Electronic Supplementary Information for

Boron Complexes of Aromatic Ring Fused Iminopyrrolyl Ligands: Synthesis, Structure, and Luminescent Properties

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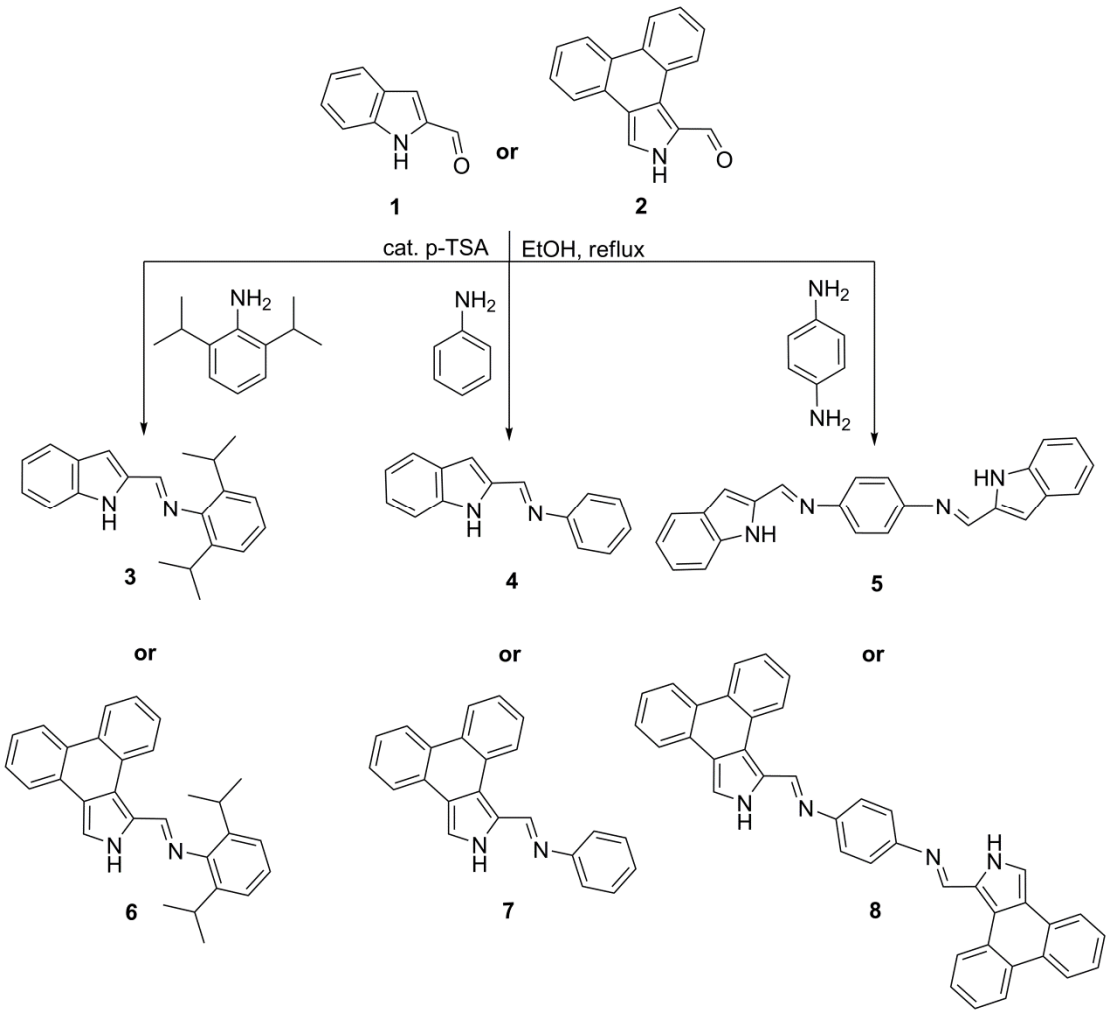
Synthesis of Ligand Precursors 3–8



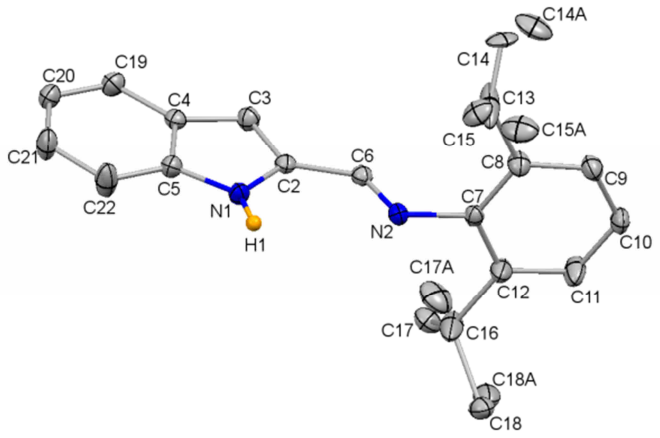
Scheme S1. Syntheses of ligand precursors **3**–**8**.

Molecular structures of ligand precursors 3 and 7

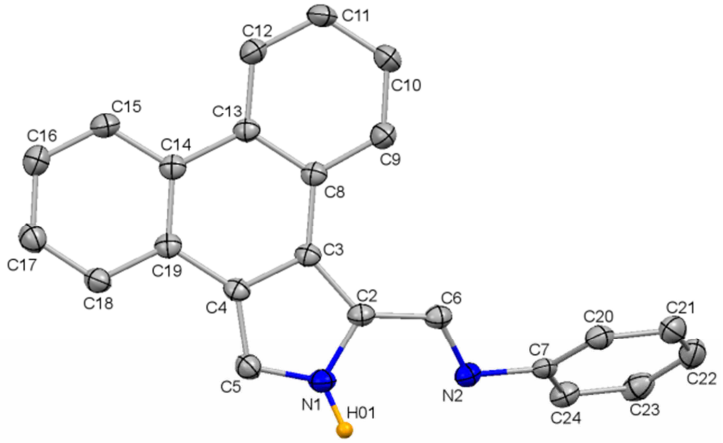
Perspective views of the molecular structures of **3** and **7** are shown in Figure S1a and b. Selected bond lengths and bond angles are given as caption in the figure. The crystals suitable for single crystal X-ray diffraction studies were obtained by cooling an ethereal solution of **3** or **7** to –20 °C, for 2 days. The ligand precursors **3** and **7** crystallized in the monoclinic crystal system, with space groups $P2_1/n$ and $P2_1/c$, respectively.

The indole and the phenanthro[9,10-*c*]pyrrole moieties in **3** and **7**, respectively, display planar backbones. The dihedral angles N1-C2-C6-N2 of -1.7(2) and 19.2(2)°, for **3** and **7**, respectively, show the imine group in **7** considerably deviated from co-planarity, which is an exception in relation to other 2-iminopyrrolyl ligand precursors. The presence of two bulky isopropyl substituents at the positions 2 and 6 of the phenyl ring in **3** resulted in twisting the *N*-aryl ring almost perpendicular with respect to the indole-aldimine moiety, with torsion angles of -96.4(5)° (C6-N2-C7A-C12), 84.2(5) (C6-N2-C7A-C8), 93.0(4) (C6-N2-C7B-C8A), and -86.5(6)º (C6-N2-C7B-C12A), while in **7**, the *N*-phenyl ring is deviated from co-planarity, dihedral angles being 44.88(19)º (C6-N2-C7-C20)° and -134.47(14)º (C6-N2-C7-C24). In **3**, the angles centered on nitrogen atoms N1 and N2 are 108.43(13)º, and 113.2(4)º and 116.3(4)º, respectively, whereas in **7** are 110.26(13)° (N1) and 116.36(13)° (N2). The imine C6=N2 distances in **3** and **7** are 1.275(2) Å and 1.2916(18) Å, respectively, being within the range reported earlier for this group.[1] The indole-to-a-dimine and phenanthro[9,10-*c*]pyrrole-to-aldimine C2-C6 single bond lengths (1.437(2) Å for **3** and 1.429(2) Å for **7**) are shorter than normal and are consistent with the conjugation of the pyrrole rings with the coplanar C=N bond.

[1] (a) S. A. Carabineiro, P. T. Gomes, L. F. Veiros, C. Freire, L. C. J. Pereira, R. T. Henriques, J. E. Warren and S. I. Pascu, *Dalton Trans.*, 2007, 5460; (b) S. A. Carabineiro, R. M. Bellabarba, P. T. Gomes, S. I. Pascu, L. F. Veiros, C. Freire, L. C. J. Pereira, R. T. Henriques, M. C. Oliveira and J. E. Warren, *Inorg. Chem.*, 2008, **47**, 8896.



