Supporting Information
for
Regulation of NH-Tautomerism in N-Confused Porphyrin by *N*-Alkylation

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Calculation Details

All density functional theory calculations[1] were achieved with a Gaussian09 program package.[2] The basis sets implemented in the program were used. The B3LYP density functional method[3] was used with the 6-31G** basis set for structural optimizations and the 6-311++G** basis set was used for nucleus-independent chemical shift (NICS) calculations. Equilibrium geometries were fully optimized and verified by the frequency calculations, where no imaginary frequency was found. The NICS values were calculated with the gauge invariant atomic orbitals (GIAO) method for the optimized structures.

[1] (a) Hohenberg, P.; Kohn, W. *Phys. Rev.* **1964**, *136*, B864. (b) Kohn, W.; Sham, L. J. *Phys. Rev.* **1965**, *140*, A1133.
[2] Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.
[3] (a) Becke, A. D. *J. Phys. Chem.* **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785. (c) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, *58*, 1200. (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623.

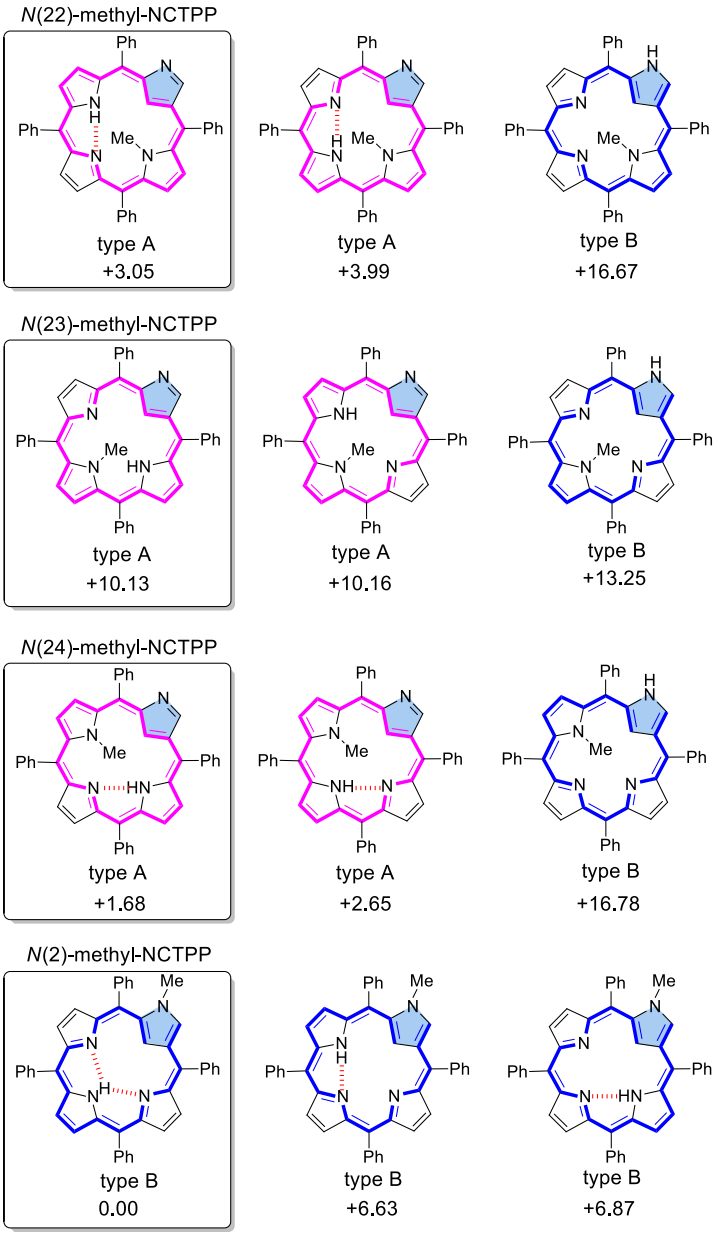
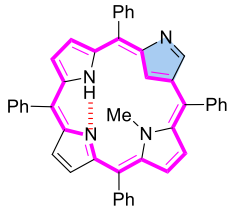


Figure S1. Structures of *N*-methyl-NCTPP isomers and NH-tautomers.

Cartesian coordinates and vibrational freqencies for the optimized structures

N(22)-Me-*N*(24)-H-NCTPP

N(22)-Me-*N*(24)-H-NCTPP



type A
+3.05

E(RB3LYP) = -1953.07408865 A.U.

Stoichiometry	C45H32N4		
Framework group	C1[X(C45H32N4)]		
Deg. of freedom	237		
Full point group	C1		
Largest Abelian subgroup	C1	NOp	1
Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

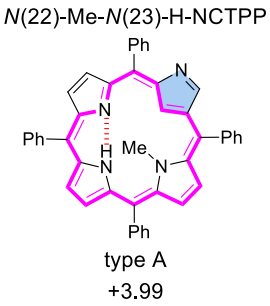
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.774956	0.921862	0.110847
2	7	0	–2.978121	2.877072	0.518278
3	7	0	–1.294540	–1.850464	0.445940
4	7	0	1.741198	–1.031921	0.089691
5	7	0	1.247545	1.798734	–0.074992
6	6	0	–1.710466	2.460757	0.023188
7	6	0	–1.709678	1.076488	–0.218948
8	6	0	–3.709041	1.800903	0.569604
9	6	0	–2.990982	0.600775	0.122570
10	6	0	–3.488322	–0.724813	0.055079
11	6	0	–2.608343	–1.830772	–0.034907
12	6	0	–2.798495	–3.027881	–0.779296
13	6	0	–1.609760	–3.721222	–0.786581
14	6	0	–0.651107	–2.979152	–0.034858
15	6	0	0.719545	–3.306765	0.137749
16	6	0	1.784226	–2.385119	0.298906
17	6	0	3.149101	–2.804807	0.624957
18	6	0	3.922590	–1.695558	0.561865
19	6	0	3.032197	–0.594552	0.202136
20	6	0	3.474223	0.731749	–0.011627
21	6	0	2.615045	1.836152	–0.199750
22	6	0	2.954804	3.188779	–0.519093
23	6	0	1.794715	3.923002	–0.548716
24	6	0	0.694353	3.056227	–0.248665
25	6	0	–0.666735	3.408810	–0.114162
26	6	0	–4.942971	–0.979924	–0.027564
27	6	0	–5.523520	–2.078506	0.636794
28	6	0	–6.893342	–2.318655	0.561713
29	6	0	–7.716719	–1.467473	–0.178172
30	6	0	–7.157561	–0.376037	–0.846186
31	6	0	–5.787542	–0.135296	–0.774991
32	6	0	1.047058	–4.755821	–0.002991
33	6	0	0.365425	–5.720198	0.761664
34	6	0	0.654029	–7.077397	0.629936
35	6	0	1.625461	–7.503382	–0.277862
36	6	0	2.303365	–6.561012	–1.053310
37	6	0	2.017279	–5.203288	–0.918625
38	6	0	4.942638	1.003616	–0.043626
39	6	0	5.769364	0.373607	–0.989293
40	6	0	7.140357	0.626892	–1.022488
41	6	0	7.713120	1.514996	–0.110529
42	6	0	6.904695	2.148242	0.834947
43	6	0	5.533458	1.895842	0.867297
44	6	0	–1.010027	4.856230	–0.074007
45	6	0	–0.335627	5.744373	0.781567
46	6	0	–0.663938	7.099320	0.809267
47	6	0	–1.671239	7.593412	–0.020006
48	6	0	–2.355227	6.720721	–0.869215
49	6	0	–2.033717	5.366370	–0.891161
50	6	0	–0.886904	–1.195161	1.692188
51	1	0	–0.934623	0.485118	–0.682580
52	1	0	–4.720166	1.821262	0.963245
53	1	0	–3.695722	–3.261140	–1.333730
54	1	0	–1.382916	–4.621911	–1.337040
55	1	0	3.453334	–3.806969	0.888670
56	1	0	4.980834	–1.613384	0.761622
57	1	0	3.956283	3.542141	–0.710221
58	1	0	1.695949	4.972967	–0.776339
59	1	0	–4.891620	–2.729705	1.231867
60	1	0	–7.320421	–3.166025	1.090197
61	1	0	–8.785005	–1.654174	–0.235354
62	1	0	–7.788544	0.283773	–1.434472
63	1	0	–5.354578	0.695859	–1.321397
64	1	0	–0.386197	–5.394070	1.473916

65	1	0	0.122645	–7.802309	1.239877
66	1	0	1.849383	–8.560900	–0.382865
67	1	0	3.050809	–6.883603	–1.772457
68	1	0	2.533835	–4.476710	–1.537092
69	1	0	5.325037	–0.309633	–1.706300
70	1	0	7.760395	0.133866	–1.765735
71	1	0	8.780878	1.711865	–0.136199
72	1	0	7.342322	2.835258	1.553607
73	1	0	4.910485	2.380459	1.612814
74	1	0	0.432264	5.361384	1.445845
75	1	0	–0.137544	7.766420	1.485910
76	1	0	–1.926461	8.649020	–0.000454
77	1	0	–3.143570	7.096225	–1.515182
78	1	0	–2.570112	4.690616	–1.547528
79	1	0	–0.086515	–0.477572	1.523487
80	1	0	–0.523511	–1.957848	2.386146
81	1	0	–1.749211	–0.692903	2.125675

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	13.9798	28.1921	31.6162
Red. masses --	6.1055	5.4792	3.9904
Frc consts --	0.0007	0.0026	0.0024
IR Inten --	0.0084	0.3994	0.0390

N(22)-Me-*N*(23)-H-NCTPP



E(RB3LYP) = -1953.07258796 A.U.

