

Electronic Computational Supplementary Information

*Subtle substitution controls the rainbow chromatic behaviour of
multi-stimuli responsive core-expanded pyrenes*

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The following contains the atomic coordinates of all density-functional theory (DFT) calculations performed for the manuscript, included here to declutter the main supporting information. For references on methods used, consult the desired section in the Electronic Supplementary Information.

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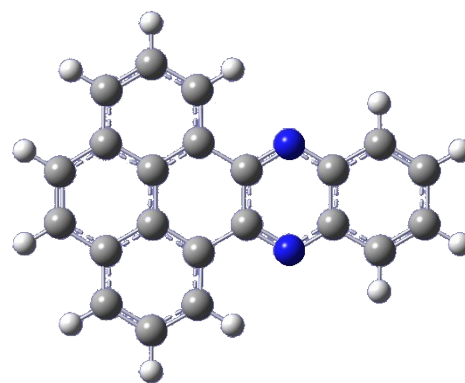
Section 1 Full Specifications for Single Molecule Calculations

Energy-minimized structures were calculated using density functional theory (DFT) with the B3LYP exchange-correlation functional and the cc-pVTZ basis sets on the Gaussian 16 Version A01 software package, solvated with the integral-equation formalism polarizable continuum model (IEFPCM). The optimized atomic cartesian coordinates are shown on the left. On the right are images captured using GaussView 6 of the optimized structure with RB3LYP energy and lowest energy vibration. Images of Kohn-Sham HOMO and LUMO surfaces with an Isovalue of 0.015 are in numbered figures immediately below their list of optimized cartesian coordinates. No keywords were added to the job input, save in the case of **NMe₂quin** derivatives. A numerical instability was observed in frequency calculations with the B3LYP functional when jobs involved many basis functions, in this case near or over 1694. The observed error "OrtVc1 failed #1" was solved by applying the keyword "FMM=NoParallelCPHF" to the input.

Electronic absorption spectra were calculated using time-dependent density functional theory (TD-DFT) with the B3LYP exchange-correlation functional and the cc-pVTZ basis set, solvated with the integral-equation formalism polarizable continuum model (IEFPCM). Geometry optimized structures were used, calculated as described above. The first 10 singlet and triplet excited states were calculated. Given the possibility for intra-molecular charge transfer (ICT) states each geometry optimization, frequency, energy and time-dependent calculation was also performed using the long range-corrected functionals CAM-B3LYP and ω B97X-D2. However, both failed to predict any absorption in the visible region, instead placing all transitions into the UV. Surprisingly, the B3LYP functional most accurately represented the positions of absorptions.

Phenanthro[4,5-*abc*]phenazine **H₂quin** in cyclohexane

Atomic Type	X	Y	Z
C	-3.955481609	-3.914351697	-0.000712145
C	-2.573218938	-3.912004308	-0.000648042
C	-1.85838173	-2.70506213	-0.000502026
C	-2.57249062	-1.476181736	-0.000418984
C	-3.989183596	-1.49563215	-0.000485032
C	-4.661031075	-2.714178409	-0.000631276
C	-0.426397411	-2.679594259	-0.000434572
C	-1.850683654	-0.23683973	-0.000270112
C	-0.429458619	-0.251602245	-0.000206938
C	0.254967266	-1.509691632	-0.000293957
C	0.267606418	0.96569065	-6.08566E-05
H	1.350027798	0.950253618	-1.33214E-05
C	-0.412395458	2.169124506	2.23009E-05
C	-1.804427957	2.190606953	-3.90195E-05
C	-2.532798313	1.004980264	-0.000184624
C	-3.995207235	1.014071467	-0.000250879
C	-4.718680825	-0.228132133	-0.00039849
H	0.103700488	-3.623420248	-0.000498889
H	-4.494430488	-4.852206371	-0.000825226
H	-2.025697714	-4.845864498	-0.000710735
H	-5.740553499	-2.70964778	-0.000681381

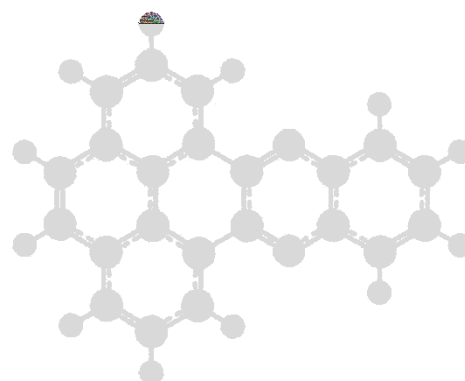


E(RB3LYP) -955.45159 a.u.
Lowest Vibration 49.5848 cm⁻¹
Imaginary 0
Frequencies

C	-6.696366779	3.384065774	-0.000153795
C	-8.112894544	0.951888687	-0.000438703
C	-8.064817004	3.372372747	-0.000215177
H	-8.613634223	4.304419157	-0.000154099
C	-8.777952283	2.147920018	-0.000358404
H	-9.859435537	2.165379256	-0.000404376
H	-6.13343984	4.307278086	-4.44557E-05
H	-8.638131121	0.006725076	-0.000548382
N	-4.630508027	2.172402478	-0.000173119
N	-6.039656925	-0.247105099	-0.000457886

Phenanthro[4,5-*abc*]phenazine **H₂quin** in CH₂Cl₂

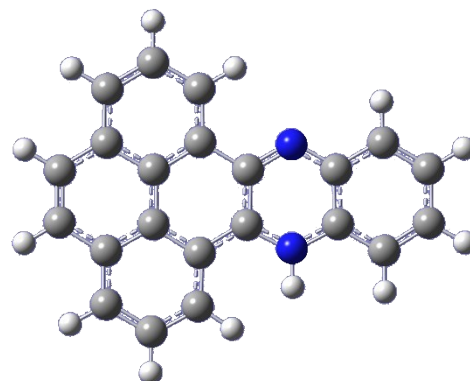
Atomic Type	X	Y	Z
C			
C			
C			
C			
C			
C	-3.954330889	-3.916009746	-0.000713325
C	-2.571879745	-3.913068158	-0.000648212
C	-1.857772708	-2.705259948	-0.00050188
C	-2.572405147	-1.476310459	-0.000418997
C	-3.989342305	-1.496021547	-0.000485331
C	-4.660265606	-2.715740808	-0.000632876
H	-0.425493698	-2.680301594	-0.000434237
C	-1.850529518	-0.236850558	-0.000270029
C	-0.428986052	-0.252034356	-0.000206877
C	0.256028412	-1.510128654	-0.000293859
C	0.269192534	0.965050767	-6.06768E-05
C	1.351450854	0.949318813	-1.30587E-05
H	-0.410385514	2.168941747	2.31242E-05
H	-1.802691299	2.190712085	-3.79655E-05
H	-2.532537932	1.005310446	-0.000184518
H	-3.995300385	1.014251881	-0.000251326
H	-4.718883710	-0.228140133	-0.000397991
H	0.104474720	-3.624032595	-0.000498395
H	-4.492784068	-4.854034021	-0.000827124
C	-2.024182460	-4.846640999	-0.000710873
C	-5.739705477	-2.714467176	-0.00068501
C	1.338374305	-1.505427955	-0.000244487
C	0.139810309	3.100126972	0.000136521
C	-2.336422215	3.128967575	2.85852E-05
H	-5.979131527	2.164092299	-0.000235109
C	-6.697874014	0.930011999	-0.000377075
H	-6.698292705	3.385301315	-0.000156397
H	-8.114919504	0.952954188	-0.00043584
H	-8.067037108	3.373731706	-0.00021642
N	-8.615952482	4.305542621	-0.000156375
N	-8.780229746	2.149180493	-0.000356941
	-9.861556601	2.166841305	-0.000401889
	-6.136924762	4.309517423	-0.000049098
	-8.641798419	0.008651275	-0.000543422
	-4.631850100	2.172341972	-0.000175243
	-6.040266511	-0.245907925	-0.000455632



E(RB3LYP) -955.454672 a.u.
Lowest Vibration 48.6963 cm⁻¹
Imaginary 0
Frequencies

Protonated Phenanthro[4,5-*abc*]phenazine **H₂quin** in CH₂Cl₂

Atomic Type	X	Y	Z
C	-1.834434846	-3.513607575	0.000373689
C	-3.029846974	-2.820234179	0.000305233
C	-3.048361982	-1.416711451	0.000164036
C	-1.816532092	-0.710062362	0.000089865
C	-0.600722025	-1.436940983	0.000163004
C	-0.622819876	-2.827834567	0.000304151
C	-4.277758418	-0.683963873	0.000093659
C	-1.823019358	0.720475353	-5.73481E-05
C	-3.062382684	1.414043239	-0.000119818
C	-4.285186001	0.669588662	-4.04568E-05
C	-3.062396942	2.816522943	-0.000258342
H	-4.009051583	3.340048213	-0.000304254
C	-1.878304575	3.531734316	-0.00033468
C	-0.661011111	2.865016845	-0.000278207
C	-0.611908889	1.468221465	-0.000142502
C	0.625963900	0.732391304	-8.07928E-05
C	0.657428317	-0.704400315	8.09188E-05
H	-5.206822746	-1.238026062	0.000150819
H	-1.836578429	-4.594533427	0.000480566
H	-3.969482313	-3.356383633	0.000360243
H	0.311283430	-3.368311026	0.000356883
H	-5.218728437	1.215654733	-9.04578E-05
H	-1.895926836	4.611859225	-0.000437239
H	0.239381460	3.46310625	-0.000338169
C	3.014362988	0.713155543	-0.000109943
C	2.972303529	-0.707944132	6.32161E-05
C	4.231500034	1.408370578	-0.000209423
C	4.195878100	-1.417995266	0.000137949
C	5.397193802	0.682862642	-0.000133348
H	6.345688251	1.200476368	-0.000206663
C	5.380353831	-0.731486353	4.16813E-05
H	6.317523877	-1.269031546	9.78516E-05
H	4.242557712	2.489899772	-0.000338503
H	4.158758263	-2.49732262	0.000268784
N	1.811960617	1.352373746	-0.000167452
N	1.799674002	-1.365587142	0.000149018
H	1.829628563	2.364543347	-0.000285778

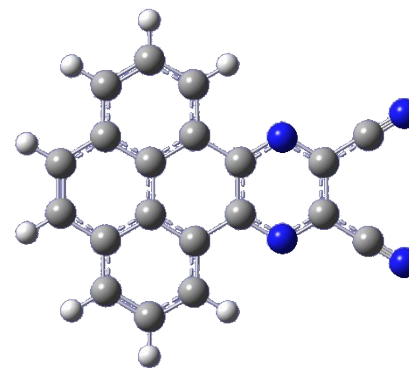


E(RB3LYP) -955.887724 a.u.
Lowest Vibration 46.5691 cm⁻¹
Imaginary 0
Frequencies

Phenanthro[4,5-*fgh*]quinoxaline-10,11-dicarbonitrile **H₂pyr** in cyclohexane

Atomic Type	X	Y	Z
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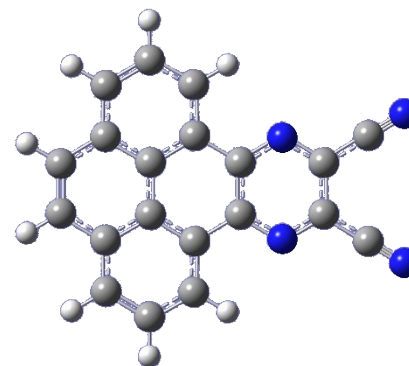
C	-3.979530382	-3.90023435	-0.000698783
C	-2.595575942	-3.89706389	-0.000334683
C	-1.876624472	-2.693544759	-0.000093949
C	-2.589499560	-1.464274846	-0.000228598
C	-4.008231213	-1.485298097	-0.000602569
C	-4.685921520	-2.702684335	-0.000833118
C	-0.444572734	-2.66897601	0.000283634
C	-1.869432808	-0.227920831	1.37656E-05
C	-0.448477808	-0.241418121	0.000386697
C	0.236763307	-1.499122596	0.00051293
C	0.243579859	0.97776427	0.000620832
H	1.325819728	0.965481357	0.000904761
C	-0.436540803	2.183075826	0.000493673
C	-1.826706868	2.206584858	0.000129304
C	-2.551185286	1.016448554	-0.000112076
C	-4.002720360	1.010664508	-0.000493805
C	-4.719424613	-0.219916097	-0.000735174
H	0.085236284	-3.61257669	0.000382449
H	-4.517033514	-4.838399727	-0.00088044
H	-2.050887755	-4.8323226	-0.000231577
H	-5.765382902	-2.70052477	-0.001116923
H	1.318917162	-1.494347651	0.000797671
H	0.114246553	3.113504318	0.000678277
H	-2.361218909	3.14442199	0.000029007
C	-5.981996435	2.155896548	-0.000964677
C	-6.692158907	0.936548179	-0.001204021
N	-4.657965364	2.175415478	-0.000615788
N	-6.055825658	-0.224709493	-0.001086745
C	-6.663625061	3.418433905	-0.001089306
N	-7.218230658	4.427304933	-0.001191481
C	-8.126631735	0.906452681	-0.001582596
N	-9.277792225	0.891039499	-0.001886049



E(RB3LYP) -986.291199 a.u.
Lowest Vibration 35.1365 cm⁻¹
Imaginary 0
Frequencies

Phenanthro[4,5-*fgh*]quinoxaline-10,11-dicarbonitrile **H₂pyr** in CH₂Cl₂

Atomic Type	X	Y	Z
C	-3.979405968	-3.900998115	-0.000698675
C	-2.595199520	-3.897222123	-0.000334632
C	-1.876872962	-2.692887277	-9.40857E-05
C	-2.590200159	-1.463805592	-0.000228825
C	-4.009175542	-1.485294173	-0.000602776
C	-4.686088096	-2.703512261	-0.000833035
C	-0.444571957	-2.669155561	0.000283439
C	-1.870186653	-0.227543	0.000013536
C	-0.449172289	-0.241526408	0.00038646
C	0.236919859	-1.49903468	0.000512809
C	0.243903227	0.977514936	0.000620971
H	1.325960933	0.964861256	0.00090484
C	-0.435815095	2.183344472	0.000494085
C	-1.826068936	2.207138261	0.000129697
C	-2.551654652	1.017267985	-0.000112119
C	-4.002557373	1.011719996	-0.000493725
C	-4.720262239	-0.220578662	-0.000735378
H	0.084762561	-3.612827858	0.000382081
H	-4.516367752	-4.839336128	-0.000880123



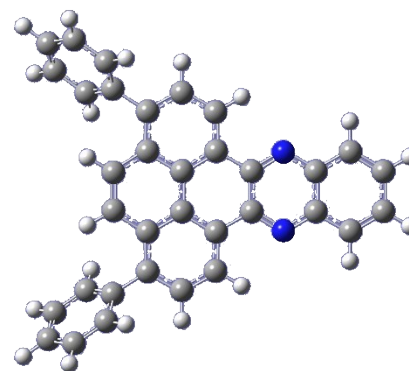
E(RB3LYP) -986.297255 a.u.
Lowest Vibration 29.0305 cm⁻¹

H	-2.050278732	-4.832139445	-0.000231522
H	-5.765441204	-2.704595621	-0.001116826
H	1.318901875	-1.493811679	0.000797455
H	0.115389534	3.113387287	0.000678883
H	-2.357706893	3.146481362	3.02924E-05
C	-5.982135075	2.154841829	-0.00096489
C	-6.691309922	0.937189204	-0.001203781
N	-4.658270853	2.176028966	-0.000615965
N	-6.056509994	-0.22474648	-0.001086882
C	-6.664731976	3.416932096	-0.001089958
N	-7.221492176	4.424682907	-0.001192885
C	-8.125871649	0.90815649	-0.001582268
N	-9.277120921	0.895170059	-0.001885562

**Imaginary
Frequencies** 0

1,8-Diphenylphenanthro[4,5-*abc*]phenazine Ph₂quin in cyclohexane

Atomic Type	X	Y	Z
C	-4.492536412	-3.762930178	0.116269357
C	-3.102482704	-3.75839583	0.145661614
C	-2.422070016	-2.514301151	0.157389501
C	-3.165664061	-1.300656213	0.0953923
C	-4.581553545	-1.351173497	0.046874284
C	-5.222125840	-2.584145154	0.067466661
C	-0.999025564	-2.425892004	0.282401502
C	-2.479468509	-0.034807757	0.092242354
C	-1.056555798	0.004709932	0.151122229
C	-0.353719171	-1.235473234	0.279439321
C	-0.385462647	1.253782135	0.133190831
C	-1.140374024	2.420914577	0.100879407
C	-2.526406129	2.388738374	0.055089486
C	-3.209990245	1.178995242	0.040577224
C	-4.668339147	1.148493951	-0.023670607
C	-5.352053562	-0.112777007	-0.020531416
H	-0.431493154	-3.336038701	0.402718657
H	-5.014211180	-4.710431709	0.106132644
H	-6.300716754	-2.608483037	0.031932247
H	0.718915565	-1.213840168	0.397436826
H	-0.631167518	3.375112765	0.086011362
H	-3.094749824	3.305670261	0.017212115
C	1.097161824	1.366526454	0.143556744
C	1.739333746	2.110029559	1.13879632
C	1.879985183	0.786293634	-0.860382911
C	3.120756424	2.261177137	1.136853711
H	1.150525639	2.560998454	1.926581289
C	3.260157426	0.942873846	-0.866524415
H	1.400831934	0.224660872	-1.650997239
C	3.886438908	1.678357795	0.133886653
H	3.598283655	2.833429628	1.921151795
H	3.846328082	0.493791979	-1.65735353
H	4.961534221	1.797708616	0.130058604
C	-2.387763279	-5.062227672	0.159547753
C	-1.476485158	-5.405410062	-0.845029814
C	-2.658157349	-6.002239986	1.159021484
C	-0.854450963	-6.647383039	-0.847692619
H	-1.269079773	-4.700462897	-1.638832385
C	-2.030878856	-7.242279229	1.160539331
H	-3.355699028	-5.751922418	1.947342349
C	-1.126785142	-7.569682341	0.156889643
H	-0.159937519	-6.896533092	-1.639056378