(a)



(b)

Fig. S1 Perspective views of the molecular structures of (a) **3** and (b) **7**. The ellipsoids were drawn at 50% probability level. All the calculated hydrogen atoms were omitted for clarity. Compound **3**: Selected bond lengths (Å): N1-C2, 1.375(2); N1-C5, 1.378(2); N2-C6, 1.275(2); N2-C7A, 1.444(6); N2-C7B, 1.414(6); N1-H1, 0.8800; C2-C6, 1.437(2). Selected bond angles (°): C2-N1-C5, 108.43(13); C6-N2-C7A, 116.3(4); C6-N2-C7B, 113.2(4); C5-N1-H1, 125.8; C2-N1-H1, 125.8; N1-C2-C6, 125.71(14); N1-C2-C3, 109.43(13); N2-C6-C2, 125.83(15); C8A-C7B-N2, 115.2(4); C12A-C7B-N2, 124.8(4); C8-C7A-N2, 125.7(4); C8-C7A-C12, 120.0. Compound **7**: Selected bond lengths (Å): N1-C2, 1.3811(19); N1-C5, 1.3495(19); N2-C6, 1.2916(18), N2 -C7, 1.4178(18), N1-H01, 0.95(2); C2-C6, 1.429(2). Selected bond angles (°): C2-N1-C5, 110.26(13); C6-N2-C7, 116.36(13); C2-N1-H01125.1(12); C5-N1-H01, 124.5(12); N1-C2-C3, 107.10(13); C3-C2-C6, 132.39(14); N1-C2-C6, 119.67(13); N1-C5-C4, 108.48(13); N2-C6-C2, 122.42(14); N2-C7-C24, 117.88(13); N2-C7-C20, 122.93(13).

Table S1 Crystallographic data for **3**, **7**, **9**, **10** and **13**.

	3	**7**	**9**	**10**	**13**
formula	$C_{21}H_{24}N_2$	$C_{23}H_{16}N_2$	$C_{33}H_{33}BN_2$	$C_{27}H_{21}BN_2$	$C_{35}H_{25}BN_2$
M / g mol^{-1}	304.42	320.37	468.42	384.27	484.38
λ /Å	0.71073	0.71073	0.71073	0.71073	0.71073
T / K	150(2)	150(2)	150(2)	150(2)	150(2)
crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	$P2_1/n$	$C2/c$	Pn	$P2_1/n$	$P2_1/c$
a / Å	9.1486(18)	26.1429(14)	10.6591(9)	8.9836(3)	12.2486(9)
b / Å	13.496(3)	5.5789(3)	8.7127(7)	13.3666(4)	9.0701(7)
c / Å	14.507(3)	22.5584(11)	14.2325(13)	17.2368(6)	21.8347(15)
α / deg	90	90	90	90	90
β / deg	97.345(6)	102.477(2)	90.856(5)	94.218(2)	91.772(4)
γ / deg	90	90	90	90	90
V / Å^3	1776.5(6)	3212.4(3)	1321.6(2)	2064.19(12)	2424.6(3)
Z	4	8	2	4	4
ρ_{calc} /g cm^{-3}	1.138	1.325	1.177	1.236	1.327
crystal size / mm	0.20 × 0.20 × 0.40	0.26 × 0.40 × 0.80	0.20 × 0.24 × 0.36	0.10 × 0.20 × 0.30	0.20 × 0.30 × 0.50
θ_{max} / deg	28.7	29.2	25.7	28.4	25.8
total data	11101	25261	12089	29573	18074
unique data	3239	4334	4881	5152	4554
R_{int}	0.049	0.074	0.041	0.038	0.052
R [I > 2σ(I)]	0.0451	0.0513	0.1080	0.0462	0.0565
wR	0.1081	0.1035	0.3148	0.1074	0.1530
goodness of fit	0.952	1.001	0.980	1.051	1.012
ρ min, ρ max	-0.25, 0.27	-0.24, 0.33	-0.47, 0.70	-0.19, 0.27	-0.22, 1.03

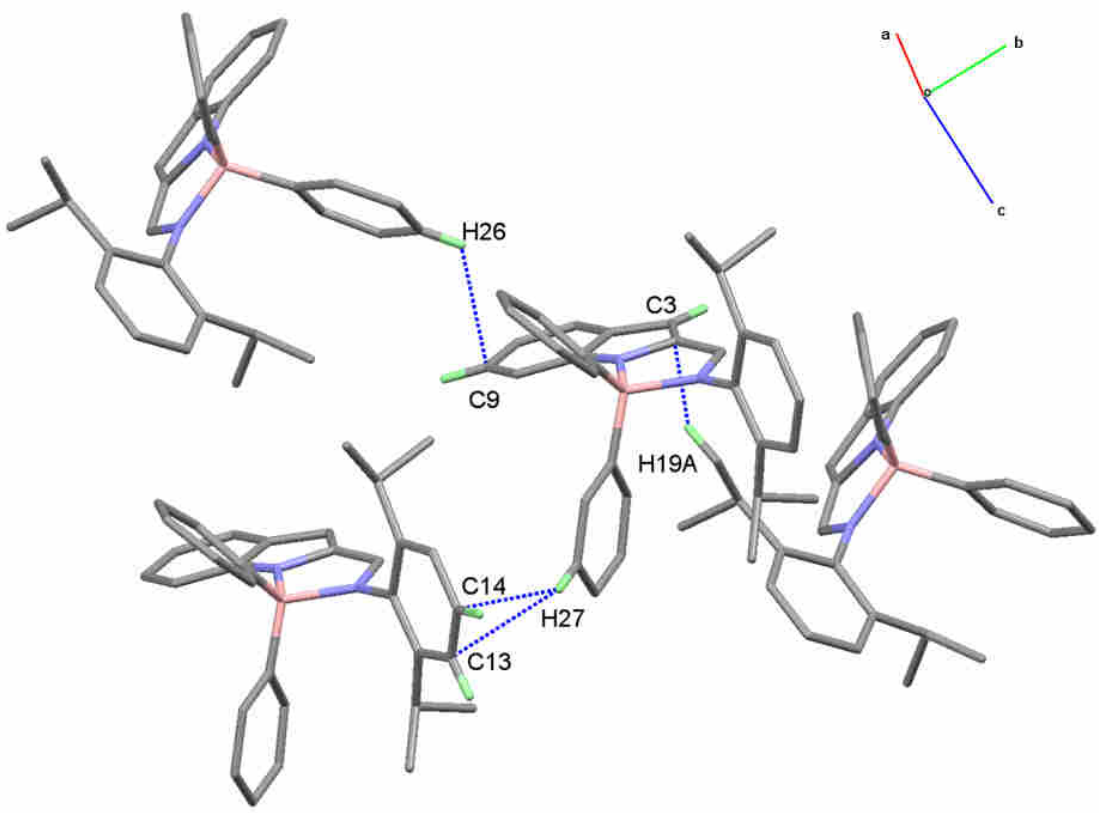


Fig. S2 View of the 3D supramolecular arrangement of compound **9**, showing the C–H···π$C_{(Ar)}$ short contacts as blue dashed lines. All hydrogen atoms, except those involved in the depicted short contacts (represented in green), were omitted for clarity.