Stoichiometry	C45H32N4			
Framework group	C1[X(C45H32N4)]			
Deg. of freedom	237			
Full point group		C1	NOp	1
Largest Abelian subgroup		C1	NOp	1
Largest concise Abelian subgroup		C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	–2.994932	2.864033	0.518974
2	7	0	–1.284213	–1.853751	0.446636
3	7	0	1.746771	–1.017777	0.090387
4	1	0	0.877511	–0.429741	–0.118179
5	7	0	1.236861	1.809995	–0.074296
6	6	0	–1.724906	2.455009	0.023884
7	6	0	–1.716163	1.070768	–0.218252
8	6	0	–3.719656	1.783682	0.570300
9	6	0	–2.994713	0.587700	0.123266
10	6	0	–3.484427	–0.740724	0.055775
11	6	0	–2.598108	–1.841608	–0.034211
12	6	0	–2.781378	–3.039790	–0.778600
13	6	0	–1.588678	–3.726289	–0.785885
14	6	0	–0.634305	–2.978723	–0.034162
15	6	0	0.738207	–3.298454	0.138445
16	6	0	1.797574	–2.370705	0.299602
17	6	0	3.164838	–2.782543	0.625653
18	6	0	3.931941	–1.668868	0.562561
19	6	0	3.035236	–0.572997	0.202832
20	6	0	3.469633	0.755822	–0.010931
21	6	0	2.604123	1.855270	–0.199054
22	6	0	2.936104	3.209827	–0.518397
23	6	0	1.771815	3.937372	–0.548020
24	6	0	0.676452	3.064288	–0.247969
25	6	0	–0.686640	3.409044	–0.113466
26	6	0	–4.937586	–1.004190	–0.026868
27	6	0	–5.511813	–2.106090	0.637490
28	6	0	–6.880232	–2.354106	0.562409
29	6	0	–7.708487	–1.507670	–0.177476
30	6	0	–7.155610	–0.413038	–0.845490
31	6	0	–5.786997	–0.164429	–0.774295
32	6	0	1.074041	–4.745604	–0.002295
33	6	0	0.397961	–5.713882	0.762360
34	6	0	0.694359	–7.069400	0.630632
35	6	0	1.668223	–7.489796	–0.277166
36	6	0	2.340701	–6.543546	–1.052614
37	6	0	2.046817	–5.187489	–0.917929
38	6	0	4.936462	1.036123	–0.042930
39	6	0	5.766794	0.410875	–0.988597
40	6	0	7.136309	0.672034	–1.021792
41	6	0	7.703959	1.563414	–0.109833
42	6	0	6.891909	2.192004	0.835643
43	6	0	5.522145	1.931729	0.867993
44	6	0	–1.038243	4.854468	–0.073311
45	6	0	–0.368958	5.746471	0.782263
46	6	0	-0.705050	7.099509	0.809963
47	6	0	–1.715173	7.587805	–0.019310
48	6	0	–2.394135	6.711198	–0.868519
49	6	0	–2.064848	5.358717	–0.890465
50	6	0	–0.880349	-1.196116	1.692884
51	1	0	–0.937723	0.483861	–0.681884
52	1	0	–4.730881	1.798230	0.963941
53	1	0	–3.677249	–3.278201	–1.333034
54	1	0	–1.356662	–4.625660	–1.336344
55	1	0	3.474825	–3.782941	0.889366
56	1	0	4.989695	–1.580614	0.762318
57	1	0	3.935536	3.568938	–0.709525
58	1	0	1.667017	4.986752	–0.775643
59	1	0	–4.876181	–2.753647	1.232563
60	1	0	–7.302435	–3.203916	1.090893
61	1	0	–8.775682	–1.700506	–0.234658
62	1	0	–7.790374	0.243135	–1.433776
63	1	0	–5.358816	0.669200	–1.320701
64	1	0	–0.355523	–5.392078	1.474612
65	1	0	0.167149	–7.797354	1.240573
66	1	0	1.898218	–8.546010	–0.382169

67	1	0	3.089986	–6.861837	–1.771761
68	1	0	2.559190	–4.457954	–1.536396
69	1	0	5.326401	–0.274907	–1.705604
70	1	0	7.759170	0.182579	–1.765039
71	1	0	8.770568	1.766416	–0.135503
72	1	0	7.325581	2.881524	1.554303
73	1	0	4.896397	2.412758	1.613510
74	1	0	0.401121	5.367901	1.446541
75	1	0	–0.182498	7.769623	1.486606
76	1	0	–1.976457	8.641929	0.000242
77	1	0	–3.184623	7.082166	–1.514486
78	1	0	–2.597351	4.679892	–1.546832
79	1	0	–0.084097	–0.473940	1.524183
80	1	0	–0.512580	–1.956702	2.386842
81	1	0	–1.745528	–0.698821	2.126371

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IR Inten --	0.0085	0.3245	0.3600

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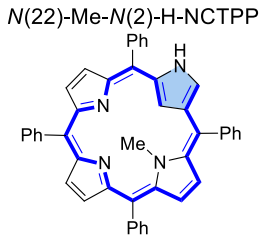

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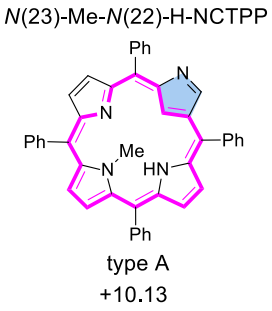
1	7	0	–4.043659	–0.206884	0.572501
2	1	0	–4.900193	0.233106	0.873626
3	7	0	0.549828	–2.149261	0.427979
4	7	0	2.026673	0.493164	–0.064179
5	7	0	–0.528001	2.095771	0.021735
6	6	0	–2.946718	0.492693	0.044322
7	6	0	–1.964637	–0.457546	–0.208919
8	6	0	–3.755056	–1.517595	0.675943
9	6	0	–2.446817	–1.731433	0.191986
10	6	0	–1.773107	–3.013321	0.117706
11	6	0	–0.384131	–3.119729	0.039628
12	6	0	0.359367	–4.169667	–0.609538
13	6	0	1.671288	–3.804176	–0.651984
14	6	0	1.811750	–2.515922	–0.020634
15	6	0	2.996832	–1.766348	0.070971
16	6	0	3.050885	–0.338880	0.194471
17	6	0	4.256843	0.406404	0.587876
18	6	0	3.919510	1.715208	0.539200
19	6	0	2.507616	1.765673	0.124675
20	6	0	1.787013	2.959022	–0.028561
21	6	0	0.362155	3.072216	–0.201568
22	6	0	–0.312389	4.308795	–0.625175
23	6	0	–1.641875	4.040364	–0.624792
24	6	0	–1.768394	2.643112	–0.213749
25	6	0	–2.959598	1.918216	–0.103950
26	6	0	–2.587617	–4.244850	0.015141
27	6	0	–2.229984	–5.410119	0.723201
28	6	0	–2.994235	–6.571282	0.631543
29	6	0	–4.140867	–6.598904	–0.164692
30	6	0	–4.513164	–5.453355	–0.871676
31	6	0	–3.748776	–4.292160	–0.783617
32	6	0	4.277565	–2.511924	–0.070628
33	6	0	4.529831	–3.670178	0.688274
34	6	0	5.725855	–4.373675	0.553855
35	6	0	6.701914	–3.934646	–0.342247
36	6	0	6.469156	–2.787502	–1.103809
37	6	0	5.272391	–2.085832	–0.971290
38	6	0	2.556058	4.239804	–0.002941
39	6	0	3.609979	4.469188	–0.904385
40	6	0	4.326132	5.665941	–0.881040
41	6	0	4.005928	6.658123	0.046686
42	6	0	2.961387	6.445892	0.948837
43	6	0	2.241923	5.252156	0.921123
44	6	0	–4.271216	2.612844	–0.122550
45	6	0	–4.501146	3.748609	0.677681
46	6	0	–5.737640	4.391175	0.668852
47	6	0	–6.775196	3.913264	–0.134312
48	6	0	–6.566129	2.786068	–0.931132
49	6	0	–5.330336	2.140633	–0.923904
50	6	0	0.339950	–1.234922	1.555181
51	1	0	–0.999668	–0.227103	–0.629091
52	1	0	–4.459661	–2.221481	1.093435
53	1	0	–0.096197	–5.026822	–1.082917
54	1	0	2.477098	–4.318318	–1.153959
55	1	0	5.200973	–0.024831	0.889213
56	1	0	4.533147	2.564533	0.801714
57	1	0	0.171877	5.233032	–0.905672
58	1	0	–2.449074	4.695083	–0.921406
59	1	0	–1.355206	–5.386876	1.364868
60	1	0	–2.700299	–7.453044	1.193791
61	1	0	–4.738407	–7.503079	–0.233547
62	1	0	–5.395936	–5.468070	–1.504750
63	1	0	–4.028990	–3.416711	–1.360219
64	1	0	3.782308	–4.005923	1.400367
65	1	0	5.899071	–5.260382	1.157219
66	1	0	7.634917	–4.480834	–0.446476