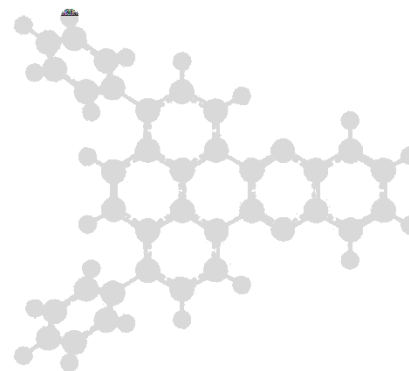


**E(RB3LYP)
Lowest Vibration
Imaginary
Frequencies** -1417.710126 a.u.
28.5586 cm⁻¹
0

H	-2.248085746	-7.951685616	1.94806229
H	-0.640050735	-8.535693472	0.155761177
N	-5.336096994	2.287234197	-0.081814058
N	-6.670804413	-0.174945248	-0.075685985
C	-6.680882566	2.235547083	-0.138609902
C	-7.361557160	0.979883938	-0.135484723
C	-7.435811250	3.43300236	-0.202597871
C	-8.777094638	0.958692114	-0.196439705
C	-8.802120024	3.37863019	-0.260541053
H	-9.378222614	4.292775731	-0.309419694
C	-9.477346570	2.133017239	-0.257440927
H	10.557860198	2.116658888	-0.304003715
H	-6.901701759	4.373146043	-0.20408241
H	-9.273372907	-0.001954895	-0.193193489

1,8-Diphenylphenanthro[4,5-*abc*]phenazine **Ph₂quin** in CH₂Cl₂

Atomic Type	X	Y	Z
C	-4.491978400	-3.763985612	0.119793424
C	-3.101719383	-3.759455887	0.146157084
C	-2.421740703	-2.514735701	0.156509708
C	-3.165529998	-1.300823498	0.095500425
C	-4.581770676	-1.351312568	0.048629055
C	-5.221510478	-2.584998347	0.071464176
C	-0.998472212	-2.426255814	0.279387849
C	-2.479256128	-0.034833553	0.092348827
C	-1.056014500	0.004660181	0.150237014
C	-0.353122135	-1.235759184	0.276423721
C	-0.384155620	1.253715071	0.133675839
C	-1.139176210	2.421029403	0.104396979
C	-2.525345369	2.388698475	0.059084394
C	-3.209988410	1.179255463	0.042330319
C	-4.668389658	1.148470719	-0.022386054
C	-5.352060947	-0.112718224	-0.019247226
H	-0.429713618	-3.335888164	0.396730575
H	-5.014906075	-4.710675076	0.112881834
H	-6.300004674	-2.613159175	0.038576844
H	0.719744496	-1.215448461	0.391451133
H	-0.631326540	3.375846226	0.092751833
H	-3.090426185	3.307646731	0.023840809
C	1.098598995	1.366961396	0.143269169
C	1.739626311	2.116832079	1.134967635
C	1.881947608	0.781821835	-0.857769101
C	3.121241853	2.269092381	1.132552822
H	1.151017929	2.573025037	1.91983236
C	3.262328221	0.939968828	-0.864607186
H	1.404737390	0.214910539	-1.645726194
C	3.887808922	1.681480342	0.132403388
H	3.597942696	2.846098975	1.91375686
H	3.848939889	0.487015334	-1.652765603
H	4.962744836	1.801775978	0.128179368
C	-2.387349218	-5.063672856	0.159281646
C	-1.471602498	-5.404573905	-0.842364624
C	-2.663766505	-6.006241196	1.155196255
C	-0.850762368	-6.647576022	-0.845712129

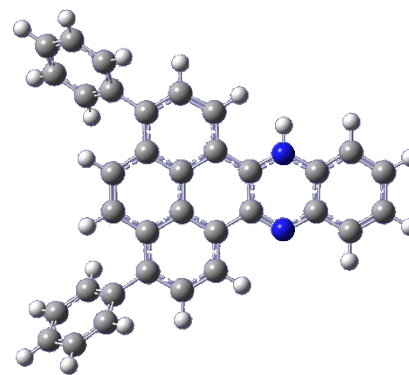


E(RB3LYP) -1417.714049 a.u.
Lowest Vibration 28.6394 cm⁻¹
Imaginary 0
Frequencies

H	-1.258660757	-4.698339865	-1.633492752
C	-2.037310428	-7.24704835	1.156251919
H	-3.365632460	-5.758977182	1.94058098
C	-1.128649244	-7.572535132	0.155449739
H	-0.152707633	-6.894947577	-1.634382341
H	-2.259003059	-7.95839077	1.940665321
H	-0.642789395	-8.538927402	0.153933037
N	-5.337011678	2.287013288	-0.081441142
N	-6.671119696	-0.174055858	-0.075316112
C	-6.682174641	2.236306595	-0.138710804
C	-7.362899123	0.98055368	-0.135585575
C	-7.436946911	3.433885519	-0.203203984
C	-8.778455900	0.959163545	-0.197045176
C	-8.803544567	3.379518762	-0.261546596
H	-9.379635435	4.2934347	-0.310712794
C	-9.478869086	2.133727311	-0.258446232
H	10.559184542	2.11748499	-0.305297588
H	-6.905071760	4.375374151	-0.20475935
H	-9.277082162	-0.000344764	-0.193869556

Protonated 1,8-Diphenylphenanthro[4,5-*abc*]phenazine **Ph₂quin** in CH₂Cl₂

Atomic Type	X	Y	Z
C	0.010693897	3.53414584	0.064795153
C	-1.205705805	2.855314389	0.060102176
C	-1.202166385	1.435406729	0.082244681
C	0.032563597	0.728668614	0.051159127
C	1.254372713	1.461981902	0.033060816
C	1.215271415	2.857671823	0.051326131
C	-2.411279130	0.679079626	0.188514662
C	0.036211113	-0.707616512	0.046291736
C	-1.193992175	-1.423056172	0.074384252
C	-2.406765242	-0.674582221	0.185052864
C	-1.184247729	-2.842807918	0.046861681
C	0.037891500	-3.505960573	0.042632609
C	1.240246324	-2.815203816	0.030578923
C	1.257901545	-1.426002158	0.021474948
C	2.518419122	-0.703540689	-0.008494608
C	2.490218513	0.731292178	0.000097265
H	-3.345914974	1.206286909	0.295350707
H	0.012743069	4.614234875	0.049207489
H	2.118590780	3.451194391	0.03838611
H	-3.339002224	-1.207481898	0.288163566



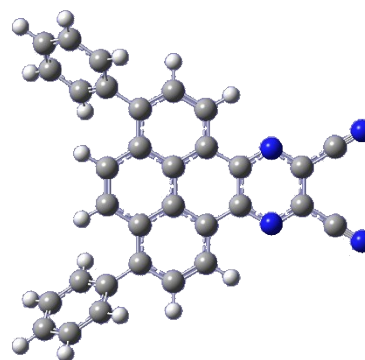
E(RB3LYP) -1418.147870 a.u.
Lowest Vibration 28.4578 cm⁻¹
Imaginary 0

Frequencies

H	0.049890689	-4.586665739	0.022890248
H	2.175636824	-3.353091526	0.013861477
C	-2.430545467	-3.650848256	0.017941595
C	-2.645366610	-4.641821763	0.981588563
C	-3.383414427	-3.484338932	-0.99317397
C	-3.785961309	-5.434444886	0.943281186
H	-1.921362501	-4.781672765	1.773207333
C	-4.518450073	-4.284032752	-1.036410276
H	-3.224771803	-2.739790413	-1.761459879
C	-4.725914850	-5.258813235	-0.066190602
H	-3.939747995	-6.188675035	1.703221628
H	-5.238860300	-4.147664815	-1.831693432
H	-5.611882917	-5.878255336	-0.098460253
C	-2.454423880	3.655259585	0.025418132
C	-3.415547319	3.463499068	-0.973861693
C	-2.662340872	4.666976975	0.969639794
C	-4.551966310	4.260078347	-1.024322165
H	-3.261484259	2.704155916	-1.728097363
C	-3.806448573	5.453297397	0.925797985
H	-1.932538296	4.825920717	1.752183417
C	-4.754045426	5.253618153	-0.072141666
H	-5.278306147	4.105923179	-1.810723159
H	-3.956882560	6.221785434	1.671827554
H	-5.642266794	5.869412174	-0.109440165
N	3.657399505	-1.369303136	-0.038663155
N	3.677753884	1.349573604	-0.021627459
C	4.832444580	-0.7143431	-0.062571704
C	4.878535727	0.706146394	-0.054337679
C	6.053222778	-1.427158675	-0.095796027
C	6.097115752	1.397573635	-0.079160749
C	7.240181374	-0.744187747	-0.119368724
H	8.174990601	-1.285277003	-0.144691543
C	7.261271894	0.669336918	-0.111291204
H	8.210499937	1.185185101	-0.130983268
H	6.013352604	-2.50643039	-0.101565524
H	6.111247791	2.4790879	-0.074138674
H	3.698908813	2.361295216	-0.012086017

1,8-Diphenylphenanthro[4,5-*fg*]quinoxaline-10,11-dicarbonitrile **Ph₂pyr** in cyclohexane

Atomic Type	X	Y	Z
C	-4.408487469	-3.583354102	-1.283888861
C	-3.081442122	-3.470132902	-1.690537171
C	-2.471816571	-2.1902176	-1.70084809
C	-3.207528653	-1.055443228	-1.254357802
C	-4.552461910	-1.220079369	-0.829970698
C	-5.135685004	-2.48319189	-0.860429386
C	-1.145916219	-1.978811553	-2.196705117
C	-2.592592391	0.242819995	-1.244087254
C	-1.245795117	0.398174395	-1.680367077
C	-0.566321877	-0.755166714	-2.187021004
C	-0.641813548	1.680438974	-1.649783323
C	-1.397430115	2.773627661	-1.233594532
C	-2.711914992	2.633908759	-0.819952545
C	-3.319872266	1.382187161	-0.809390342
C	-4.689353835	1.220958076	-0.364801807
C	-5.298050385	-0.064140549	-0.374957559



H	-0.606320848	-2.818124819	-2.607559184
H	-4.872307968	-4.5600361	-1.275543727
H	-6.159245108	-2.595622227	-0.536632123
H	0.427416062	-0.635691363	-2.590285415
H	-0.935673817	3.751033048	-1.20978828
H	-3.275370276	3.492862879	-0.488476325
C	0.773701287	1.906648414	-2.041848069
C	1.086476490	2.840185864	-3.035024537
C	1.822962934	1.241896964	-1.398155093
C	2.407583471	3.093180516	-3.382882909
H	0.287358988	3.359615443	-3.547060647
C	3.143825219	1.501877098	-1.739800316
H	1.602682836	0.532949188	-0.611492176
C	3.440887675	2.425520871	-2.735959507
H	2.628561608	3.81196381	-4.160569348
H	3.941850061	0.985623899	-1.223073364
H	4.469680277	2.625028729	-3.003637345
C	-2.357291575	-4.703528295	-2.094157562
C	-1.182221500	-5.102633206	-1.448316162
C	-2.875300192	-5.523967598	-3.10126569
C	-0.544478002	-6.284841356	-1.801382064
H	-0.778110378	-4.493342791	-0.6511788
C	-2.231958417	-6.701859578	-3.460455279
H	-3.780278012	-5.228060918	-3.61510531
C	-1.064766042	-7.086816194	-2.81125027
H	0.357319952	-6.581976624	-1.282885335
H	-2.643294132	-7.318038447	-4.248746772
H	-0.565721086	-8.005702444	-3.087784533
N	-5.372742554	2.291841399	0.050907433
N	-6.562069259	-0.21911376	0.031078293
C	-6.624326045	2.124960326	0.450825866
C	-7.228325195	0.849768257	0.440760613
C	-7.339206985	3.287618185	0.892834697
N	-7.919523765	4.216089023	1.248807647
C	-8.583456676	0.660685267	0.872114314
N	-9.671624389	0.516944835	1.219637167

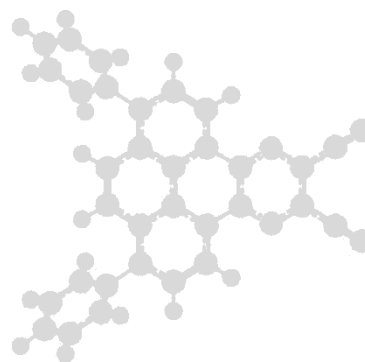
E(RB3LYP)
Lowest Vibration
Imaginary
Frequencies

-1448.550237 a.u.
24.4666 cm⁻¹
0

1,8-Diphenylphenanthro[4,5-*fg*h]quinoxaline-10,11-dicarbonitrile **Ph₂pyr** in CH₂Cl₂

Atomic Type	X	Y	Z
C	-4.409179125	-3.58357533	-1.287702686
C	-3.081200015	-3.470649838	-1.691850495
C	-2.471456203	-2.190390366	-1.701555551
C	-3.207452971	-1.055419624	-1.255841974
C	-4.553019162	-1.219971641	-0.832510497
C	-5.136252380	-2.483236669	-0.86477311
C	-1.145249964	-1.979168446	-2.196444681
C	-2.592553057	0.242760484	-1.245569256
C	-1.245427258	0.398006201	-1.681070356
C	-0.565627739	-0.755468651	-2.186759363
C	-0.641247135	1.6805869	-1.651082381
C	-1.397667024	2.774343529	-1.237389708
C	-2.712206211	2.634425564	-0.824279862
C	-3.320289144	1.382577793	-0.811919664

C	-4.688962452	1.221647916	-0.366961625
C	-5.298327287	-0.06485126	-0.377136455
H	-0.603934799	-2.817935974	-2.605807358
H	-4.874834415	-4.559255544	-1.281272159
H	-6.160139556	-2.598146423	-0.543345988
H	0.428768037	-0.63769161	-2.588550968
H	-0.937834185	3.752557466	-1.215495922
H	-3.273933007	3.495234025	-0.495134912
C	0.774563377	1.907629913	-2.041495497
C	1.087648169	2.850217036	-3.026553555
C	1.823509252	1.235977315	-1.403906201
C	2.409086534	3.105005214	-3.37288944
H	0.289385711	3.376093572	-3.533194192
C	3.144791271	1.498044454	-1.743773143
H	1.604041207	0.519658602	-0.623837426
C	3.442378075	2.430425903	-2.732135995
H	2.630212927	3.830540574	-4.14419248
H	3.942332315	0.975999665	-1.232271513
H	4.471224109	2.631168654	-2.998614672
C	-2.357516374	-4.704822149	-2.09383471
C	-1.177228030	-5.099190261	-1.45405517
C	-2.882413868	-5.53137399	-3.092897562
C	-0.540838398	-6.283064771	-1.805373159
H	-0.766829715	-4.485742347	-0.66345989
C	-2.240253880	-6.710675111	-3.450590689
H	-3.791902580	-5.240313561	-3.601393311
C	-1.067637923	-7.091118618	-2.807513606
H	0.365198926	-6.576057033	-1.292062051
H	-2.656786060	-7.331357395	-4.232550578
H	-0.569517455	-8.010841325	-3.082865829
N	-5.372149166	2.291982856	0.04980792
N	-6.561805681	-0.219642192	0.029950607
C	-6.623190554	2.123487144	0.45030904
C	-7.226467411	0.849835335	0.440242127
C	-7.338627586	3.2855493	0.893275435
N	-7.921677563	4.211915035	1.250451273
C	-8.581503981	0.661553826	0.872542615
N	-9.669788428	0.521251263	1.221293943

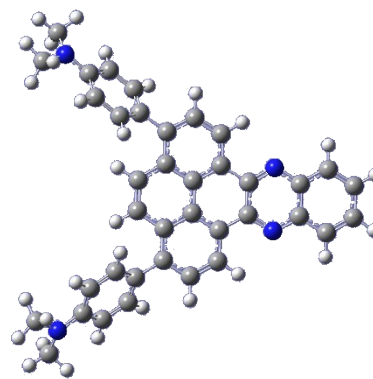


E(RB3LYP) -1448.556970 a.u.
Lowest Vibration 15.8677 cm⁻¹
Imaginary 0
Frequencies

1,8-Bis(4-N,N-dimethylaminophenyl)phenanthro[4,5-abc]phenazine NMe₂quin in cyclohexane

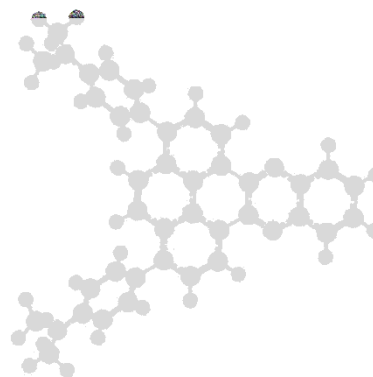
Atomic Type	X	Y	Z
C	-4.789762632	-3.183610443	-2.483634401
C	-3.669322617	-2.909559433	-3.263737416
C	-3.131554413	-1.594817619	-3.237165543
C	-3.701510744	-0.609664302	-2.379697938
C	-4.830182732	-0.941368895	-1.588136776
C	-5.363268116	-2.223042106	-1.665434372
C	-2.058762596	-1.194119921	-4.095187032
C	-3.139296025	0.715791888	-2.329088367
C	-2.012007080	1.044593914	-3.136388903
C	-1.441144465	2.34351455	-3.063167832
C	-2.044893064	3.287564605	-2.236544004
C	-3.155921369	2.980887235	-1.466727295
C	-3.707690670	1.704964738	-1.487089504
C	-4.861376151	1.379857416	-0.655439987