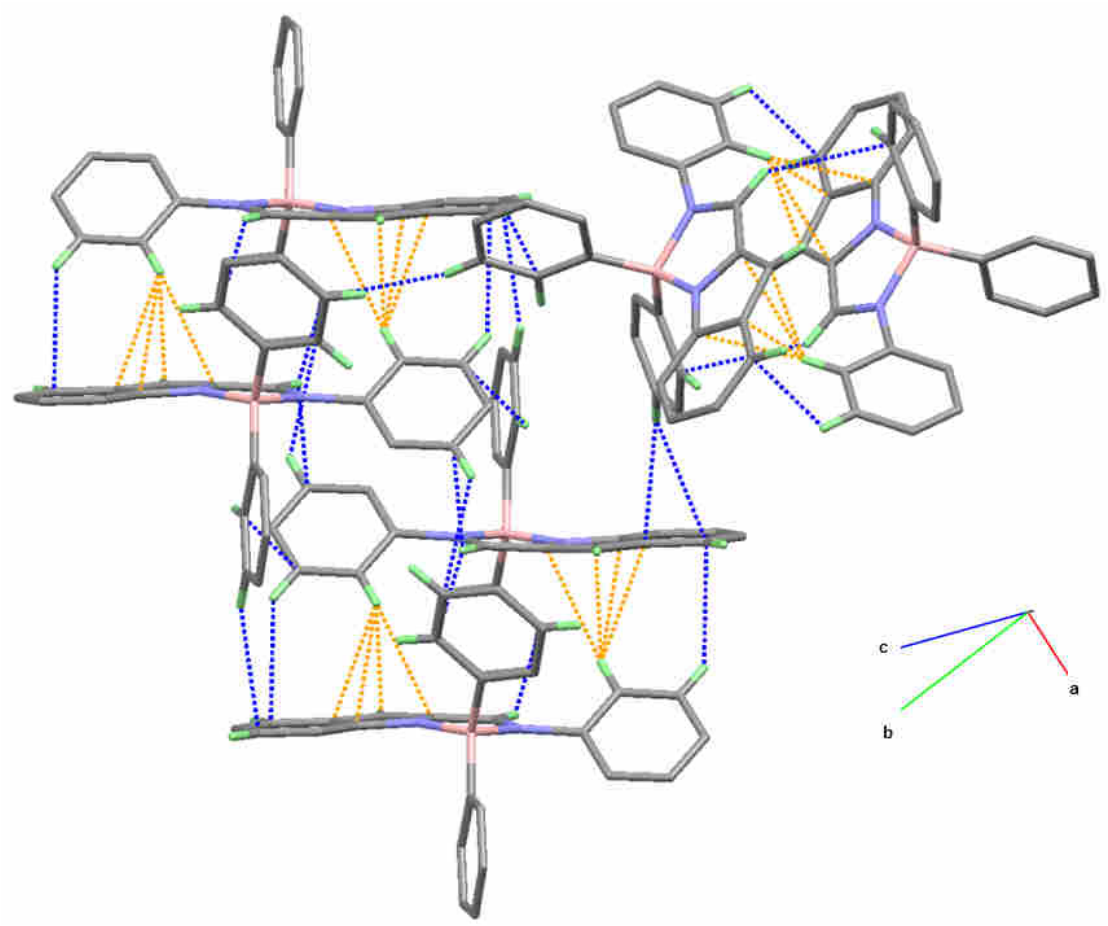


Fig. S3 View of the 3D supramolecular arrangement of compound **10**, showing all the short contacts: C–H··· $\pi C_{(Ar)}$ (blue dashed lines) and C–H··· $\pi C_{(Pyrr)}$ (orange dashed lines) responsible for the formation of head-to-tail dimers. All hydrogen atoms, except those (represented in green) involved in the depicted short contacts, were omitted for clarity.

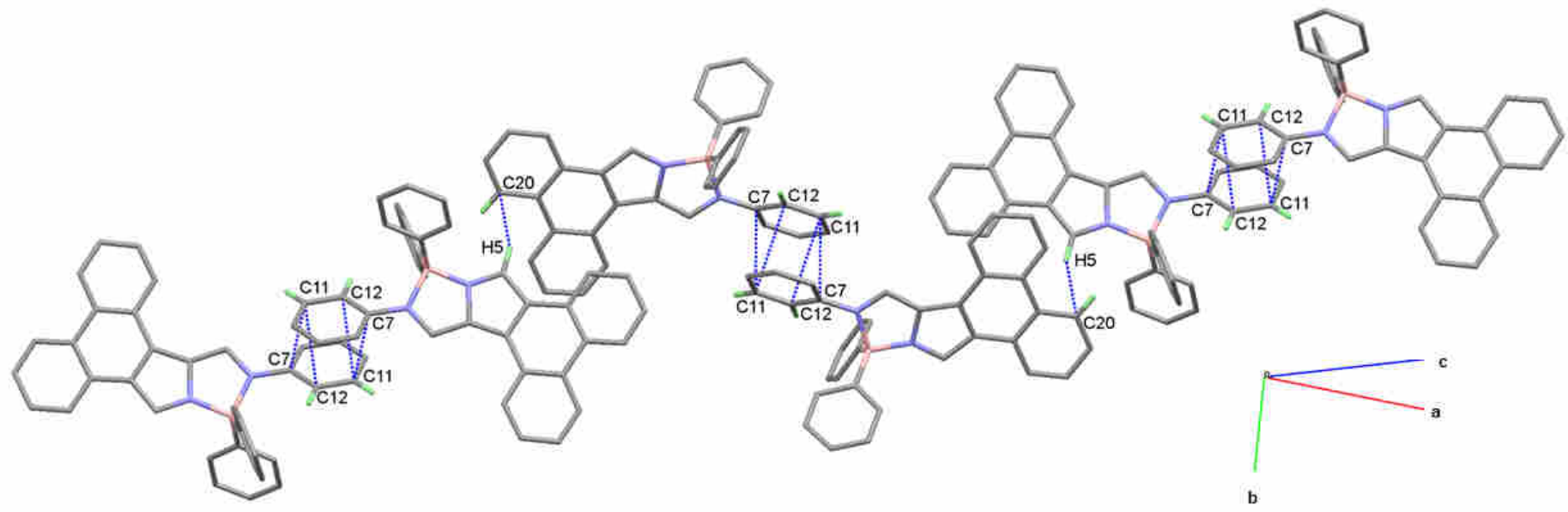


Fig. S4 Detail of the supramolecular arrangement of compound **13**, showing the formation of a 1D chain of head-to-tail dimers, through π-stacking between two iminic phenyl rings (*ca.* 3.34 Å). All hydrogen atoms, except those (represented in green) involved in the depicted short contacts, were omitted for clarity.

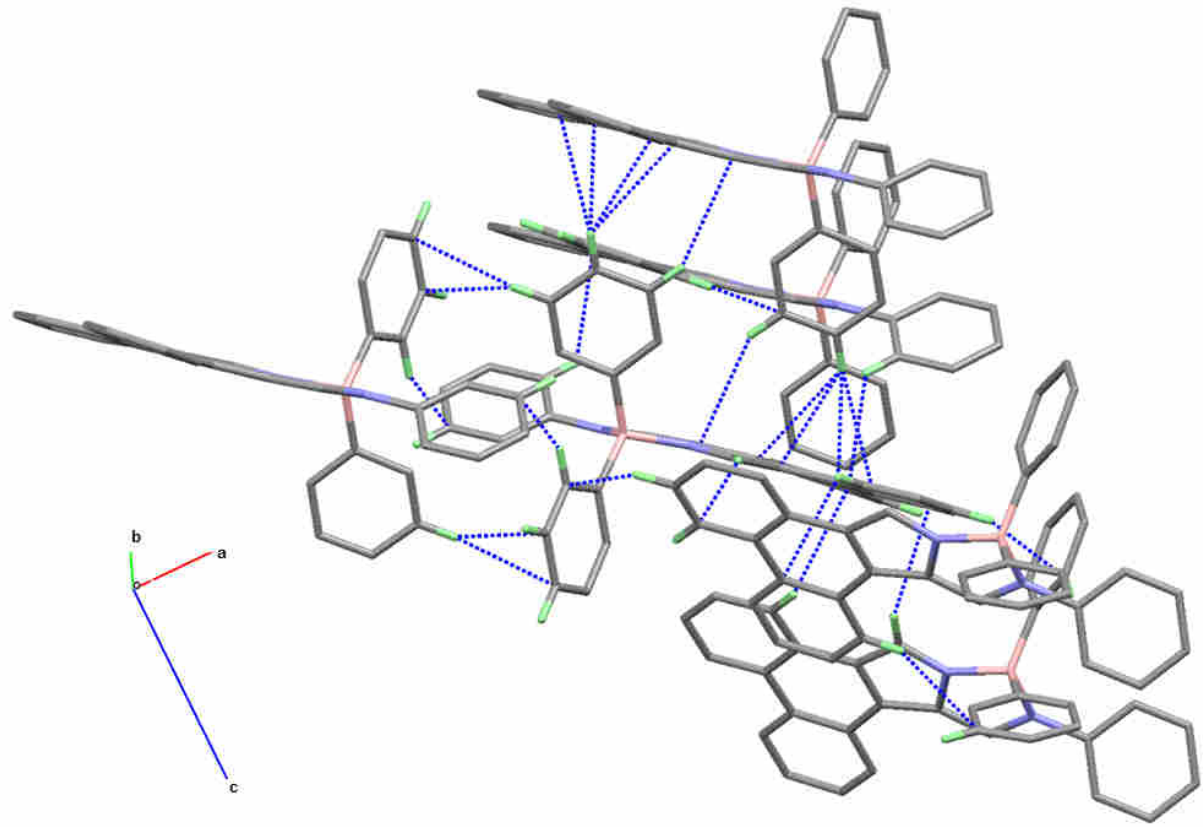
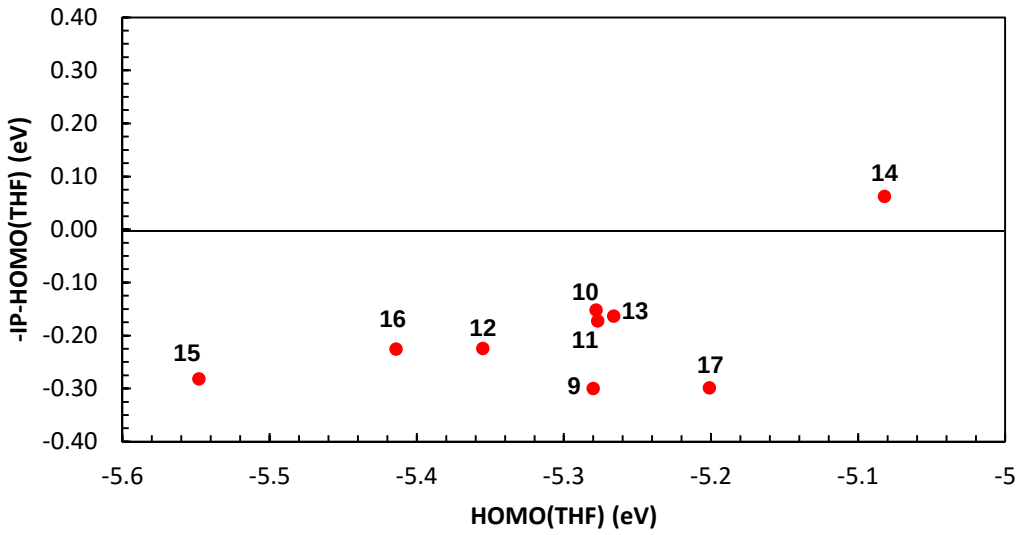


