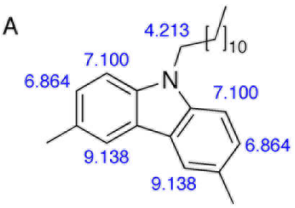
B



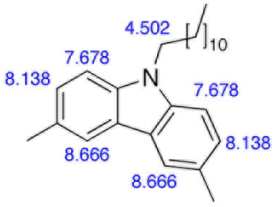


(*E*,*E*,*Z*,*Z*)

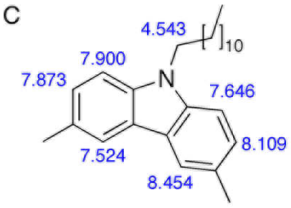
A

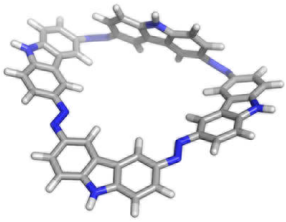


B

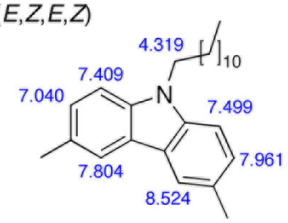


C



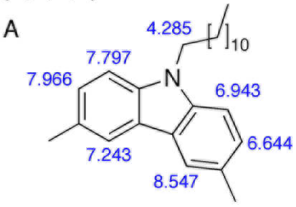


(*E*,*Z*,*E*,*Z*)

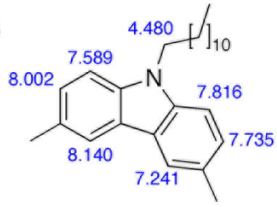


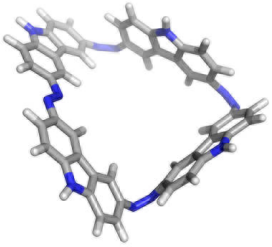
(*E*,*Z*,*Z*,*Z*)

A

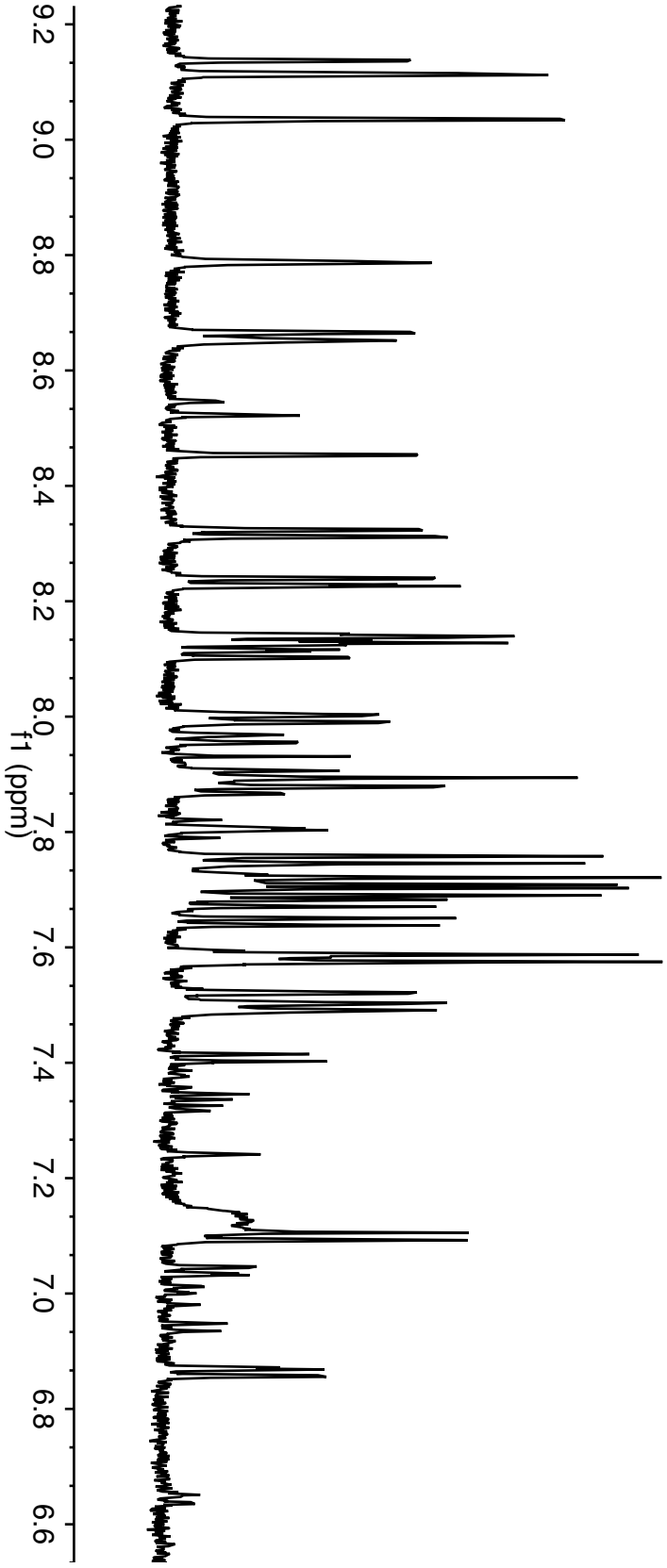


B

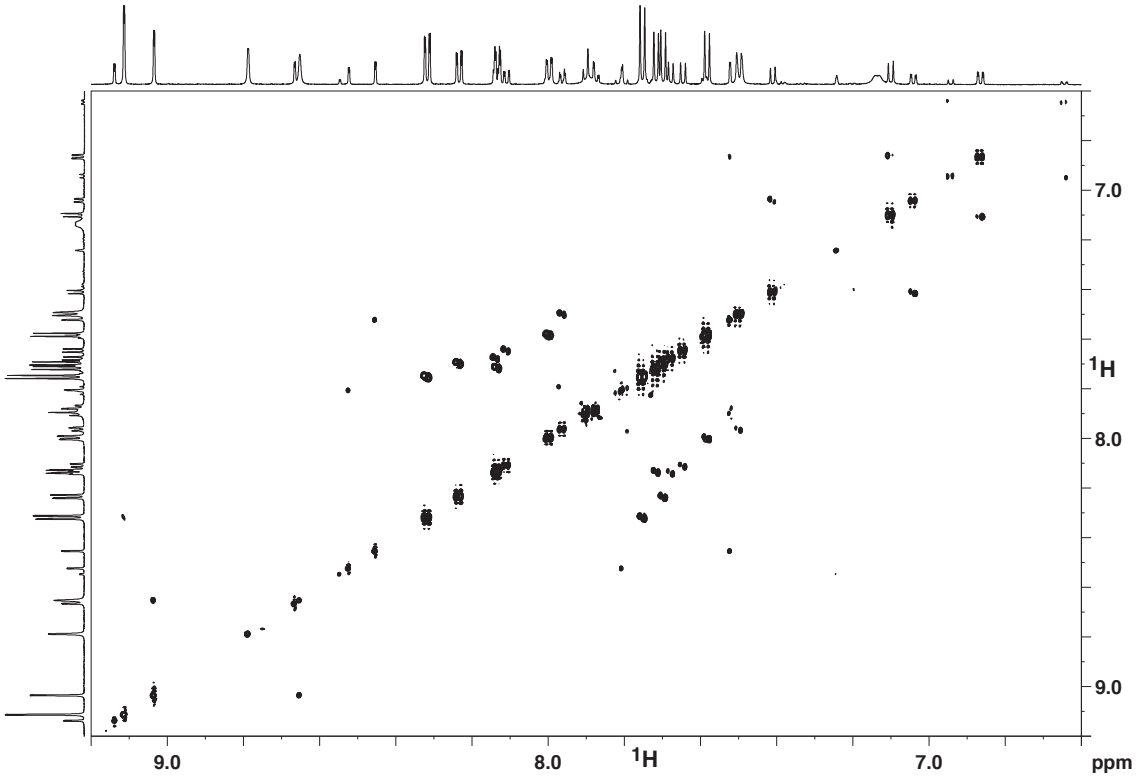


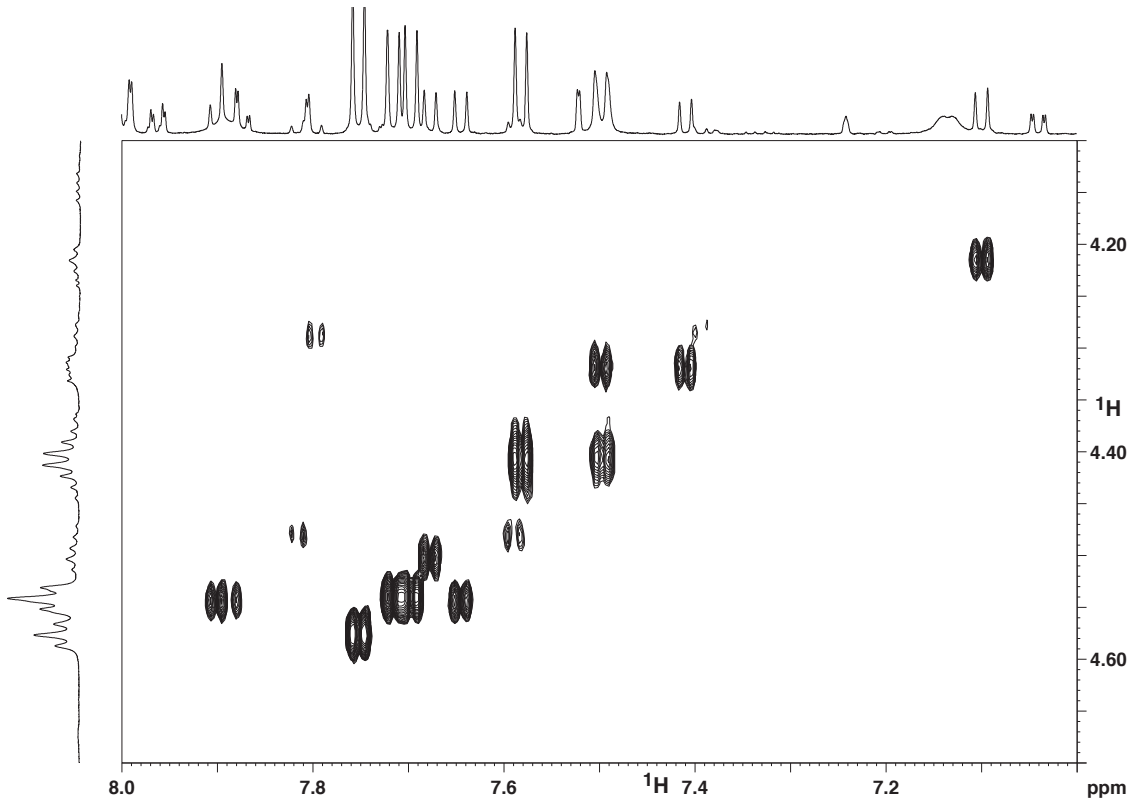


^{1}H-NMR spectrum in THF-d_8 (700MHz) ca. 15 μM, in the photostationary state (aromatic region)