C	-5.421812142	0.058603597	-0.705892109
H	-1.681990352	-1.902544517	-4.816850769
H	-5.202940573	-4.183195068	-2.495333877
H	-6.223619683	-2.463098436	-1.059109388
H	-1.614106451	4.277673	-2.172274222
H	-3.598456703	3.725848631	-0.822788716
C	-0.230293384	2.735302021	-3.822502047
C	-0.214416212	3.900258913	-4.596108613
C	0.962554372	2.007328013	-3.760215169
C	0.916335555	4.316737244	-5.278077742
H	-1.119074744	4.487790095	-4.686376173
C	2.106556596	2.412720077	-4.426142584
H	1.007235311	1.109377841	-3.158349701
C	2.121496164	3.589149428	-5.203494324
H	0.855776657	5.212943017	-5.875360657
H	2.996595775	1.810682836	-4.331046754
C	-3.087803485	-4.001474779	-4.079705254
C	-1.737257351	-4.357677737	-4.003168022
C	-3.892089910	-4.770097257	-4.927164582
C	-1.214563979	-5.417058023	-4.725004529
H	-1.077886715	-3.806468843	-3.345938045
C	-3.386131510	-5.826606204	-5.665358438
H	-4.940612678	-4.521729805	-5.030419651
C	-2.027637499	-6.192706294	-5.576925326
H	-0.165925284	-5.645192188	-4.615588167
H	-4.055417851	-6.365510913	-6.317461367
N	-5.374755309	2.309446447	0.131266413
N	-6.467922029	-0.267746591	0.032857347
C	-6.441318560	1.986548638	0.888747612
C	-6.998516883	0.672926461	0.838587641
C	-7.022231521	2.953071863	1.74655205
C	-8.120062129	0.364882841	1.647723534
C	-8.105647129	2.624187134	2.516131629
H	-8.548353837	3.362777206	3.170790212
C	-8.658409003	1.321024105	2.466371098
H	-9.514597275	1.084811348	3.083807381
H	-6.585210715	3.941907888	1.770116229
H	-8.526876964	-0.635664558	1.595324287
N	-1.519822036	-7.265037582	-6.281368609
N	3.263984360	4.013064302	-5.850819901
C	-2.340996866	-7.924075548	-7.279332749
H	-2.621473666	-7.257879805	-8.104626412
H	-1.790330205	-8.764037597	-7.693707912
H	-3.258699821	-8.317423872	-6.838186083
C	-0.087161008	-7.49113084	-6.313562131
H	0.312034745	-7.643166883	-5.308934716
H	0.117310977	-8.391144813	-6.886803336
H	0.462218827	-6.660183105	-6.773077458
C	3.193570227	5.123935748	-6.781196468
H	4.191039800	5.337291847	-7.155376035
H	2.542731714	4.917092587	-7.639810991
H	2.825812283	6.026995991	-6.290536261
C	4.423465947	3.142981321	-5.907643854
H	5.227692561	3.656849846	-6.426872604
H	4.782685918	2.896670015	-4.906624476
H	4.221368652	2.202416793	-6.43484626
C	-1.530183908	0.052036952	-4.047605208
H	-0.739669699	0.319028555	-4.732021602



E(RB3LYP) -1685.741729 a.u.
Lowest Vibration 20.3405 cm⁻¹
Imaginary 0
Frequencies

Atomic Type	X	Y	Z
C	-4.793358168	-3.182507083	-2.494236708
C	-3.671320654	-2.909892506	-3.27364347
C	-3.134798234	-1.59365036	-3.246933374
C	-3.703841713	-0.608536367	-2.388256094
C	-4.832542746	-0.940080927	-1.595978835
C	-5.366410145	-2.221743557	-1.676064034
C	-2.065143586	-1.191028657	-4.107945381
C	-3.141493469	0.717225784	-2.337635926
C	-2.014829899	1.04672755	-3.146118817
C	-1.442014796	2.345802133	-3.072971001
C	-2.047893505	3.29005431	-2.247101795
C	-3.158747949	2.982922446	-1.477339237
C	-3.710042105	1.706265877	-1.49493594
C	-4.861805972	1.380263296	-0.661124613
C	-5.422248106	0.058995238	-0.711573437
H	-1.689356866	-1.897450617	-4.831869073
H	-5.209164006	-4.180871497	-2.506013008
H	-6.227394450	-2.464929771	-1.071988827
H	-1.619806013	4.281208114	-2.182914994
H	-3.599414256	3.730655239	-0.835428646
C	-0.230443183	2.737775727	-3.829703376
C	-0.204993918	3.918287998	-4.58108116
C	0.956498538	1.99707278	-3.785702995
C	0.926765086	4.336397447	-5.25997517
H	-1.102943399	4.51819865	-4.656248911
C	2.102232149	2.403573054	-4.447663197
H	0.996646367	1.087968753	-3.200491862
C	2.126370868	3.594676302	-5.205069483
H	0.873198343	5.244604847	-5.839537716
H	2.986892072	1.791670669	-4.366612976
C	-3.089510485	-4.002611969	-4.087063972
C	-1.733413747	-4.344523352	-4.027842213
C	-3.898931259	-4.790349688	-4.913583308
C	-1.210416308	-5.406157219	-4.745857183
H	-1.068719422	-3.781224877	-3.386413792
C	-3.393526048	-5.848898807	-5.648858262
H	-4.952104899	-4.556389297	-5.002713264
C	-2.028186958	-6.199895034	-5.579048494
H	-0.158037015	-5.622655217	-4.649710652
H	-4.067064911	-6.402314724	-6.284215907
N	-5.374309669	2.308695294	0.128088382
N	-6.466986468	-0.267339765	0.029729895
C	-6.439841627	1.986021202	0.887941567
C	-6.997087760	0.672288212	0.837780379
C	-7.019052673	2.951903041	1.747626131
C	-8.117039491	0.363349656	1.648789545
C	-8.101287939	2.622297473	2.519161278
H	-8.542853940	3.360116589	3.175156928
C	-8.654099150	1.319020118	2.469399297
H	-9.508976435	1.082439288	3.088190229
H	-6.583854041	3.941571325	1.772898853
H	-8.525767128	-0.636576184	1.598095277
N	-1.520546403	-7.269080263	-6.280527012
N	3.266406670	4.016385096	-5.849605768
C	-2.354539127	-7.963177159	-7.245743613

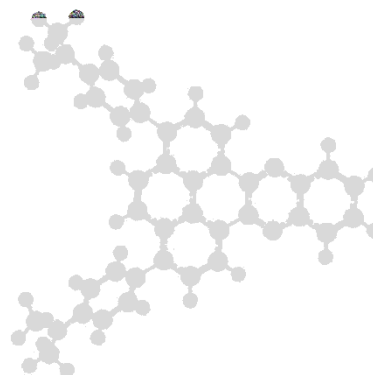


E(RB3LYP) -1685.747766 a.u.
Lowest Vibration 20.6871 cm⁻¹
Imaginary 0
Frequencies

H	-2.669983664	-7.315067487	-8.071872535
H	-1.795930635	-8.796216759	-7.662232073
H	-3.251748980	-8.368598203	-6.774344005
C	-0.086314367	-7.494229714	-6.318439516
H	0.318332898	-7.643782664	-5.315587995
H	0.115939273	-8.393515062	-6.892669625
H	0.457080601	-6.662402475	-6.781690643
C	3.211283643	5.158539471	-6.744819305
H	4.209375363	5.361648656	-7.12167766
H	2.549258087	4.989216596	-7.602196708
H	2.865428941	6.053285345	-6.223880256
C	4.426449793	3.144877612	-5.912310912
H	5.228642710	3.659934854	-6.432469406
H	4.787725032	2.892969855	-4.913394854
H	4.219654920	2.208284908	-6.443206114
C	-1.536497483	0.055279188	-4.060359102
H	-0.748047485	0.32173024	-4.747136789

1,8-Bis(4-*N,N*-dimethylaminophenyl)phenanthro[4,5-*abc*]phenazine **NMe₂quin** in CHCl₃

Atomic Type	X	Y	Z
C	-4.792520842	-3.18266484	-2.4914468
C	-3.67111782	-2.909460385	-3.271292729
C	-3.134452624	-1.593628137	-3.244792011
C	-3.70369731	-0.608572669	-2.386356125
C	-4.832188062	-0.940284263	-1.594084719
C	-5.365681282	-2.22201	-1.673185869
C	-2.064017393	-1.191506828	-4.105098498
C	-3.141397043	0.717092729	-2.335716019
C	-2.014649399	1.04642857	-3.1439561
C	-1.442283291	2.34534296	-3.070590236
C	-2.047234772	3.289442068	-2.244201579
C	-3.158091456	2.982432305	-1.474351436
C	-3.709679128	1.706069669	-1.492983533
C	-4.861892289	1.380259129	-0.659662786
C	-5.422344398	0.05898552	-0.710146281
H	-1.688181593	-1.898519878	-4.828487318
H	-5.207272358	-4.181509021	-2.503052654
H	-6.226271879	-2.46429257	-1.068166575
H	-1.618072646	4.28015785	-2.179816356
H	-3.599155738	3.729172928	-0.831540238
C	-0.230829982	2.737139593	-3.828085864



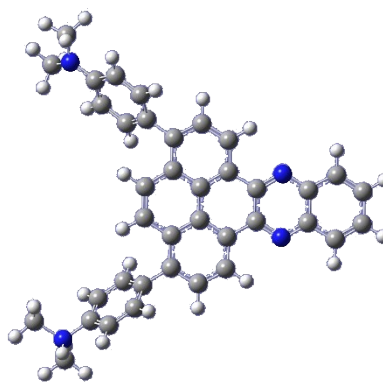
E(RB3LYP) -1685.745841 a.u.
Lowest Vibration 20.5379 cm⁻¹
Imaginary 0
Frequencies

H	0.867956179	5.234638662	-5.851416668
H	2.989468505	1.79719515	-4.355517078
C	-3.089289018	-4.001953277	-4.085414206
C	-1.734903463	-4.348259622	-4.020310855
C	-3.896917715	-4.783757064	-4.918683527
C	-1.211770449	-5.40924061	-4.739286831
H	-1.072101569	-3.788679758	-3.373688097
C	-3.391106267	-5.841727318	-5.654654559
H	-4.948644086	-4.545265443	-5.012605842
C	-2.027883783	-6.197421831	-5.578523823
H	-0.160578115	-5.629422847	-4.638606893
H	-4.063102187	-6.390629554	-6.295533676
N	-5.374482614	2.308939474	0.129019932
N	-6.467320395	-0.267448473	0.030585368
C	-6.440081575	1.986053627	0.888453122
C	-6.997310905	0.672372144	0.838262824
C	-7.019482378	2.951981858	1.747981876
C	-8.117438682	0.363522643	1.649088422
C	-8.101771011	2.622429292	2.519281309
H	-8.543419113	3.360357485	3.175192735
C	-8.65457459	1.31918084	2.469490107
H	-9.50959662	1.082569651	3.088168815
H	-6.583681692	3.941378173	1.772798224
H	-8.525545213	-0.636612955	1.597893672
N	-1.51993408	-7.267586134	-6.280684655
N	3.265671688	4.01482331	-5.850065426
C	-2.350022695	-7.951826889	-7.255483384
H	-2.654308968	-7.299026575	-8.082397551
H	-1.793999539	-8.787712703	-7.670112722
H	-3.253905282	-8.352823137	-6.793160749
C	-0.086256552	-7.49335283	-6.316022424
H	0.316132071	-7.644352963	-5.31247052
H	0.116891851	-8.39254743	-6.890359936
H	0.45944537	-6.661676898	-6.777345448
C	3.206550865	5.148193261	-6.755295965
H	4.204813018	5.354863478	-7.130188339
H	2.548737257	4.968012766	-7.613982113
H	2.853429936	6.045216012	-6.243241769
C	4.425628417	3.143889892	-5.910284384
H	5.228362164	3.658186734	-6.43066992
H	4.786448952	2.894513665	-4.91055718
H	4.220355533	2.205645618	-6.43929763
C	-1.535396536	0.054755923	-4.057491314
H	-0.746481989	0.321582322	-4.743666356

Aniline-Protonated 1,8-Bis(4-*N,N*-dimethylaminophenyl)phenanthro[4,5-*abc*]phenazine NMe₂quin in CH₂Cl₂

Atomic Type	X	Y	Z
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C	-4.253003864	-3.742071376	0.541079496
C	-2.882493436	-3.745813642	0.328277111
C	-2.190146431	-2.557517751	0.127875509
C	-2.891965999	-1.325607944	0.157951155
C	-4.298097079	-1.325330956	0.390542937
C	-4.979259746	-2.556999155	0.560780385
C	-0.748068037	-2.567683369	-0.106550932
C	-2.192701068	-0.081165576	-0.034437109
C	-0.791066809	-0.071726792	-0.246520175
C	-0.051300868	-1.327791901	-0.290284682
C	-0.137754456	1.145087216	-0.409529816
H	0.930110257	1.144393525	-0.567497052
C	-0.840938100	2.339200066	-0.39792192
C	-2.221997761	2.378031355	-0.217658993
C	-2.907033057	1.15146906	-0.000535166
C	-4.301795278	1.107116346	0.314988285
C	-4.960433642	-0.06184181	0.500539454
H	-6.007178070	-0.039790321	0.762952372
H	-4.835255727	2.037779068	0.430531138
H	-4.770989979	-4.682849653	0.669166623
H	-2.337307626	-4.676821137	0.304878774
H	-0.308542749	3.265519516	-0.564963069
C	-2.909183649	3.688791211	-0.265080005
C	-2.430603068	4.776047775	0.475325239
C	-4.008091941	3.931787751	-1.097542942
C	-3.020603101	6.026501941	0.413729583
H	-1.579771910	4.638666683	1.130262312
C	-4.604704956	5.177823386	-1.182798535
H	-4.390495840	3.135491457	-1.722394722
C	-4.139528376	6.266181079	-0.412977978
H	-2.607280757	6.820611303	1.01539069
H	-5.432426391	5.305838903	-1.862471557
C	-6.450568611	-2.637208635	0.752606633
C	-7.339985042	-2.095302831	-0.18280206
C	-6.980292425	-3.31416966	1.854234071
C	-8.712427703	-2.218941274	-0.028013237
H	-6.956302462	-1.584458898	-1.053965384
C	-8.352537309	-3.442796329	2.023607244
H	-6.316525923	-3.736706039	2.594895396
C	-9.202244672	-2.892550803	1.080212122
H	-9.372226466	-1.795902887	-0.771842946
H	-8.743595502	-3.96424697	2.887845956
N	-4.748900347	7.498262433	-0.463245101
N	10.665059120	-3.042025455	1.278263792
C	-5.784892584	7.753117497	-1.448848048
H	-6.174585202	8.75598321	-1.301351971
H	-5.414683812	7.67720422	-2.477988155
H	-6.616381183	7.054987962	-1.337238321
C	-4.134891641	8.636612006	0.198435179
H	-3.149369253	8.881277233	-0.214450834
H	-4.777740063	9.503813714	0.079663152
H	-4.017021626	8.455789088	1.268296441
C	11.313848782	-3.886667614	0.2120123
H	10.805226805	-4.844391582	0.180217403
H	12.360342366	-4.016508675	0.468985229
H	11.220324039	-3.376853943	-0.740073375
C	11.371219227	-1.722909357	1.45542203
H	12.408032119	-1.923099837	1.707213347
H	10.881567781	-1.178610295	2.255724361
H	11.310220212	-1.166808177	0.526801567
N	1.254577895	-1.304693801	-0.498016136

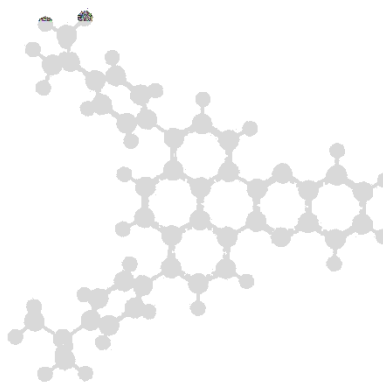


E(RB3LYP) -1686.183847 a.u.
Lowest Vibration 19.7559 cm⁻¹
Imaginary 0
Frequencies

N	-0.109084500	-3.723632477	-0.140830833
C	1.916919392	-2.477013962	-0.533570469
C	3.316875713	-2.496667309	-0.753059815
C	1.221570747	-3.711901466	-0.352005756
C	3.987531012	-3.689401519	-0.789454272
H	3.827505183	-1.553222664	-0.88839209
C	1.945604123	-4.929127664	-0.395603284
C	3.297521019	-4.91406877	-0.609603517
H	5.055826942	-3.704023193	-0.956928914
H	1.402506469	-5.853691597	-0.256113497
H	3.850572798	-5.842765073	-0.642788224
H	10.778000056	-3.548133765	2.156426404

Aniline-Protonated 1,8-Bis(4-*N,N*-dimethylaminophenyl)phenanthro[4,5-*abc*]phenazine NMe₂quin in CHCl₃

Atomic Type	X	Y	Z
C	-4.25043856	-3.742544296	0.548787031
C	-2.880433953	-3.746005565	0.333941022
C	-2.189365225	-2.557317812	0.131594629
C	-2.891284954	-1.325590681	0.161904835
C	-4.297077664	-1.325240347	0.396744221
C	-4.976891178	-2.557436999	0.568279095
C	-0.747596427	-2.567405529	-0.105504712
C	-2.192432415	-0.081351674	-0.032844529
C	-0.79151211	-0.072004921	-0.247881308
C	-0.051689797	-1.327951922	-0.291926265
C	-0.138608455	1.144553138	-0.413673491
H	0.928860691	1.142561908	-0.574363969
C	-0.841785916	2.338673471	-0.401367106
C	-2.222270985	2.377490336	-0.21791544
C	-2.906525442	1.151214806	0.001315729
C	-4.300377623	1.107252874	0.319904035
C	-4.958816716	-0.061510777	0.507667099
H	-6.004566705	-0.038559706	0.774171106
H	-4.83251193	2.038629331	0.436526358
H	-4.768060793	-4.683656454	0.676850966
H	-2.333700724	-4.676071698	0.309595544
H	-0.310305035	3.265104188	-0.570694575
C	-2.910490403	3.687709804	-0.264561276
C	-2.436370492	4.77348179	0.480408771
C	-4.005993092	3.931061566	-1.100948817
C	-3.027575498	6.023271902	0.4189758
H	-1.588118514	4.635282145	1.138494236
C	-4.603517833	5.176641996	-1.186081569
H	-4.383976188	3.13546088	-1.729451353
C	-4.142534667	6.263572219	-0.412309223
H	-2.617293675	6.816631731	1.023659582
H	-5.428006777	5.305646417	-1.869521358
C	-6.447905976	-2.638156386	0.758188307
C	-7.335832228	-2.088500713	-0.174598549
C	-6.981056105	-3.322364754	1.854014235
C	-8.708618079	-2.210116027	-0.022719336
H	-6.94930481	-1.572427487	-1.041350693
C	-8.353832899	-3.450109705	2.020384557