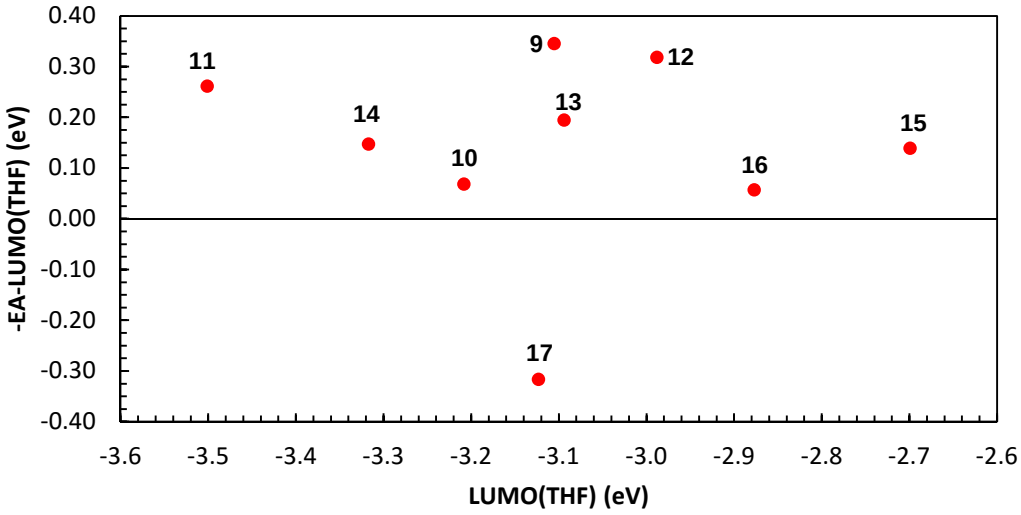
Fig. S5 View of the overall interactions of each boron complex with the neighboring molecules in the crystalline structure of **13**, showing the complexity of the packing, and highlighting the formation of 2D sheets containing the phenanthro[9,10-*c*]pyrrolyl-boron moieties. All hydrogen atoms, except those involved in the depicted short contacts (represented in green), were omitted for clarity.

Table S2 List of short contacts for compounds **9**, **10** and **13**, and corresponding symmetry operations in relation to the asymmetric unit

	D–H···A	**d(H···A) (Å)**	**d(D···A) (Å)**	**(D–H···A) (º)**	**Symmetry operation**
9	C27–H27···πC13	2.963	3.807	149	*x* , - 1 + *y* , *z*
	C27–H27··· πC14	2.926	3.771	149	*x* , - 1 + *y* , *z*
	C19–H19A···πC3	2.997	3.505	114	½ + *x* , 1 – *y*, ½ + *z*
	C26–H26···πC9	2.879	3.463	121	½ + *x* , - *y*, - ½ + *z*
10	C12–H12···πC2	2.933	3.634	132	2 – *x*, 1 – *y*, 1 – *z*
	C12–H12···πC3	2.943	3.387	110	2 – *x*, 1 – *y*, 1 – *z*
	C12–H12···πC4	2.911	3.398	113	2 – *x*, 1 – *y*, 1 – *z*
	C12–H12···πC5	2.914	3.684	139	2 – *x*, 1 – *y*, 1 – *z*
	C9–H9···πC19	2.918	3.681	138	- 1 + *x* , *y* , *z*
	C6–H6···πC9	2.860	3.384	116	1 – *x*, 1 – *y*, 1 – *z*
	C6–H6···πC18	2.975	3.772	142	2 – *x*, 1 – *y*, 1 – *z*
	C11–H11···πC13	2.887	3.512	124	2 – *x*, 1 – *y*, 1 – *z*
	C20–H20···πC4	2.835	3.578	136	- ½ + *x* , ½ - *y*, - ½ + *z*
	C20–H20···πC13	2.992	3.658	128	- ½ + *x* , ½ - *y*, - ½ + *z*
	C28–H28···πC11	2.971	3.594	125	1 – *x*, 1 – *y*, 1 – *z*
13	C23–H23···πC18	2.950	3.439	113	2 – *x*, - ½ + *y*, ½ – *z*
	C5–H5···πC20	2.878	3.679	143	2 – *x*, - ½ + *y*, ½ – *z*
	C21–H21···πC32	2.929	3.589	128	2 – *x*, ½ + *y*, ½ – *z*
	C32–H32···πC11	2.712	3.516	143	1 – *x*, 1 – *y*, – *z*
	C29–H29···πC33	2.785	3.448	128	1 – *x*, 1 – *y*, – *z*
	C29–H29···πC34	2.923	3.747	146	1 – *x*, 1 – *y*, – *z*
	C8–H8···πC18	2.973	3.668	131	2 – *x*, – *y*, – *z*
	C27–H27···πC2	2.937	3.782	149	2 – *x*, 1 – *y*, – *z*
	C28–H28···πC3	2.965	3.644	126	2 – *x*, 1 – *y*, – *z*
	C28–H28···πC4	2.931	3.479	118	2 – *x*, 1 – *y*, – *z*
	C28–H28···πC19	2.996	3.855	151	2 – *x*, 1 – *y*, – *z*
	C28–H28···πC24	2.921	3.577	127	2 – *x*, 1 – *y*, – *z*



(a)



(b)

Fig. S6 Plots of (a) the difference between –IP and HOMO versus the energies of the HOMOs, and of (b) the difference between –EA and LUMO versus the energies of the LUMOs of compounds **9**–**17**. IP and EA were estimated from cyclic voltammetry measurements, and the energies of the HOMOs and LUMOs were determined by DFT (THF).

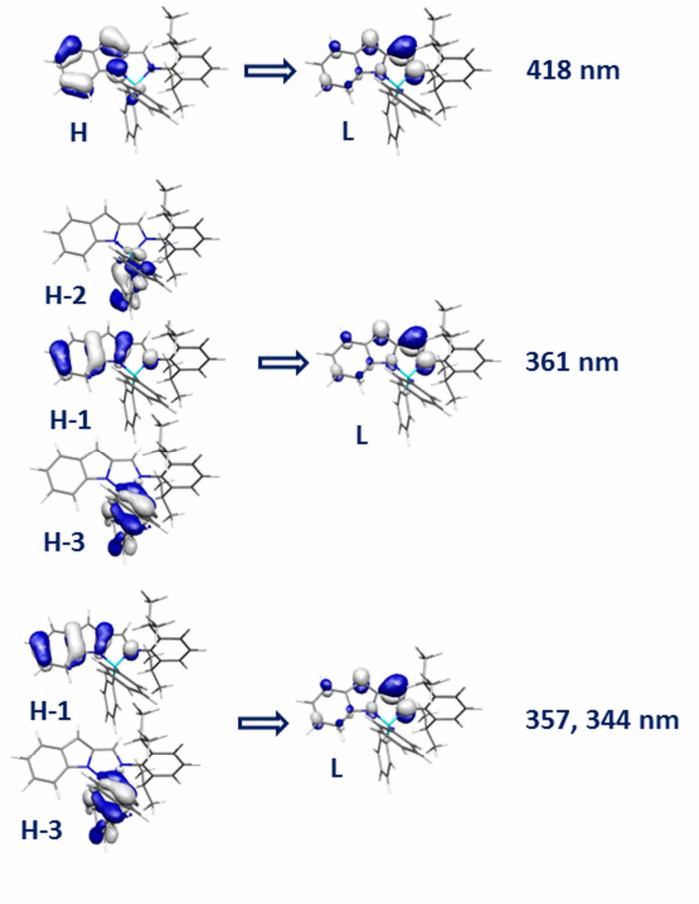


Fig. S7 The frontier orbitals of **9** involved in the low energy transitions.