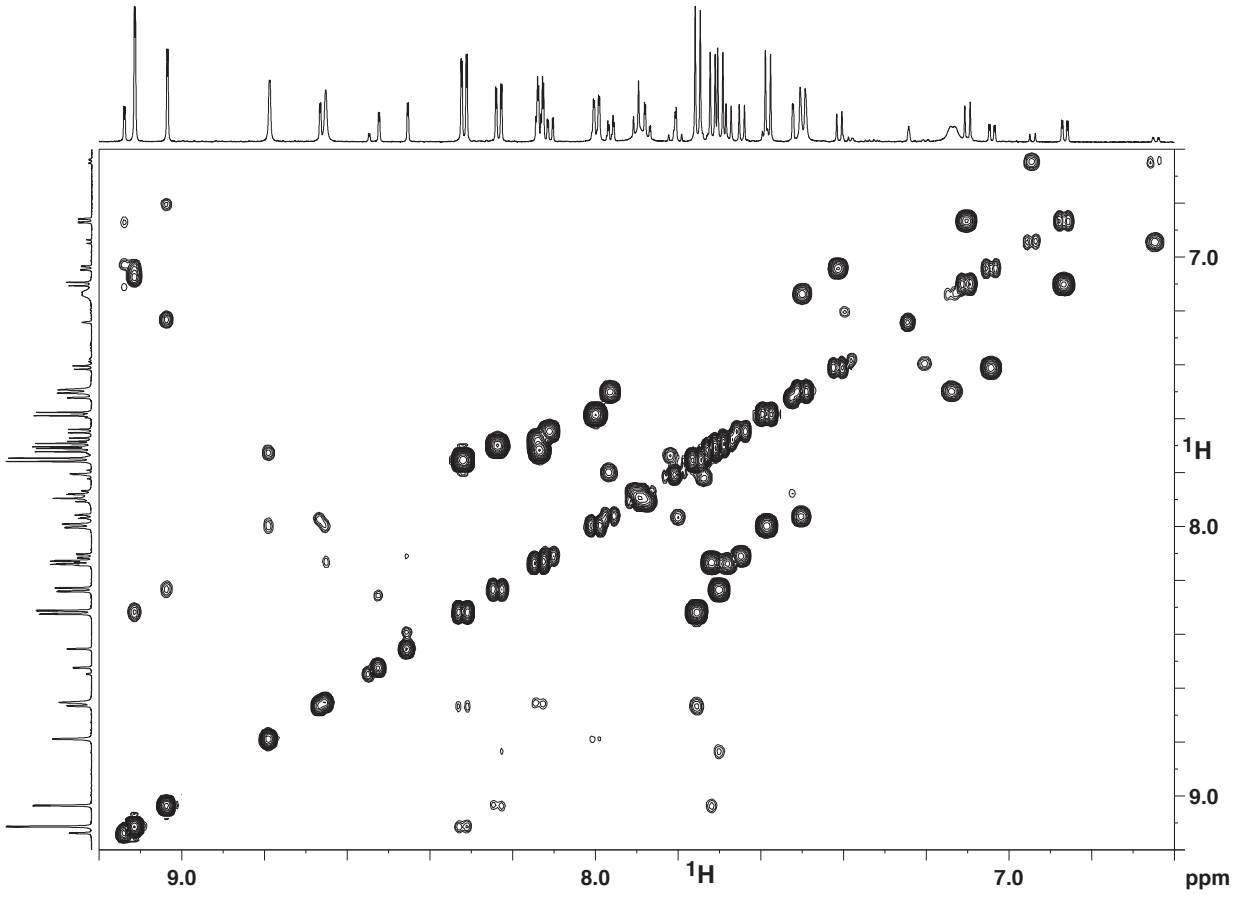


ROESY-NMR in THF-d_8 (700MHz) ca. 125 μM, in the photostationary state:

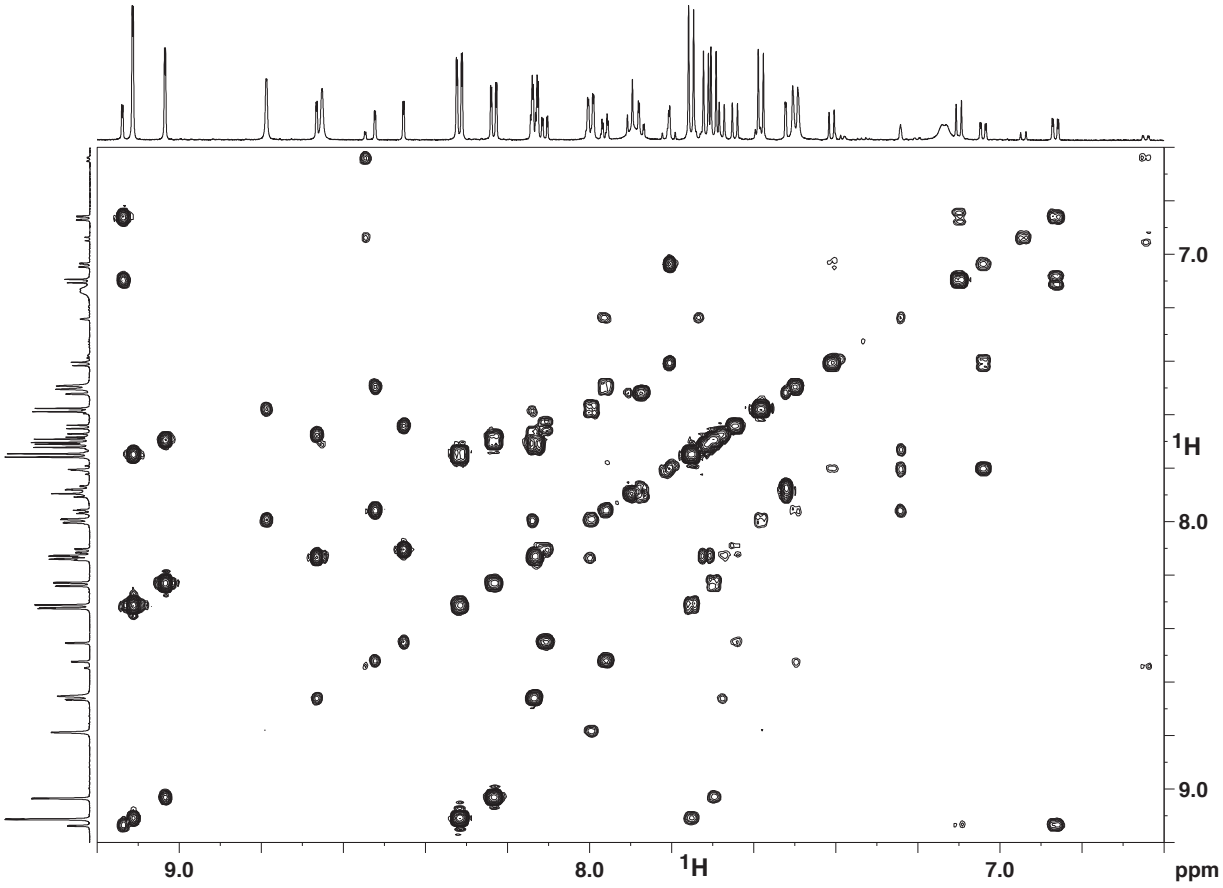




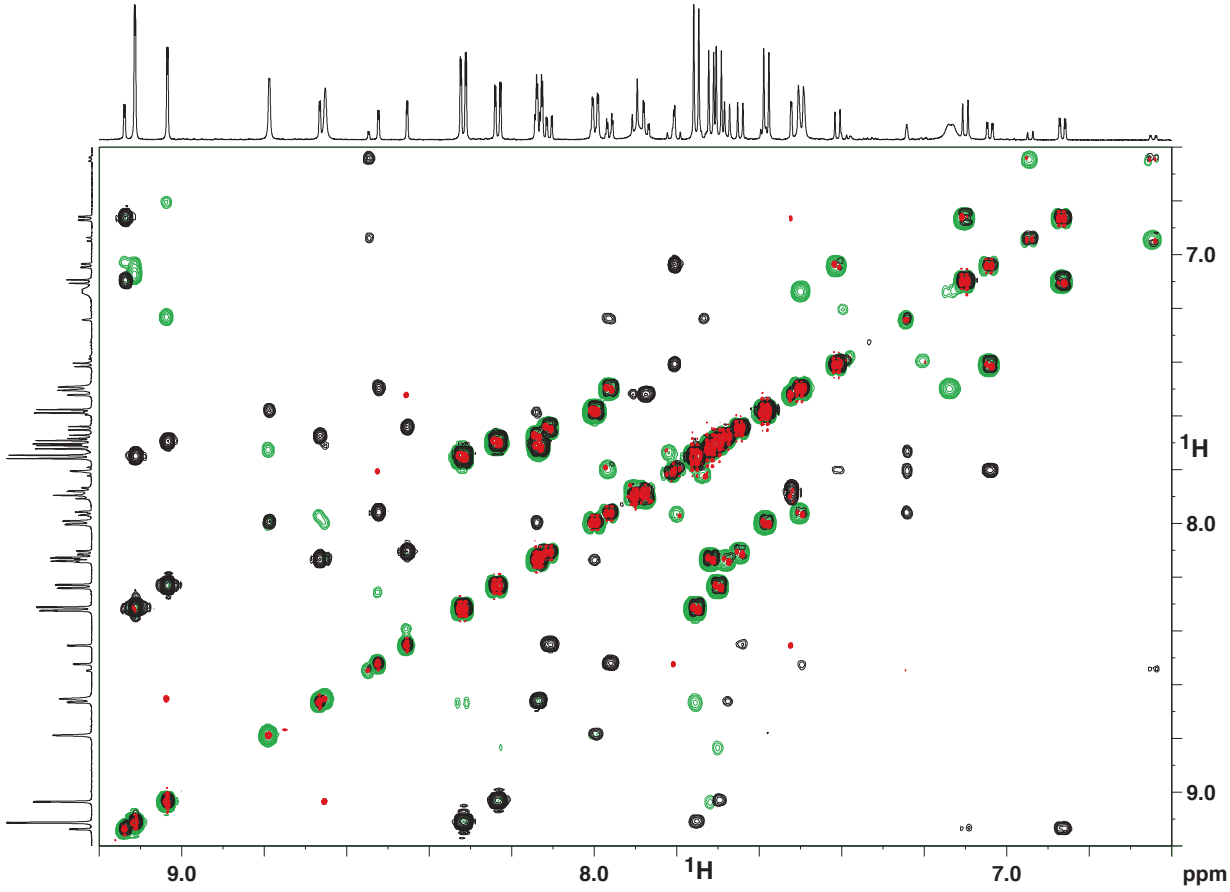
COSY-NMR in THF-d_8 (700MHz) ca. 125 μM, in the photostationary state:



Long-range COSY-NMR (^{4}J-coupling) in THF-d_8 (700MHz) ca. 125 μM, in the photostationary state:



Overlay of the 2D NMR spectra (long-range COSY (black), COSY(green) and ROESY (red)), in the photostationary state:



Data DFT-calculations[2,3]

Calculations were conducted for the electronic ground state. The absence of imaginary frequencies or in case of transition states the existence of one imaginary frequency was checked after every calculation. All possible conformers of the *E*-isomerized azo units in a macrocyclic ring system were analyzed. The geometries with the lowest energies were chosen.
The initial structures for the transition state optimizations were generated using a bottom up approach starting from calculations on B3LYP level with a 6-31G basis set and the QST3 keyword. The resulting geometries were then re-optimized on B3LYP level with a 6-311G(d,p) basis set.
IRC (intrinsic reaction coordinate) calculations were not conducted with the optimized transition state geometries because they were too time-consuming due to the large number of atoms in the molecule.

all-*E*

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opt=tight freq b3lyp/6-311g(d,p) geom=connectivity int=ultrafine
---

XYZ coordinates of the optimized species:

Tag	Symbol	X	Y	Z
1	C	3.0480770	5.8387410	-0.0000520
2	C	4.0575500	6.8223380	-0.0000610
3	C	5.4022820	6.4859120	-0.0000570
4	C	5.7260530	5.1293800	-0.0000430
5	C	4.7244960	4.1181420	-0.0000330
6	C	3.3827820	4.4786940	-0.0000380
7	H	3.7451680	7.8593850	-0.0000720
8	H	6.1695640	7.2515470	-0.0000650
9	H	2.5892110	3.7431280	-0.0000310
10	H	7.8490390	4.9982560	-0.0000400
11	C	6.8097120	3.1420020	-0.0000220
12	C	7.7806380	2.1350470	-0.0000110
13	C	7.3524190	0.8205790	0.0000020
14	C	5.9749840	0.5008740	0.0000040
15	C	5.0134520	1.5142280	-0.0000070
16	C	5.4236420	2.8452890	-0.0000200
17	H	8.8383050	2.3747720	-0.0000130
18	H	8.0623350	0.0048250	0.0000110
19	H	3.9664150	1.2359770	-0.0000040
20	N	6.9655890	4.5164240	-0.0000360
21	N	1.7266540	6.3389410	-0.0000590
22	N	0.8183490	5.4704930	-0.0000500
23	C	-5.1293810	5.7260530	-0.0000330
24	H	-4.9982560	7.8490390	-0.0000480
25	C	-3.1420020	6.8097100	-0.0000470
26	C	-6.4859130	5.4022820	-0.0000260

27	C	-4.1181430	4.7244950	-0.0000290
28	C	-2.1350470	7.7806360	-0.0000570
29	C	-2.8452890	5.4236400	-0.0000380
30	C	-6.8223390	4.0575500	-0.0000160
31	H	-7.2515470	6.1695650	-0.0000290
32	C	-4.4786960	3.3827810	-0.0000180
33	C	-0.8205790	7.3524170	-0.0000580
34	H	-2.3747710	8.8383030	-0.0000630
35	C	-1.5142280	5.0134500	-0.0000390
36	C	-5.8387440	3.0480770	-0.0000110
37	H	-7.8593870	3.7451680	-0.0000100
38	H	-3.7431300	2.5892090	-0.0000150
39	C	-0.5008740	5.9749820	-0.0000490
40	H	-0.0048240	8.0623330	-0.0000650
41	H	-1.2359780	3.9664130	-0.0000320
42	N	-4.5164240	6.9655880	-0.0000440
43	N	5.4704960	-0.8183490	0.0000180
44	N	6.3389440	-1.7266530	0.0000270
45	C	5.1293810	-5.7260530	0.0000490
46	H	4.9982560	-7.8490390	0.0000630
47	C	3.1420020	-6.8097100	0.0000500
48	C	6.4859130	-5.4022820	0.0000520
49	C	4.1181430	-4.7244950	0.0000390
50	C	2.1350470	-7.7806360	0.0000530
51	C	2.8452890	-5.4236400	0.0000400
52	C	6.8223390	-4.0575500	0.0000440
53	H	7.2515470	-6.1695650	0.0000590
54	C	4.4786960	-3.3827810	0.0000310
55	C	0.8205790	-7.3524170	0.0000460
56	H	2.3747710	-8.8383030	0.0000610
57	C	1.5142280	-5.0134500	0.0000330
58	C	5.8387440	-3.0480770	0.0000340
59	H	7.8593870	-3.7451680	0.0000450
60	H	3.7431300	-2.5892090	0.0000240
61	C	0.5008740	-5.9749820	0.0000360
62	H	0.0048240	-8.0623330	0.0000480
63	H	1.2359780	-3.9664130	0.0000250
64	N	4.5164240	-6.9655880	0.0000560
65	C	-6.8097120	-3.1420020	0.0000190
66	H	-7.8490390	-4.9982560	0.0000260
67	C	-5.7260530	-5.1293800	0.0000270
68	C	-7.7806380	-2.1350470	0.0000150
69	C	-5.4236420	-2.8452890	0.0000180
70	C	-5.4022820	-6.4859120	0.0000320
71	C	-4.7244960	-4.1181420	0.0000230
72	C	-7.3524190	-0.8205790	0.0000100
73	H	-8.8383050	-2.3747720	0.0000160
74	C	-5.0134520	-1.5142280	0.0000120
75	C	-4.0575500	-6.8223380	0.0000330
76	H	-6.1695640	-7.2515470	0.0000350
77	C	-3.3827820	-4.4786940	0.0000240

78	C	-5.9749840	-0.5008740	0.0000090
79	H	-8.0623350	-0.0048250	0.0000070
80	H	-3.9664150	-1.2359770	0.0000110
81	C	-3.0480770	-5.8387410	0.0000290
82	H	-3.7451680	-7.8593850	0.0000370
83	H	-2.5892110	-3.7431280	0.0000210
84	N	-6.9655890	-4.5164240	0.0000240
85	N	-6.3389440	1.7266530	0.0000000
86	N	-5.4704960	0.8183490	0.0000040
87	N	-1.7266540	-6.3389410	0.0000310
88	N	-0.8183490	-5.4704930	0.0000280

E(RB3LYP) = -2503.52387201

Zero-point vibrational energy 1737452.0 (Joules/Mol)
415.26099 (Kcal/Mol)

Zero-point correction=	0.661761 (Hartree/Particle)
Thermal correction to Energy=	0.704788
Thermal correction to Enthalpy=	0.705733
Thermal correction to Gibbs Free Energy=	0.585996
Sum of electronic and zero-point Energies=	-2502.862111
Sum of electronic and thermal Energies=	-2502.819084
Sum of electronic and thermal Enthalpies=	-2502.818139
Sum of electronic and thermal Free Energies=	-2502.937876

(*E*,*E*,*E*,*Z*)

---
opt=tight freq b3lyp/6-311g(d,p) geom=connectivity int=ultrafine
---

XYZ coordinates of the optimized species:

Tag	Symbol	X	Y	Z
1	C	6.6609350	0.8002670	0.7120760
2	C	8.0369780	0.5977950	0.9372020
3	C	8.5989900	-0.6722930	0.9310730
4	C	7.7516270	-1.7535320	0.6847340
5	C	6.3580780	-1.5682980	0.4761880
6	C	5.8150380	-0.2931150	0.4933270
7	H	8.6531750	1.4732830	1.1025530
8	H	9.6615170	-0.8101770	1.0953340
9	H	4.7628920	-0.1157360	0.3159600
10	H	8.9524970	-3.5096850	0.6197750
11	C	6.8730760	-3.8028170	0.2620020
12	C	6.6821900	-5.1567370	-0.0221460
13	C	5.3997980	-5.5727270	-0.3556930
14	C	4.3146770	-4.6751240	-0.3587580
15	C	4.5140670	-3.3221770	-0.0698050
16	C	5.7966660	-2.8793840	0.2200990

17	H	7.5062770	-5.8607270	-0.0053770
18	H	5.2037930	-6.6072940	-0.6104480
19	H	3.6698900	-2.6464230	-0.1054550
20	N	8.0328180	-3.1049680	0.5658870
21	N	6.2282720	2.1472630	0.6721470
22	N	4.9946840	2.2933750	0.4796040
23	C	1.3820780	6.9252880	-0.4271640
24	H	3.0663160	8.2187820	-0.3033310
25	C	3.4692110	6.1494550	-0.0151180
26	C	0.2733170	7.7251570	-0.7036350
27	C	1.2722630	5.5132910	-0.2892260
28	C	4.8459880	6.0296300	0.2044850
29	C	2.6136140	5.0194550	-0.0344010
30	C	-0.9545820	7.0945740	-0.8314430
31	H	0.3633910	8.7994780	-0.8160390
32	C	0.0286130	4.9038250	-0.4067190
33	C	5.3673260	4.7619380	0.3903890
34	H	5.4896540	6.9023020	0.2203020
35	C	3.1587030	3.7525460	0.1517640
36	C	-1.0917760	5.7007130	-0.6722650
37	H	-1.8509560	7.6640070	-1.0443310
38	H	-0.1011430	3.8353590	-0.2944660
39	C	4.5344680	3.6200810	0.3576840
40	H	6.4266700	4.6140650	0.5516290
41	H	2.5503240	2.8564950	0.1287960
42	N	2.7075810	7.2799820	-0.2519660
43	N	3.0503280	-5.1806410	-0.7449850
44	N	2.0811220	-4.5259070	-0.2859250
45	C	-1.7547440	-5.2289870	-1.7697490
46	H	-3.5145400	-5.5949080	-2.9064380
47	C	-3.8105130	-4.6488630	-1.0214790
48	C	-0.6758170	-5.6999160	-2.5250830
49	C	-1.5702540	-4.6151540	-0.5031610
50	C	-5.1817250	-4.4430320	-0.8762450
51	C	-2.8896150	-4.2715510	-0.0098470
52	C	0.5990490	-5.5251880	-2.0156800
53	H	-0.8284330	-6.1708820	-3.4898350
54	C	-0.2776770	-4.4104030	-0.0297580
55	C	-5.6315220	-3.8583370	0.2985710
56	H	-5.8830140	-4.7369810	-1.6489790
57	C	-3.3675570	-3.7501600	1.1912170
58	C	0.8059570	-4.8657320	-0.7835550
59	H	1.4687250	-5.8562650	-2.5678470
60	H	-0.0805160	-3.8934150	0.9017480
61	C	-4.7358840	-3.5222090	1.3348390
62	H	-6.6920080	-3.7008390	0.4437690
63	H	-2.7036750	-3.5326950	2.0198290
64	N	-3.1053990	-5.2306050	-2.0625170
65	C	-6.4995410	2.5549530	-0.5637360
66	H	-8.5992740	2.2406410	-0.6353640
67	C	-7.4723090	0.7377790	0.3685080

68	C	-6.2523320	3.7818820	-1.1905030
69	C	-5.4585780	1.7983410	0.0335220
70	C	-8.3866690	-0.1787700	0.8888730
71	C	-6.0813180	0.6272900	0.6205080
72	C	-4.9583020	4.2672490	-1.1812370
73	H	-7.0534650	4.3455620	-1.6558960
74	C	-4.1565040	2.2964520	0.0117730
75	C	-7.8956600	-1.2051390	1.6829410
76	H	-9.4518290	-0.0754470	0.7151660
77	C	-5.6005310	-0.4532560	1.3611070
78	C	-3.9091160	3.5407440	-0.5709860
79	H	-4.7204850	5.2227040	-1.6286200
80	H	-3.3297590	1.7650720	0.4678570
81	C	-6.5130740	-1.3656540	1.8909090
82	H	-8.5751760	-1.9021660	2.1591150
83	H	-4.5430400	-0.5609630	1.5687190
84	N	-7.6938490	1.8870310	-0.3753660
85	N	-2.4132660	5.2137370	-0.7915350
86	N	-2.5795880	4.0099230	-0.4710670
87	N	-6.0863530	-2.3295320	2.8676990
88	N	-5.2178440	-3.1916620	2.6470920

E(RB3LYP) = -2503.48808521

Zero-point vibrational energy 1734786.7 (Joules/Mol)
414.62396 (Kcal/Mol)

Zero-point correction=	0.660745 (Hartree/Particle)
Thermal correction to Energy=	0.703809
Thermal correction to Enthalpy=	0.704754
Thermal correction to Gibbs Free Energy=	0.585489
Sum of electronic and zero-point Energies=	-2502.827340
Sum of electronic and thermal Energies=	-2502.784276
Sum of electronic and thermal Enthalpies=	-2502.783332
Sum of electronic and thermal Free Energies=	-2502.902597

(*E*,*E*,*Z*,*Z*)

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opt=tight freq b3lyp/6-311g(d,p) geom=connectivity int=ultrafine
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XYZ coordinates of the optimized species:

Tag	Symbol	X	Y	Z
1	C	4.9621240	2.1932920	0.1956690
2	C	6.1789170	2.6325470	0.7670950
3	C	7.2258920	1.7571380	0.9803500
4	C	7.0524670	0.4227810	0.5993180
5	C	5.8427120	-0.0417370	0.0204880
6	C	4.7897360	0.8548150	-0.1624660