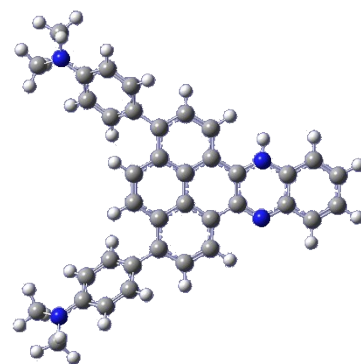
**E(RB3LYP)
Lowest Vibration
Imaginary
Frequencies**

-1686.174744 a.u.
19.0865 cm⁻¹
0

H	-6.318980625	-3.750787983	2.592815504
C	-9.201086981	-2.890579167	1.080192914
H	-9.366275434	-1.779851211	-0.764487971
H	-8.746384085	-3.976765867	2.881182776
N	-4.752798847	7.49589956	-0.463591926
N	-10.66529771	-3.037878504	1.276026764
C	-5.778059459	7.753030516	-1.459297909
H	-6.1647619	8.758022175	-1.318116276
H	-5.398650475	7.673155235	-2.484834372
H	-6.614044445	7.059041326	-1.35403437
C	-4.143881268	8.632831093	0.204730205
H	-3.157488904	8.882252421	-0.203446878
H	-4.788723555	9.498978431	0.088094289
H	-4.029563384	8.447472585	1.274175325
C	-11.31259022	-3.885745414	0.211275227
H	-10.80605748	-4.845001743	0.186480107
H	-12.36111977	-4.011842079	0.462565382
H	-11.21240028	-3.381857561	-0.74332249
C	-11.37098745	-1.718120365	1.450457441
H	-12.40827722	-1.915814108	1.70328665
H	-10.88032829	-1.171531395	2.248673914
H	-11.30996246	-1.16346106	0.520851992
N	1.253745696	-1.30461072	-0.502111855
N	-0.109182984	-3.723638563	-0.139244027
C	1.915714405	-2.476784346	-0.537330463
C	3.315250029	-2.496511754	-0.759640299
C	1.22083467	-3.711816656	-0.352758426
C	3.985704358	-3.689116146	-0.795785046
H	3.82481299	-1.552887644	-0.897185379
C	1.945018331	-4.928992805	-0.39614077
C	3.296280233	-4.913742676	-0.612869447
H	5.053679832	-3.703876687	-0.965444725
H	1.401896284	-5.853127016	-0.254280669
H	3.84958092	-5.842328011	-0.645944067
H	-10.77879042	-3.542059808	2.155148085

**Quinoxaline-Protonated 1,8-Bis(4-*N,N*-dimethylaminophenyl)
phenanthro[4,5-*abc*]phenazine NMe₂quin in CH₂Cl₂**

Atomic Type	X	Y	Z
C	-4.255782224	-3.661759542	0.617889296
C	-2.884088527	-3.676715254	0.431361217
C	-2.182099589	-2.496205547	0.211266893
C	-2.878140775	-1.26030857	0.21029891
C	-4.284428982	-1.249369095	0.431963708
C	-4.989357927	-2.476250131	0.601771958
C	-0.748268683	-2.52166629	-0.010378045
C	-2.171833485	-0.026570485	0.001655039
C	-0.758842103	-0.024469201	-0.20023435
C	-0.063316739	-1.272669336	-0.211662085
C	-0.099483032	1.198926579	-0.372238917
H	0.970153057	1.247854882	-0.522621191
C	-0.795246506	2.386829721	-0.391100685
C	-2.186300485	2.431341198	-0.240359284
C	-2.877356641	1.207637225	0.010044899
C	-4.265296267	1.181544813	0.349724137
C	-4.930701052	0.018520561	0.5499852
H	-5.970260579	0.046737814	0.835788009
H	-4.784666016	2.116771142	0.482906664



E(RB3LYP) -1686.186402 a.u.
Lowest Vibration 21.9148 cm⁻¹

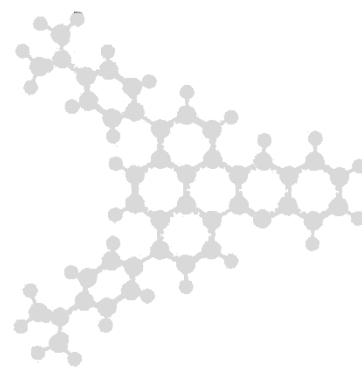
H	-4.778298853	-4.599537332	0.743977202
H	-2.346864488	-4.612845654	0.431614706
H	-0.256892225	3.304603131	-0.576340656
C	-2.860374598	3.72981986	-0.360325092
C	-2.307455293	4.880979537	0.224792214
C	-4.029541990	3.909270611	-1.117563209
C	-2.891055455	6.123898452	0.095443707
H	-1.412023458	4.794721791	0.826000006
C	-4.614613528	5.148215787	-1.279626522
H	-4.469685127	3.065007658	-1.629565565
C	-4.071708388	6.301409155	-0.664676614
H	-2.431664627	6.964441858	0.590828671
H	-5.494786227	5.225304254	-1.898004648
C	-6.455871691	-2.546141673	0.755136369
C	-7.336721721	-1.888113662	-0.113725363
C	-7.034346917	-3.349163706	1.747321177
C	-8.708981845	-2.011855982	-9.73632E-05
H	-6.941389955	-1.290794791	-0.924284533
C	-8.403852154	-3.472469612	1.888328256
H	-6.395275574	-3.876881938	2.44338302
C	-9.291294806	-2.798200559	1.01953383
H	-9.332756528	-1.500930634	-0.716430469
H	-8.786480365	-4.09474742	2.681847037
N	-4.655898203	7.527030558	-0.801403538
N	10.650759685	-2.901784773	1.159272278
C	-5.852325846	7.685112225	-1.61267666
H	-6.175462177	8.7201176	-1.569429944
H	-5.671409237	7.42866658	-2.66062632
H	-6.670239211	7.060432215	-1.246033593
C	-4.046783772	8.703342651	-0.201207456
H	-3.046688720	8.89293496	-0.6013092
H	-4.665117317	9.56953034	-0.413043716
H	-3.965628741	8.603976017	0.883954588
C	11.533854102	-2.283530803	0.185304578
H	11.411756352	-2.709335072	-0.816603791
H	12.563469893	-2.434691813	0.494521966
H	11.360156482	-1.207556847	0.118678704
C	11.216486429	-3.818322318	2.134615293
H	12.298659760	-3.734634037	2.113266161
H	10.950094331	-4.860452368	1.928276734
H	10.883208726	-3.578315939	3.146517411
N	1.262507119	-1.347219969	-0.404875551
N	-0.101678815	-3.671321984	-0.016272336
C	1.973190025	-2.51327618	-0.420493329
C	3.357590607	-2.541408367	-0.629437806
C	1.232562354	-3.705942185	-0.21422135
C	3.998085289	-3.758379036	-0.630114536
H	3.903171263	-1.620987107	-0.788054251
C	1.926082970	-4.93655561	-0.221478322
C	3.282227553	-4.957347038	-0.425523631
H	5.066021706	-3.797332839	-0.790304795
H	1.358589195	-5.842059776	-0.063818935
H	3.813529704	-5.898195793	-0.431577992
H	1.779971509	-0.490587857	-0.549793509

**Imaginary
Frequencies**

0

Quinoxaline-Protonated 1,8-Bis(4-*N,N*-dimethylaminophenyl)
phenanthro[4,5-*abc*]phenazine **NMe₂quin** in CHCl₃

Atomic Type	X	Y	Z
C	-4.25665011	-3.663093116	0.61026472
C	-2.885413555	-3.67797943	0.422211272
C	-2.182670264	-2.496686372	0.207464817
C	-2.878285104	-1.260358644	0.213166616
C	-4.284158423	-1.24962576	0.436178134
C	-4.989959525	-2.477101729	0.600636213
C	-0.749367309	-2.521955735	-0.013947342
C	-2.172021926	-0.026223949	0.009337271
C	-0.758583696	-0.024104008	-0.192192513
C	-0.06379928	-1.271212916	-0.207129015
C	-0.099242505	1.200558933	-0.360783898
H	0.970411479	1.249414624	-0.512773544
C	-0.794312409	2.388110096	-0.37733467
C	-2.186301027	2.432417031	-0.227984669
C	-2.877133927	1.207977315	0.021623052
C	-4.264051656	1.181542257	0.364652051
C	-4.92932371	0.017834728	0.562068328
H	-5.967756804	0.044747406	0.852010996
H	-4.78192772	2.11667341	0.504114351
H	-4.779959585	-4.60105024	0.731377879
H	-2.348370178	-4.614237068	0.416739186
H	-0.256672275	3.30634914	-0.562236913
C	-2.860253426	3.729179338	-0.351565057
C	-2.30474306	4.884442077	0.223795574
C	-4.033102553	3.903905475	-1.104854969
C	-2.888856863	6.12596194	0.089149636
H	-1.407654474	4.802005246	0.82304221
C	-4.618234603	5.141454597	-1.272775223
H	-4.474735965	3.056489077	-1.610187151
C	-4.072478844	6.298617889	-0.667698524
H	-2.427994668	6.969602515	0.577760441
H	-5.500404269	5.214866983	-1.888675546
C	-6.455671598	-2.54654882	0.754459815
C	-7.33636188	-1.879904604	-0.108065267
C	-7.034369034	-3.357343559	1.740319895
C	-8.708365494	-2.00294871	0.005579447
H	-6.940736688	-1.277277883	-0.91452795
C	-8.403553951	-3.479598229	1.881568878
H	-6.395422363	-3.891071315	2.431863092
C	-9.290697752	-2.79706049	1.019046951
H	-9.332139745	-1.486107334	-0.706457344
H	-8.786478745	-4.107581591	2.670388092
N	-4.656429867	7.523182933	-0.810848911
N	-10.65005439	-2.900591508	1.158597927
C	-5.85528738	7.676456786	-1.619606395
H	-6.177171065	8.712105039	-1.583299423
H	-5.677495734	7.412093696	-2.666073085
H	-6.672734657	7.055642108	-1.245566714
C	-4.04598239	8.703407919	-0.219491354
H	-3.048021497	8.892096988	-0.625234924
H	-4.66629027	9.56780004	-0.432953137
H	-3.960331054	8.609636865	0.865752836

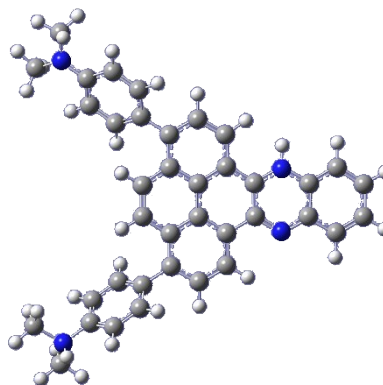


E(RB3LYP) -1686.180359 a.u.
Lowest Vibration 21.6172 cm⁻¹
Imaginary 0
Frequencies

C	-11.5331446	-2.271019161	0.19214256
H	-11.41326449	-2.687156551	-0.814089822
H	-12.56274248	-2.423137324	0.501044201
H	-11.35757726	-1.194708883	0.136220824
C	-11.21639489	-3.823110132	2.127839138
H	-12.29849524	-3.737506115	2.108369151
H	-10.95205212	-4.864129579	1.913567068
H	-10.8818045	-3.590754905	3.141091778
N	1.263704554	-1.345189767	-0.395875055
N	-0.102480092	-3.671464133	-0.025298333
C	1.974518581	-2.512098702	-0.417307571
C	3.359070305	-2.539765035	-0.622846231
C	1.232517064	-3.705331745	-0.220952733
C	3.999467979	-3.757255517	-0.630004689
H	3.90621263	-1.618830158	-0.77487668
C	1.925445505	-4.935945058	-0.234790226
C	3.282414365	-4.956580931	-0.435434093
H	5.067802855	-3.795497098	-0.787839123
H	1.356580125	-5.841854276	-0.084714119
H	3.812779349	-5.897923212	-0.446407464
H	1.781645272	-0.48757611	-0.531010031

Quinoxaline & Aniline-Protonated 1,8-Bis(4-*N,N*-dimethylaminophenyl)
phenanthro[4,5-*abc*]phenazine **NMe₂quin** in CH₂Cl₂

Atomic Type	X	Y	Z
C	-4.25406813	-3.729971984	0.496336953
C	-2.882773047	-3.732945053	0.284969498
C	-2.191640195	-2.54097966	0.114680605
C	-2.887965407	-1.30732529	0.170446639
C	-4.292943643	-1.309552299	0.402103934
C	-4.976595788	-2.544945268	0.544198114
C	-0.753218904	-2.549423004	-0.112427868
C	-2.187031328	-0.064046937	0.006249937
C	-0.773752983	-0.048329924	-0.190792532
C	-0.073667743	-1.291911303	-0.255184364
C	-0.120376125	1.184513942	-0.309247786
H	0.949756177	1.24471897	-0.451150394
C	-0.822018657	2.368533234	-0.285691236
C	-2.214953736	2.401123135	-0.146524441
C	-2.89970093	1.164373045	0.054561636
C	-4.291108678	1.119431625	0.379898239
C	-4.952349097	-0.050878754	0.54539153
H	-5.996043004	-0.03254185	0.818516475
H	-4.818016058	2.04797265	0.528367696
H	-4.773038888	-4.6722593	0.602961861
H	-2.341975301	-4.66558754	0.240961285



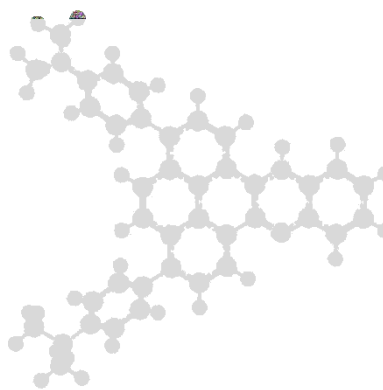
E(RB3LYP) -1686.615324 a.u.
Lowest Vibration 18.9824 cm⁻¹
Imaginary 0
Frequencies

H	-5.518880082	5.235785846	-1.740638024
C	-6.44826878	-2.625080391	0.73708309
C	-7.335789478	-2.071023279	-0.192010374
C	-6.975108184	-3.314914612	1.831438696
C	-8.708126706	-2.199317609	-0.03906165
H	-6.952927517	-1.549169068	-1.057013342
C	-8.347263819	-3.445554702	1.999392117
H	-6.311111344	-3.746667326	2.56654332
C	-9.197104225	-2.887110864	1.06070625
H	-9.368101777	-1.768276784	-0.77793411
H	-8.737554896	-3.977172823	2.857602603
N	-4.695830444	7.502658514	-0.562500572
N	-10.6594921	-3.046633848	1.252580581
C	-5.881552784	7.685936828	-1.384740824
H	-6.207815281	8.718095483	-1.310498017
H	-5.685072531	7.465863658	-2.438042474
H	-6.702543912	7.047458773	-1.050587842
C	-4.093098944	8.6619215	0.077502031
H	-3.092402237	8.867657769	-0.312607076
H	-4.714115931	9.531931893	-0.108811417
H	-4.01624092	8.527459983	1.158957565
C	-11.29767291	-3.892506634	0.17994554
H	-10.782623	-4.846862141	0.147840403
H	-12.34418366	-4.030207664	0.432388501
H	-11.2037334	-3.378942667	-0.770061785
C	-11.37640611	-1.733314184	1.432435221
H	-12.4116493	-1.94332967	1.682608663
H	-10.89253912	-1.187409485	2.23510638
H	-11.31978594	-1.174218054	0.505383297
N	1.253372603	-1.355100874	-0.450187551
N	-0.108177162	-3.695633354	-0.17273794
C	1.964519146	-2.517508893	-0.521162767
C	3.348950287	-2.535229511	-0.731855753
C	1.225782082	-3.720884423	-0.372484097
C	3.988414989	-3.750957063	-0.790665416
H	3.894652363	-1.608650798	-0.847780316
C	1.918413097	-4.950024481	-0.438759815
C	3.274021609	-4.959853058	-0.643619072
H	5.056268092	-3.781960888	-0.953142122
H	1.350925066	-5.861951766	-0.32475269
H	3.806720188	-5.898376833	-0.695110091
H	-10.77317288	-3.557381375	2.127963286
H	1.769983074	-0.491828159	-0.55407208

Quinoxaline & Aniline-Protonated 1,8-Bis(4-*N,N*-dimethylaminophenyl)
phenanthro[4,5-*abc*]phenazine **NMe₂quin** in CHCl₃

Atomic Type	X	Y	Z
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C	-4.246209312	-3.736569488	0.503360423
C	-2.875141101	-3.737366138	0.289360731
C	-2.186126489	-2.544100298	0.120378954
C	-2.883611341	-1.31127666	0.181619563
C	-4.288226568	-1.315665833	0.415540642
C	-4.970052742	-2.552691741	0.554389301
C	-0.747937483	-2.550244565	-0.110654422
C	-2.184310431	-0.066829187	0.019948822
C	-0.770717206	-0.049488065	-0.177293066
C	-0.070000933	-1.29090653	-0.247233174
C	-0.119118662	1.18559055	-0.291220115
H	0.95118428	1.247367514	-0.433088528
C	-0.821414499	2.368334854	-0.265668104
C	-2.215630189	2.399278794	-0.13043705
C	-2.897990662	1.16041911	0.070795616
C	-4.288251993	1.113396219	0.399712226
C	-4.948119251	-0.057942296	0.563954101
H	-5.990840594	-0.040669598	0.840845495
H	-4.814555487	2.04144994	0.553084437
H	-4.763465463	-4.680067887	0.608136845
H	-2.332925824	-4.669056996	0.241658926
H	-0.287684629	3.295931216	-0.410020006
C	-2.896551655	3.69350157	-0.217427669
C	-2.349361562	4.834355406	0.395532239
C	-4.065929326	3.88572645	-0.972953169
C	-2.938550636	6.075700535	0.295157302
H	-1.45522853	4.738774022	0.997070718
C	-4.655532439	5.124671747	-1.107510147
H	-4.497872622	3.053438574	-1.510914838
C	-4.118870663	6.266152538	-0.46397605
H	-2.483903097	6.90639919	0.810751909
H	-5.531588648	5.213609161	-1.729953845
C	-6.442538105	-2.633043713	0.74200537
C	-7.323471164	-2.072995259	-0.189802144
C	-6.978398343	-3.324712195	1.830917383
C	-8.697116418	-2.193925745	-0.044084569
H	-6.933430805	-1.55046602	-1.051154574
C	-8.352309881	-3.448911554	1.991632233
H	-6.320607403	-3.762536807	2.568063504
C	-9.195333683	-2.882632618	1.050923408
H	-9.349110203	-1.754756346	-0.784678218
H	-8.748273441	-3.98078932	2.847500333
N	-4.706029527	7.490743796	-0.574423729
N	-10.66027321	-3.030343215	1.241938793
C	-5.895854284	7.665910295	-1.392935781
H	-6.22155968	8.698773208	-1.327803532
H	-5.703615388	7.435417583	-2.44464557
H	-6.715285466	7.031133738	-1.048230258
C	-4.104672021	8.656333073	0.056322585
H	-3.108096561	8.865453839	-0.342084556
H	-4.731609852	9.52217949	-0.129293355
H	-4.020206706	8.526604545	1.137649831
C	-11.31469963	-3.864670311	0.168875505
H	-10.78773055	-4.810949731	0.103826359
H	-12.35216291	-4.02315262	0.446497216
H	-11.25753723	-3.331570476	-0.773587538
C	-11.36464475	-1.711662763	1.434948749
H	-12.40093758	-1.912148167	1.690153063
H	-10.87085727	-1.174693481	2.237609295
H	-11.30836718	-1.147441162	0.510818626
N	1.258283492	-1.352418421	-0.442408361