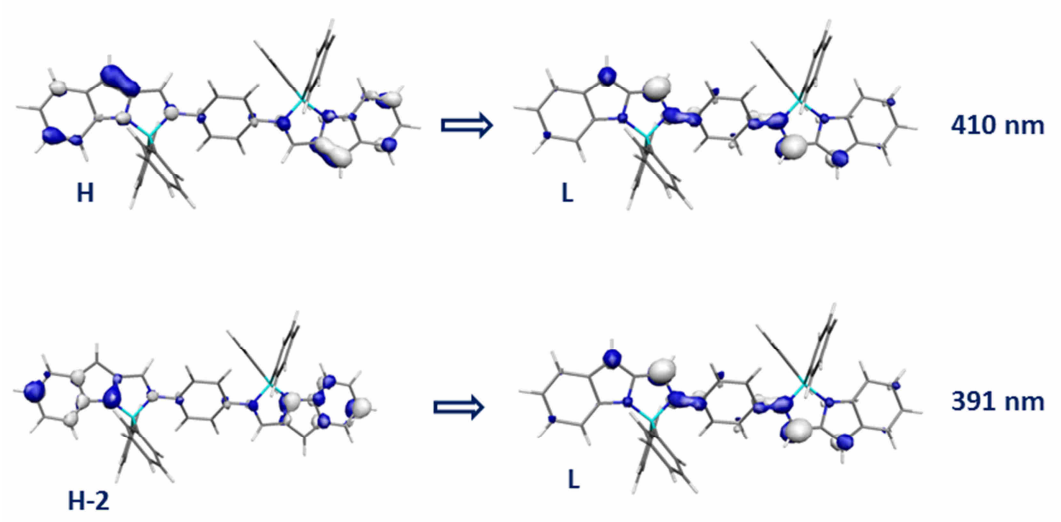


Fig. S8 The frontier orbitals of **11** involved in the low energy transitions.

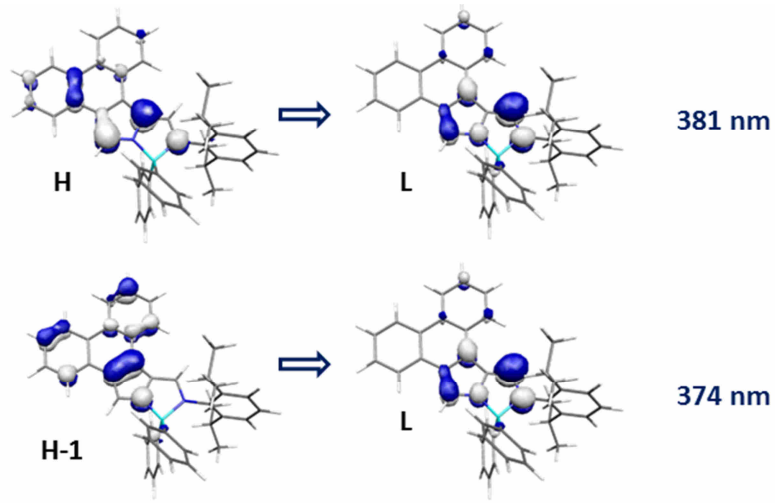


Fig. S9 The frontier orbitals of **12** involved in the low energy transitions.

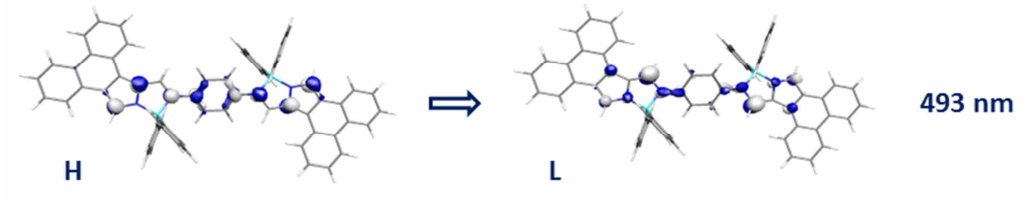


Fig. S10 The frontier orbitals of **14** involved in the low energy transition.

Table S2 Calculated GP, THF and TDDFT maximum emission wavelength (E_{em}^{max}) and energy (λ_{em}^{max}) (in nm and eV, respectively) for complexes **9**–**14**.

Complex	GP		THF		TDDFT	
	nm	eV	nm	eV	nm	eV
9	712	1.74	691	1.79	589	2.10
10	785	1.58	748	1.66	609	2.04
11	930	1.33	874	1.42	649	1.91
12	634	1.96	624	1.99	420	2.95
13	725	1.71	705	1.76	446	2.78
14	935	1.32	899	1.38	474	2.62

DFT Optimized Structures of Boron Complexes 9–14 in the Ground State (S_0) and First Singlet State (S_1)

9 (Ground state)

N	1.066824	1.736566	9.976769
N	1.103137	0.373517	11.932180
C	2.035435	2.161107	10.872262
H	3.561048	3.776681	10.870468
C	1.165280	2.530692	8.868663
C	0.430068	2.511298	7.669184
C	2.483586	4.465088	8.089848
C	2.209257	3.505270	9.091598
C	-0.002734	0.303325	14.130910
C	0.783700	-2.379223	14.448869
H	1.095811	-3.413649	14.586459
C	2.755784	3.248384	10.373300
C	-0.418825	1.769613	14.040012
H	-0.276571	2.105909	13.005671
C	1.990028	1.342195	12.020784
C	1.161382	-1.704320	13.281557
C	0.743248	-0.363718	13.128109
C	0.032042	-1.752642	15.438191
H	-0.251985	-2.298152	16.337672
C	-0.345249	-0.424269	15.279079
H	-0.924935	0.065630	16.061052
C	3.555329	-2.203918	12.689372
H	3.823974	-1.142474	12.784833
H	4.218697	-2.655037	11.937404
H	3.753659	-2.688419	13.657349
C	-1.904814	1.986500	14.373042
H	-2.169124	3.042035	14.218126
H	-2.125872	1.743487	15.422373
H	-2.549717	1.373513	13.730524
C	0.458016	2.649102	14.955970
H	0.175002	3.706601	14.853617
H	1.528134	2.559196	14.722160
H	0.326977	2.363208	16.010113
C	2.079597	-2.384963	12.277391
H	1.945046	-1.887057	11.311378
C	1.762013	-3.872834	12.066233
H	2.372105	-4.267383	11.242427
H	0.705923	-4.026239	11.808263
H	1.988899	-4.474383	12.958605
H	2.583667	1.489943	12.921806
B	0.326738	0.441111	10.453930
C	-1.257845	0.629647	10.698842
C	-1.927444	1.816422	10.350477
C	-2.043862	-0.404717	11.246598
C	-3.309347	1.959277	10.513147
C	-3.423791	-0.270790	11.417957
C	-4.065036	0.913230	11.044818
H	-1.360867	2.652130	9.937162
H	-1.569795	-1.339907	11.548392
H	-3.794654	2.891977	10.223840
H	-3.999307	-1.093725	11.842772
H	-5.142792	1.019921	11.171676
C	0.749292	-0.792241	9.472568
C	2.083266	-0.904893	9.026526
C	-0.164294	-1.733233	8.968276
C	2.489845	-1.912312	8.151107
C	0.231053	-2.746488	8.087077
C	1.560877	-2.844208	7.678475
H	2.827643	-0.181897	9.367770
H	-1.214230	-1.669790	9.254226
H	3.530157	-1.964740	7.828240
H	-0.508149	-3.455825	7.713315
H	1.870434	-3.629829	6.988484
C	1.747743	4.437077	6.919854
C	0.732774	3.466450	6.713069
H	3.263977	5.210629	8.240995
H	1.946584	5.169048	6.137936
H	0.180355	3.472424	5.774096
H	-0.345896	1.766351	7.503931

9 (Singlet state)