67	1	0	7.218212	–2.442662	–1.811090
68	1	0	5.090685	–1.205922	–1.579865
69	1	0	3.854046	3.703663	–1.634044
70	1	0	5.132001	5.824407	–1.592136
71	1	0	4.564416	7.589532	0.066206
72	1	0	2.708512	7.209729	1.678808
73	1	0	1.435346	5.088385	1.628967
74	1	0	–3.703747	4.110036	1.318257
75	1	0	–5.893983	5.262469	1.298215
76	1	0	–7.738404	4.414699	–0.139019
77	1	0	–7.363130	2.414028	–1.568529
78	1	0	–5.165086	1.282426	–1.568299
79	1	0	0.169249	–0.210519	1.221940
80	1	0	1.236084	–1.253293	2.179501
81	1	0	–0.507652	–1.597392	2.138276

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	14.5302	27.9792	30.9453
Red. masses --	6.0786	5.3542	4.3929
Frc consts --	0.0008	0.0025	0.0025
IR Inten --	0.0455	0.6927	0.2129

N(23)-Me-*N*(22)-H-NCTPP



E(RB3LYP) = -1953.05783441 A.U.

Stoichiometry	C45H32N4			
Framework group	C1[X(C45H32N4)]			
Deg. of freedom	237			
Full point group		C1	NOp	1
Largest Abelian subgroup		C1	NOp	1
Largest concise Abelian subgroup		C1	NOp	1

Standard orientation:

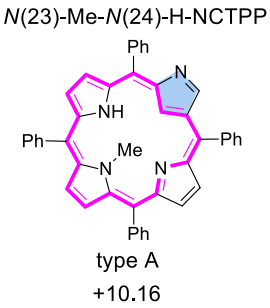
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.717881	–1.668044	0.157623
2	7	0	3.982837	–0.996527	–0.006926
3	7	0	0.187705	2.150415	0.030539
4	7	0	–2.119374	0.149073	0.456937
5	7	0	–0.162818	–2.165274	–0.000098
6	6	0	2.633877	–1.345247	–0.212670
7	6	0	1.942577	–0.144053	–0.361590
8	6	0	4.124805	0.337034	0.010526
9	6	0	2.859580	0.932346	–0.199723
10	6	0	2.620445	2.352040	–0.086816
11	6	0	1.344388	2.898848	0.045988
12	6	0	1.019898	4.317347	0.210841
13	6	0	–0.329917	4.388796	0.315254
14	6	0	–0.827867	3.012686	0.179252
15	6	0	–2.216260	2.650035	0.121125
16	6	0	–2.723482	1.342417	0.056012
17	6	0	–3.971399	0.986639	–0.569965
18	6	0	–4.079449	–0.370390	–0.578271
19	6	0	–2.904910	–0.926724	0.042701
20	6	0	–2.611015	–2.300656	0.094480
21	6	0	–1.296635	–2.870103	0.140998
22	6	0	–1.005115	–4.304431	0.269646
23	6	0	0.342654	–4.428980	0.174257
24	6	0	0.867426	–3.071552	0.018678
25	6	0	2.213243	–2.710459	–0.099020
26	6	0	3.813719	3.244976	–0.055686
27	6	0	4.067787	4.092697	1.036959
28	6	0	5.194724	4.913933	1.058489
29	6	0	6.093078	4.905103	–0.009967
30	6	0	5.857425	4.065274	–1.099855
31	6	0	4.732960	3.240791	–1.120551
32	6	0	–3.219373	3.746316	–0.023860
33	6	0	–4.320660	3.825313	0.846999
34	6	0	–5.269155	4.839348	0.717453
35	6	0	–5.139395	5.796479	–0.289843
36	6	0	–4.054947	5.729431	–1.167221
37	6	0	–3.105956	4.716842	–1.036091
38	6	0	–3.773521	–3.224895	–0.052876
39	6	0	–3.810989	–4.203909	–1.062810
40	6	0	–4.907179	–5.054727	–1.195785
41	6	0	–5.992617	–4.946947	–0.323777
42	6	0	–5.974008	–3.977958	0.680482
43	6	0	–4.877612	–3.126597	0.812700
44	6	0	3.274459	–3.756669	–0.037091
45	6	0	3.388166	–4.616591	1.070244
46	6	0	4.391830	–5.582921	1.125201
47	6	0	5.309294	–5.706873	0.080079
48	6	0	5.215581	–4.855981	–1.022421
49	6	0	4.211090	–3.889311	–1.079955
50	1	0	0.889368	–0.056387	–0.548009
51	1	0	5.081175	0.800706	0.199817
52	1	0	1.725268	5.135026	0.241280
53	1	0	–0.931553	5.272715	0.470446
54	1	0	–4.631963	1.697799	–1.042074
55	1	0	–4.844565	–0.962183	–1.057450
56	1	0	–1.729217	–5.092178	0.419475
57	1	0	0.922300	–5.340373	0.205541
58	1	0	3.381593	4.089714	1.877713
59	1	0	5.374584	5.556245	1.915885
60	1	0	6.969869	5.545754	0.007414
61	1	0	6.547039	4.055411	–1.939199
62	1	0	4.546763	2.598725	–1.976086
63	1	0	–4.419902	3.088154	1.637855
64	1	0	–6.107094	4.883856	1.407390
65	1	0	–5.877450	6.586740	–0.392108
66	1	0	–3.951550	6.462886	–1.961896

67	1	0	–2.273990	4.661522	–1.730794
68	1	0	–2.978705	–4.281013	–1.755007
69	1	0	–4.917566	–5.797375	–1.988599
70	1	0	–6.845862	–5.610874	–0.427957
71	1	0	–6.811637	–3.887248	1.366262
72	1	0	–4.862483	–2.380398	1.601064
73	1	0	2.687773	–4.511552	1.892326
74	1	0	4.462172	–6.234903	1.991122
75	1	0	6.091099	–6.459197	0.125016
76	1	0	5.919141	–4.949466	–1.844747
77	1	0	4.128232	–3.244938	–1.950474
78	6	0	–1.196455	0.069161	1.591548
79	1	0	–1.475292	–0.794467	2.198332
80	1	0	–0.165692	–0.034115	1.267410
81	1	0	–1.304721	0.978382	2.184816

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	15.0397	28.8217	31.1930
Red. masses --	6.0454	5.6648	4.1566
Frc consts --	0.0008	0.0028	0.0024
IR Inten --	0.0163	0.6618	0.0429

N(23)-Me-*N*(24)-H-NCTPP



E(RB3LYP) = -1953.06275571 A.U.