E(RB3LYP) -1686.596885 a.u.
Lowest Vibration 10.4684 cm⁻¹
Imaginary 0
Frequencies

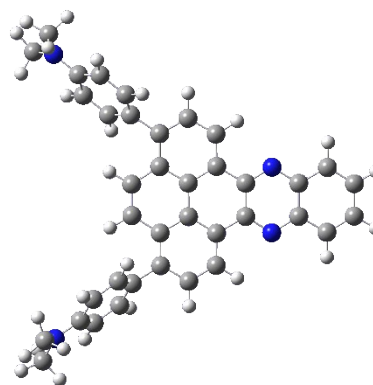
N	-0.102289582	-3.695369508	-0.178548042
C	1.970221549	-2.514626209	-0.521803223
C	3.353980063	-2.530848619	-0.734560879
C	1.23180121	-3.719103078	-0.380385463
C	3.99387632	-3.74629019	-0.802378025
H	3.899901687	-1.603543668	-0.846360603
C	1.924406739	-4.947403732	-0.455957533
C	3.279955561	-4.955946827	-0.662708961
H	5.061499413	-3.775794118	-0.966810227
H	1.356753663	-5.859915222	-0.347843819
H	3.812452891	-5.894138284	-0.72157891
H	-10.77435551	-3.545860356	2.114223192
H	1.774222256	-0.488178562	-0.539159351

Section 2 Full Specifications for Crystal Packing Calculations

DFT Simulations were performed on the crystal structures of the two polymorphs of **NMe₂quin** to compare the relative energies of intermolecular (i.e. dispersive) interactions. Cartesian coordinates were extracted from the crystal structures and all C-H bonds lengths were manually set to those obtained of a single molecule of **NMe₂quin** at the B3LYP/cc-pVTZ level. The structures were not optimized *in-silico* but left frozen to acquire the best simulation of a collective of molecules in the crystal structures. Energy calculations were performed using the 6-311G++(d,p) basis set to adequately model dispersive interactions with lesser computational cost than cc-pVTZ. The energies of the crystal structures were obtained using multiple functionals that include Grimme's empirical dispersion with Becke-Johnson damping, if implemented: B3LYP-D3(BJ), B97-D3(BJ), ω B97X-D2, and M06-2X-D2. The crystal structure energies were then compared to multiple times the individual molecule energies, at the same level of theory, and the difference was assumed to represent the stabilization incurred from dispersive intermolecular interactions. Such comparison is summed in a table, below.

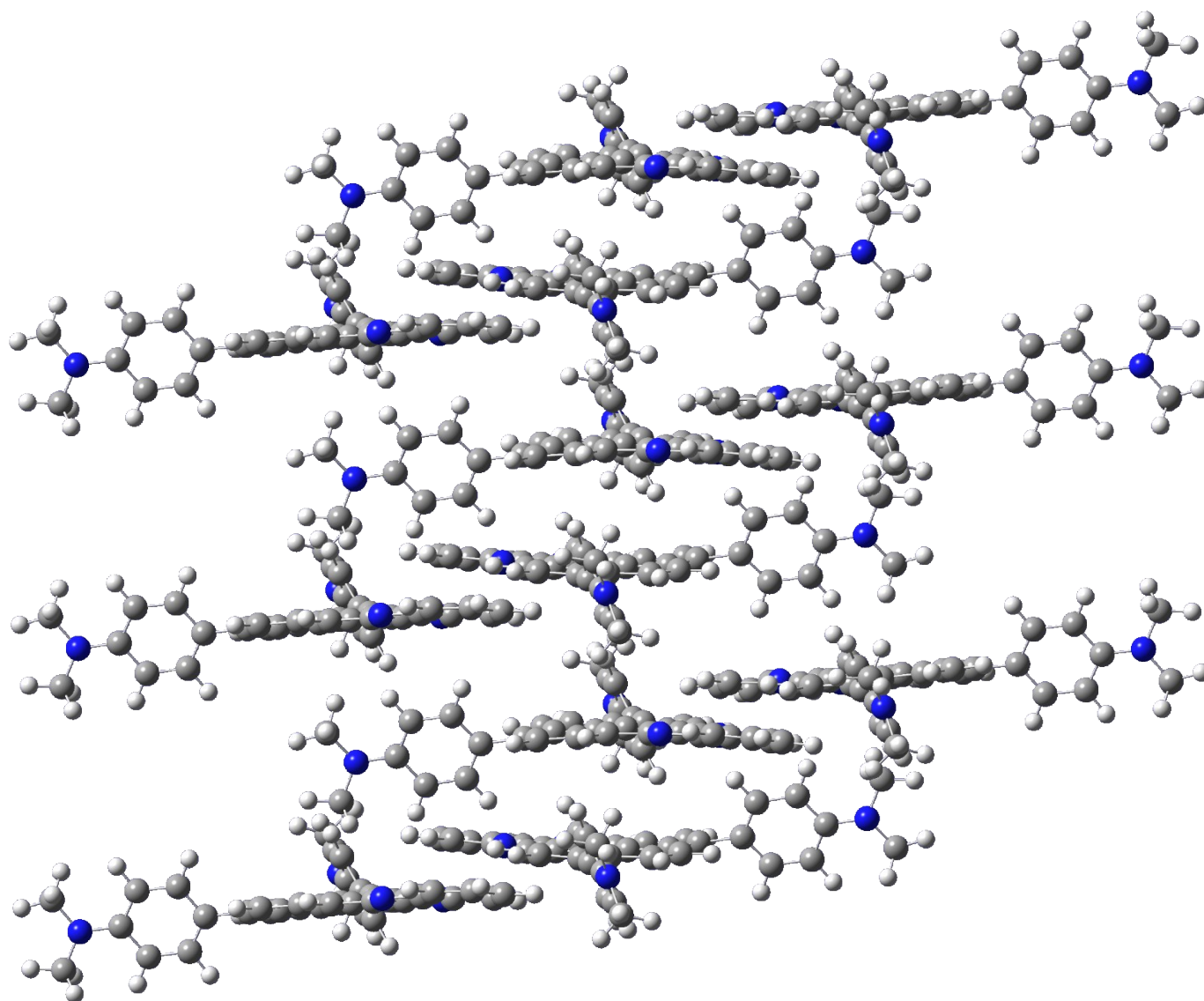
1,8-Bis(4-*N,N*-dimethylaminophenyl)phenanthro[4,5-*abc*]phenazine **NMe₂quin** in Polymorph **NMe₂quin-grou**

Atomic Type	X	Y	Z
N	4.836	14.3641	12.0124
N	4.7778	14.3113	9.185
N	3.9535	4.8752	16.7165
N	5.8187	4.8569	4.5079
C	4.7863	15.5209	11.2868
C	4.7891	16.7644	11.9519
H	4.8837	16.8061	13.0284
C	4.6707	17.9171	11.2285
H	4.6747	18.8713	11.7376
C	4.5448	17.8809	9.8309
H	4.4192	18.806	9.2848
C	4.5776	16.7021	9.1516
H	4.4978	16.6956	8.0731
C	4.7173	15.4828	9.862
C	5.2017	9.4528	7.833
C	4.8542	13.2238	11.3311
C	4.8483	11.9618	12.0769
C	4.7423	11.9572	13.4592



H	4.7262	12.8933	13.9966
C	4.7157	9.532	13.5075
C	4.9148	9.5128	12.1045
C	5.0709	8.2873	11.3805
H	5.094	7.3548	11.9229
C	5.154	9.4757	9.2512
C	5.0848	10.6521	7.1438
H	5.0849	10.64	6.0623
C	4.9671	11.8692	7.8077
H	4.8854	12.7816	7.2365
C	4.9539	11.9261	9.1986
C	4.8668	13.1981	9.901
C	5.0254	10.7177	9.9366
C	4.5396	8.2826	14.2982
C	5.4753	7.8966	15.2553
H	6.3694	8.4918	15.3851
C	5.2958	6.7755	16.0445
H	6.0545	6.5023	16.761
C	4.1414	5.9889	15.9275
C	3.1851	6.387	14.9751
H	2.2742	5.8196	14.8653
C	3.3989	7.4966	14.1782
H	2.6553	7.7617	13.4375
C	4.9224	4.5073	17.7041
H	5.9056	4.4251	17.2377
H	4.6477	3.5465	18.1427
H	4.9528	5.2676	18.4864
C	2.6567	4.2283	16.7763
H	1.9085	4.9444	17.1203
H	2.7014	3.3879	17.471
H	2.3846	3.8657	15.7836
C	5.3431	8.1924	7.0517
C	6.4953	7.4117	7.0864
H	7.2862	7.673	7.7768
C	6.6584	6.3159	6.2672
H	7.5726	5.7458	6.3198
C	5.6529	5.928	5.364
C	4.4796	6.6997	5.3449
H	3.6735	6.4257	4.6826
C	4.344	7.8057	6.1631
H	3.4329	8.388	6.1114
C	7.083	4.1725	4.4328
H	7.8739	4.8903	4.2085
H	7.0424	3.4175	3.6459
H	7.2917	3.6889	5.3886
C	4.7575	4.4556	3.6208
H	3.8406	4.309	4.1941
H	5.0303	3.5216	3.1266
H	4.5974	5.2313	2.8701
C	4.6567	10.7632	14.1586
H	4.5424	10.7875	15.2338
C	5.1909	8.27	10.0309
H	5.3173	7.3239	9.5277
C	4.9401	10.7394	11.3789

1,8-Bis(4-*N,N*-dimethylaminophenyl)phenanthro[4,5-*abc*]phenazine **NMe₂quin** in Polymorph
NMe₂quin-grou



Atomic Type	X	Y	Z
N	4.836	14.3641	12.0124
N	4.7778	14.3113	9.185
N	3.9535	4.8752	16.7165
N	5.8187	4.8569	4.5079
C	4.7863	15.5209	11.2868
C	4.7891	16.7644	11.9519
H	4.88373871	16.80614568	13.02830153
C	4.6707	17.9171	11.2285
H	4.6746841	18.87146222	11.73766772
C	4.5448	17.8809	9.8309
H	4.4191684	18.80610899	9.28474992
C	4.5776	16.7021	9.1516
H	4.49784109	16.69561461	8.07320494
C	4.7173	15.4828	9.862

C	5.2017	9.4528	7.833
C	4.8542	13.2238	11.3311
C	4.8483	11.9618	12.0769
C	4.7423	11.9572	13.4592
H	4.72616311	12.89336673	13.9966038
C	4.7157	9.532	13.5075
C	4.9148	9.5128	12.1045
C	5.0709	8.2873	11.3805
H	5.09395757	7.35466087	11.92297771
C	5.154	9.4757	9.2512
C	5.0848	10.6521	7.1438
H	5.08491385	10.64003148	6.06218733
C	4.9671	11.8692	7.8077
H	4.88540201	12.78162678	7.23649584
C	4.9539	11.9261	9.1986
C	4.8668	13.1981	9.901
C	5.0254	10.7177	9.9366
C	4.5396	8.2826	14.2982
C	5.4753	7.8966	15.2553
H	6.3699	8.4921	15.3852
C	5.2958	6.7755	16.0445
H	6.0545	6.5023	16.761
C	4.1414	5.9889	15.9275
C	3.1851	6.387	14.9751
H	2.2742	5.8196	14.8653
C	3.3989	7.4966	14.1782
H	2.6557	7.7616	13.4379
C	4.9224	4.5073	17.7041
H	5.9056	4.4251	17.2377
H	4.6477	3.5465	18.1427
H	4.9528	5.2676	18.4864
C	2.6567	4.2283	16.7763
H	1.9085	4.9444	17.1203
H	2.7014	3.3879	17.471
H	2.3846	3.8657	15.7836
C	5.3431	8.1924	7.0517
C	6.4953	7.4117	7.0864
H	7.2867	7.6732	7.7772
C	6.6584	6.3159	6.2672
H	7.5726	5.7457	6.3198
C	5.6529	5.928	5.364
C	4.4796	6.6997	5.3449
H	3.6735	6.4257	4.6826
C	4.344	7.8057	6.1631
H	3.4334	8.3877	6.1114
C	7.083	4.1725	4.4328
H	7.8739	4.8903	4.2085
H	7.0424	3.4175	3.6459
H	7.2917	3.6889	5.3886
C	4.7575	4.4556	3.6208
H	3.8406	4.309	4.1941
H	5.0303	3.5216	3.1266
H	4.5974	5.2313	2.8701
C	4.6567	10.7632	14.1586
H	4.54237877	10.78745341	15.23394834
C	5.1909	8.27	10.0309
H	5.31734433	7.32376927	9.52762204
C	4.9401	10.7394	11.3789
N	14.2001	14.3641	12.0124
N	14.1419	14.3113	9.185
N	13.3176	4.8752	16.7165

N	15.1828	4.8569	4.5079
C	14.1504	15.5209	11.2868
C	14.1532	16.7644	11.9519
H	14.24783871	16.80614568	13.02830153
C	14.0348	17.9171	11.2285
H	14.0387841	18.87146222	11.73766772
C	13.9089	17.8809	9.8309
H	13.7832684	18.80610899	9.28474992
C	13.9417	16.7021	9.1516
H	13.86194109	16.69561461	8.07320494
C	14.0814	15.4828	9.862
C	14.5658	9.4528	7.833
C	14.2183	13.2238	11.3311
C	14.2124	11.9618	12.0769
C	14.1064	11.9572	13.4592
H	14.09026311	12.89336673	13.9966038
C	14.0798	9.532	13.5075
C	14.2789	9.5128	12.1045
C	14.435	8.2873	11.3805
H	14.45805757	7.35466087	11.92297771
C	14.5181	9.4757	9.2512
C	14.4489	10.6521	7.1438
H	14.44901385	10.64003148	6.06218733
C	14.3312	11.8692	7.8077
H	14.24950201	12.78162678	7.23649584
C	14.318	11.9261	9.1986
C	14.2309	13.1981	9.901
C	14.3895	10.7177	9.9366
C	13.9037	8.2826	14.2982
C	14.8394	7.8966	15.2553
H	15.734	8.4921	15.3852
C	14.6599	6.7755	16.0445
H	15.4186	6.5023	16.761
C	13.5055	5.9889	15.9275
C	12.5492	6.387	14.9751
H	11.6383	5.8196	14.8653
C	12.763	7.4966	14.1782
H	12.0198	7.7616	13.4379
C	14.2865	4.5073	17.7041
H	15.2697	4.4251	17.2377
H	14.0118	3.5465	18.1427
H	14.3169	5.2676	18.4864
C	12.0208	4.2283	16.7763
H	11.2726	4.9444	17.1203
H	12.0655	3.3879	17.471
H	11.7487	3.8657	15.7836
C	14.7072	8.1924	7.0517
C	15.8594	7.4117	7.0864
H	16.6508	7.6732	7.7772
C	16.0225	6.3159	6.2672
H	16.9367	5.7457	6.3198
C	15.017	5.928	5.364
C	13.8437	6.6997	5.3449
H	13.0376	6.4257	4.6826
C	13.7081	7.8057	6.1631
H	12.7975	8.3877	6.1114
C	16.4471	4.1725	4.4328
H	17.238	4.8903	4.2085
H	16.4065	3.4175	3.6459
H	16.6558	3.6889	5.3886
C	14.1216	4.4556	3.6208

H	13.2047	4.309	4.1941
H	14.3944	3.5216	3.1266
H	13.9615	5.2313	2.8701
C	14.0208	10.7632	14.1586
H	13.90647877	10.78745341	15.23394834
C	14.555	8.27	10.0309
H	14.68144433	7.32376927	9.52762204
C	14.3042	10.7394	11.3789
N	23.5642	14.3641	12.0124
N	23.506	14.3113	9.185
N	22.6817	4.8752	16.7165
N	24.5469	4.8569	4.5079
C	23.5145	15.5209	11.2868
C	23.5173	16.7644	11.9519
H	23.61193871	16.80614568	13.02830153
C	23.3989	17.9171	11.2285
H	23.4028841	18.87146222	11.73766772
C	23.273	17.8809	9.8309
H	23.1473684	18.80610899	9.28474992
C	23.3058	16.7021	9.1516
H	23.22604109	16.69561461	8.07320494
C	23.4455	15.4828	9.862
C	23.9299	9.4528	7.833
C	23.5824	13.2238	11.3311
C	23.5765	11.9618	12.0769
C	23.4705	11.9572	13.4592
H	23.45436311	12.89336673	13.9966038
C	23.4439	9.532	13.5075
C	23.643	9.5128	12.1045
C	23.7991	8.2873	11.3805
H	23.82215757	7.35466087	11.92297771
C	23.8822	9.4757	9.2512
C	23.813	10.6521	7.1438
H	23.81311385	10.64003148	6.06218733
C	23.6953	11.8692	7.8077
H	23.61360201	12.78162678	7.23649584
C	23.6821	11.9261	9.1986
C	23.595	13.1981	9.901
C	23.7536	10.7177	9.9366
C	23.2678	8.2826	14.2982
C	24.2035	7.8966	15.2553
H	25.0981	8.4921	15.3852
C	24.024	6.7755	16.0445
H	24.7827	6.5023	16.761
C	22.8696	5.9889	15.9275
C	21.9133	6.387	14.9751
H	21.0024	5.8196	14.8653
C	22.1271	7.4966	14.1782
H	21.3839	7.7616	13.4379
C	23.6506	4.5073	17.7041
H	24.6338	4.4251	17.2377
H	23.3759	3.5465	18.1427
H	23.681	5.2676	18.4864
C	21.3849	4.2283	16.7763
H	20.6367	4.9444	17.1203
H	21.4296	3.3879	17.471
H	21.1128	3.8657	15.7836
C	24.0713	8.1924	7.0517
C	25.2235	7.4117	7.0864
H	26.0149	7.6732	7.7772
C	25.3866	6.3159	6.2672