N	1.071029	1.726937	10.044215
N	1.144541	0.317797	11.947774

C	2.053387	2.139546	10.901502
H	3.558969	3.809530	10.789396
C	1.114112	2.522089	8.890551
C	0.339738	2.476929	7.751053
C	2.369020	4.457067	8.058496
C	2.148224	3.503174	9.069055
C	0.128708	0.452608	14.196401
C	0.556405	-2.301655	14.552911
H	0.720939	-3.368016	14.700857
C	2.744444	3.260978	10.329885
C	-0.185803	1.940151	14.059975
H	0.031651	2.242443	13.029036
C	2.082184	1.321212	12.039847
C	0.944274	-1.712299	13.344731
C	0.724363	-0.321714	13.165065
C	-0.016067	-1.551319	15.576469
H	-0.303165	-2.028909	16.512961
C	-0.221314	-0.188738	15.392226
H	-0.684986	0.394666	16.188423
C	3.200174	-2.408423	12.475778
H	3.519654	-1.358963	12.425509
H	3.727585	-2.964367	11.687107
H	3.511833	-2.813024	13.450767
C	-1.676088	2.235282	14.311547
H	-1.881763	3.301778	14.138709
H	-1.963302	2.006144	15.347958
H	-2.315871	1.647873	13.639943
C	0.690783	2.793395	14.997746
H	0.470827	3.862227	14.860493
H	1.762512	2.638064	14.811655
H	0.497156	2.543400	16.051389
C	1.673634	-2.540070	12.297378
H	1.427374	-2.122487	11.314549
C	1.267219	-4.020745	12.277951
H	1.721919	-4.516675	11.409691
H	0.177939	-4.143550	12.207521
H	1.612365	-4.555727	13.174853
H	2.704346	1.446441	12.918445
B	0.395222	0.399768	10.526983
C	-1.212549	0.481979	10.707062
C	-1.949052	1.652100	10.455828
C	-1.931078	-0.646176	11.145024
C	-3.337765	1.694252	10.621366
C	-3.316420	-0.611269	11.322204
C	-4.027712	0.561462	11.055647
H	-1.434841	2.555800	10.125659
H	-1.400220	-1.578082	11.346317
H	-3.878982	2.618206	10.414500
H	-3.840983	-1.503679	11.664735
H	-5.109710	0.591113	11.187372
C	0.875191	-0.733267	9.422569
C	2.250037	-0.952141	9.201301
C	-0.027213	-1.442664	8.613339
C	2.703371	-1.869277	8.253039
C	0.418791	-2.363506	7.658358
C	1.785051	-2.581933	7.475676
H	2.984394	-0.403703	9.795065
H	-1.099168	-1.283814	8.735444
H	3.773959	-2.022354	8.112805
H	-0.306897	-2.909696	7.054757
H	2.133831	-3.294175	6.727332
C	1.578781	4.412746	6.894383
C	0.589416	3.447512	6.739681
H	3.139219	5.218370	8.175464
H	1.745940	5.144637	6.105628
H	-0.009449	3.426004	5.830932
H	-0.432898	1.721727	7.623510

9 (TD-DFT optimized geometry – Singlet)

N	1.103701	1.760939	10.027853
N	1.229851	0.398725	11.949205
C	2.145139	2.237518	10.848424
H	3.579199	3.910146	10.673728
C	1.071318	2.556544	8.841566
C	0.254073	2.457476	7.714867
C	2.259599	4.482578	7.950701
C	2.083018	3.558698	8.973295
C	0.086656	0.400021	14.171855
C	0.788207	-2.304285	14.552888
H	1.067168	-3.351061	14.708647
C	2.751150	3.323805	10.268265

C	-0.310484	1.880693	14.009239
H	-0.040375	2.190915	12.988664
C	2.241733	1.356050	12.043008
C	1.184829	-1.660106	13.368042
C	0.820582	-0.301706	13.174883
C	0.060833	-1.627147	15.534090
H	-0.236872	-2.143415	16.452944
C	-0.278406	-0.284962	15.343291
H	-0.842639	0.245618	16.116409
C	3.405580	-2.828196	12.947665
H	3.946808	-1.944873	13.310005
H	4.021401	-3.325072	12.186787
H	3.270289	-3.520459	13.788268
C	-1.838960	2.082791	14.178058
H	-2.097901	3.132461	13.988670
H	-2.160451	1.828732	15.195531
H	-2.390602	1.454817	13.467805
C	0.468592	2.775109	15.011884
H	0.202039	3.829385	14.861837
H	1.551976	2.668030	14.874453
H	0.224069	2.501081	16.045901
C	2.038110	-2.420103	12.337570
H	2.227892	-1.734399	11.498955
C	1.291570	-3.660051	11.781022
H	1.914282	-4.164492	11.031072
H	0.351556	-3.360015	11.301026
H	1.063438	-4.375986	12.580702
H	2.655321	1.658775	13.006636
B	0.447281	0.433943	10.565212
C	-1.148326	0.538179	10.766542
C	-1.898265	1.687617	10.442892
C	-1.862653	-0.560451	11.295793
C	-3.287164	1.739604	10.624649
C	-3.249178	-0.516730	11.488035
C	-3.970118	0.635446	11.147652
H	-1.391352	2.570581	10.040902
H	-1.321059	-1.472963	11.568330
H	-3.838266	2.648766	10.360335
H	-3.770618	-1.386562	11.902336
H	-5.054996	0.672387	11.291811
C	0.915811	-0.712016	9.505743
C	2.287760	-0.882100	9.203840
C	0.001611	-1.522627	8.801481
C	2.727219	-1.830931	8.273032
C	0.431080	-2.476041	7.868242
C	1.796995	-2.635474	7.601408
H	3.030811	-0.255758	9.711422
H	-1.070964	-1.409231	8.992033
H	3.797346	-1.941469	8.066201
H	-0.303962	-3.097482	7.344767
H	2.134403	-3.378230	6.870510
C	1.422119	4.397876	6.793073
C	0.449248	3.413539	6.676517
H	3.024660	5.266127	8.014406
H	1.560437	5.126209	5.985999
H	-0.178532	3.362504	5.780887
H	-0.507345	1.671992	7.629418

10 (Ground state)

N	1.101684	1.881841	9.783163
N	1.076885	0.633312	11.800457
C	1.966081	2.423669	10.721692
H	3.369722	4.148645	10.733850
C	1.207990	2.635545	8.650427
C	0.549788	2.514148	7.412840
C	2.443225	4.620052	7.856671
C	2.165507	3.693769	8.889310
C	0.775384	0.315384	14.213713
C	0.310130	-2.402450	13.804620
H	0.129156	-3.463574	13.637997
C	2.640338	3.538706	10.213637
H	0.901705	1.386067	14.370251
C	1.904779	1.658823	11.900952
C	0.550274	-1.573173	12.710525
C	0.799383	-0.208470	12.910437
C	0.309972	-1.886726	15.102314
H	0.120437	-2.539879	15.953253
C	0.539556	-0.523005	15.300854
H	0.514779	-0.103449	16.305787
H	0.576839	-1.977592	11.701419
H	2.472929	1.854079	12.808284
B	0.368090	0.600261	10.310162

C	-1.223810	0.822294	10.494458
C	-1.795139	2.105911	10.418307
C	-2.098003	-0.245215	10.778068
C	-3.164291	2.316708	10.605855
C	-3.466861	-0.045771	10.972110
C	-4.007039	1.239481	10.885036
H	-1.158266	2.964570	10.200054
H	-1.704799	-1.260524	10.841844
H	-3.572133	3.325497	10.533232
H	-4.113388	-0.896450	11.189818
H	-5.075660	1.399057	11.032315
C	0.833364	-0.710334	9.472961
C	2.144059	-1.215256	9.574394
C	-0.016968	-1.334853	8.543557
C	2.580387	-2.297104	8.807764
C	0.410165	-2.416696	7.766223
C	1.710091	-2.906160	7.899261
H	2.845775	-0.754929	10.273337
H	-1.038237	-0.970393	8.425656
H	3.601139	-2.664871	8.916703
H	-0.276667	-2.877487	7.055585
H	2.045152	-3.752188	7.298610
C	1.789462	4.485363	6.646677
C	0.851648	3.441044	6.429660
H	3.162407	5.423021	8.016647
H	1.992692	5.188860	5.840188
H	0.357568	3.369316	5.461328
H	-0.168875	1.715719	7.240280

10 (Singlet state)