Stoichiometry	C45H32N4			
Framework group	C1[X(C45H32N4)]			
Deg. of freedom	237			
Full point group		C1	NOp	1
Largest Abelian subgroup		C1	NOp	1
Largest concise Abelian subgroup		C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	–4.042380	1.237398	0.026314
2	7	0	–0.319783	–2.125555	–0.002376
3	7	0	2.098795	–0.260786	0.429608
4	7	0	0.251944	2.178058	–0.015522
5	1	0	0.124180	1.181592	–0.059827
6	6	0	–2.663165	1.456511	–0.255666
7	6	0	–2.000822	0.223542	–0.433412
8	6	0	–4.196387	–0.053339	0.055627
9	6	0	–2.949056	–0.789432	–0.202165
10	6	0	–2.773338	–2.187172	–0.064670
11	6	0	–1.501384	–2.807804	0.020091
12	6	0	–1.256193	–4.241347	0.140774
13	6	0	0.092784	–4.395635	0.203169
14	6	0	0.662726	–3.053689	0.098635
15	6	0	2.055975	–2.763973	0.040434
16	6	0	2.643831	–1.482707	0.001669
17	6	0	3.909731	–1.185015	–0.589272
18	6	0	4.107938	0.170341	–0.551849
19	6	0	2.971005	0.774098	0.063833
20	6	0	2.738753	2.167548	0.126363
21	6	0	1.473667	2.801481	0.119296
22	6	0	1.190540	4.203439	0.149067
23	6	0	–0.166447	4.376855	0.004151
24	6	0	–0.785993	3.092918	–0.084652
25	6	0	–2.159669	2.777606	–0.177130
26	6	0	–3.995944	–3.034237	0.044566
27	6	0	–4.211731	–3.875936	1.149695
28	6	0	–5.367733	–4.649829	1.242544
29	6	0	–6.329876	–4.601385	0.232069
30	6	0	–6.130625	–3.768090	–0.869680
31	6	0	–4.978076	–2.988682	–0.960164
32	6	0	3.002911	–3.909140	–0.118634
33	6	0	4.077412	–4.073997	0.772546
34	6	0	4.969085	–5.136662	0.632452
35	6	0	4.809680	–6.052514	–0.408616
36	6	0	3.752489	–5.897472	–1.307514
37	6	0	2.857071	–4.838515	–1.163649
38	6	0	3.950719	3.038003	0.046841
39	6	0	4.114537	3.983512	–0.980527
40	6	0	5.258486	4.778361	–1.044296
41	6	0	6.263835	4.642743	–0.085066
42	6	0	6.119526	3.701785	0.935711
43	6	0	4.976103	2.906636	0.999017
44	6	0	–3.132446	3.905981	–0.112176
45	6	0	–3.112481	4.828830	0.946192
46	6	0	–4.022828	5.884818	0.990938
47	6	0	–4.968158	6.038313	–0.023168
48	6	0	–5.004677	5.121317	–1.076023
49	6	0	–4.101386	4.062401	–1.116802
50	1	0	–0.993584	0.009866	–0.747363
51	1	0	–5.153208	–0.501689	0.300800
52	1	0	–2.007365	–5.017021	0.164343
53	1	0	0.644698	–5.317016	0.318101
54	1	0	4.537537	–1.918567	–1.072058
55	1	0	4.917033	0.724410	–1.003243
56	1	0	1.934472	4.976172	0.263727
57	1	0	–0.697754	5.314753	–0.036432
58	1	0	–3.474819	–3.903787	1.945961
59	1	0	–5.520078	–5.286084	2.109670
60	1	0	–7.229276	–5.205795	0.304756
61	1	0	–6.872592	–3.724770	–1.661766
62	1	0	–4.822048	–2.347058	–1.821792
63	1	0	4.200872	–3.367097	1.587233
64	1	0	5.786258	–5.250664	1.338893
65	1	0	5.504760	–6.879493	–0.520330
66	1	0	3.627309	–6.599028	–2.127241

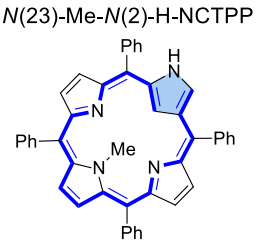
67	1	0	2.043414	–4.715371	–1.871022
68	1	0	3.344860	4.080537	–1.739643
69	1	0	5.368401	5.497634	–1.850745
70	1	0	7.154126	5.262572	–0.135493
71	1	0	6.895793	3.588968	1.686990
72	1	0	4.864469	2.179887	1.797837
73	1	0	–2.395400	4.700526	1.750898
74	1	0	–3.997521	6.581621	1.823924
75	1	0	–5.676526	6.861055	0.009822
76	1	0	–5.741982	5.228858	–1.866345
77	1	0	–4.138044	3.346050	–1.930119
78	6	0	1.255835	–0.181960	1.633760
79	1	0	1.360188	0.810163	2.071507
80	1	0	0.213653	–0.401658	1.398331
81	1	0	1.600787	–0.924409	2.358610

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	15.5885	29.4282	30.8388
Red. masses --	6.0611	5.6434	4.2303
Frc consts --	0.0009	0.0029	0.0024
IR Inten --	0.0156	0.5035	0.1395

N(23)-Me-*N*(2)-H-NCTPP

E(RB3LYP) = -1953.06279144 A.U.



Stoichiometry	C45H32N4
Framework group	C1[X(C45H32N4)]
Deg. of freedom	237
Full point group	C1 NOp 1
Largest Abelian subgroup	C1 NOp 1
Largest concise Abelian subgroup	C1 NOp 1

Standard orientation:

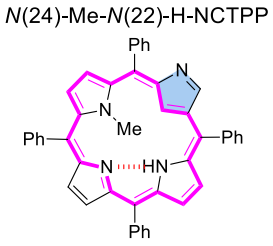
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.238706	–0.025544	0.073940
2	7	0	–0.344936	2.172820	–0.005360
3	1	0	–0.185455	1.185156	–0.108603
4	7	0	–2.084959	–0.341550	0.422051
5	7	0	0.410294	–2.104263	–0.015542
6	6	0	2.993498	–0.666310	–0.173204
7	6	0	1.989811	0.292855	–0.434008
8	6	0	3.996107	1.248704	0.000645
9	6	0	2.583527	1.558328	–0.294262
10	6	0	2.029118	2.864579	–0.220959
11	6	0	0.656133	3.129366	–0.077955
12	6	0	–0.010262	4.388017	0.070530
13	6	0	–1.351672	4.158439	0.249998
14	6	0	–1.585645	2.745044	0.178625
15	6	0	–2.822619	2.067260	0.190574
16	6	0	–2.997355	0.663634	0.078439
17	6	0	–4.101217	0.034342	–0.563219
18	6	0	–3.845367	–1.312467	–0.636531
19	6	0	–2.576410	–1.573443	–0.041673
20	6	0	–1.937433	–2.834611	–0.032631
21	6	0	–0.539675	–3.075290	0.033287
22	6	0	0.082951	–4.394264	0.100011
23	6	0	1.425855	–4.181663	0.073187
24	6	0	1.613777	–2.735866	0.009014
25	6	0	2.872341	–2.063898	–0.025156
26	6	0	2.965128	4.027815	–0.227227
27	6	0	3.009329	4.946347	0.835510
28	6	0	3.900510	6.018780	0.815774
29	6	0	4.766202	6.193281	–0.265176
30	6	0	4.739498	5.283375	–1.323392
31	6	0	3.850608	4.209354	–1.303245
32	6	0	–4.070513	2.887510	0.160881
33	6	0	–5.076743	2.675977	1.119279
34	6	0	–6.252210	3.425219	1.102222
35	6	0	–6.449302	4.399428	0.121998
36	6	0	–5.464220	4.613973	–0.843600
37	6	0	–4.288177	3.864840	–0.826085
38	6	0	–2.841110	–4.008817	–0.229362
39	6	0	–2.653887	–4.902773	–1.298157
40	6	0	–3.508368	–5.989895	–1.477046
41	6	0	–4.564123	–6.208640	–0.589874
42	6	0	–4.764143	–5.328057	0.474467
43	6	0	–3.914441	–4.236642	0.649105
44	6	0	4.113788	–2.864747	0.160828
45	6	0	4.260139	–3.733223	1.255757
46	6	0	5.423396	–4.484148	1.422462
47	6	0	6.459878	–4.386205	0.493705
48	6	0	6.329942	–3.522217	–0.595739
49	6	0	5.173655	–2.763174	–0.756192
50	1	0	0.994401	0.010783	–0.731439
51	1	0	4.768161	1.984802	0.197709
52	1	0	0.483994	5.346912	0.049507
53	1	0	–2.120505	4.897187	0.414564
54	1	0	–4.930176	0.567053	–1.004239
55	1	0	–4.438902	–2.057319	–1.144684
56	1	0	–0.430857	–5.341813	0.168383
57	1	0	2.208217	–4.925783	0.082264
58	1	0	2.355983	4.801289	1.690130
59	1	0	3.925596	6.712197	1.651475
60	1	0	5.460577	7.028137	–0.279752
61	1	0	5.410840	5.409519	–2.167806
62	1	0	3.828406	3.505532	–2.129473
63	1	0	–4.924748	1.923018	1.886594
64	1	0	–7.012640	3.250478	1.857848
65	1	0	–7.364865	4.983282	0.107738
66	1	0	–5.614931	5.359125	-1.619410