H	26.3008	5.7457	6.3198
C	24.3811	5.928	5.364
C	23.2078	6.6997	5.3449
H	22.4017	6.4257	4.6826
C	23.0722	7.8057	6.1631
H	22.1616	8.3877	6.1114
C	25.8112	4.1725	4.4328
H	26.6021	4.8903	4.2085
H	25.7706	3.4175	3.6459
H	26.0199	3.6889	5.3886
C	23.4857	4.4556	3.6208
H	22.5688	4.309	4.1941
H	23.7585	3.5216	3.1266
H	23.3256	5.2313	2.8701
C	23.3849	10.7632	14.1586
H	23.27057877	10.78745341	15.23394834
C	23.9191	8.27	10.0309
H	24.04554433	7.32376927	9.52762204
C	23.6683	10.7394	11.3789
N	-0.6127	5.736	13.5223
N	-0.5545	5.6832	16.3497
N	0.2698	-3.7529	8.8182
N	-1.5954	-3.7712	21.0268
C	-0.563	6.8928	14.2479
C	-0.5658	8.1363	13.5828
H	-0.66043871	8.17804568	12.50639847
C	-0.4474	9.289	14.3062
H	-0.4513841	10.24336222	13.79703228
C	-0.3215	9.2528	15.7038
H	-0.1958684	10.17800899	16.24995008
C	-0.3543	8.074	16.3831
H	-0.27465425	8.06751456	17.46150342
C	-0.4941	6.8547	15.6727
C	-0.9784	0.8247	17.7017
C	-0.6309	4.5957	14.2036
C	-0.625	3.3337	13.4578
C	-0.519	3.3291	12.0755
H	-0.50286311	4.26526673	11.5380962
C	-0.4924	0.9039	12.0272
C	-0.6915	0.8847	13.4302
C	-0.8476	-0.3408	14.1542
H	-0.87065757	-1.27343913	13.61172229
C	-0.9307	0.8476	16.2835
C	-0.8615	2.024	18.3909
H	-0.86172771	2.01193148	19.47251265
C	-0.7438	3.2411	17.727
H	-0.66210201	4.15352678	18.29820416
C	-0.7306	3.298	16.3361
C	-0.6435	4.57	15.6337
C	-0.8021	2.0896	15.5981
C	-0.3163	-0.3455	11.2365
C	-1.252	-0.7315	10.2794
H	-2.1462	-0.1364	10.1496
C	-1.0725	-1.8526	9.4902
H	-1.8312	-2.1258	8.7737
C	0.0819	-2.6392	9.6072
C	1.0382	-2.2411	10.5596
H	1.9491	-2.8085	10.6694
C	0.8244	-1.1315	11.3565
H	1.568	-0.8664	12.0971
C	-0.6991	-4.1208	7.8306

H	-1.6823	-4.203	8.297
H	-0.4245	-5.0816	7.392
H	-0.7295	-3.3605	7.0483
C	1.5666	-4.3998	8.7584
H	2.3148	-3.6837	8.4144
H	1.5219	-5.2402	8.0637
H	1.8387	-4.7624	9.7511
C	-1.1198	-0.4357	18.483
C	-2.2721	-1.2164	18.4483
H	-3.063	-0.955	17.7578
C	-2.4351	-2.3122	19.2675
H	-3.3493	-2.8824	19.2149
C	-1.4296	-2.7001	20.1707
C	-0.2564	-1.9284	20.1898
H	0.5498	-2.2024	20.8521
C	-0.1207	-0.8224	19.3716
H	0.7903	-0.2401	19.4233
C	-2.8597	-4.4556	21.1019
H	-3.6506	-3.7378	21.3262
H	-2.8191	-5.2106	21.8888
H	-3.0684	-4.9392	20.1461
C	-0.5342	-4.1725	21.9139
H	0.3827	-4.3191	21.3406
H	-0.8071	-5.1064	22.4081
H	-0.3741	-3.3968	22.6646
C	-0.4334	2.1351	11.376
H	-0.3190668	2.15935595	10.30065299
C	-0.9676	-0.3581	15.5038
H	-1.09415637	-1.30431906	16.00707175
C	-0.7168	2.1113	14.1558
N	8.7514	5.736	13.5223
N	8.8096	5.6832	16.3497
N	9.6339	-3.7529	8.8182
N	7.7687	-3.7712	21.0268
C	8.8011	6.8928	14.2479
C	8.7983	8.1363	13.5828
H	8.70366129	8.17804568	12.50639847
C	8.9167	9.289	14.3062
H	8.9127159	10.24336222	13.79703228
C	9.0426	9.2528	15.7038
H	9.1682316	10.17800899	16.24995008
C	9.0098	8.074	16.3831
H	9.08944575	8.06751456	17.46150342
C	8.87	6.8547	15.6727
C	8.3857	0.8247	17.7017
C	8.7332	4.5957	14.2036
C	8.7391	3.3337	13.4578
C	8.8451	3.3291	12.0755
H	8.86123689	4.26526673	11.5380962
C	8.8717	0.9039	12.0272
C	8.6726	0.8847	13.4302
C	8.5165	-0.3408	14.1542
H	8.49344243	-1.27343913	13.61172229
C	8.4334	0.8476	16.2835
C	8.5026	2.024	18.3909
H	8.50237229	2.01193148	19.47251265
C	8.6203	3.2411	17.727
H	8.70199799	4.15352678	18.29820416
C	8.6335	3.298	16.3361
C	8.7206	4.57	15.6337
C	8.562	2.0896	15.5981

C	9.0478	-0.3455	11.2365
C	8.1121	-0.7315	10.2794
H	7.2179	-0.1364	10.1496
C	8.2916	-1.8526	9.4902
H	7.5329	-2.1258	8.7737
C	9.446	-2.6392	9.6072
C	10.4023	-2.2411	10.5596
H	11.3132	-2.8085	10.6694
C	10.1885	-1.1315	11.3565
H	10.9321	-0.8664	12.0971
C	8.665	-4.1208	7.8306
H	7.6818	-4.203	8.297
H	8.9396	-5.0816	7.392
H	8.6346	-3.3605	7.0483
C	10.9307	-4.3998	8.7584
H	11.6789	-3.6837	8.4144
H	10.886	-5.2402	8.0637
H	11.2028	-4.7624	9.7511
C	8.2443	-0.4357	18.483
C	7.092	-1.2164	18.4483
H	6.3011	-0.955	17.7578
C	6.929	-2.3122	19.2675
H	6.0148	-2.8824	19.2149
C	7.9345	-2.7001	20.1707
C	9.1077	-1.9284	20.1898
H	9.9139	-2.2024	20.8521
C	9.2434	-0.8224	19.3716
H	10.1544	-0.2401	19.4233
C	6.5044	-4.4556	21.1019
H	5.7135	-3.7378	21.3262
H	6.545	-5.2106	21.8888
H	6.2957	-4.9392	20.1461
C	8.8299	-4.1725	21.9139
H	9.7468	-4.3191	21.3406
H	8.557	-5.1064	22.4081
H	8.99	-3.3968	22.6646
C	8.9307	2.1351	11.376
H	9.0450332	2.15935595	10.30065299
C	8.3965	-0.3581	15.5038
H	8.26994363	-1.30431906	16.00707175
C	8.6473	2.1113	14.1558
N	18.1155	5.736	13.5223
N	18.1737	5.6832	16.3497
N	18.998	-3.7529	8.8182
N	17.1328	-3.7712	21.0268
C	18.1652	6.8928	14.2479
C	18.1624	8.1363	13.5828
H	18.06776129	8.17804568	12.50639847
C	18.2808	9.289	14.3062
H	18.2768159	10.24336222	13.79703228
C	18.4067	9.2528	15.7038
H	18.5323316	10.17800899	16.24995008
C	18.3739	8.074	16.3831
H	18.45354575	8.06751456	17.46150342
C	18.2341	6.8547	15.6727
C	17.7498	0.8247	17.7017
C	18.0973	4.5957	14.2036
C	18.1032	3.3337	13.4578
C	18.2092	3.3291	12.0755
H	18.22533689	4.26526673	11.5380962
C	18.2358	0.9039	12.0272

C	18.0367	0.8847	13.4302
C	17.8806	-0.3408	14.1542
H	17.85754243	-1.27343913	13.61172229
C	17.7975	0.8476	16.2835
C	17.8667	2.024	18.3909
H	17.86647229	2.01193148	19.47251265
C	17.9844	3.2411	17.727
H	18.06609799	4.15352678	18.29820416
C	17.9976	3.298	16.3361
C	18.0847	4.57	15.6337
C	17.9261	2.0896	15.5981
C	18.4119	-0.3455	11.2365
C	17.4762	-0.7315	10.2794
H	16.582	-0.1364	10.1496
C	17.6557	-1.8526	9.4902
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C	19.7664	-2.2411	10.5596
H	20.6773	-2.8085	10.6694
C	19.5526	-1.1315	11.3565
H	20.2962	-0.8664	12.0971
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H	18.3037	-5.0816	7.392
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C	16.2931	-2.3122	19.2675
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H	19.278	-2.2024	20.8521
C	18.6075	-0.8224	19.3716
H	19.5185	-0.2401	19.4233
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H	15.0776	-3.7378	21.3262
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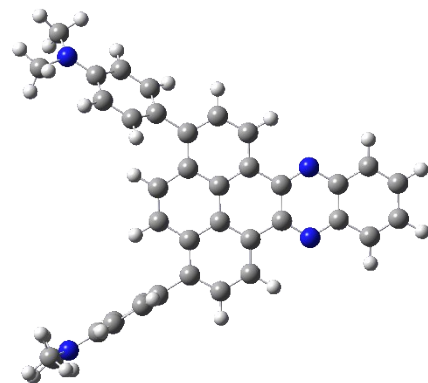
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H	26.8117	17.3922	6.8737
C	25.7376	19.1088	7.5329
H	26.4963	19.382	8.2494
C	24.5832	19.8954	7.416
C	23.6269	19.4973	6.4635
H	22.716	20.0647	6.3537
C	23.8407	18.3877	5.6667
H	23.0975	18.1227	4.9264
C	25.3642	21.377	9.1925
H	26.3474	21.4592	8.7261
H	25.0895	22.3378	9.6311
H	25.3946	20.6167	9.9748
C	23.0985	21.656	8.2647
H	22.3503	20.9399	8.6087
H	23.1432	22.4964	8.9594
H	22.8263	22.0186	7.272
C	25.7849	17.6919	-1.4599
C	26.9372	18.4726	-1.4252
H	27.7285	18.2111	-0.7344
C	27.1002	19.5684	-2.2443
H	28.0144	20.1386	-2.1918
C	26.0947	19.9563	-3.1476
C	24.9215	19.1846	-3.1666
H	24.1154	19.4586	-3.829
C	24.7858	18.0786	-2.3485
H	23.8752	17.4966	-2.4002
C	27.5248	21.7118	-4.0787
H	28.3156	20.994	-4.3031
H	27.4842	22.4667	-4.8657
H	27.7336	22.1954	-3.1229
C	25.1993	21.4287	-4.8907
H	24.2823	21.5753	-4.3175
H	25.4721	22.3627	-5.3849
H	25.0392	20.6531	-5.6415
C	25.0985	15.1211	5.6471
H	24.98417877	15.09684659	6.72244834
C	25.6327	17.6143	1.5193
H	25.75925637	18.56051906	1.01602825
C	25.3819	15.1449	2.8674

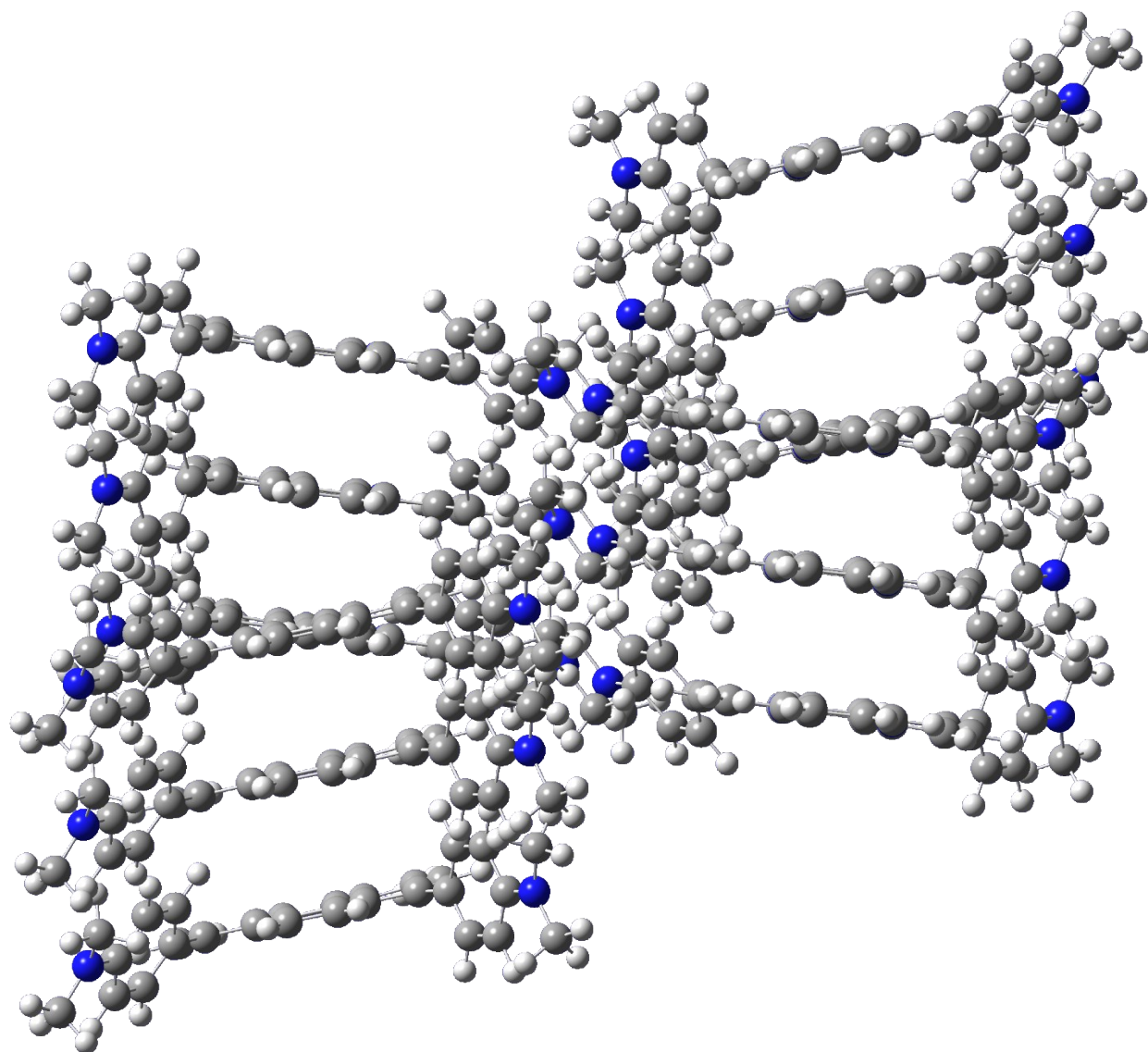
1,8-Bis(4-*N,N*-dimethylaminophenyl)phenanthro[4,5-*abc*]phenazine **NMe₂quin** in Polymorph **NMe₂quin-pris**

Atomic Type	X	Y	Z
N	-0.3266		
N	-0.1088	8.7896	2.6121
N	7.8792	6.0057	2.1807
N	8.6021	13.2841	7.7282
C	-1.3119	1.6014	6.5095
C	-2.4683	8.0977	1.9903
H	-2.5635	8.7821	1.5412
C	-3.4606	9.8472	1.702
H	-4.3351	8.0957	0.9056
C	-3.3612	8.6258	0.5536
H	-4.1632	6.6987	0.7005
C	-2.2637	6.1721	0.2013
H	-2.2002	6.0113	1.1268
C	-1.2047	4.9433	0.9695
C	0.7416	6.6965	1.7764
C	1.8207	8.1052	2.9986
C	1.7193	8.8206	3.6839
H	0.8385	10.1827	3.9368
C	2.734	10.7202	3.6195
H	2.6277	10.8593	4.5906
C	3.8887	11.9204	4.7708
C	4.007	10.2121	5.0227
C	5.1113	8.8126	4.8062
H	5.8867	8.0499	5.3181
C	5.2035	8.5548	5.8731
H	6.0541	6.7181	5.1224
C	4.2029	6.1873	5.5211
C	4.3158	5.9874	4.3995
C	3.3417	4.5901	4.1838
H	3.4456	3.9551	3.4378
C	2.2309	2.8998	3.2248
H	1.4906	4.637	2.9536
C	2.0643	4.1077	2.373
C	0.8581	5.9899	3.2089
C	3.076	6.6962	2.7735
C	2.9694	6.6932	3.9069
C	4.938	8.1163	4.1247
C	4.6045	11.0031	5.7161
H	3.5664	11.8629	6.7578
C	5.5529	11.9508	7.0496
H	5.245	12.6098	7.4339
C	6.9136	13.2606	8.2372
C	7.2501	12.5309	7.0875
H	8.2836	11.6714	6.0332
C	6.2897	11.5806	5.7379
H	6.5903	10.9359	5.3614
C	7.5664	10.2941	4.5431
H	6.6107	14.0743	8.8864
H	8.3496	14.5789	8.7352
H	7.5009	14.8181	9.042
C	9.2835	13.4263	9.7621
H	9.4886	12.9671	7.5392
H	9.8962	11.9722	7.9379
H	9.521	13.7025	8.0633