N	1.086617	1.880454	9.818300
N	1.065943	0.667690	11.853190
C	1.937049	2.443956	10.719785
H	3.315800	4.223185	10.617272
C	1.149781	2.611407	8.628785
C	0.471181	2.448053	7.437789
C	2.341408	4.580809	7.754466
C	2.094042	3.683776	8.815245
C	1.291107	0.136877	14.238486
C	-0.128645	-2.229609	13.816122
H	-0.680271	-3.153269	13.644662
C	2.590161	3.581305	10.130518
H	1.816990	1.068422	14.432136
C	1.920251	1.748087	11.934144
C	0.106524	-1.375277	12.748293
C	0.826462	-0.169141	12.931422
C	0.336908	-1.919476	15.100560
H	0.147318	-2.592665	15.935347
C	1.044695	-0.727852	15.297279
H	1.400712	-0.463304	16.292893
H	-0.243726	-1.636247	11.754870
H	2.515341	1.974866	12.807358
B	0.385594	0.599007	10.396698
C	-1.228429	0.813211	10.496332
C	-1.750209	2.086003	10.794966
C	-2.153974	-0.233144	10.343344
C	-3.122508	2.306472	10.930068
C	-3.530281	-0.024478	10.476210
C	-4.020836	1.248981	10.768167
H	-1.069375	2.929130	10.925805
H	-1.799691	-1.237986	10.109100
H	-3.491132	3.306725	11.160055
H	-4.218983	-0.860553	10.350599
H	-5.093447	1.416369	10.870077
C	0.882230	-0.700836	9.542118
C	2.042914	-1.413051	9.895554
C	0.218513	-1.104586	8.369187
C	2.504502	-2.490065	9.134424
C	0.673897	-2.177785	7.598665
C	1.820296	-2.878031	7.980935
H	2.596173	-1.128860	10.791711
H	-0.685321	-0.580536	8.055900
H	3.402839	-3.025298	9.443481
H	0.129545	-2.469544	6.699939
H	2.178293	-3.716822	7.383395
C	1.657712	4.406088	6.545947
C	0.740575	3.363598	6.389985
H	3.052712	5.396408	7.878590
H	1.840188	5.090271	5.718928
H	0.216799	3.245988	5.442753
H	-0.248028	1.644424	7.302459

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10 (TD-DFT optimized geometry – Singlet)

N	1.081747	1.888136	9.822237
N	1.078231	0.712537	11.875731
C	1.966941	2.524198	10.716665
H	3.293027	4.285826	10.557867
C	1.116013	2.595062	8.584637
C	0.414495	2.372223	7.397960
C	2.264631	4.535432	7.668332
C	2.042073	3.675922	8.736318
C	1.216702	0.148642	14.296894
C	-0.132655	-2.259226	13.802240
H	-0.658084	-3.200072	13.606008
C	2.566681	3.601272	10.113271
H	1.719277	1.095805	14.505319
C	1.915894	1.812520	12.007538
C	0.126672	-1.389430	12.744220
C	0.811297	-0.166433	12.971781
C	0.275600	-1.943039	15.107723
H	0.068255	-2.629683	15.934002
C	0.948232	-0.734804	15.342324
H	1.262312	-0.472550	16.358511
H	-0.180601	-1.647962	11.728598
H	2.591945	1.962214	12.846004
B	0.396216	0.608573	10.436626
C	-1.204430	0.822139	10.527697
C	-1.731295	2.098722	10.826630
C	-2.132753	-0.227015	10.365777
C	-3.108172	2.320727	10.950679
C	-3.512733	-0.017576	10.491669
C	-4.007038	1.259821	10.782341
H	-1.047164	2.942989	10.968594
H	-1.773937	-1.235595	10.135514
H	-3.482382	3.324157	11.181352
H	-4.205586	-0.856318	10.362616
H	-5.085078	1.427153	10.878969
C	0.922137	-0.662443	9.580566
C	2.120946	-1.326562	9.920498
C	0.253607	-1.105379	8.418800
C	2.612533	-2.396038	9.161053
C	0.738333	-2.170998	7.649857
C	1.921205	-2.823509	8.020217
H	2.677931	-1.004871	10.807285
H	-0.674878	-0.613921	8.109810
H	3.540910	-2.896095	9.458248
H	0.190807	-2.495236	6.758055
H	2.303326	-3.657679	7.422103
C	1.555877	4.312665	6.443448
C	0.656569	3.263187	6.312273
H	2.966908	5.374572	7.747164
H	1.732058	4.989841	5.599970
H	0.122111	3.109878	5.369020
H	-0.296309	1.542816	7.301528

11 (Ground state)

N	-0.091130	0.488301	18.123132
N	-1.896630	0.427155	16.584319
C	-1.928466	1.580347	17.353897
C	2.034171	-0.633793	13.385510
H	2.681226	-0.662010	12.508404
C	-2.998930	2.407043	16.993709
H	-3.256267	3.363414	17.433805
C	0.357615	-0.564720	15.677741
C	-2.941742	0.494095	15.709669
C	-3.357228	-0.412905	14.717690
C	-3.661419	1.728130	15.944755
C	-4.800682	2.024680	15.159870
C	0.395285	-1.684038	14.826570
H	-0.230004	-2.548577	15.053551
C	2.109093	-0.481681	18.542939
H	2.147897	-0.811917	17.508335
C	2.010469	0.495132	14.208757
H	2.639133	1.354851	13.975323
C	-1.118459	-1.902037	17.586788
C	1.179736	0.524438	15.330614
H	1.178378	1.421238	15.953788
C	0.989318	0.230655	18.997923
C	0.974208	0.691646	20.325628
H	0.090144	1.189254	20.720703
C	-0.851895	1.565292	18.255515
H	-0.630335	2.343054	18.982867
C	1.218044	-1.722485	13.696229

H	1.221508	-2.607076	13.058583
C	-2.420126	-2.090604	18.087517
H	-3.149550	-1.283574	18.001832
C	-0.607015	-4.185389	18.320890
H	0.110832	-5.002003	18.405042
C	-1.907436	-4.345144	18.804806
H	-2.211213	-5.284030	19.268652
C	-2.814763	-3.290915	18.684992
H	-3.834318	-3.402546	19.055350
C	-0.224849	-2.982054	17.722712
H	0.792708	-2.889349	17.340935
B	-0.672592	-0.491437	16.929730
N	4.258378	-0.489065	21.585988
N	6.075240	-0.405210	23.109967
C	6.107638	-1.564536	22.349599
C	2.168190	0.634483	26.340390
H	1.531102	0.660418	27.224747
C	7.187502	-2.380591	22.705999
H	7.447262	-3.338813	22.271404
C	3.820278	0.570780	24.030244
C	7.130334	-0.456645	23.973509
C	7.550420	0.462578	24.952237
C	7.856774	-1.687208	23.741132
C	9.007664	-1.967527	24.514942
C	3.793129	1.687260	24.885632
H	4.417340	2.551624	24.655081
C	2.053701	0.471242	21.168921
H	2.015127	0.801575	22.203490
C	2.181588	-0.491607	25.513170
H	1.554610	-1.351470	25.750562
C	5.269039	1.913051	22.104214
C	3.000483	-0.518357	24.382490
H	2.994471	-1.413420	23.756906
C	3.174183	-0.239555	20.713474
C	3.187993	-0.703562	19.386801
H	4.071947	-1.201494	18.991912
C	5.024488	-1.562542	21.455721
H	4.802869	-2.346155	20.734649
C	2.982567	1.723092	26.024688
H	2.987472	2.605381	26.665516
C	6.561590	2.106560	21.582310
H	7.295619	1.302594	21.656973
C	4.736033	4.193488	21.376321
H	4.013559	5.007130	21.303305
C	6.027620	4.358104	20.871006
H	6.319839	5.297811	20.401377
C	6.941299	3.307785	20.977071
H	7.954088	3.423283	20.589834
C	4.368829	2.989232	21.982016
H	3.358241	2.892592	22.380960
B	4.840503	0.501224	22.769930
C	-5.193073	1.123981	14.188401
C	-4.476235	-0.083083	13.971946
H	-6.066769	1.336903	13.573745
H	-4.818541	-0.766849	13.196009
H	-5.354522	2.949053	15.321745
H	-2.812332	-1.338580	14.545459
C	9.404824	-1.054622	25.473031
C	8.681042	0.148634	25.687184
H	7.000606	1.385736	25.122395
H	9.027396	0.842390	26.452455
H	10.287640	-1.254908	26.078829
H	9.566478	-2.889252	24.355323

11 (Singlet state)

N	-0.122301	0.483934	18.185563
N	-1.903444	0.404452	16.606627
C	-1.974559	1.537594	17.376272
C	2.073266	-0.590304	13.460207
H	2.727956	-0.607544	12.588524
C	-3.074778	2.344447	16.989948
H	-3.363083	3.291985	17.430161
C	0.373859	-0.550262	15.737379
C	-2.943215	0.443625	15.701853
C	-3.317131	-0.461823	14.709404
C	-3.696139	1.658426	15.927308
C	-4.826018	1.935061	15.121270
C	0.263651	-1.548970	14.751267
H	-0.485560	-2.333605	14.865540
C	1.888181	-0.768703	18.703166
H	1.750254	-1.347146	17.795686
C	2.199685	0.417551	14.418368