67	1	0	–3.534783	4.022635	-1.591345
68	1	0	–1.840682	–4.729746	–1.995403
69	1	0	–3.352167	–6.663618	–2.314567
70	1	0	–5.227072	–7.057596	–0.728704
71	1	0	–5.580746	–5.491781	1.171704
72	1	0	–4.069722	–3.556235	1.480621
73	1	0	3.463757	–3.800031	1.989963
74	1	0	5.520522	–5.141624	2.281763
75	1	0	7.364742	–4.973685	0.620540
76	1	0	7.133935	–3.436056	–1.321070
77	1	0	5.079356	–2.086301	–1.597683
78	6	0	–1.246001	–0.250575	1.629029
79	1	0	–1.557379	–1.023461	2.336919
80	1	0	–0.195335	–0.415894	1.390079
81	1	0	–1.397053	0.726344	2.086945

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	14.4250	27.0442	27.9266
Red. masses --	6.0414	4.6314	4.9612
Frc consts --	0.0007	0.0020	0.0023
IR Inten --	0.0110	0.4340	0.1335

N(24)-Me-*N*(22)-H-NCTPP



E(RB3LYP) = -1953.07626031 A.U.

Stoichiometry	C45H32N4		
Framework group	C1[X(C45H32N4)]		
Deg. of freedom	237		
Full point group	C1		
Largest Abelian subgroup	C1	NOp	1
Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

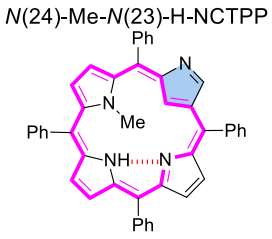
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.944893	–1.169196	1.673304
2	7	0	3.687790	1.919737	0.607413
3	7	0	–1.372426	1.725774	–0.076007
4	7	0	–1.695731	–1.115367	0.073086
5	7	0	1.396317	–1.759452	0.409119
6	6	0	2.959274	0.789312	0.162242
7	6	0	1.647240	1.163547	–0.223694
8	6	0	2.866761	2.925514	0.495436
9	6	0	1.543936	2.543633	–0.024295
10	6	0	0.442311	3.432958	–0.173535
11	6	0	–0.895152	3.015905	–0.250748
12	6	0	–2.058593	3.828986	–0.477775
13	6	0	–3.171851	3.035312	–0.402573
14	6	0	–2.745116	1.691810	–0.131497
15	6	0	–3.532622	0.542475	0.060666
16	6	0	–3.002800	–0.763619	0.230855
17	6	0	–3.815433	–1.924353	0.587678
18	6	0	–2.976350	–2.986847	0.599576
19	6	0	–1.648792	–2.478155	0.250336
20	6	0	–0.534053	–3.320290	0.047851
21	6	0	0.814977	–2.895685	–0.130079
22	6	0	1.800892	–3.532920	–0.931447
23	6	0	2.951846	–2.772096	–0.889263
24	6	0	2.701337	–1.641502	–0.072743
25	6	0	3.534893	–0.495964	0.098067
26	6	0	0.727552	4.895557	–0.211263
27	6	0	0.101769	5.794681	0.670474
28	6	0	0.394779	7.157135	0.629172
29	6	0	1.319953	7.649872	–0.292912
30	6	0	1.955119	6.768682	–1.169633
31	6	0	1.665395	5.405840	–1.126722
32	6	0	–5.014947	0.726001	0.082818
33	6	0	–5.627396	1.556510	1.036637
34	6	0	–7.011430	1.728926	1.053601
35	6	0	–7.812130	1.073549	0.116897
36	6	0	–7.218368	0.244380	–0.836366
37	6	0	–5.834535	0.072666	–0.853350
38	6	0	–0.764148	–4.783425	–0.125862
39	6	0	–1.735255	–5.271691	–1.019697
40	6	0	–1.932683	–6.641790	–1.184914
41	6	0	–1.163187	–7.555551	–0.462838
42	6	0	–0.189015	–7.088370	0.421800
43	6	0	0.011739	–5.718984	0.583521
44	6	0	4.998002	–0.698403	0.112577
45	6	0	5.552101	–1.847679	0.710916
46	6	0	6.928699	–2.060111	0.719152
47	6	0	7.784040	–1.129407	0.127793
48	6	0	7.251041	0.016213	–0.468396
49	6	0	5.876657	0.232495	–0.477005
50	1	0	–0.848233	0.867453	0.052884
51	1	0	0.931009	0.504078	–0.689779
52	1	0	3.149105	3.923773	0.813152
53	1	0	–2.029005	4.887410	–0.686071
54	1	0	–4.199685	3.337304	–0.532570
55	1	0	–4.870578	–1.910599	0.818016
56	1	0	–3.212454	–4.011390	0.846598
57	1	0	1.621092	–4.413559	–1.529773
58	1	0	3.859468	–2.922678	–1.455109
59	1	0	–0.600455	5.413865	1.405224
60	1	0	–0.092940	7.832949	1.325796
61	1	0	1.547672	8.711263	–0.324364
62	1	0	2.675826	7.142582	–1.891078
63	1	0	2.154409	4.724213	–1.815604
64	1	0	–5.009953	2.056430	1.776730
65	1	0	–7.464479	2.370094	1.804397
66	1	0	–8.889858	1.207122	0.130080

67	1	0	–7.832550	–0.265713	–1.572967
68	1	0	–5.375234	–0.564519	–1.602716
69	1	0	–2.321738	–4.565884	–1.598391
70	1	0	–2.682407	–6.995545	–1.886785
71	1	0	–1.317688	–8.622799	–0.591770
72	1	0	0.413468	–7.791348	0.989832
73	1	0	0.766939	–5.361724	1.276541
74	1	0	4.894054	–2.564763	1.190335
75	1	0	7.333330	–2.948774	1.194851
76	1	0	8.857761	–1.293495	0.133000
77	1	0	7.910258	0.743123	–0.933864
78	1	0	5.469239	1.121805	–0.940277
79	1	0	0.136309	–0.457945	1.518384
80	1	0	1.788137	–0.673299	2.150229
81	1	0	0.579425	–1.969803	2.321205

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	14.0110	27.8391	31.8274
Red. masses --	6.1187	5.6139	4.1442
Frc consts --	0.0007	0.0026	0.0025
IR Inten --	0.0083	0.4471	0.0605

N(24)-Me-*N*(23)-H-NCTPP



E(RB3LYP) = -1953.07471250 A.U.