C	5.4451	3.8047	4.7778
C	6.617	3.5567	4.0875
H	6.7258	3.9405	3.0812
C	7.6536	2.8332	4.6458
H	8.5491	2.6621	4.0693
C	7.5658	2.3193	5.9399
C	6.3888	2.5784	6.638
H	6.2787	2.2087	7.6454
C	5.356	3.3038	6.0607
H	4.455	3.4814	6.6327
C	8.502	1.0903	7.8425
H	8.5307	1.9183	8.5528
H	9.3369	0.4151	8.0376
H	7.5617	0.5479	7.9548
C	9.868	1.5028	5.8716
H	9.7379	1.0982	4.8664
H	10.5161	0.8413	6.449
H	10.3216	2.4934	5.8087

1,8-Bis(4-*N,N*-dimethylaminophenyl)phenanthro[4,5-*abc*]phenazine **NMe₂quin** in Polymorph
NMe₂quin-pris



Atomic Type	X	Y	Z
N	-0.3266		
N	-0.1088	8.7896	2.6121
N	7.8792	6.0057	2.1807
N	8.6021	13.2841	7.7282
C	-1.3119	1.6014	6.5095
C	-2.4683	8.0977	1.9903
H	-2.5635	8.7821	1.5412
C	-3.4606	9.8472	1.702
H	-4.3353	8.0957	0.9056
C	-3.3612	8.6258	0.5535
H	-4.1633	6.6987	0.7005
C	-2.2637	6.172	0.2012
H	-2.2002	6.0113	1.1268
C	-1.2047	4.9433	0.9695
C	0.7416	6.6965	1.7764
C	1.8207	8.1052	2.9986
C	1.7193	8.8206	3.6839
H	0.8385	10.1827	3.9368
C	2.734	10.7202	3.6194
H	2.6277	10.8593	4.5906
C	3.8887	11.9205	4.7708
C	4.007	10.2121	5.0227
C	5.1113	8.8126	4.8062
H	5.8869	8.0499	5.3181
C	5.2035	8.5549	5.8732
H	6.0542	6.7181	5.1224
C	4.2029	6.1872	5.5212
C	4.3158	5.9874	4.3995
C	3.3417	4.5901	4.1838
H	3.4456	3.9551	3.4378
C	2.2309	2.8997	3.2248
H	1.4906	4.637	2.9536
C	2.0643	4.1077	2.3729
C	0.8581	5.9899	3.2089
C	3.076	6.6962	2.7735
C	2.9694	6.6932	3.9069
C	4.938	8.1163	4.1247
C	4.6045	11.0031	5.7161
H	3.5659	11.8629	6.7578
C	5.5529	11.9509	7.0497
H	5.245	12.6098	7.4339
C	6.9136	13.2606	8.2372
C	7.2501	12.5309	7.0875
H	8.2836	11.6714	6.0332
C	6.2897	11.5805	5.7379
H	6.5901	10.9359	5.3614
C	7.5664	10.2945	4.5436
H	6.6107	14.0743	8.8864
H	8.3496	14.5789	8.7352
H	7.5009	14.8181	9.042
C	9.2835	13.4263	9.7621
H	9.4886	12.9671	7.5392
H	9.8962	11.9722	7.9379
H	9.521	13.7025	8.0633
C	5.4451	12.9884	6.4743
C	6.617	3.8047	4.7778
H	6.7258	3.5567	4.0875

C	7.6536	2.8332	4.6458
H	8.5491	2.6621	4.0692
C	7.5658	2.3193	5.9399
C	6.3888	2.5784	6.638
H	6.2787	2.2087	7.6454
C	5.356	3.3038	6.0607
H	4.4546	3.4815	6.633
C	8.502	1.0903	7.8425
H	8.5307	1.9183	8.5528
H	9.3369	0.4151	8.0376
H	7.5617	0.5479	7.9548
C	9.868	1.5028	5.8716
H	9.7379	1.0982	4.8664
H	10.5161	0.8413	6.449
H	10.3216	2.4934	5.8087
N	7.8139	8.7896	2.6121
N	8.0317	6.0057	2.1807
N	16.0197	13.2841	7.7282
N	16.7426	1.6014	6.5095
C	6.8286	8.0977	1.9903
C	5.6722	8.7821	1.5412
H	5.577	9.8472	1.702
C	4.6799	8.0957	0.9056
H	3.8052	8.6258	0.5535
C	4.7793	6.6987	0.7005
H	3.9772	6.172	0.2012
C	5.8768	6.0113	1.1268
H	5.9403	4.9433	0.9695
C	6.9358	6.6965	1.7764
C	8.8821	8.1052	2.9986
C	9.9612	8.8206	3.6839
C	9.8598	10.1827	3.9368
H	8.979	10.7202	3.6194
C	10.8745	10.8593	4.5906
H	10.7682	11.9205	4.7708
C	12.0292	10.2121	5.0227
C	12.1475	8.8126	4.8062
C	13.2518	8.0499	5.3181
H	14.0274	8.5549	5.8732
C	13.344	6.7181	5.1224
H	14.1947	6.1872	5.5212
C	12.3434	5.9874	4.3995
C	12.4563	4.5901	4.1838
C	11.4822	3.9551	3.4378
H	11.5861	2.8997	3.2248
C	10.3714	4.637	2.9536
H	9.6311	4.1077	2.3729
C	10.2048	5.9899	3.2089
C	8.9986	6.6962	2.7735
C	11.2165	6.6932	3.9069
C	11.1099	8.1163	4.1247
C	13.0785	11.0031	5.7161
C	12.745	11.8629	6.7578
H	11.7064	11.9509	7.0497
C	13.6934	12.6098	7.4339
H	13.3855	13.2606	8.2372
C	15.0541	12.5309	7.0875
C	15.3906	11.6714	6.0332
H	16.4241	11.5805	5.7379
C	14.4302	10.9359	5.3614
H	14.7306	10.2945	4.5436

C	15.7069	14.0743	8.8864
H	14.7512	14.5789	8.7352
H	16.4901	14.8181	9.042
H	15.6414	13.4263	9.7621
C	17.424	12.9671	7.5392
H	17.6291	11.9722	7.9379
H	18.0367	13.7025	8.0633
H	17.6615	12.9884	6.4743
C	13.5856	3.8047	4.7778
C	14.7575	3.5567	4.0875
H	14.8663	3.9402	3.0817
C	15.7941	2.8332	4.6458
H	16.6896	2.6621	4.0692
C	15.7063	2.3193	5.9399
C	14.5293	2.5784	6.638
H	14.4192	2.2087	7.6454
C	13.4965	3.3038	6.0607
H	12.5951	3.4815	6.633
C	16.6425	1.0903	7.8425
H	16.6712	1.9183	8.5528
H	17.4774	0.4151	8.0376
H	15.7022	0.5479	7.9548
C	18.0085	1.5028	5.8716
H	17.8784	1.0982	4.8664
H	18.6566	0.8413	6.449
H	18.4621	2.4934	5.8087
N	15.9544	8.7896	2.6121
N	16.1722	6.0057	2.1807
N	24.1602	13.2841	7.7282
N	24.8831	1.6014	6.5095
C	14.9691	8.0977	1.9903
C	13.8127	8.7821	1.5412
H	13.7175	9.8472	1.702
C	12.8204	8.0957	0.9056
H	11.9457	8.6258	0.5535
C	12.9198	6.6987	0.7005
H	12.1177	6.172	0.2012
C	14.0173	6.0113	1.1268
H	14.0808	4.9433	0.9695
C	15.0763	6.6965	1.7764
C	17.0226	8.1052	2.9986
C	18.1017	8.8206	3.6839
C	18.0003	10.1827	3.9368
H	17.1195	10.7202	3.6194
C	19.015	10.8593	4.5906
H	18.9087	11.9205	4.7708
C	20.1697	10.2121	5.0227
C	20.288	8.8126	4.8062
C	21.3923	8.0499	5.3181
H	22.1679	8.5549	5.8732
C	21.4845	6.7181	5.1224
H	22.3352	6.1872	5.5212
C	20.4839	5.9874	4.3995
C	20.5968	4.5901	4.1838
C	19.6227	3.9551	3.4378
H	19.7266	2.8997	3.2248
C	18.5119	4.637	2.9536
H	17.7716	4.1077	2.3729
C	18.3453	5.9899	3.2089
C	17.1391	6.6962	2.7735
C	19.357	6.6932	3.9069

C	19.2504	8.1163	4.1247
C	21.219	11.0031	5.7161
C	20.8855	11.8629	6.7578
H	19.8469	11.9509	7.0497
C	21.8339	12.6098	7.4339
H	21.526	13.2606	8.2372
C	23.1946	12.5309	7.0875
C	23.5311	11.6714	6.0332
H	24.5646	11.5805	5.7379
C	22.5707	10.9359	5.3614
H	22.8711	10.2945	4.5436
C	23.8474	14.0743	8.8864
H	22.8917	14.5789	8.7352
H	24.6306	14.8181	9.042
H	23.7819	13.4263	9.7621
C	25.5645	12.9671	7.5392
H	25.7696	11.9722	7.9379
H	26.1772	13.7025	8.0633
H	25.802	12.9884	6.4743
C	21.7261	3.8047	4.7778
C	22.898	3.5567	4.0875
H	23.0068	3.9402	3.0817
C	23.9346	2.8332	4.6458
H	24.8301	2.6621	4.0692
C	23.8468	2.3193	5.9399
C	22.6698	2.5784	6.638
H	22.5597	2.2087	7.6454
C	21.637	3.3038	6.0607
H	20.7356	3.4815	6.633
C	24.783	1.0903	7.8425
H	24.8117	1.9183	8.5528
H	25.6179	0.4151	8.0376
H	23.8427	0.5479	7.9548
C	26.149	1.5028	5.8716
H	26.0189	1.0982	4.8664
H	26.7971	0.8413	6.449
H	26.6026	2.4934	5.8087
N	12.391	22.6712	3.3892
N	12.1732	19.8873	3.8205
N	4.1852	27.1657	-1.7269
N	3.4623	15.483	-0.5082
C	13.3763	21.9793	4.011
C	14.5327	22.6637	4.46
H	14.6279	23.7288	4.2992
C	15.525	21.9773	5.0957
H	16.3997	22.5074	5.4478
C	15.4256	20.5803	5.3008
H	16.2278	20.0536	5.8
C	14.3281	19.8929	4.8745
H	14.2646	18.8249	5.0318
C	13.2691	20.5781	4.2249
C	11.3228	21.9868	3.0027
C	10.2437	22.7022	2.3173
C	10.3451	24.0643	2.0644
H	11.2259	24.6018	2.3818
C	9.3304	24.7409	1.4107
H	9.4367	25.8021	1.2305
C	8.1757	24.0937	0.9786
C	8.0574	22.6942	1.1951
C	6.9531	21.9315	0.6832
H	6.1775	22.4365	0.1281

C	6.8609	20.5997	0.8788
H	6.0101	20.0688	0.4801
C	7.8615	19.869	1.6017
C	7.7486	18.4717	1.8174
C	8.7227	17.8367	2.5635
H	8.6188	16.7813	2.7764
C	9.8335	18.5186	3.0477
H	10.5738	17.9893	3.6284
C	10.0001	19.8715	2.7924
C	11.2063	20.5778	3.2277
C	8.9884	20.5748	2.0943
C	9.095	21.9979	1.8766
C	7.1264	24.8847	0.2852
C	7.4599	25.7445	-0.7565
H	8.4985	25.8325	-1.0484
C	6.5115	26.4914	-1.4326
H	6.8194	27.1422	-2.2359
C	5.1508	26.4125	-1.0862
C	4.8143	25.553	-0.0319
H	3.7807	25.4621	0.2633
C	5.7747	24.8175	0.6399
H	5.4742	24.176	1.4577
C	4.498	27.9559	-2.8852
H	5.4537	28.4605	-2.7339
H	3.7147	28.6997	-3.0407
H	4.5635	27.3079	-3.7608
C	2.7809	26.8487	-1.5379
H	2.5758	25.8538	-1.9366
H	2.1682	27.5841	-2.062
H	2.5434	26.87	-0.473
C	6.6193	17.6863	1.2234
C	5.4474	17.4383	1.9138
H	5.3386	17.8218	2.9196
C	4.4108	16.7148	1.3554
H	3.5153	16.5437	1.932
C	4.4986	16.2009	0.0613
C	5.6756	16.46	-0.6367
H	5.7857	16.0903	-1.6441
C	6.7084	17.1854	-0.0594
H	7.6098	17.3631	-0.6317
C	3.5624	14.9719	-1.8412
H	3.5337	15.7999	-2.5515
H	2.7275	14.2967	-2.0363
H	4.5027	14.4295	-1.9537
C	2.1964	15.3844	0.1296
H	2.3265	14.9799	1.1348
H	1.5483	14.7229	-0.4477
H	1.7428	16.3749	0.1926
N	20.5315	22.6712	3.3892
N	20.3137	19.8873	3.8205
N	12.3257	27.1657	-1.7269
N	11.6028	15.483	-0.5082
C	21.5168	21.9793	4.011
C	22.6732	22.6637	4.46
H	22.7684	23.7288	4.2992
C	23.6655	21.9773	5.0957
H	24.5402	22.5074	5.4478
C	23.5661	20.5803	5.3008
H	24.3683	20.0536	5.8
C	22.4686	19.8929	4.8745
H	22.4051	18.8249	5.0318

C	21.4096	20.5781	4.2249
C	19.4633	21.9868	3.0027
C	18.3842	22.7022	2.3173
C	18.4856	24.0643	2.0644
H	19.3664	24.6018	2.3818
C	17.4709	24.7409	1.4107
H	17.5772	25.8021	1.2305
C	16.3162	24.0937	0.9786
C	16.1979	22.6942	1.1951
C	15.0936	21.9315	0.6832
H	14.318	22.4365	0.1281
C	15.0014	20.5997	0.8788
H	14.1506	20.0688	0.4801
C	16.002	19.869	1.6017
C	15.8891	18.4717	1.8174
C	16.8632	17.8367	2.5635
H	16.7593	16.7813	2.7764
C	17.974	18.5186	3.0477
H	18.7143	17.9893	3.6284
C	18.1406	19.8715	2.7924
C	19.3468	20.5778	3.2277
C	17.1289	20.5748	2.0943
C	17.2355	21.9979	1.8766
C	15.2669	24.8847	0.2852
C	15.6004	25.7445	-0.7565
H	16.639	25.8325	-1.0484
C	14.652	26.4914	-1.4326
H	14.9599	27.1422	-2.2359
C	13.2913	26.4125	-1.0862
C	12.9548	25.553	-0.0319
H	11.9212	25.4621	0.2633
C	13.9152	24.8175	0.6399
H	13.6147	24.176	1.4577
C	12.6385	27.9559	-2.8852
H	13.5942	28.4605	-2.7339
H	11.8552	28.6997	-3.0407
H	12.704	27.3079	-3.7608
C	10.9214	26.8487	-1.5379
H	10.7163	25.8538	-1.9366
H	10.3087	27.5841	-2.062
H	10.6839	26.87	-0.473
C	14.7598	17.6863	1.2234
C	13.5879	17.4383	1.9138
H	13.4791	17.8218	2.9196
C	12.5513	16.7148	1.3554
H	11.6558	16.5437	1.932
C	12.6391	16.2009	0.0613
C	13.8161	16.46	-0.6367
H	13.9262	16.0903	-1.6441
C	14.8489	17.1854	-0.0594
H	15.7503	17.3631	-0.6317
C	11.7029	14.9719	-1.8412
H	11.6742	15.7999	-2.5515
H	10.868	14.2967	-2.0363
H	12.6432	14.4295	-1.9537
C	10.3369	15.3844	0.1296
H	10.467	14.9799	1.1348
H	9.6888	14.7229	-0.4477
H	9.8833	16.3749	0.1926
N	28.672	22.6712	3.3892
N	28.4542	19.8873	3.8205

N	20.4662	27.1657	-1.7269
N	19.7433	15.483	-0.5082
C	29.6573	21.9793	4.011
C	30.8137	22.6637	4.46
H	30.9089	23.7288	4.2992
C	31.806	21.9773	5.0957
H	32.6807	22.5074	5.4478
C	31.7066	20.5803	5.3008
H	32.5088	20.0536	5.8
C	30.6091	19.8929	4.8745
H	30.5456	18.8249	5.0318
C	29.5501	20.5781	4.2249
C	27.6038	21.9868	3.0027
C	26.5247	22.7022	2.3173
C	26.6261	24.0643	2.0644
H	27.5069	24.6018	2.3818
C	25.6114	24.7409	1.4107
H	25.7177	25.8021	1.2305
C	24.4567	24.0937	0.9786
C	24.3384	22.6942	1.1951
C	23.2341	21.9315	0.6832
H	22.4585	22.4365	0.1281
C	23.1419	20.5997	0.8788
H	22.2911	20.0688	0.4801
C	24.1425	19.869	1.6017
C	24.0296	18.4717	1.8174
C	25.0037	17.8367	2.5635
H	24.8998	16.7813	2.7764
C	26.1145	18.5186	3.0477
H	26.8548	17.9893	3.6284
C	26.2811	19.8715	2.7924
C	27.4873	20.5778	3.2277
C	25.2694	20.5748	2.0943
C	25.376	21.9979	1.8766
C	23.4074	24.8847	0.2852
C	23.7409	25.7445	-0.7565
H	24.7795	25.8325	-1.0484
C	22.7925	26.4914	-1.4326
H	23.1004	27.1422	-2.2359
C	21.4318	26.4125	-1.0862
C	21.0953	25.553	-0.0319
H	20.0617	25.4621	0.2633
C	22.0557	24.8175	0.6399
H	21.7552	24.176	1.4577
C	20.779	27.9559	-2.8852
H	21.7347	28.4605	-2.7339
H	19.9957	28.6997	-3.0407
H	20.8445	27.3079	-3.7608
C	19.0619	26.8487	-1.5379
H	18.8568	25.8538	-1.9366
H	18.4492	27.5841	-2.062
H	18.8244	26.87	-0.473
C	22.9003	17.6863	1.2234
C	21.7284	17.4383	1.9138
H	21.6196	17.8218	2.9196
C	20.6918	16.7148	1.3554
H	19.7963	16.5437	1.932
C	20.7796	16.2009	0.0613
C	21.9566	16.46	-0.6367
H	22.0667	16.0903	-1.6441
C	22.9894	17.1854	-0.0594