7	H	6.2642080	3.6763670	1.0360040
8	H	8.1525790	2.0967820	1.4297820
9	H	3.8421020	0.5498930	-0.5904160
10	H	8.8775680	-0.5751550	1.0335300
11	C	7.3456990	-1.7781420	0.1748720
12	C	7.8777840	-3.0576820	0.0196400
13	C	7.0813340	-4.0159440	-0.5866280
14	C	5.7577460	-3.7314970	-0.9774190
15	C	5.2319170	-2.4460950	-0.8261780
16	C	6.0316450	-1.4549980	-0.2553630
17	H	8.8896150	-3.2918530	0.3305290
18	H	7.4645700	-5.0107440	-0.7793270
19	H	4.2282210	-2.2232610	-1.1667900
20	N	7.9324420	-0.6365950	0.6939270
21	N	3.8602000	3.0508430	-0.0337350
22	N	4.1265460	4.2752370	0.0603350
23	C	-1.1313040	7.1444200	-0.3839490
24	H	-0.0000050	8.9358130	-0.5569340
25	C	1.1312950	7.1444200	-0.3839450
26	C	-2.4733760	7.5215440	-0.3870290
27	C	-0.7278810	5.7870650	-0.2427220
28	C	2.4733680	7.5215460	-0.3870210
29	C	0.7278730	5.7870650	-0.2427200
30	C	-3.4171010	6.5193830	-0.2350190
31	H	-2.7699690	8.5589640	-0.4901920
32	C	-1.6941440	4.7948970	-0.1140320
33	C	3.4170930	6.5193850	-0.2350090
34	H	2.7699600	8.5589660	-0.4901840
35	C	1.6941360	4.7948990	-0.1140270
36	C	-3.0453340	5.1658690	-0.1077630
37	H	-4.4749410	6.7504570	-0.2131180
38	H	-1.4349320	3.7498410	-0.0033430
39	C	3.0453260	5.1658710	-0.1077540
40	H	4.4749320	6.7504600	-0.2131040
41	H	1.4349240	3.7498420	-0.0033390
42	N	-0.0000040	7.9325900	-0.4785800
43	N	5.1047970	-4.7657200	-1.7227950
44	N	3.9211220	-5.1266210	-1.5788670
45	C	1.1315710	-4.3200120	1.4554320
46	H	0.0000040	-4.0242890	3.2337870
47	C	-1.1315640	-4.3200130	1.4554330
48	C	2.4802980	-4.3181430	1.8187400
49	C	0.7245540	-4.5513450	0.1168690
50	C	-2.4802900	-4.3181450	1.8187410
51	C	-0.7245470	-4.5513460	0.1168700
52	C	3.4272610	-4.5182810	0.8261230
53	H	2.7860190	-4.1761420	2.8491670
54	C	1.6893890	-4.7836350	-0.8584980
55	C	-3.4272540	-4.5182840	0.8261260
56	H	-2.7860110	-4.1761450	2.8491690
57	C	-1.6893830	-4.7836370	-0.8584970

58	C	3.0430180	-4.7346780	-0.5170160
59	H	4.4744560	-4.5346180	1.0933950
60	H	1.4244150	-5.0221690	-1.8816160
61	C	-3.0430110	-4.7346810	-0.5170130
62	H	-4.4744490	-4.5346220	1.0933990
63	H	-1.4244090	-5.0221710	-1.8816150
64	N	0.0000040	-4.1706190	2.2382000
65	C	-7.0524670	0.4227730	0.5993190
66	H	-8.8775640	-0.5751660	1.0335380
67	C	-7.3456960	-1.7781510	0.1748770
68	C	-7.2258940	1.7571300	0.9803500
69	C	-5.8427130	-0.0417430	0.0204860
70	C	-7.8777780	-3.0576930	0.0196480
71	C	-6.0316430	-1.4550050	-0.2553620
72	C	-6.1789210	2.6325410	0.7670910
73	H	-8.1525810	2.0967720	1.4297830
74	C	-4.7897390	0.8548110	-0.1624720
75	C	-7.0813280	-4.0159540	-0.5866200
76	H	-8.8896070	-3.2918650	0.3305410
77	C	-5.2319140	-2.4461010	-0.8261770
78	C	-4.9621290	2.1932880	0.1956610
79	H	-6.2642140	3.6763620	1.0359990
80	H	-3.8421050	0.5498900	-0.5904240
81	C	-5.7577410	-3.7315050	-0.9774150
82	H	-7.4645610	-5.0107550	-0.7793170
83	H	-4.2282200	-2.2232650	-1.1667920
84	N	-7.9324390	-0.6366050	0.6939320
85	N	-4.1265540	4.2752340	0.0603240
86	N	-3.8602070	3.0508410	-0.0337460
87	N	-5.1047910	-4.7657280	-1.7227900
88	N	-3.9211160	-5.1266270	-1.5788630

E(RB3LYP) = -2503.46512938

Zero-point vibrational energy 1733702.3 (Joules/Mol)
414.36480 (Kcal/Mol)

Zero-point correction= 0.660332 (Hartree/Particle)
Thermal correction to Energy= 0.703381
Thermal correction to Enthalpy= 0.704325
Thermal correction to Gibbs Free Energy= 0.585067
Sum of electronic and zero-point Energies= -2502.804797
Sum of electronic and thermal Energies= -2502.761749
Sum of electronic and thermal Enthalpies= -2502.760804
Sum of electronic and thermal Free Energies= -2502.880062

(*E*,*Z*,*E*,*Z*)

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opt=tight freq b3lyp/6-311g(d,p) geom=connectivity int=ultrafine

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XYZ coordinates of the optimized species:

Tag	Symbol	X	Y	Z
1	C	0.5180260	-3.7121440	-1.1938920
2	C	0.2156210	-4.1837850	-2.4918710
3	C	-1.0936670	-4.3692300	-2.8953720
4	C	-2.1112290	-4.0908260	-1.9757850
5	C	-1.8287940	-3.6464820	-0.6575540
6	C	-0.5036020	-3.4423820	-0.2806190
7	H	1.0385830	-4.3757150	-3.1672200
8	H	-1.3228420	-4.7079410	-3.8997450
9	H	-0.2348120	-3.0718550	0.7013710
10	H	-3.9553240	-4.4264860	-2.9779350
11	C	-4.1054670	-3.7693710	-0.9572790
12	C	-5.4640090	-3.6784380	-0.6574780
13	C	-5.8225750	-3.2516460	0.6122960
14	C	-4.8451850	-2.9568980	1.5845170
15	C	-3.4889450	-3.0939330	1.2935390
16	C	-3.1071840	-3.4580430	0.0015850
17	H	-6.2229750	-3.9308810	-1.3893410
18	H	-6.8695500	-3.1706500	0.8747670
19	H	-2.7570600	-2.9096710	2.0715090
20	N	-3.4813250	-4.1582540	-2.1319670
21	N	1.8248600	-3.4296860	-0.7438160
22	N	2.7597490	-3.8649030	-1.4622790
23	C	7.5987170	-1.2787950	0.9649510
24	H	8.7692290	-2.7731210	-0.0034100
25	C	6.6703130	-2.8859010	-0.3365120
26	C	8.4697070	-0.4797020	1.7070780
27	C	6.1999300	-1.0486370	0.9690230
28	C	6.4409740	-3.9647000	-1.1927520
29	C	5.6021680	-2.0856950	0.1520160
30	C	7.9230840	0.5589230	2.4490830
31	H	9.5363430	-0.6722440	1.7283140
32	C	5.6763930	0.0295450	1.6764950
33	C	5.1274040	-4.2388030	-1.5454300
34	H	7.2567250	-4.5667570	-1.5762210
35	C	4.2922150	-2.3939390	-0.1913280
36	C	6.5454110	0.8440350	2.4040030
37	H	8.5547780	1.1778690	3.0751750
38	H	4.6116830	0.2234240	1.6816840
39	C	4.0531530	-3.4818840	-1.0365520
40	H	4.8936060	-5.0589500	-2.2134030
41	H	3.4519510	-1.8167000	0.1712550
42	N	7.8576850	-2.3824410	0.1658370
43	N	-5.2206370	-2.7186990	2.9524060
44	N	-6.0549970	-1.8584870	3.2925760
45	C	-7.5987130	1.2787910	0.9649780
46	H	-8.7692290	2.7731170	-0.0033770
47	C	-6.6703140	2.8858990	-0.3364860

48	C	-8.4697010	0.4796970	1.7071080
49	C	-6.1999270	1.0486330	0.9690460
50	C	-6.4409780	3.9646990	-1.1927250
51	C	-5.6021670	2.0856930	0.1520380
52	C	-7.9230760	-0.5589290	2.4491100
53	H	-9.5363370	0.6722380	1.7283470
54	C	-5.6763870	-0.0295500	1.6765150
55	C	-5.1274100	4.2388030	-1.5454070
56	H	-7.2567300	4.5667560	-1.5761900
57	C	-4.2922160	2.3939380	-0.1913090
58	C	-6.5454030	-0.8440400	2.4040250
59	H	-8.5547680	-1.1778760	3.0752020
60	H	-4.6116770	-0.2234290	1.6817000
61	C	-4.0531570	3.4818840	-1.0365320
62	H	-4.8936140	5.0589510	-2.2133800
63	H	-3.4519500	1.8166980	0.1712700
64	N	-7.8576850	2.3824380	0.1658670
65	C	4.1054630	3.7693770	-0.9572860
66	H	3.9553130	4.4264980	-2.9779400
67	C	2.1112210	4.0908330	-1.9757840
68	C	5.4640070	3.6784450	-0.6574900
69	C	3.1071840	3.4580440	0.0015800
70	C	1.0936570	4.3692390	-2.8953670
71	C	1.8287910	3.6464840	-0.6575540
72	C	5.8225770	3.2516480	0.6122810
73	H	6.2229700	3.9308910	-1.3893540
74	C	3.4889500	3.0939300	1.2935310
75	C	-0.2156300	4.1837910	-2.4918620
76	H	1.3228270	4.7079530	-3.8997400
77	C	0.5036010	3.4423820	-0.2806150
78	C	4.8451910	2.9568960	1.5845050
79	H	6.8695530	3.1706540	0.8747490
80	H	2.7570670	2.9096660	2.0715030
81	C	-0.5180300	3.7121460	-1.1938840
82	H	-1.0385950	4.3757230	-3.1672080
83	H	0.2348140	3.0718520	0.7013750
84	N	3.4813170	4.1582630	-2.1319700
85	N	6.0550090	1.8584800	3.2925570
86	N	5.2206480	2.7186940	2.9523920
87	N	-1.8248630	3.4296870	-0.7438030
88	N	-2.7597540	3.8649040	-1.4622630

E(RB3LYP) = -2503.46336525

Zero-point vibrational energy 1733139.3 (Joules/Mol)
414.23023 (Kcal/Mol)

Zero-point correction= 0.660118 (Hartree/Particle)
Thermal correction to Energy= 0.703194
Thermal correction to Enthalpy= 0.704139
Thermal correction to Gibbs Free Energy= 0.584977

Sum of electronic and zero-point Energies= -2502.803247
Sum of electronic and thermal Energies= -2502.760171
Sum of electronic and thermal Enthalpies= -2502.759227
Sum of electronic and thermal Free Energies= -2502.878389

(*E*,*Z*,*Z*,*Z*)

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opt=tight freq b3lyp/6-311g(d,p) geom=connectivity int=ultrafine
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XYZ coordinates of the optimized species:

Tag	Symbol	X	Y	Z
1	C	-6.5472680	-0.4807030	1.7059580
2	C	-7.8654160	-0.0281180	1.5049520
3	C	-8.1285920	1.1464410	0.8154580
4	C	-7.0392860	1.8976140	0.3754380
5	C	-5.7021100	1.4953390	0.6320850
6	C	-5.4596720	0.2943740	1.2984690
7	H	-8.6757950	-0.6322570	1.8948630
8	H	-9.1482230	1.4719950	0.6433240
9	H	-4.4477750	-0.0391570	1.4923750
10	H	-7.8228430	3.6103050	-0.6190070
11	C	-5.7027610	3.4832800	-0.5285280
12	C	-5.2011500	4.6124570	-1.1857610
13	C	-3.8300790	4.7740330	-1.2452260
14	C	-2.9561610	3.8301990	-0.6563560
15	C	-3.4659520	2.7035050	-0.0073730
16	C	-4.8456790	2.5171270	0.0587060
17	H	-5.8665950	5.3441620	-1.6306940
18	H	-3.3924160	5.6338360	-1.7337740
19	H	-2.7692640	2.0035180	0.4382200
20	N	-7.0116380	3.0934940	-0.3236900
21	N	-6.4130100	-1.6758690	2.4881540
22	N	-5.6605900	-2.6292380	2.2030030
23	C	-1.4606890	-4.2632380	-1.7002210
24	H	-2.6169950	-3.4022060	-3.2649410
25	C	-3.4508140	-3.2656240	-1.3132320
26	C	-0.3230680	-4.8080820	-2.2928700
27	C	-1.7020350	-4.3710140	-0.3050860
28	C	-4.6920400	-2.6402740	-1.4467740
29	C	-2.9703190	-3.7106410	-0.0547960
30	C	0.5863450	-5.4615030	-1.4767190
31	H	-0.1537050	-4.7378980	-3.3613280
32	C	-0.8030330	-5.0826350	0.4882010
33	C	-5.4251220	-2.3934730	-0.2986650
34	H	-5.0760900	-2.3524570	-2.4188350
35	C	-3.7365130	-3.4739490	1.0851440
36	C	0.3550660	-5.6039310	-0.0917520
37	H	1.4648300	-5.9075270	-1.9192000

38	H	-0.9871400	-5.2561400	1.5419710
39	C	-4.9373500	-2.7695380	0.9733450
40	H	-6.3898600	-1.9138090	-0.3825040
41	H	-3.4264260	-3.8134920	2.0662900
42	N	-2.5241870	-3.5984180	-2.2824690
43	N	-1.5502790	3.9633960	-0.6366420
44	N	-1.0941610	4.9563620	-1.2580750
45	C	2.9811440	5.8443300	-0.9938110
46	H	4.8754240	6.8029910	-0.9579260
47	C	4.7185320	5.0219050	0.2026980
48	C	2.1394360	6.6318570	-1.7810070
49	C	2.5041700	4.6833920	-0.3215950
50	C	5.9330740	4.8573420	0.8679980
51	C	3.6265790	4.1480290	0.4259810
52	C	0.8040690	6.2677400	-1.8538930
53	H	2.5066890	7.5111370	-2.2976980
54	C	1.1626040	4.3342310	-0.4134160
55	C	6.0443340	3.8041500	1.7666280
56	H	6.7573780	5.5459860	0.7202430
57	C	3.7803080	3.0531740	1.2769210
58	C	0.3034760	5.1415800	-1.1686090
59	H	0.0994790	6.8585140	-2.4264360
60	H	0.7536590	3.4803310	0.1105400
61	C	4.9942370	2.8842570	1.9411140
62	H	6.9515940	3.6728350	2.3447810
63	H	2.9626910	2.3660420	1.4590110
64	N	4.3164210	6.0123290	-0.6847340
65	C	4.9567070	-3.7517220	-1.1305830
66	H	6.4161170	-2.7023430	-2.2760350
67	C	5.6099340	-1.6477390	-0.6177640
68	C	4.8564260	-5.0345380	-1.6687700
69	C	4.2298240	-3.3735770	0.0253180
70	C	6.2670290	-0.4176720	-0.5592490
71	C	4.6728710	-2.0379550	0.3757580
72	C	3.9977670	-5.9340920	-1.0506730
73	H	5.4457550	-5.3353760	-2.5276290
74	C	3.3153720	-4.2669620	0.5866810
75	C	6.0004900	0.4171220	0.5145130
76	H	6.9873810	-0.1271420	-1.3156750
77	C	4.4631280	-1.2090880	1.4751790
78	C	3.1934960	-5.5388060	0.0327060
79	H	3.9226610	-6.9530040	-1.4127500
80	H	2.7265630	-3.9956990	1.4547270
81	C	5.1150270	0.0248960	1.5439780
82	H	6.5231600	1.3596710	0.5889130
83	H	3.8390810	-1.5132220	2.3073000
84	N	5.7516060	-2.6828660	-1.5209540
85	N	1.1433560	-6.4808580	0.7285850
86	N	2.3865870	-6.5250470	0.7076900
87	N	5.0351230	0.6827780	2.8158460
88	N	5.0982900	1.9124230	2.9945540

E(RB3LYP) = -2503.43120954

Zero-point vibrational energy 1731194.5 (Joules/Mol)
413.76541 (Kcal/Mol)

Zero-point correction= 0.659377 (Hartree/Particle)
Thermal correction to Energy= 0.702566
Thermal correction to Enthalpy= 0.703511
Thermal correction to Gibbs Free Energy= 0.583717
Sum of electronic and zero-point Energies= -2502.771832
Sum of electronic and thermal Energies= -2502.728643
Sum of electronic and thermal Enthalpies= -2502.727699
Sum of electronic and thermal Free Energies= -2502.847493

all-*Z*

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opt=tight freq b3lyp/6-311g(d,p) geom=connectivity int=ultrafine
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XYZ coordinates of the optimized species:

Tag	Symbol	X	Y	Z
1	C	-3.0457370	-3.7533490	-0.3788940
2	C	-3.4276370	-3.3407620	0.9188540
3	C	-2.4789510	-2.9862350	1.8656510
4	C	-1.1316170	-3.0322110	1.5019770
5	C	-0.7251260	-3.4523170	0.2102410
6	C	-1.6911170	-3.8319150	-0.7158880
7	H	-4.4720000	-3.3280850	1.1941420
8	H	-2.7831530	-2.6967650	2.8653220
9	H	-1.4282170	-4.2178480	-1.6934570
10	H	0.0000080	-2.5205450	3.2291040
11	C	1.1316280	-3.0322120	1.5019740
12	C	2.4789620	-2.9862390	1.8656450
13	C	3.4276450	-3.3407660	0.9188450
14	C	3.0457410	-3.7533510	-0.3789020
15	C	1.6911200	-3.8319160	-0.7158930
16	C	0.7251320	-3.4523180	0.2102390
17	H	2.7831670	-2.6967700	2.8653140
18	H	4.4720090	-3.3280910	1.1941290
19	H	1.4282160	-4.2178480	-1.6934620
20	N	0.0000060	-2.7641580	2.2528570
21	N	-3.9074290	-4.3230600	-1.3724090
22	N	-5.1202920	-4.0840550	-1.5225240
23	C	-7.5847220	1.1302500	0.1414580
24	H	-9.2060810	-0.0000190	0.9267750
25	C	-7.5847210	-1.1302580	0.1414190
26	C	-7.9369020	2.4749320	0.2591250
27	C	-6.3812840	0.7259290	-0.4939620

28	C	-7.9368990	-2.4749440	0.2590400
29	C	-6.3812830	-0.7259140	-0.4939870
30	C	-7.0756350	3.4174820	-0.2801000
31	H	-8.8685000	2.7770300	0.7241600
32	C	-5.5022040	1.6945430	-0.9843350
33	C	-7.0756300	-3.4174750	-0.2802180
34	H	-8.8684960	-2.7770600	0.7240640
35	C	-5.5022020	-1.6945090	-0.9843940
36	C	-5.8508800	3.0406320	-0.8657320
37	H	-7.3311410	4.4702300	-0.2626780
38	H	-4.5775950	1.4136250	-1.4743930
39	C	-5.8508760	-3.0406030	-0.8658370
40	H	-7.3311350	-4.4702240	-0.2628320
41	H	-4.5775930	-1.4135730	-1.4744420
42	N	-8.2789600	-0.0000110	0.5362300
43	N	3.9074300	-4.3230620	-1.3724200
44	N	5.1202930	-4.0840550	-1.5225380
45	C	7.5847190	-1.1302530	0.1413990
46	H	9.2060780	-0.0000120	0.9267530
47	C	7.5847180	1.1302550	0.1414370
48	C	7.9368990	-2.4749390	0.2590210
49	C	6.3812800	-0.7259110	-0.4940060
50	C	7.9368970	2.4749370	0.2591030
51	C	6.3812800	0.7259320	-0.4939820
52	C	7.0756310	-3.4174710	-0.2802360
53	H	8.8684970	-2.7770530	0.7240440
54	C	5.5021990	-1.6945080	-0.9844110
55	C	7.0756270	3.4174860	-0.2801220
56	H	8.8684940	2.7770360	0.7241370
57	C	5.5021980	1.6945440	-0.9843550
58	C	5.8508760	-3.0406020	-0.8658540
59	H	7.3311380	-4.4702200	-0.2628500
60	H	4.5775900	-1.4135730	-1.4744580
61	C	5.8508730	3.0406340	-0.8657530
62	H	7.3311330	4.4702340	-0.2627000
63	H	4.5775890	1.4136250	-1.4744110
64	N	8.2789580	-0.0000060	0.5362090
65	C	-1.1316200	3.0321580	1.5020790
66	H	0.0000070	2.5204310	3.2291860
67	C	1.1316250	3.0321580	1.5020740
68	C	-2.4789530	2.9861700	1.8657520
69	C	-0.7251300	3.4523090	0.2103570
70	C	2.4789600	2.9861710	1.8657410
71	C	0.7251290	3.4523090	0.2103540
72	C	-3.4276400	3.3407300	0.9189680
73	H	-2.7831540	2.6966660	2.8654130
74	C	-1.6911210	3.8319400	-0.7157580
75	C	3.4276420	3.3407310	0.9189530
76	H	2.7831650	2.6966670	2.8654000
77	C	1.6911150	3.8319400	-0.7157660
78	C	-3.0457410	3.7533620	-0.3787660

79	H	-4.4720030	3.3280450	1.1942560
80	H	-1.4282210	4.2179060	-1.6933140
81	C	3.0457370	3.7533630	-0.3787790
82	H	4.4720060	3.3280460	1.1942360
83	H	1.4282110	4.2179060	-1.6933210
84	N	0.0000040	2.7640780	2.2529480
85	N	-5.1202970	4.0841080	-1.5223830
86	N	-3.9074340	4.3231080	-1.3722600
87	N	3.9074260	4.3231090	-1.3722770
88	N	5.1202880	4.0841090	-1.5224030

E(RB3LYP) = -2503.40542059

Zero-point vibrational energy 1729658.5 (Joules/Mol)
413.39829 (Kcal/Mol)

Zero-point correction= 0.658792 (Hartree/Particle)
Thermal correction to Energy= 0.702003
Thermal correction to Enthalpy= 0.702947
Thermal correction to Gibbs Free Energy= 0.582852
Sum of electronic and zero-point Energies= -2502.746628
Sum of electronic and thermal Energies= -2502.703418
Sum of electronic and thermal Enthalpies= -2502.702473
Sum of electronic and thermal Free Energies= -2502.822569

Transition-state all-*Z* → (*E*,*Z*,*Z*,*Z*)

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opt=(calcfc,tight,ts,noeigen) freq b3lyp/6-311g(d,p) geom=connectivity int=ultrafine scf=(maxcycle=1000)

XYZ coordinates of the optimized species:

Tag	Symbol	X	Y	Z
1	C	-1.3038540	-3.6163590	-0.5453430
2	C	-1.8664980	-3.1266520	0.6605210
3	C	-1.0583740	-2.6995870	1.7027110
4	C	0.3292720	-2.7609330	1.5427260
5	C	0.9162650	-3.2604650	0.3508320
6	C	0.0891890	-3.6855930	-0.6809090
7	H	-2.9364910	-3.0878510	0.7853940
8	H	-1.5010520	-2.3320550	2.6218850
9	H	0.4823120	-4.0897530	-1.6056210
10	H	1.2042070	-2.0575360	3.3459660
11	C	2.5732450	-2.6802910	1.8333150
12	C	3.8592150	-2.5271630	2.3521780
13	C	4.9331330	-2.8920870	1.5528430
14	C	4.7343070	-3.4232430	0.2608990
15	C	3.4437920	-3.6150480	-0.2319860
16	C	2.3534220	-3.2143690	0.5399230