Stoichiometry	C45H32N4			
Framework group	C1[X(C45H32N4)]			
Deg. of freedom	237			
Full point group		C1	NOp	1
Largest Abelian subgroup		C1	NOp	1
Largest concise Abelian subgroup		C1	NOp	1

Standard orientation:

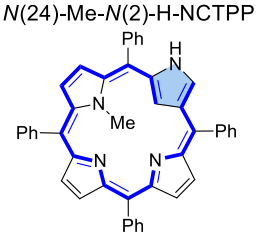
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.130497	–0.867185	1.582380
2	7	0	3.166137	2.705974	0.599912
3	7	0	–1.659375	1.324827	–0.101735
4	7	0	–1.452838	–1.535513	0.014152
5	1	0	–0.899689	–0.715331	–0.210413
6	7	0	1.727638	–1.382881	0.340798
7	6	0	2.712573	1.451297	0.115006
8	6	0	1.359285	1.534032	–0.283874
9	6	0	2.138930	3.502791	0.503044
10	6	0	0.940898	2.842684	–0.042825
11	6	0	–0.346303	3.427641	–0.187689
12	6	0	–1.540528	2.682840	–0.298635
13	6	0	–2.845431	3.261487	–0.595398
14	6	0	–3.744643	2.245444	–0.538657
15	6	0	–2.983436	1.048676	–0.204954
16	6	0	–3.562744	–0.239057	0.005395
17	6	0	–2.822480	–1.415288	0.168160
18	6	0	–3.301010	–2.725849	0.508320
19	6	0	–2.236441	–3.582349	0.521618
20	6	0	–1.042920	–2.846325	0.189026
21	6	0	0.242585	–3.389077	0.022105
22	6	0	1.450497	–2.652408	–0.156163
23	6	0	2.575496	–3.062702	–0.917991
24	6	0	3.511940	–2.048621	–0.888676
25	6	0	2.987830	–0.979749	–0.123427
26	6	0	3.549644	0.318719	0.050031
27	6	0	–0.422315	4.915374	–0.178209
28	6	0	–1.286065	5.604766	0.692007
29	6	0	–1.328624	6.998066	0.701393
30	6	0	–0.511505	7.732894	–0.159726
31	6	0	0.354537	7.063609	–1.026111
32	6	0	0.403358	5.670638	–1.030826
33	6	0	–5.050193	–0.350905	0.067134
34	6	0	–5.786283	0.381278	1.014886
35	6	0	–7.174975	0.275781	1.079074
36	6	0	–7.858299	–0.562674	0.196265
37	6	0	–7.141753	–1.293885	–0.752128
38	6	0	–5.752343	–1.188414	–0.816256
39	6	0	0.365537	–4.871825	–0.093764
40	6	0	–0.425678	–5.606915	–0.995104
41	6	0	–0.291354	–6.990477	–1.103379
42	6	0	0.639801	–7.670405	–0.316629
43	6	0	1.439499	–6.954474	0.576492
44	6	0	1.306122	–5.571508	0.683796
45	6	0	5.021776	0.440832	0.087086
46	6	0	5.809390	–0.554557	0.698759
47	6	0	7.198434	–0.453558	0.727899
48	6	0	7.832662	0.644536	0.145410
49	6	0	7.066030	1.642257	–0.462003
50	6	0	5.678443	1.545521	–0.491099
51	1	0	0.776519	0.763559	–0.757233
52	1	0	2.186502	4.529122	0.852051
53	1	0	–3.036001	4.295037	–0.843951
54	1	0	–4.808469	2.291932	–0.719659
55	1	0	–4.329955	–2.960397	0.734127
56	1	0	–2.250219	–4.634214	0.761744
57	1	0	2.624983	–3.982943	–1.480481
58	1	0	4.445759	–2.005299	–1.429851
59	1	0	–1.909311	5.038341	1.376115
60	1	0	–1.995791	7.510424	1.388637
61	1	0	–0.546573	8.818370	–0.152602
62	1	0	0.992451	7.626283	–1.701570
63	1	0	1.071474	5.153328	–1.712155
64	1	0	–5.258395	1.026823	1.709742
65	1	0	–7.723303	0.845142	1.824126
66	1	0	–8.940159	–0.643859	0.246089

67	1	0	–7.664584	–1.941994	–1.449696
68	1	0	–5.200803	–1.745858	–1.567048
69	1	0	–1.136863	–5.082010	–1.624897
70	1	0	–0.907801	–7.535998	–1.812087
71	1	0	0.744834	–8.747921	–0.401916
72	1	0	2.165855	–7.474139	1.194665
73	1	0	1.927135	–5.021005	1.383601
74	1	0	5.321400	–1.399080	1.173576
75	1	0	7.784351	–1.228391	1.213800
76	1	0	8.915660	0.724990	0.167256
77	1	0	7.552767	2.498928	–0.918918
78	1	0	5.088801	2.322250	–0.960931
79	1	0	0.354348	–0.122330	1.400272
80	1	0	1.915136	–0.401869	2.179625
81	1	0	0.706370	–1.706496	2.135513

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	14.1608	28.7921	35.7856
Red. masses --	6.1256	5.6399	4.2250
Frc consts --	0.0007	0.0028	0.0032
IR Inten --	0.0069	0.4041	0.3672

N(24)-Me-*N*(2)-H-NCTPP



E(RB3LYP) = -1953.05220867 A.U.

Stoichiometry	C45H32N4			
Framework group	C1[X(C45H32N4)]			
Deg. of freedom	237			
Full point group		C1	NOp	1
Largest Abelian subgroup		C1	NOp	1
Largest concise Abelian subgroup		C1	NOp	1

Standard orientation:

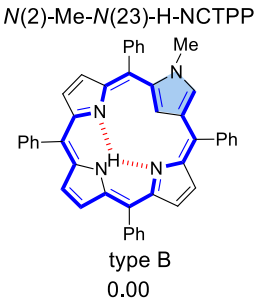
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	–0.504084	–1.206117	1.573422
2	7	0	3.520224	–1.921911	0.683655
3	1	0	4.006169	–2.727666	1.047273
4	7	0	0.754209	2.017418	0.026093
5	7	0	–1.969464	0.690340	–0.069631
6	7	0	–0.792560	–2.088525	0.438007
7	6	0	2.204170	–1.953471	0.192062
8	6	0	1.900014	–0.655517	–0.191096
9	6	0	4.014507	–0.670526	0.618413
10	6	0	3.023377	0.173901	0.078327
11	6	0	3.158560	1.600564	–0.098423
12	6	0	2.047217	2.437174	–0.214314
13	6	0	2.056901	3.840004	–0.626512
14	6	0	0.762019	4.241787	–0.615576
15	6	0	–0.030925	3.079380	–0.187914
16	6	0	–1.462315	3.115100	–0.008261
17	6	0	–2.308385	2.007712	0.133884
18	6	0	–3.717125	2.106235	0.549355
19	6	0	–4.195637	0.841447	0.581599
20	6	0	–3.078076	–0.025930	0.180603
21	6	0	–3.179228	–1.452561	0.047357
22	6	0	–2.081764	–2.324093	–0.026353
23	6	0	–2.064777	–3.620214	–0.657497
24	6	0	–0.795591	–4.114529	–0.604354
25	6	0	0.040546	–3.143987	0.053287
26	6	0	1.435349	–3.169909	0.135719
27	6	0	4.528073	2.168488	–0.154109
28	6	0	4.880319	3.293364	0.616098
29	6	0	6.170687	3.817350	0.568503
30	6	0	7.139061	3.232012	–0.249677
31	6	0	6.807413	2.114564	–1.018125
32	6	0	5.519216	1.585027	–0.967101
33	6	0	–2.086809	4.471554	0.037939
34	6	0	–1.656204	5.432564	0.970057
35	6	0	–2.242311	6.696301	1.018930
36	6	0	–3.265709	7.031480	0.129874
37	6	0	–3.699337	6.091648	–0.806217
38	6	0	–3.117223	4.824825	–0.850421
39	6	0	–4.531544	-2.050848	–0.118153
40	6	0	–5.463065	–1.505098	–1.022127
41	6	0	–6.727754	–2.069150	–1.177920
42	6	0	–7.093955	–3.194620	–0.436614
43	6	0	–6.182938	–3.750394	0.463089
44	6	0	–4.918760	–3.184452	0.621049
45	6	0	2.141277	–4.468329	0.049021
46	6	0	1.680477	–5.591884	0.764800
47	6	0	2.342277	–6.815308	0.686769
48	6	0	3.489812	–6.948023	–0.097745
49	6	0	3.964856	–5.844988	–0.810592
50	6	0	3.300685	–4.622044	–0.740675
51	1	0	0.967883	–0.315520	–0.610656
52	1	0	5.004011	–0.432359	0.978555
53	1	0	2.923509	4.409979	-0.929619
54	1	0	0.371395	5.209501	-0.895447
55	1	0	–4.235124	3.013891	0.822301
56	1	0	–5.181791	0.512538	0.877425
57	1	0	–2.912513	–4.051961	–1.168054
58	1	0	–0.423273	–5.012905	–1.074450
59	1	0	4.136003	3.738255	1.267918
60	1	0	6.422590	4.680130	1.178433
61	1	0	8.143852	3.642494	–0.287012
62	1	0	7.551245	1.658207	–1.665040
63	1	0	5.260652	0.729113	–1.582200
64	1	0	–0.865527	5.174481	1.667704
65	1	0	–1.901973	7.419135	1.755069
66	1	0	–3.719854	8.017512	0.165730

67	1	0	–4.489227	6.345202	–1.507592
68	1	0	–3.448692	4.099103	–1.586166
69	1	0	–5.178762	–0.641528	–1.614536
70	1	0	–7.425977	–1.633880	–1.887299
71	1	0	–8.079945	–3.633463	–0.558720
72	1	0	–6.459841	–4.620820	1.051320
73	1	0	–4.222107	–3.609379	1.337027
74	1	0	0.804746	–5.488157	1.397147
75	1	0	1.967924	–7.664493	1.251286
76	1	0	4.008255	–7.900480	–0.153460
77	1	0	4.847769	–5.940813	–1.436245
78	1	0	3.656374	–3.782338	–1.329668
79	1	0	–0.222482	–0.204064	1.249572
80	1	0	0.293898	–1.657398	2.164680
81	1	0	–1.405830	–1.136504	2.185572

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	14.6425	28.3874	31.9812
Red. masses --	6.0709	5.6037	4.2574
Frc consts --	0.0008	0.0027	0.0026
IR Inten --	0.0359	0.4457	0.6038

N(2)-Me-*N*(23)-H-NCTPP



E(RB3LYP) = -1953.07894218 A.U.