H	23.8908	17.3631	-0.6317
C	19.8434	14.9719	-1.8412
H	19.8147	15.7999	-2.5515
H	19.0085	14.2967	-2.0363
H	20.7837	14.4295	-1.9537
C	18.4774	15.3844	0.1296
H	18.6075	14.9799	1.1348
H	17.8293	14.7229	-0.4477
H	18.0238	16.3749	0.1926
N	8.1744	18.9736	9.3904
N	7.9566	21.7575	9.8218
N	-0.0314	14.4791	4.2743
N	-0.7543	26.1618	5.4931
C	9.1597	19.6655	10.0123
C	10.3161	18.9811	10.4613
H	10.4113	17.916	10.3005
C	11.3084	19.6675	11.0969
H	12.1831	19.1374	11.449
C	11.209	21.0645	11.3021
H	12.0112	21.5912	11.8013
C	10.1115	21.7519	10.8757
H	10.048	22.8199	11.033
C	9.0525	21.0667	10.2262
C	7.1062	19.658	9.0039
C	6.0271	18.9426	8.3186
C	6.1285	17.5805	8.0657
H	7.0093	17.043	8.3831
C	5.1138	16.9039	7.4119
H	5.2201	15.8426	7.2318
C	3.9591	17.5511	6.9798
C	3.8408	18.9506	7.1964
C	2.7365	19.7133	6.6844
H	1.9609	19.2083	6.1293
C	2.6443	21.0451	6.8801
H	1.7935	21.576	6.4814
C	3.6449	21.7758	7.603
C	3.532	23.1731	7.8187
C	4.5061	23.8081	8.5648
H	4.4022	24.8635	8.7777
C	5.6169	23.1262	9.0489
H	6.3572	23.6555	9.6296
C	5.7835	21.7733	8.7937
C	6.9897	21.067	9.229
C	4.7718	21.07	8.0956
C	4.8784	19.6469	7.8779
C	2.9098	16.7601	6.2864
C	3.2433	15.9003	5.2447
H	4.2819	15.8123	4.9528
C	2.2949	15.1534	4.5686
H	2.6028	14.5026	3.7653
C	0.9342	15.2323	4.915
C	0.5977	16.0918	5.9693
H	-0.4358	16.1827	6.2646
C	1.5581	16.8273	6.6411
H	1.2577	17.4687	7.4589
C	0.2814	13.6889	3.1161
H	1.2371	13.1843	3.2673
H	-0.5019	12.9451	2.9606
H	0.3469	14.3369	2.2405
C	-1.4358	14.7961	4.4634
H	-1.6408	15.7911	4.0647

H	-2.0484	14.0606	3.9393
H	-1.6732	14.7748	5.5283
C	2.4027	23.9585	7.2247
C	1.2307	24.2065	7.9151
H	1.1221	23.8229	8.9209
C	0.1942	24.93	7.3567
H	-0.7013	25.1011	7.9333
C	0.282	25.4439	6.0626
C	1.459	25.1848	5.3645
H	1.5691	25.5545	4.3571
C	2.4918	24.4594	5.9419
H	3.3932	24.2817	5.3695
C	-0.6542	26.6729	4.1601
H	-0.6829	25.8449	3.4498
H	-1.4891	27.3481	3.965
H	0.2861	27.2153	4.0476
C	-2.0202	26.2604	6.1309
H	-1.8901	26.6649	7.1361
H	-2.6683	26.9219	5.5536
H	-2.4738	25.2698	6.1938
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N	16.0971	21.7575	9.8218
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C	17.3002	19.6655	10.0123
C	18.4566	18.9811	10.4613
H	18.5518	17.916	10.3005
C	19.4489	19.6675	11.0969
H	20.3236	19.1374	11.449
C	19.3495	21.0645	11.3021
H	20.1517	21.5912	11.8013
C	18.252	21.7519	10.8757
H	18.1885	22.8199	11.033
C	17.193	21.0667	10.2262
C	15.2467	19.658	9.0039
C	14.1676	18.9426	8.3186
C	14.269	17.5805	8.0657
H	15.1498	17.043	8.3831
C	13.2543	16.9039	7.4119
H	13.3606	15.8426	7.2318
C	12.0996	17.5511	6.9798
C	11.9813	18.9506	7.1964
C	10.877	19.7133	6.6844
H	10.1014	19.2083	6.1293
C	10.7848	21.0451	6.8801
H	9.934	21.576	6.4814
C	11.7854	21.7758	7.603
C	11.6725	23.1731	7.8187
C	12.6466	23.8081	8.5648
H	12.5427	24.8635	8.7777
C	13.7574	23.1262	9.0489
H	14.4977	23.6555	9.6296
C	13.924	21.7733	8.7937
C	15.1302	21.067	9.229
C	12.9123	21.07	8.0956
C	13.0189	19.6469	7.8779
C	11.0503	16.7601	6.2864
C	11.3838	15.9003	5.2447
H	12.4224	15.8123	4.9528
C	10.4354	15.1534	4.5686
H	10.7433	14.5026	3.7653

C	9.0747	15.2323	4.915
C	8.7382	16.0918	5.9693
H	7.7047	16.1827	6.2646
C	9.6986	16.8273	6.6411
H	9.3982	17.4687	7.4589
C	8.4219	13.6889	3.1161
H	9.3776	13.1843	3.2673
H	7.6386	12.9451	2.9606
H	8.4874	14.3369	2.2405
C	6.7047	14.7961	4.4634
H	6.4997	15.7911	4.0647
H	6.0921	14.0606	3.9393
H	6.4673	14.7748	5.5283
C	10.5432	23.9585	7.2247
C	9.3712	24.2065	7.9151
H	9.2626	23.8229	8.9209
C	8.3347	24.93	7.3567
H	7.4392	25.1011	7.9333
C	8.4225	25.4439	6.0626
C	9.5995	25.1848	5.3645
H	9.7096	25.5545	4.3571
C	10.6323	24.4594	5.9419
H	11.5337	24.2817	5.3695
C	7.4863	26.6729	4.1601
H	7.4576	25.8449	3.4498
H	6.6514	27.3481	3.965
H	8.4266	27.2153	4.0476
C	6.1203	26.2604	6.1309
H	6.2504	26.6649	7.1361
H	5.4722	26.9219	5.5536
H	5.6667	25.2698	6.1938
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C	26.5971	18.9811	10.4613
H	26.6923	17.916	10.3005
C	27.5894	19.6675	11.0969
H	28.4641	19.1374	11.449
C	27.49	21.0645	11.3021
H	28.2922	21.5912	11.8013
C	26.3925	21.7519	10.8757
H	26.329	22.8199	11.033
C	25.3335	21.0667	10.2262
C	23.3872	19.658	9.0039
C	22.3081	18.9426	8.3186
C	22.4095	17.5805	8.0657
H	23.2903	17.043	8.3831
C	21.3948	16.9039	7.4119
H	21.5011	15.8426	7.2318
C	20.2401	17.5511	6.9798
C	20.1218	18.9506	7.1964
C	19.0175	19.7133	6.6844
H	18.2419	19.2083	6.1293
C	18.9253	21.0451	6.8801
H	18.0745	21.576	6.4814
C	19.9259	21.7758	7.603
C	19.813	23.1731	7.8187
C	20.7871	23.8081	8.5648
H	20.6832	24.8635	8.7777

C	21.8979	23.1262	9.0489
H	22.6382	23.6555	9.6296
C	22.0645	21.7733	8.7937
C	23.2707	21.067	9.229
C	21.0528	21.07	8.0956
C	21.1594	19.6469	7.8779
C	19.1908	16.7601	6.2864
C	19.5243	15.9003	5.2447
H	20.5629	15.8123	4.9528
C	18.5759	15.1534	4.5686
H	18.8838	14.5026	3.7653
C	17.2152	15.2323	4.915
C	16.8787	16.0918	5.9693
H	15.8452	16.1827	6.2646
C	17.8391	16.8273	6.6411
H	17.5387	17.4687	7.4589
C	16.5624	13.6889	3.1161
H	17.5181	13.1843	3.2673
H	15.7791	12.9451	2.9606
H	16.6279	14.3369	2.2405
C	14.8452	14.7961	4.4634
H	14.6402	15.7911	4.0647
H	14.2326	14.0606	3.9393
H	14.6078	14.7748	5.5283
C	18.6837	23.9585	7.2247
C	17.5117	24.2065	7.9151
H	17.4031	23.8229	8.9209
C	16.4752	24.93	7.3567
H	15.5797	25.1011	7.9333
C	16.563	25.4439	6.0626
C	17.74	25.1848	5.3645
H	17.8501	25.5545	4.3571
C	18.7728	24.4594	5.9419
H	19.6742	24.2817	5.3695
C	15.6268	26.6729	4.1601
H	15.5981	25.8449	3.4498
H	14.7919	27.3481	3.965
H	16.5671	27.2153	4.0476
C	14.2608	26.2604	6.1309
H	14.3909	26.6649	7.1361
H	13.6127	26.9219	5.5536
H	13.8072	25.2698	6.1938
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C	-5.5285	5.7839	7.9915
C	-6.6849	5.0995	7.5425
H	-6.7801	4.0344	7.7033
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H	-8.5519	5.2558	6.5548
C	-7.5778	7.1829	6.7017
H	-8.38	7.7096	6.2025
C	-6.4803	7.8703	7.1281
H	-6.4168	8.9383	6.9708
C	-5.4213	7.1851	7.7776
C	-3.475	5.7764	8.9999
C	-2.3959	5.061	9.6852
C	-2.4973	3.6989	9.9381
H	-3.3781	3.1614	9.6207
C	-1.4826	3.0223	10.5919

H	-1.5889	1.961	10.772
C	-0.3279	3.6695	11.024
C	-0.2096	5.069	10.8074
C	0.8947	5.8317	11.3193
H	1.6702	5.3267	11.8745
C	0.9869	7.1635	11.1237
H	1.8377	7.6944	11.5224
C	-0.0137	7.8942	10.4008
C	0.0992	9.2915	10.1851
C	-0.8749	9.9265	9.439
H	-0.771	10.9819	9.2261
C	-1.9857	9.2446	8.9548
H	-2.7261	9.7739	8.3742
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C	-3.3585	7.1854	8.7748
C	-1.1406	7.1884	9.9082
C	-1.2472	5.7653	10.1259
C	0.7214	2.8785	11.7174
C	0.3879	2.0187	12.7591
H	-0.6507	1.9307	13.051
C	1.3363	1.2718	13.4352
H	1.0284	0.621	14.2385
C	2.697	1.3507	13.0888
C	3.0335	2.2102	12.0345
H	4.067	2.3011	11.7392
C	2.0731	2.9457	11.3627
H	2.3735	3.5871	10.5449
C	3.3498	-0.1927	14.8877
H	2.394	-0.6973	14.7365
H	4.1331	-0.9365	15.0432
H	3.2843	0.4553	15.7633
C	5.0669	0.9145	13.5404
H	5.272	1.9094	13.9391
H	5.6796	0.1791	14.0645
H	5.3044	0.8932	12.4755
C	1.2285	10.0769	10.7791
C	2.4004	10.3249	10.0887
H	2.509	9.9413	9.0829
C	3.4369	11.0484	10.6471
H	4.3324	11.2195	10.0705
C	3.3492	11.5623	11.9412
C	2.1722	11.3032	12.6393
H	2.0621	11.6729	13.6467
C	1.1394	10.5778	12.0619
H	0.238	10.4001	12.6343
C	4.2854	12.7913	13.8437
H	4.3141	11.9633	14.554
H	5.1203	13.4665	14.0388
H	3.3451	13.3337	13.9562
C	5.6514	12.3788	11.8729
H	5.5213	12.7833	10.8677
H	6.2995	13.0403	12.4502
H	6.105	11.3882	11.81
N	3.5973	5.092	8.6134
N	3.8151	7.8759	8.182
N	11.8031	0.5975	13.7295
N	12.526	12.2802	12.5107
C	2.612	5.7839	7.9915
C	1.4556	5.0995	7.5425
H	1.3604	4.0344	7.7033
C	0.4633	5.7859	6.9069

H	-0.4114	5.2558	6.5548
C	0.5627	7.1829	6.7017
H	-0.2395	7.7096	6.2025
C	1.6602	7.8703	7.1281
H	1.7237	8.9383	6.9708
C	2.7192	7.1851	7.7776
C	4.6655	5.7764	8.9999
C	5.7446	5.061	9.6852
C	5.6432	3.6989	9.9381
H	4.7624	3.1614	9.6207
C	6.6579	3.0223	10.5919
H	6.5516	1.961	10.772
C	7.8126	3.6695	11.024
C	7.9309	5.069	10.8074
C	9.0352	5.8317	11.3193
H	9.8107	5.3267	11.8745
C	9.1274	7.1635	11.1237
H	9.9782	7.6944	11.5224
C	8.1268	7.8942	10.4008
C	8.2397	9.2915	10.1851
C	7.2656	9.9265	9.439
H	7.3695	10.9819	9.2261
C	6.1548	9.2446	8.9548
H	5.4144	9.7739	8.3742
C	5.9882	7.8917	9.2101
C	4.782	7.1854	8.7748
C	6.9999	7.1884	9.9082
C	6.8933	5.7653	10.1259
C	8.8619	2.8785	11.7174
C	8.5284	2.0187	12.7591
H	7.4898	1.9307	13.051
C	9.4768	1.2718	13.4352
H	9.1689	0.621	14.2385
C	10.8375	1.3507	13.0888
C	11.174	2.2102	12.0345
H	12.2075	2.3011	11.7392
C	10.2136	2.9457	11.3627
H	10.514	3.5871	10.5449
C	11.4903	-0.1927	14.8877
H	10.5345	-0.6973	14.7365
H	12.2736	-0.9365	15.0432
H	11.4248	0.4553	15.7633
C	13.2074	0.9145	13.5404
H	13.4125	1.9094	13.9391
H	13.8201	0.1791	14.0645
H	13.4449	0.8932	12.4755
C	9.369	10.0769	10.7791
C	10.5409	10.3249	10.0887
H	10.6495	9.9413	9.0829
C	11.5774	11.0484	10.6471
H	12.4729	11.2195	10.0705
C	11.4897	11.5623	11.9412
C	10.3127	11.3032	12.6393
H	10.2026	11.6729	13.6467
C	9.2799	10.5778	12.0619
H	8.3785	10.4001	12.6343
C	12.4259	12.7913	13.8437
H	12.4546	11.9633	14.554
H	13.2608	13.4665	14.0388
H	11.4856	13.3337	13.9562
C	13.7919	12.3788	11.8729

H	13.6618	12.7833	10.8677
H	14.44	13.0403	12.4502
H	14.2455	11.3882	11.81
N	11.7378	5.092	8.6134
N	11.9556	7.8759	8.182
N	19.9436	0.5975	13.7295
N	20.6665	12.2802	12.5107
C	10.7525	5.7839	7.9915
C	9.5961	5.0995	7.5425
H	9.5009	4.0344	7.7033
C	8.6038	5.7859	6.9069
H	7.7291	5.2558	6.5548
C	8.7032	7.1829	6.7017
H	7.901	7.7096	6.2025
C	9.8007	7.8703	7.1281
H	9.8642	8.9383	6.9708
C	10.8597	7.1851	7.7776
C	12.806	5.7764	8.9999
C	13.8851	5.061	9.6852
C	13.7837	3.6989	9.9381
H	12.9029	3.1614	9.6207
C	14.7984	3.0223	10.5919
H	14.6921	1.961	10.772
C	15.9531	3.6695	11.024
C	16.0714	5.069	10.8074
C	17.1757	5.8317	11.3193
H	17.9512	5.3267	11.8745
C	17.2679	7.1635	11.1237
H	18.1187	7.6944	11.5224
C	16.2673	7.8942	10.4008
C	16.3802	9.2915	10.1851
C	15.4061	9.9265	9.439
H	15.51	10.9819	9.2261
C	14.2953	9.2446	8.9548
H	13.5549	9.7739	8.3742
C	14.1287	7.8917	9.2101
C	12.9225	7.1854	8.7748
C	15.1404	7.1884	9.9082
C	15.0338	5.7653	10.1259
C	17.0024	2.8785	11.7174
C	16.6689	2.0187	12.7591
H	15.6303	1.9307	13.051
C	17.6173	1.2718	13.4352
H	17.3094	0.621	14.2385
C	18.978	1.3507	13.0888
C	19.3145	2.2102	12.0345
H	20.348	2.3011	11.7392
C	18.3541	2.9457	11.3627
H	18.6545	3.5871	10.5449
C	19.6308	-0.1927	14.8877
H	18.675	-0.6973	14.7365
H	20.4141	-0.9365	15.0432
H	19.5653	0.4553	15.7633
C	21.3479	0.9145	13.5404
H	21.553	1.9094	13.9391
H	21.9606	0.1791	14.0645
H	21.5854	0.8932	12.4755
C	17.5095	10.0769	10.7791
C	18.6814	10.3249	10.0887
H	18.79	9.9413	9.0829
C	19.7179	11.0484	10.6471

H	20.6134	11.2195	10.0705
C	19.6302	11.5623	11.9412
C	18.4532	11.3032	12.6393
H	18.3431	11.6729	13.6467
C	17.4204	10.5778	12.0619
H	16.519	10.4001	12.6343
C	20.5664	12.7913	13.8437
H	20.5951	11.9633	14.554
H	21.4013	13.4665	14.0388
H	19.6261	13.3337	13.9562
C	21.9324	12.3788	11.8729
H	21.8023	12.7833	10.8677
H	22.5805	13.0403	12.4502
H	22.386	11.3882	11.81