17	H	4.0235930	-2.1411220	3.3519940
18	H	5.9422780	-2.7874150	1.9309090
19	H	3.3140380	-4.0799510	-1.2022480
20	N	1.3391790	-2.4100590	2.4134150
21	N	-1.9534410	-4.1537060	-1.7009530
22	N	-3.1731920	-4.2045910	-1.9416200
23	C	-7.7063460	-0.8205740	0.0306490
24	H	-8.5708990	-2.5940380	0.8196020
25	C	-6.6216150	-2.8043080	-0.0121040
26	C	-8.6591660	0.1911850	0.1646710
27	C	-6.4672420	-0.5947880	-0.6261540
28	C	-6.2795220	-4.1519900	0.0897760
29	C	-5.7790520	-1.8716320	-0.6674120
30	C	-8.3592030	1.4384090	-0.3615590
31	H	-9.6174820	0.0052670	0.6362910
32	C	-6.1587050	0.6852110	-1.0887490
33	C	-5.0953530	-4.5688460	-0.5012210
34	H	-6.9293160	-4.8650030	0.5848200
35	C	-4.5757030	-2.3058120	-1.2342460
36	C	-7.1034780	1.7013000	-0.9411400
37	H	-9.0866610	2.2406950	-0.3248260
38	H	-5.2151520	0.8872570	-1.5804970
39	C	-4.2387840	-3.6558360	-1.1475590
40	H	-4.8204770	-5.6168530	-0.4900680
41	H	-3.9266270	-1.6196410	-1.7660240
42	N	-7.7640480	-2.1451280	0.4202980
43	N	5.8056250	-3.9989690	-0.5000350
44	N	6.8904290	-3.4381930	-0.7548460
45	C	8.1506710	0.5487520	-0.3744210
46	H	9.2570360	2.3532200	-0.2632000
47	C	7.1466030	2.5706800	-0.5476790
48	C	9.0601680	-0.5058640	-0.2514990
49	C	6.7648610	0.3064770	-0.5945020
50	C	6.8582060	3.9322070	-0.6012920
51	C	6.1246260	1.6042480	-0.6988870
52	C	8.5693230	-1.7956490	-0.3596790
53	H	10.1191340	-0.3252200	-0.1056180
54	C	6.2887760	-0.9989530	-0.6668500
55	C	5.5491790	4.3315080	-0.8230570
56	H	7.6363580	4.6801920	-0.4948920
57	C	4.7973060	1.9928900	-0.8534670
58	C	7.1922880	-2.0598280	-0.5337530
59	H	9.2383900	-2.6467690	-0.3219070
60	H	5.2401620	-1.1874090	-0.8522630
61	C	4.4958980	3.3741090	-0.9310480
62	H	5.3040160	5.3829860	-0.8974450
63	H	3.9999950	1.2650500	-0.9305590
64	N	8.3590150	1.9076400	-0.3432820
65	C	-3.0390610	3.2408790	1.6683920
66	H	-1.9012200	2.9931620	3.4523660
67	C	-0.7825590	3.3815010	1.6893230

68	C	-4.3800670	3.0885410	2.0185190
69	C	-2.6411270	3.5187710	0.3365240
70	C	0.5663210	3.3766140	2.0620920
71	C	-1.1941960	3.6107570	0.3485160
72	C	-5.3268060	3.1755680	1.0106090
73	H	-4.6802460	2.9032840	3.0436060
74	C	-3.6140110	3.6554580	-0.6539230
75	C	1.5098390	3.5800000	1.0724180
76	H	0.8641060	3.2135740	3.0919320
77	C	-0.2264970	3.8425140	-0.6266900
78	C	-4.9506840	3.4415980	-0.3229980
79	H	-6.3746060	3.0583830	1.2522190
80	H	-3.3575530	3.9148630	-1.6744010
81	C	1.1164860	3.8045740	-0.2616600
82	H	2.5666750	3.5719820	1.3101580
83	H	-0.4779970	4.0284090	-1.6644200
84	N	-1.9045620	3.1734090	2.4624270
85	N	-6.9241940	2.9921390	-1.5441350
86	N	-5.9252950	3.7085580	-1.3441560
87	N	2.0522160	3.9965250	-1.3430990
88	N	3.2320610	3.7702320	-1.1010220

E(RB3LYP) = -2503.36427308

Zero-point vibrational energy 1723772.3 (Joules/Mol)
411.99147 (Kcal/Mol)

Zero-point correction=	0.656550 (Hartree/Particle)
Thermal correction to Energy=	0.699938
Thermal correction to Enthalpy=	0.700883
Thermal correction to Gibbs Free Energy=	0.580174
Sum of electronic and zero-point Energies=	-2502.707723
Sum of electronic and thermal Energies=	-2502.664335
Sum of electronic and thermal Enthalpies=	-2502.663391
Sum of electronic and thermal Free Energies=	-2502.784099

Imaginary frequency: -452.81

Transition-state (*E*,*Z*,*Z*,*Z*)→ (*E*,*E*,*Z*,*Z*)

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opt=(calcfc,tight,ts,noeigen) freq b3lyp/6-311g(d,p) geom=connectivity int=ultrafine scf=(maxcycle=1000)

XYZ coordinates of the optimized species:

Tag	Symbol	X	Y	Z
1	C	4.5712570	2.5326840	-1.1668550
2	C	5.2944820	3.2988080	-0.2330480
3	C	6.2459910	2.7066020	0.5815020

4	C	6.4238670	1.3220780	0.4808870
5	C	5.6581590	0.5329690	-0.4193760
6	C	4.7628170	1.1585870	-1.2811150
7	H	5.1176230	4.3665980	-0.1845350
8	H	6.8354390	3.3008610	1.2706570
9	H	4.1962820	0.6134180	-2.0271100
10	H	7.9662740	0.7896290	1.8424300
11	C	7.1019870	-0.8225110	0.7447160
12	C	7.7633790	-1.9903390	1.1262420
13	C	7.3534270	-3.1856040	0.5500270
14	C	6.2592320	-3.2292960	-0.3340390
15	C	5.6279810	-2.0575800	-0.7447760
16	C	6.0674380	-0.8413700	-0.2228050
17	H	8.5809220	-1.9722530	1.8379390
18	H	7.8581980	-4.1128350	0.7946450
19	H	4.8146720	-2.0998630	-1.4589820
20	N	7.2932300	0.4901460	1.1570570
21	N	3.6055680	3.0825000	-2.0846880
22	N	3.0480790	4.1285740	-1.7684150
23	C	-1.6321970	6.8913270	0.5671210
24	H	-0.5018320	8.6856640	0.6419150
25	C	0.5208590	6.9760170	-0.1453640
26	C	-2.9079130	7.1693060	1.0673500
27	C	-1.2900370	5.5845810	0.1133480
28	C	1.8108480	7.3600740	-0.5020600
29	C	0.0855240	5.6441580	-0.3386840
30	C	-3.8293600	6.1324090	1.1025380
31	H	-3.1754300	8.1610240	1.4140370
32	C	-2.2258930	4.5643480	0.1555700
33	C	2.6785760	6.4042880	-1.0173710
34	H	2.1555240	8.3798230	-0.3691520
35	C	0.9216130	4.6970030	-0.9121220
36	C	-3.5068650	4.8356290	0.6508880
37	H	-4.8319820	6.2978550	1.4782920
38	H	-1.9985840	3.5635480	-0.1864290
39	C	2.2506160	5.0631300	-1.2357100
40	H	3.6901310	6.6810790	-1.2863850
41	H	0.5859120	3.6858860	-1.1013860
42	N	-0.5347480	7.7083480	0.4073640
43	N	5.9266260	-4.4856010	-0.9462130
44	N	4.7900690	-4.9925910	-0.8875010
45	C	1.5979410	-4.0767900	1.6798180
46	H	0.2659960	-3.7312920	3.3025600
47	C	-0.6457640	-4.2113030	1.4422130
48	C	2.8914210	-3.9534070	2.1867830
49	C	1.3557920	-4.4275580	0.3256450
50	C	-2.0230050	-4.2650030	1.6681210
51	C	-0.0866560	-4.4965590	0.1702220
52	C	3.9536490	-4.1700280	1.3241250
53	H	3.0682390	-3.7081990	3.2278790
54	C	2.4388080	-4.6921670	-0.5114260

55	C	-2.8527520	-4.5535610	0.5974510
56	H	-2.4381130	-4.0922220	2.6546290
57	C	-0.9389060	-4.7999970	-0.8884050
58	C	3.7385200	-4.5356730	-0.0229380
59	H	4.9629640	-4.0960730	1.7030250
60	H	2.3013480	-5.0344550	-1.5304060
61	C	-2.3242080	-4.7904980	-0.6932620
62	H	-3.9182170	-4.6117250	0.7626430
63	H	-0.5651880	-5.0572020	-1.8722380
64	N	0.3824900	-3.9474010	2.3266620
65	C	-7.0965780	-0.3037100	0.4183420
66	H	-8.7850340	-1.5788800	0.6326470
67	C	-7.0525670	-2.4728160	-0.2236600
68	C	-7.4673330	0.9497530	0.9187950
69	C	-5.8041860	-0.5439110	-0.1148020
70	C	-7.3777810	-3.7978080	-0.5123490
71	C	-5.7739090	-1.9352050	-0.5271400
72	C	-6.5317800	1.9671960	0.8850200
73	H	-8.4592160	1.1206320	1.3228580
74	C	-4.8765290	0.4953420	-0.1368980
75	C	-6.4059320	-4.5841310	-1.1119190
76	H	-8.3625280	-4.1987990	-0.3006140
77	C	-4.7992100	-2.7531620	-1.1012410
78	C	-5.2361160	1.7497010	0.3615180
79	H	-6.7684160	2.9540630	1.2593680
80	H	-3.8759380	0.3648730	-0.5313780
81	C	-5.1128060	-4.0872490	-1.3714520
82	H	-6.6224500	-5.6070380	-1.3954490
83	H	-3.8168440	-2.3636970	-1.3394380
84	N	-7.8270480	-1.4742320	0.3435840
85	N	-4.5371010	3.8730160	0.7302450
86	N	-4.2277370	2.7331250	0.2965670
87	N	-4.2544990	-4.9725240	-2.1020950
88	N	-3.0556670	-5.2080630	-1.8523630

E(RB3LYP) = -2503.39178748

Zero-point vibrational energy 1726228.9 (Joules/Mol)
412.57860 (Kcal/Mol)

Zero-point correction=	0.657486 (Hartree/Particle)
Thermal correction to Energy=	0.700670
Thermal correction to Enthalpy=	0.701614
Thermal correction to Gibbs Free Energy=	0.581856
Sum of electronic and zero-point Energies=	-2502.734302
Sum of electronic and thermal Energies=	-2502.691118
Sum of electronic and thermal Enthalpies=	-2502.690173
Sum of electronic and thermal Free Energies=	-2502.809932

Imaginary frequency: -539.60

Transition-state (*E*,*Z*,*Z*,*Z*)→ (*E*,*Z*,*E*,*Z*)

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opt=(calcfc,tight,ts,noeigen) freq b3lyp/6-311g(d,p) geom=connectivity int=ultrafine scf=maxcycle=1000

XYZ coordinates of the optimized species:

Tag	Symbol	X	Y	Z
1	C	4.1444960	3.0926100	0.0781630
2	C	5.2269050	3.9727290	-0.1459360
3	C	6.5248590	3.5963920	0.1605520
4	C	6.7367420	2.3093310	0.6711440
5	C	5.6586210	1.4174190	0.9005620
6	C	4.3604060	1.8271460	0.6256730
7	H	5.0164640	4.9475350	-0.5661980
8	H	7.3519430	4.2778130	-0.0054890
9	H	3.5060430	1.1807000	0.7851620
10	H	8.8359580	2.0514290	0.9043610
11	C	7.6378760	0.3549150	1.3857580
12	C	8.4961720	-0.6837980	1.7479570
13	C	7.9293200	-1.9190190	2.0367560
14	C	6.5416460	-2.1386910	1.9324050
15	C	5.6847730	-1.0785360	1.6325670
16	C	6.2330020	0.1680610	1.3498660
17	H	9.5692900	-0.5410380	1.8049990
18	H	8.5525360	-2.7534850	2.3353410
19	H	4.6144760	-1.2310850	1.5912590
20	N	7.9138590	1.6599200	0.9987610
21	N	2.7979130	3.3651870	-0.2278790
22	N	2.5745550	4.3061870	-1.0295810
23	C	-3.4192730	4.1977870	-1.0772460
24	H	-3.3346600	5.0983700	-3.0050320
25	C	-1.4566360	4.7757050	-2.0537480
26	C	-4.7647390	3.9858800	-0.7735550
27	C	-2.3923680	3.8642210	-0.1574160
28	C	-0.4637590	5.2537380	-2.9106720
29	C	-1.1362650	4.2087540	-0.7913070
30	C	-5.0783320	3.4376460	0.4628650
31	H	-5.5504240	4.2503410	-1.4722480
32	C	-2.7289360	3.3767700	1.1005390
33	C	0.8575710	5.1223730	-2.5036680
34	H	-0.7085270	5.7081040	-3.8638660
35	C	0.1916710	4.0574430	-0.4175300
36	C	-4.0705380	3.1405650	1.4051120
37	H	-6.1158860	3.2807650	0.7252650
38	H	-1.9782310	3.1954300	1.8606510
39	C	1.1927770	4.4951700	-1.2887520
40	H	1.6676890	5.4670470	-3.1349290
41	H	0.4746310	3.5899070	0.5159760

42	N	-2.8336930	4.7502610	-2.2049510
43	N	6.0819110	-3.4495900	2.2931430
44	N	5.1605730	-4.0558970	1.7044680
45	C	3.2578960	-2.8542610	-1.8494120
46	H	2.6562990	-2.0710620	-3.7269750
47	C	1.0927530	-2.8495270	-2.4968590
48	C	4.6504530	-2.7435990	-1.7893770
49	C	2.5095360	-3.4181910	-0.7799020
50	C	-0.1019150	-2.6943690	-3.1958340
51	C	1.1203720	-3.4377330	-1.2070360
52	C	5.2868460	-3.1195530	-0.6196860
53	H	5.2209080	-2.3679270	-2.6314380
54	C	3.1780750	-3.8232910	0.3761420
55	C	-1.2769490	-3.1298100	-2.6082230
56	H	-0.1277300	-2.2276840	-4.1746300
57	C	-0.0461820	-3.9563340	-0.6471790
58	C	4.5546080	-3.6158030	0.4822170
59	H	6.3628500	-3.0333690	-0.5481220
60	H	2.6538010	-4.2708800	1.2125910
61	C	-1.2643720	-3.8173100	-1.3530550
62	H	-2.2220940	-3.0087220	-3.1215850
63	H	-0.0357280	-4.4766810	0.3018630
64	N	2.3928290	-2.5159190	-2.8644830
65	C	-7.4960190	-0.8299330	1.1832560
66	H	-8.9956520	-2.2256670	0.6045900
67	C	-7.0002940	-2.7767170	0.1480830
68	C	-8.1524400	0.1959500	1.8620230
69	C	-6.0833920	-0.8754550	1.0752960
70	C	-7.0688570	-4.0555610	-0.4086360
71	C	-5.7588360	-2.1265120	0.4082730
72	C	-7.3738980	1.1697220	2.4673500
73	H	-9.2323020	0.2108230	1.9565550
74	C	-5.3204150	0.1534900	1.6337880
75	C	-5.8738730	-4.6953910	-0.6827060
76	H	-8.0201480	-4.5431250	-0.5879620
77	C	-4.5688690	-2.7698050	0.0685430
78	C	-5.9722250	1.1691390	2.3355870
79	H	-7.8341840	1.9462720	3.0667390
80	H	-4.2386460	0.1421830	1.5770190
81	C	-4.6380620	-4.0561260	-0.4713520
82	H	-5.8529320	-5.7065860	-1.0710240
83	H	-3.6017190	-2.3141050	0.2501000
84	N	-8.0237350	-1.9652870	0.5866130
85	N	-4.3475760	2.8431110	2.7788640
86	N	-5.2420120	2.0764690	3.1751080
87	N	-3.5044740	-4.8918730	-0.7689000
88	N	-2.3978100	-4.3855800	-0.9256340

E(RB3LYP) = -2503.38890375

Zero-point vibrational energy 1725645.9 (Joules/Mol)

412.43926 (Kcal/Mol)

Zero-point correction=	0.657264 (Hartree/Particle)
Thermal correction to Energy=	0.700437
Thermal correction to Enthalpy=	0.701382
Thermal correction to Gibbs Free Energy=	0.581674
Sum of electronic and zero-point Energies=	-2502.731640
Sum of electronic and thermal Energies=	-2502.688466
Sum of electronic and thermal Enthalpies=	-2502.687522
Sum of electronic and thermal Free Energies=	-2502.807230

Imaginary frequency: -486.91

Transition-state (*E*,*E*,*Z*,*Z*)→ (*E*,*E*,*E*,*Z*)

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opt=(calcfc,tight,ts,noeigen) freq b3lyp/6-311g(d,p) geom=connectivity int=ultrafine scf=maxcycle=1000

XYZ coordinates of the optimized species:

Tag	Symbol	X	Y	Z
1	C	6.1645210	1.8181210	-0.5849540
2	C	7.5047700	2.0076220	-0.9766530
3	C	8.3424710	0.9377340	-1.2483240
4	C	7.8141080	-0.3436810	-1.1015390
5	C	6.4725180	-0.5619750	-0.6838150
6	C	5.6448230	0.5266660	-0.4316890
7	H	7.8584310	3.0270450	-1.0694860
8	H	9.3684600	1.0956590	-1.5599390
9	H	4.6143950	0.4084530	-0.1223820
10	H	9.3691080	-1.7065400	-1.6036230
11	C	7.5252800	-2.5873480	-1.0230690
12	C	7.7039420	-3.9689010	-1.0991420
13	C	6.6252870	-4.7704250	-0.7622830
14	C	5.4067110	-4.2128120	-0.3400340
15	C	5.2259240	-2.8291620	-0.2734340
16	C	6.2888650	-2.0034580	-0.6236180
17	H	8.6472310	-4.4011000	-1.4124070
18	H	6.6908110	-5.8509240	-0.8068650
19	H	4.2712510	-2.4240510	0.0425100
20	N	8.4191690	-1.5724920	-1.2995600
21	N	5.4393450	3.0096220	-0.3619900
22	N	4.2011640	2.8736370	-0.1970010
23	C	-0.2288220	6.7792850	0.5749030
24	H	1.2264780	8.3053510	0.8534730
25	C	1.9920200	6.3554580	0.4885060
26	C	-1.4782100	7.3875670	0.6891450
27	C	-0.0901170	5.3874030	0.3121140
28	C	3.3863090	6.4637590	0.4998070

29	C	1.3369320	5.1183740	0.2609360
30	C	-2.5961880	6.5837380	0.5334760
31	H	-1.5757630	8.4480710	0.8909390
32	C	-1.2259220	4.6012190	0.1564480
33	C	4.1268660	5.3194270	0.2724850
34	H	3.8742590	7.4150660	0.6813370
35	C	2.1028510	3.9739970	0.0483190
36	C	-2.4854150	5.2042740	0.2661860
37	H	-3.5935030	6.9988880	0.6107990
38	H	-1.1683340	3.5402000	-0.0484280
39	C	3.4964030	4.0746340	0.0438510
40	H	5.2077290	5.3496560	0.2649540
41	H	1.6511940	3.0046810	-0.1257070
42	N	1.0339800	7.3331800	0.6787640
43	N	4.3958410	-5.1911260	-0.0225940
44	N	3.3389230	-4.8025960	0.4657830
45	C	-0.0556130	-3.6203980	2.5008870
46	H	-1.5445430	-3.0057460	3.9060290
47	C	-2.2646490	-3.6386770	2.0126130
48	C	1.1864900	-3.4985310	3.1208350
49	C	-0.1667930	-4.0993840	1.1720770
50	C	-3.6613280	-3.5746860	2.0574160
51	C	-1.5822680	-4.0984500	0.8537450
52	C	2.3230490	-3.8351060	2.4045880
53	H	1.2783270	-3.1279380	4.1360470
54	C	0.9628840	-4.5208710	0.4766140
55	C	-4.3722480	-3.9165630	0.9190990
56	H	-4.1809240	-3.2698150	2.9589830
57	C	-2.3191150	-4.4714660	-0.2665300
58	C	2.2328060	-4.3843690	1.0860460
59	H	3.3018660	-3.7276350	2.8542820
60	H	0.8916300	-4.9466270	-0.5158400
61	C	-3.7095930	-4.3360260	-0.2579760
62	H	-5.4525600	-3.8775760	0.9398990
63	H	-1.8460780	-4.8645250	-1.1587740
64	N	-1.3336950	-3.3490380	2.9845620
65	C	-7.2265700	1.1846010	-0.5080560
66	H	-9.2187770	0.4479690	-0.5803170
67	C	-7.6874110	-0.9851670	-0.9519490
68	C	-7.3102650	2.5466650	-0.1974430
69	C	-5.9796590	0.5376920	-0.7087150
70	C	-8.3188210	-2.2045460	-1.1938360
71	C	-6.2747260	-0.8540830	-0.9963680
72	C	-6.1326870	3.2595670	-0.0805730
73	H	-8.2696400	3.0299190	-0.0482000
74	C	-4.8040190	1.2754230	-0.5832610
75	C	-7.5161360	-3.2977680	-1.4815890
76	H	-9.3989650	-2.2964310	-1.1805160
77	C	-5.4852250	-1.9721340	-1.2627140
78	C	-4.8775450	2.6340250	-0.2674900
79	H	-6.1426870	4.3133740	0.1616020

80	H	-3.8269440	0.8270950	-0.7182990
81	C	-6.1099920	-3.2027890	-1.4819350
82	H	-7.9566100	-4.2590380	-1.7173490
83	H	-4.4063870	-1.8912520	-1.3014590
84	N	-8.2347470	0.2543470	-0.6611920
85	N	-3.7173170	4.5262650	0.1307250
86	N	-3.6395180	3.3026890	-0.1455360
87	N	-5.4229840	-4.3828180	-1.9172000
88	N	-4.3527920	-4.8149680	-1.4418910

E(RB3LYP) = -2503.42573205

Zero-point vibrational energy 1728280.7 (Joules/Mol)
413.06899 (Kcal/Mol)

Zero-point correction=	0.658267 (Hartree/Particle)
Thermal correction to Energy=	0.701385
Thermal correction to Enthalpy=	0.702330
Thermal correction to Gibbs Free Energy=	0.582458
Sum of electronic and zero-point Energies=	-2502.767465
Sum of electronic and thermal Energies=	-2502.724347
Sum of electronic and thermal Enthalpies=	-2502.723402
Sum of electronic and thermal Free Energies=	-2502.843274

Imaginary frequency: -443.72

Transition-state (*E*,*Z*,*E*,*Z*)→ (*E*,*E*,*E*,*Z*)

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opt=(calcfc,tight,ts,noeigen) freq b3lyp/6-311g(d,p) geom=connectivity int=ultrafine scf=(maxcycle=1000)