Stoichiometry	C45H32N4			
Framework group	C1[X(C45H32N4)]			
Deg. of freedom	237			
Full point group		C1	NOp	1
Largest Abelian subgroup		C1	NOp	1
Largest concise Abelian subgroup		C1	NOp	1

Standard orientation:

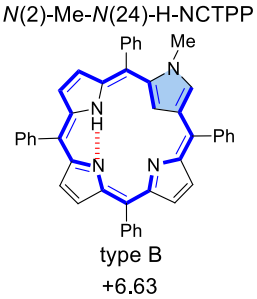
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	–3.848501	–0.684767	0.648701
2	7	0	0.842504	–1.997941	–0.057853
3	7	0	2.077760	0.677579	0.042839
4	7	0	–0.561619	2.002918	0.073715
5	6	0	–2.864556	0.161365	0.069848
6	6	0	–1.803541	–0.656269	–0.298160
7	6	0	–3.391353	–1.951843	0.627519
8	6	0	–2.112745	–1.994510	0.040933
9	6	0	–1.309337	–3.186116	–0.071572
10	6	0	0.078462	–3.145522	–0.184681
11	6	0	0.942037	–4.298784	–0.432446
12	6	0	2.214495	–3.833259	–0.422240
13	6	0	2.120314	–2.393681	–0.167135
14	6	0	3.254346	–1.526642	–0.053120
15	6	0	3.196037	–0.139304	0.069146
16	6	0	4.330765	0.740362	0.234190
17	6	0	3.880718	2.022392	0.277179
18	6	0	2.442022	2.009089	0.137899
19	6	0	1.620036	3.135520	0.078342
20	6	0	0.195105	3.106588	–0.038568
21	6	0	–0.622466	4.287696	–0.330359
22	6	0	–1.904410	3.854612	–0.384504
23	6	0	–1.867145	2.416660	–0.111217
24	6	0	–2.990011	1.587790	–0.052052
25	6	0	–2.017120	–4.492364	–0.022707
26	6	0	–1.619642	–5.508568	0.866359
27	6	0	–2.300408	–6.724096	0.914568
28	6	0	–3.393532	–6.953036	0.076881
29	6	0	–3.805038	–5.953235	–0.806575
30	6	0	–3.129548	–4.734820	–0.851157
31	6	0	4.611563	–2.159531	–0.068576
32	6	0	5.010135	–3.022948	0.965300
33	6	0	6.270046	–3.621034	0.952732
34	6	0	7.156951	–3.369099	–0.095680
35	6	0	6.773775	–2.515887	–1.131442
36	6	0	5.512802	–1.918418	–1.118129
37	6	0	2.280857	4.478275	0.113795
38	6	0	3.153293	4.890422	–0.907061
39	6	0	3.757426	6.147560	–0.869724
40	6	0	3.497722	7.020122	0.188095
41	6	0	2.628281	6.626880	1.207194
42	6	0	2.025677	5.369632	1.169275
43	6	0	–4.343597	2.192712	–0.193156
44	6	0	–4.785974	3.224879	0.652609
45	6	0	–6.056374	3.780105	0.498763
46	6	0	–6.909763	3.317619	–0.504225
47	6	0	–6.483348	2.293774	–1.354009
48	6	0	–5.216369	1.734405	–1.197091
49	1	0	1.119785	0.339245	0.040699
50	1	0	–0.907628	–0.313374	–0.779077
51	1	0	–3.961921	–2.752688	1.074532
52	1	0	0.611444	–5.309758	–0.621115
53	1	0	3.124951	–4.391263	–0.585433
54	1	0	5.352500	0.403256	0.314529
55	1	0	4.469646	2.917904	0.399632
56	1	0	–0.255109	5.290922	–0.490737
57	1	0	–2.785675	4.435170	–0.614060
58	1	0	–0.783640	–5.326866	1.533436
59	1	0	–1.981083	–7.490800	1.614686
60	1	0	–3.922214	–7.900997	0.114582
61	1	0	–4.650590	–6.123994	–1.466863
62	1	0	–3.443913	–3.965956	–1.549850
63	1	0	4.325113	–3.216186	1.785344
64	1	0	6.560736	–4.280748	1.765434
65	1	0	8.137930	–3.835233	–0.105858
66	1	0	7.453971	–2.318906	–1.955294

67	1	0	5.212663	–1.264364	–1.931298
68	1	0	3.346566	4.220007	–1.739095
69	1	0	4.425658	6.447463	–1.672072
70	1	0	3.967145	7.999155	0.217194
71	1	0	2.421947	7.297880	2.036290
72	1	0	1.354486	5.064239	1.966317
73	1	0	–4.128848	3.578997	1.440538
74	1	0	–6.380931	4.572483	1.167139
75	1	0	–7.898170	3.751227	–0.624081
76	1	0	–7.136322	1.934984	–2.144561
77	1	0	–4.883212	0.945401	–1.865085
78	6	0	–5.063811	–0.306360	1.365912
79	1	0	–5.863284	–0.020427	0.680542
80	1	0	–5.386590	–1.161885	1.961396
81	1	0	–4.863085	0.531791	2.034646

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	12.5781	26.4228	28.9439
Red. masses --	6.0642	4.1382	5.6036
Frc consts --	0.0006	0.0017	0.0028
IR Inten --	0.0205	0.3310	0.4553

N(2)-Me-*N*(24)-H-NCTPP



E(RB3LYP) = -1953.06836899 A.U.

Stoichiometry	C45H32N4			
Framework group	C1[X(C45H32N4)]			
Deg. of freedom	237			
Full point group		C1	NOp	1
Largest Abelian subgroup		C1	NOp	1
Largest concise Abelian subgroup		C1	NOp	1

Standard orientation:

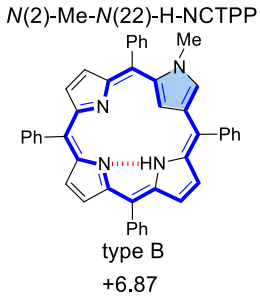
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	–3.842464	–0.697716	0.648015
2	7	0	0.852255	–1.997548	–0.058539
3	7	0	2.079900	0.681473	0.042153
4	7	0	–0.563237	1.999303	0.073029
5	1	0	–0.221661	1.003868	0.266250
6	6	0	–2.860929	0.151210	0.069162
7	6	0	–1.797593	–0.663404	–0.298846
8	6	0	–3.381716	–1.963487	0.626833
9	6	0	–2.102992	–2.002519	0.040247
10	6	0	–1.296199	–3.191836	–0.072258
11	6	0	0.091479	–3.147297	–0.185367
12	6	0	0.958329	–4.298099	–0.433132
13	6	0	2.229459	–3.828958	–0.422926
14	6	0	2.131185	–2.389654	–0.167821
15	6	0	3.262748	–1.519394	–0.053806
16	6	0	3.200495	–0.132227	0.068460
17	6	0	4.332717	0.750661	0.233504
18	6	0	3.879027	2.031407	0.276493
19	6	0	2.440375	2.014013	0.137213
20	6	0	1.615189	3.138103	0.077656
21	6	0	0.190346	3.105120	–0.039254
22	6	0	–0.630579	4.283898	–0.331045
23	6	0	–1.911287	3.847172	–0.385190
24	6	0	–1.869934	2.409331	–0.111903
25	6	0	–2.990439	1.577272	–0.052738
26	6	0	–2.000265	–4.500091	–0.023393
27	6	0	–1.599900	–5.515161	0.865673
28	6	0	–2.277207	–6.732620	0.913882
29	6	0	–3.369676	–6.964666	0.076195
30	6	0	–3.784023	–5.966039	–0.807261
31	6	0	–3.112000	–4.745709	–0.851843
32	6	0	4.621758	–2.148422	–0.069262
33	6	0	5.022784	–3.010702	0.964614
34	6	0	6.284390	–3.605204	0.952046
35	6	0	7.170575	–3.350748	–0.096366
36	6	0	6.784975	–2.498629	–1.132128
37	6	0	5.522308	–1.904747	–1.118815
38	6	0	2.272190	4.482731	0.113109
39	6	0	3.143451	4.897357	–0.907747
40	6	0	3.744007	6.156207	–0.870410
41	6	0	3.481824	7.028027	0.187409
42	6	0	2.613504	6.632315	1.206508
43	6	0	2.014477	5.373359	1.168589
44	6	0	–4.345739	2.178344	–0.193842
45	6	0	–4.791049	3.209249	0.651923
46	6	0	–6.063022	3.760861	0.498077
47	6	0	–6.915093	3.295950	–0.504911
48	6	0	–6.485769	2.273322	–1.354695
49	6	0	–5.217205	1.717557	–1.197777
50	1	0	–0.902659	–0.317964	–0.779763
51	1	0	–3.950004	–2.765951	1.073846
52	1	0	0.630612	–5.310009	–0.621801
53	1	0	3.141497	–4.384371	–0.586119
54	1	0	5.355406	0.416461	0.313843
55	1	0	4.465407	2.928589	0.398946
56	1	0	–0.266076	5.288165	–0.491423
57	1	0	–2.794199	4.425222	–0.614746
58	1	0	–0.764418	–5.331083	1.532750
59	1	0	–1.955704	–7.498413	1.614000
60	1	0	–3.895661	–7.914127	0.113896
61	1	0	–4.629086	–6.139202	–1.467549
62	1	0	–3.428549	–3.977742	–1.550536
63	1	0	4.338314	–3.205887	1.784658
64	1	0	6.576954	–4.264089	1.764748
65	1	0	8.152875	–3.814091	–0.106544
66	1	0	7.464608	–2.299715	–1.955980

67	1	0	5.220311	–1.251549	–1.931984
68	1	0	3.338629	4.227494	–1.739781
69	1	0	4.411384	6.458009	–1.672758
70	1	0	3.948461	8.008391	0.216508
71	1	0	2.405263	7.302726	2.035604
72	1	0	1.344157	5.066059	1.965631
73	1	0	–4.134932	3.565233	1.439852
74	1	0	–6.389831	4.552313	1.166453
75	1	0	–7.904729	3.726746	–0.624767
76	1	0	–7.137720	1.912677	–2.145247
77	1	0	–4.881806	0.929503	–1.865771
78	6	0	–5.058845	–0.322766	1.365226
79	1	0	–5.859128	–0.039107	0.679856
80	1	0	–5.379190	–1.179205	1.960710
81	1	0	–4.860503	0.515952	2.033960

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	13.8084	29.2319	30.5815
Red. masses --	6.1089	4.2969	5.5510
Frc consts --	0.0007	0.0022	0.0031
IR Inten --	0.0193	0.4479	0.8682

N(2)-Me-*N*(22)-H-NCTPP



E(RB3LYP) = -1953.06798634 A.U.

Stoichiometry	C45H32N4			
Framework group	C1[X(C45H32N4)]			
Deg. of freedom	237			
Full point group		C1	NOp	1
Largest Abelian subgroup		C1	NOp	1
Largest concise Abelian subgroup		C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	–3.843756	–0.696502	0.648534
2	7	0	0.852604	–1.990396	–0.058020
3	1	0	0.493249	–0.994318	0.095579
4	7	0	2.076859	0.690175	0.042672
5	7	0	–0.567941	2.004662	0.073548
6	6	0	–2.863295	0.153665	0.069681
7	6	0	–1.798930	–0.659604	–0.298327
8	6	0	–3.381407	–1.961690	0.627352
9	6	0	–2.102634	–1.999104	0.040766
10	6	0	–1.294339	–3.187400	–0.071739
11	6	0	0.093282	–3.141106	–0.184848
12	6	0	0.961587	–4.290811	–0.432613
13	6	0	2.232122	–3.820063	–0.422407
14	6	0	2.132029	–2.380884	–0.167302
15	6	0	3.262489	–1.509194	–0.053287
16	6	0	3.198482	–0.122107	0.068979
17	6	0	4.329587	0.762212	0.234023
18	6	0	3.874278	2.042383	0.277012
19	6	0	2.435649	2.023170	0.137732
20	6	0	1.609043	3.146215	0.078175
21	6	0	0.184243	3.111431	–0.038735
22	6	0	–0.638173	4.289170	–0.330526
23	6	0	–1.918327	3.850824	–0.384671
24	6	0	–1.875156	2.413037	–0.111384
25	6	0	–2.994608	1.579562	–0.052219
26	6	0	–1.996750	–4.496544	–0.022874
27	6	0	–1.595101	–5.511107	0.866192
28	6	0	–2.270869	–6.729421	0.914401
29	6	0	–3.363043	–6.962849	0.076714
30	6	0	–3.778652	–5.964747	–0.806742
31	6	0	–3.108173	–4.743568	–0.851324
32	6	0	4.622295	–2.136503	–0.068743
33	6	0	5.024410	–2.998275	0.965133
34	6	0	6.286767	–3.591181	0.952565
35	6	0	7.172630	–3.335605	–0.095847
36	6	0	6.785952	–2.483974	–1.131609
37	6	0	5.522536	–1.891690	–1.118296
38	6	0	2.264343	4.491673	0.113628
39	6	0	3.135079	4.907401	–0.907228
40	6	0	3.734043	6.167010	–0.869891
41	6	0	3.470757	7.038497	0.187928
42	6	0	2.602938	6.641687	1.207027
43	6	0	2.005504	5.381975	1.169108
44	6	0	–4.350667	2.178919	–0.193323
45	6	0	–4.797280	3.209260	0.652442
46	6	0	–6.069950	3.759263	0.498596
47	6	0	–6.921432	3.293276	–0.504392
48	6	0	–6.490815	2.271191	–1.354176
49	6	0	–5.221549	1.717031	–1.197258
50	1	0	–0.904433	–0.313032	–0.779244
51	1	0	–3.948681	–2.764871	1.074365
52	1	0	0.635149	–5.303134	–0.621282
53	1	0	3.144862	–4.374323	–0.585600
54	1	0	5.352699	0.429306	0.314362
55	1	0	4.459523	2.940306	0.399465
56	1	0	–0.274940	5.293897	–0.490904
57	1	0	–2.801969	4.427757	–0.614227
58	1	0	–0.759853	–5.325973	1.533269
59	1	0	–1.948397	–7.494807	1.614519
60	1	0	–3.887827	–7.912974	0.114415
61	1	0	–4.623496	–6.138978	–1.467030
62	1	0	–3.425693	–3.976001	–1.550017
63	1	0	4.340187	–3.194326	1.785177
64	1	0	6.580164	–4.249696	1.765267
65	1	0	8.155515	–3.797706	–0.106025
66	1	0	7.465333	–2.284201	–1.955461

67	1	0	5.219713	–1.238874	–1.931465
68	1	0	3.331104	4.237785	–1.739262
69	1	0	4.401037	6.469655	–1.672239
70	1	0	3.936154	8.019450	0.217027
71	1	0	2.393850	7.311834	2.036123
72	1	0	1.335573	5.073827	1.966150
73	1	0	–4.141614	3.566074	1.440371
74	1	0	–6.397759	4.550301	1.166972
75	1	0	–7.911612	3.722820	–0.624248
76	1	0	–7.142310	1.909722	–2.144728
77	1	0	–4.885154	0.929402	–1.865252
78	6	0	–5.060610	–0.323090	1.365745
79	1	0	–5.861251	–0.040444	0.680375
80	1	0	–5.379872	–1.179934	1.961229
81	1	0	–4.863328	0.515878	2.034479

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	12.8729	26.3484	28.6626
Red. masses --	6.0947	4.0959	5.7611
Frc consts --	0.0006	0.0017	0.0028
IR Inten --	0.0279	0.4483	0.6284