XYZ coordinates of the optimized species:

Tag	Symbol	X	Y	Z
1	C	4.8464080	3.4315310	0.9871950
2	C	5.6062820	4.3755850	0.2244780
3	C	5.0052870	5.1610260	-0.7402990
4	C	3.6284550	5.0621580	-0.9227500
5	C	2.8454090	4.1620830	-0.1608290
6	C	3.4534050	3.3236010	0.7783680
7	H	6.6700990	4.4494060	0.4081330
8	H	5.6054370	5.8520820	-1.3224230
9	H	2.8746670	2.6169670	1.3594610
10	H	3.0926920	6.4724140	-2.4367890
11	C	1.5001260	5.3384760	-1.6229540
12	C	0.3361590	5.7625690	-2.2765370
13	C	-0.8622170	5.1877890	-1.9088660
14	C	-0.9186120	4.1906480	-0.9049180
15	C	0.2494190	3.7620110	-0.2669820

16	C	1.4730200	4.3373870	-0.6109270
17	H	0.3753320	6.5215340	-3.0505210
18	H	-1.7893700	5.4851180	-2.3788430
19	H	0.1693290	2.9949870	0.4944910
20	N	2.7956710	5.7533610	-1.7995280
21	N	5.5124450	2.7055340	1.8946360
22	N	6.3654990	2.1180660	2.5526730
23	C	6.8288770	-3.3435160	0.0672440
24	H	8.8119050	-3.4107450	0.8455850
25	C	7.7033420	-1.6562060	1.3028670
26	C	6.6239480	-4.5217900	-0.6517850
27	C	5.8124970	-2.3615870	0.1910000
28	C	8.5167810	-0.8549620	2.1071990
29	C	6.3809250	-1.2653840	0.9500530
30	C	5.3715110	-4.7219840	-1.2166100
31	H	7.4092680	-5.2599950	-0.7661080
32	C	4.5534940	-2.5992280	-0.3460480
33	C	7.9999080	0.3588830	2.5351500
34	H	9.5129790	-1.1693610	2.3960650
35	C	5.9053380	-0.0190650	1.3385720
36	C	4.3288300	-3.7945840	-1.0326850
37	H	5.1570050	-5.6206150	-1.7821680
38	H	3.7401620	-1.8941950	-0.2364610
39	C	6.7284380	0.7913030	2.1204180
40	H	8.5764400	1.0203370	3.1708150
41	H	4.9173450	0.3267020	1.0579040
42	N	7.9530420	-2.8957130	0.7466180
43	N	-2.1211050	3.5800240	-0.4876630
44	N	-3.1659440	4.0883520	-0.9708010
45	C	-6.9161400	2.5653950	0.0698130
46	H	-8.9856640	2.2421410	0.4384440
47	C	-7.6701530	0.7382000	1.1731730
48	C	-6.8115920	3.7689730	-0.6272150
49	C	-5.7684180	1.8043440	0.4258790
50	C	-8.4569000	-0.2066190	1.8325960
51	C	-6.2567060	0.6256780	1.1197230
52	C	-5.5392340	4.2102480	-0.9529040
53	H	-7.6894220	4.3413430	-0.9045240
54	C	-4.4993760	2.2739160	0.1006970
55	C	-7.8118470	-1.2731640	2.4415400
56	H	-9.5340440	-0.1012390	1.8955600
57	C	-5.6334190	-0.4833380	1.6876090
58	C	-4.3846110	3.4888080	-0.5847880
59	H	-5.3954550	5.1380570	-1.4929130
60	H	-3.5994240	1.7338940	0.3653460
61	C	-6.4181470	-1.4386380	2.3372150
62	H	-8.3739940	-2.0061960	3.0078410
63	H	-4.5570780	-0.5933630	1.6516910
64	N	-8.0423850	1.9028000	0.5231590
65	C	-1.7957150	-4.1535490	-2.3269570
66	H	-3.6218110	-4.4160150	-3.3839380

67	C	-3.8103180	-3.9129710	-1.3215270
68	C	-0.7561290	-4.3753100	-3.2378940
69	C	-1.5414450	-3.8078740	-0.9739270
70	C	-5.1732660	-3.8624990	-1.0298460
71	C	-2.8295820	-3.6750220	-0.3257170
72	C	0.5452770	-4.2390180	-2.7866240
73	H	-0.9606130	-4.6379590	-4.2698680
74	C	-0.2281830	-3.6343400	-0.5518950
75	C	-5.5504530	-3.5595460	0.2705550
76	H	-5.9222490	-4.0570360	-1.7891320
77	C	-3.2273150	-3.4342580	0.9882840
78	C	0.8142680	-3.8595310	-1.4526290
79	H	1.3839390	-4.3988780	-3.4514600
80	H	0.0176910	-3.3319220	0.4588770
81	C	-4.5873450	-3.3462390	1.2786990
82	H	-6.6013650	-3.5186500	0.5259910
83	H	-2.5059460	-3.3196410	1.7889840
84	N	-3.1634390	-4.2036070	-2.5137750
85	N	3.0633960	-4.1326460	-1.5745340
86	N	2.1047830	-3.6325990	-0.9352100
87	N	-4.9568500	-3.2652970	2.6651380
88	N	-5.8364740	-2.5013500	3.1042400

E(RB3LYP) = -2503.41895608

Zero-point vibrational energy 1727608.5 (Joules/Mol)
412.90834 (Kcal/Mol)

Zero-point correction= 0.658011 (Hartree/Particle)
Thermal correction to Energy= 0.701164
Thermal correction to Enthalpy= 0.702108
Thermal correction to Gibbs Free Energy= 0.582345
Sum of electronic and zero-point Energies= -2502.760945
Sum of electronic and thermal Energies= -2502.717792
Sum of electronic and thermal Enthalpies= -2502.716848
Sum of electronic and thermal Free Energies= -2502.836611

Imaginary frequency: -529.41

Transition-state (*E*,*E*,*E*,*Z*)→ all-*E*

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opt=(calcfc,tight,ts,noeigen) freq b3lyp/6-311g(d,p) geom=connectivity int=ultrafine scf=(maxcycle=1000)

XYZ coordinates of the optimized species:

Tag	Symbol	X	Y	Z
1	C	4.0913030	4.0681110	0.0262700

2	C	4.8536080	5.2323810	0.2732460
3	C	4.2461220	6.4164190	0.6492930
4	C	2.8529600	6.4298520	0.7679880
5	C	2.0669530	5.2784470	0.5122020
6	C	2.7000080	4.0919740	0.1502210
7	H	5.9282770	5.1662710	0.1705970
8	H	4.8355250	7.3042280	0.8504830
9	H	2.1472330	3.1796490	-0.0389540
10	H	2.3065530	8.4009490	1.3557990
11	C	0.6983560	7.0343940	1.1048440
12	C	-0.4746940	7.7397870	1.3728490
13	C	-1.6735050	7.0607780	1.2317890
14	C	-1.7173350	5.7058510	0.8424220
15	C	-0.5331630	4.9995720	0.5926900
16	C	0.6815850	5.6632550	0.7200930
17	H	-0.4539070	8.7827420	1.6672060
18	H	-2.6181070	7.5602850	1.4081090
19	H	-0.5932730	3.9631620	0.2867390
20	N	2.0099610	7.4663080	1.1295460
21	N	4.6496560	2.8171520	-0.3131910
22	N	5.8832480	2.8186150	-0.5546900
23	C	7.2042220	-3.0147750	-0.9958970
24	H	9.1676400	-2.4251290	-1.5758640
25	C	7.7896200	-0.8385790	-1.2497690
26	C	7.2057080	-4.4055340	-0.8808460
27	C	6.0525870	-2.2453810	-0.6872940
28	C	8.4782090	0.3583250	-1.4526550
29	C	6.4274110	-0.8527570	-0.8409630
30	C	6.0391710	-5.0162770	-0.4415910
31	H	8.0895110	-4.9919050	-1.1049300
32	C	4.8826870	-2.8785480	-0.2875580
33	C	7.7922180	1.5418010	-1.2192260
34	H	9.5164980	0.3690590	-1.7638710
35	C	5.7554590	0.3414960	-0.6278310
36	C	4.8766940	-4.2710310	-0.1630050
37	H	5.9933710	-6.0904880	-0.3090730
38	H	3.9848260	-2.3254300	-0.0450420
39	C	6.4437530	1.5470750	-0.8099420
40	H	8.2837500	2.4994330	-1.3407620
41	H	4.7243650	0.3690540	-0.3015480
42	N	8.2271010	-2.1470100	-1.3512860
43	N	-3.0174600	5.1852580	0.6802330
44	N	-3.1028220	3.9655140	0.3894330
45	C	-6.9243410	2.5588710	-0.5538230
46	H	-8.9407850	2.2821310	-1.1696190
47	C	-7.7083910	0.5556920	-1.2435720
48	C	-6.7953980	3.9130380	-0.2340420
49	C	-5.8276200	1.6623390	-0.4983750
50	C	-8.4986980	-0.4626300	-1.7784530
51	C	-6.3341630	0.3647740	-0.9173800
52	C	-5.5418300	4.3779590	0.1101500

53	H	-7.6468830	4.5833110	-0.2746030
54	C	-4.5680280	2.1559600	-0.1521050
55	C	-7.8979870	-1.6912540	-1.9875570
56	H	-9.5353420	-0.2924720	-2.0450810
57	C	-5.7735520	-0.9034740	-1.0643990
58	C	-4.4221310	3.5145500	0.1377730
59	H	-5.3807770	5.4211430	0.3436950
60	H	-3.6889900	1.5229800	-0.1266200
61	C	-6.5668360	-1.9205430	-1.5980660
62	H	-8.4409980	-2.5147920	-2.4354060
63	H	-4.7401740	-1.1045890	-0.8055810
64	N	-8.0408790	1.8690190	-0.9893650
65	C	-0.7340210	-6.0807990	1.9357920
66	H	-2.1899750	-7.0910370	3.0964270
67	C	-2.9459930	-5.7556080	1.6058820
68	C	0.5187050	-6.5157040	2.3877080
69	C	-0.8623440	-5.1418850	0.8728420
70	C	-4.3359530	-5.8039270	1.6672820
71	C	-2.2841870	-4.9518600	0.6490090
72	C	1.6461210	-5.9995980	1.7791800
73	H	0.6031270	-7.2306430	3.1989770
74	C	0.2892140	-4.6047700	0.3037390
75	C	-5.0704700	-5.0848300	0.7418880
76	H	-4.8507700	-6.4040220	2.4098350
77	C	-3.0152990	-4.2021100	-0.2762270
78	C	1.5416900	-5.0375670	0.7469620
79	H	2.6363270	-6.3007140	2.0940200
80	H	0.2492720	-3.8589880	-0.4815200
81	C	-4.4228000	-4.2903570	-0.2567620
82	H	-6.1516430	-5.1292580	0.7479020
83	H	-2.5214600	-3.6014110	-1.0291200
84	N	-1.9896640	-6.4204690	2.3743180
85	N	3.7595320	-4.9935750	0.3160840
86	N	2.6551820	-4.4140180	0.1516370
87	N	-5.2002690	-3.7269720	-1.1933540
88	N	-6.1117180	-3.2628110	-1.8637730

E(RB3LYP) = -2503.44631590

Zero-point vibrational energy 1729419.8 (Joules/Mol)
413.34125 (Kcal/Mol)

Zero-point correction= 0.658701 (Hartree/Particle)
Thermal correction to Energy= 0.701862
Thermal correction to Enthalpy= 0.702806
Thermal correction to Gibbs Free Energy= 0.582710
Sum of electronic and zero-point Energies= -2502.787615
Sum of electronic and thermal Energies= -2502.744454
Sum of electronic and thermal Enthalpies= -2502.743510
Sum of electronic and thermal Free Energies= -2502.863606

Imaginary frequency: -527.89

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