H	2.954727	1.194874	14.297907
C	-1.139301	-1.916408	17.605480
C	1.357541	0.435102	15.533013
H	1.478176	1.237809	16.262612
C	0.956473	0.254983	19.014185
C	1.196072	1.025755	20.187177
H	0.491301	1.792947	20.497111
C	-0.929850	1.565171	18.311023
H	-0.753879	2.353629	19.032251
C	1.096779	-1.573952	13.629511
H	0.984046	-2.365326	12.887778
C	-2.344726	-2.007488	18.327340
H	-2.971702	-1.120855	18.437990
C	-0.799304	-4.301602	18.061052
H	-0.187055	-5.196672	17.946342
C	-1.999738	-4.361424	18.770700
H	-2.331652	-5.300523	19.214294
C	-2.772830	-3.205594	18.903152
H	-3.713991	-3.237680	19.452975
C	-0.380916	-3.095573	17.491280
H	0.555748	-3.082090	16.931919
B	-0.668859	-0.492086	16.980586
N	4.304258	-0.459872	21.500212
N	6.083481	-0.381416	23.081485
C	6.161816	-1.508616	22.303934
C	2.094386	0.551019	26.230838
H	1.438066	0.554296	27.101456
C	7.266827	-2.311455	22.684952
H	7.561358	-3.253821	22.237795
C	3.797831	0.547654	23.956296
C	7.123016	-0.420786	23.986578
C	7.491010	0.479807	24.985609
C	7.883378	-1.629376	23.752900
C	9.014476	-1.904954	24.557555
C	3.899083	1.536615	24.953151
H	4.642593	2.327971	24.848490
C	2.292063	0.790802	20.984288
H	2.429538	1.368676	21.892132
C	1.976842	-0.447405	25.261782
H	1.227161	-1.231330	25.372524
C	5.304383	1.943549	22.104863
C	2.820965	-0.446929	24.148505
H	2.707515	-1.242756	23.410327
C	3.224405	-0.232177	20.672722
C	2.984480	-1.003200	19.499868
H	3.688569	-1.771015	19.190064
C	5.117990	-1.535831	21.368340
H	4.947823	-2.320041	20.641183
C	3.063956	1.543497	26.073681
H	3.169684	2.327684	26.824019
C	6.509613	2.050031	21.384870
H	7.141849	1.168421	21.264535
C	4.950586	4.331823	21.676208
H	4.333045	5.221966	21.800699
C	6.151094	4.406809	20.968110
H	6.477740	5.352838	20.535410
C	6.931002	3.257127	20.823012
H	7.872294	3.300974	20.274316
C	4.538931	3.116890	22.231794
H	3.602086	3.091592	22.790456
B	4.842833	0.509615	22.714214
C	-5.183136	1.028897	14.134431
C	-4.438175	-0.153869	13.933565
H	-6.048635	1.226503	13.503804
H	-4.744966	-0.846768	13.151144
H	-5.401467	2.846838	15.277871
H	-2.753562	-1.376392	14.542000
C	9.365582	-1.003776	25.551096
C	8.613450	0.173041	25.759928
H	6.921939	1.389827	25.159080
H	8.915684	0.862170	26.547446
H	10.231913	-1.200661	26.180787
H	9.595477	-2.812088	24.394680

11 (TD-DFT optimized geometry – Singlet)

N	-0.147595	0.533690	18.138491
N	-1.921367	0.427877	16.567560
C	-2.017544	1.612663	17.333483
C	2.095551	-0.576832	13.462593
H	2.762663	-0.603527	12.594666
C	-3.123924	2.377956	16.935726

H	-3.437205	3.333537	17.355249	C	7.146941	-0.359296	24.045435
C	0.363806	-0.511714	15.726111	C	7.460661	0.608141	25.004426
C	-2.980190	0.438846	15.667367	C	7.932513	-1.542426	23.863293
C	-3.359887	-0.505434	14.677579	C	9.046371	-1.751335	24.670432
C	-3.746076	1.650737	15.882592	C	3.921055	1.427476	24.955155
C	-4.896871	1.889158	15.076457	H	4.666466	2.224858	24.867843
C	0.251008	-1.510564	14.734543	C	2.310656	0.779823	20.976257
H	-0.520177	-2.281926	14.835013	H	2.468565	1.356423	21.890628
C	1.883048	-0.750523	18.662712	C	2.000766	-0.578556	25.226895
H	1.719901	-1.320889	17.744870	H	1.250451	-1.370731	25.326367
C	2.224824	0.432436	14.424354	C	5.292919	1.877886	22.082145
H	2.995302	1.202612	14.309261	C	2.848177	-0.557152	24.111591
C	-1.127618	-1.858932	17.606908	H	2.742743	-1.340630	23.353373
C	1.367364	0.461845	15.531592	C	3.220845	-0.262614	20.644729
H	1.486597	1.265693	16.266079	C	2.977743	-1.023161	19.463209
C	0.970305	0.289753	18.994075	H	3.670036	-1.812882	19.161052
C	1.214225	1.048274	20.175655	C	5.134209	-1.624053	21.351476
H	0.522222	1.838423	20.477397	H	4.969443	-2.409820	20.614350
C	-0.945563	1.633647	18.270581	C	3.081353	1.411743	26.075960
H	-0.753014	2.419128	19.008751	H	3.180599	2.186884	26.843823
C	1.099972	-1.548497	13.620806	C	6.462094	1.968173	21.294369
H	0.983967	-2.339782	12.872140	H	7.058986	1.068474	21.107273
C	-2.322482	-1.945340	18.355407	C	4.973503	4.285222	21.725196
H	-2.948402	-1.052552	18.464653	H	4.380439	5.190415	21.896044
C	-0.774120	-4.244563	18.087310	C	6.140069	4.347991	20.952849
H	-0.160274	-5.144636	17.973123	H	6.465419	5.299775	20.519152
C	-1.963741	-4.298688	18.822827	C	6.884825	3.181365	20.737744
H	-2.285697	-5.236800	19.287005	H	7.797115	3.217275	20.132229
C	-2.739800	-3.140172	18.954357	C	4.560932	3.066452	22.280485
H	-3.674887	-3.169695	19.524266	H	3.646287	3.045661	22.882245
C	-0.368137	-3.042163	17.492578	B	4.829360	0.450642	22.677159
H	0.561738	-3.032908	16.914129	C	-5.249645	0.958881	14.115601
B	-0.682409	-0.444744	16.956352	C	-4.485997	-0.230438	13.918928
N	4.336377	-0.525100	21.495361	H	-6.131164	1.128506	13.489161
N	6.088724	-0.399640	23.092636	H	-4.803250	-0.940589	13.147800
C	6.224793	-1.581902	22.342550	H	-5.489250	2.798769	15.222232
C	2.114246	0.407917	26.214927	H	-2.775546	-1.417784	14.526758
H	1.454753	0.392783	27.089423	C	9.372863	-0.770357	25.660047
C	7.317300	-2.305238	22.765331	C	8.603816	0.376352	25.821425
H	7.671460	-3.259675	22.366987	H	6.851585	1.512243	25.125273
C	3.817775	0.454006	23.938418	H	8.872582	1.116564	26.582597

H	10.249713	-0.933318	26.297321
H	9.672052	-2.646016	24.559504

12 (Ground state)

N	1.156590	1.780250	9.732830
N	1.095130	0.444570	11.700430
C	4.083830	5.422060	9.896560
C	2.016190	2.283180	10.702490
C	3.646630	4.337590	10.717510
C	1.258280	2.529160	8.624200
H	0.686040	2.294520	7.734400
C	2.612740	4.659150	8.012840
C	2.184270	3.575520	8.857050
C	-0.170940	0.377860	13.816040
C	0.646500	-2.282240	14.224760
H	0.969660	-3.308230	14.397090
C	2.679360	3.422970	10.176580
C	3.560680	5.587040	8.535270
C	-0.618330	1.831050	13.676610
H	-0.394140	2.165110	12.656340
C	4.169580	4.200690	12.021850
H	3.838640	3.369430	12.641280
C	1.918230	1.475220	11.843340
C	1.094380	-1.610640	13.080650
C	0.662990	-0.279990	12.877630
C	-0.187650	-1.661860	15.149660
H	-0.525270	-2.203400	16.032990
C	5.027950	6.318430	10.443880
H	5.383040	7.155810	9.848400
C	3.965320	6.651920	7.700300
H	4.684920	7.381280	8.063980
C	-0.579980	-0.343940	14.946200
H	-1.225660	0.141590	15.677680
C	2.537470	5.882120	5.909530
H	2.145530	5.997260	4.899820
C	3.468540	6.802220	6.415670
H	3.802420	7.636560	5.800190
C	5.524930	6.167500	11.728120
H	6.252600	6.879780	12.114800
C	5.093540	5.097480	12.526790
H	5.483890	4.972570	13.535870
C	3.527280	-2.130380	12.709650
H	3.794630	-1.073630	12.849900
H	4.255170	-2.575680	12.016140
H	3.628110	-2.634260	13.682760
C	2.119410	4.827490	6.701710
H	1.396770	4.112250	6.311260
C	-2.133280	2.007000	13.877970
H	-2.413590	3.053660	13.693470
H	-2.436940	1.762210	14.905950
H	-2.703630	1.372410	13.187480
C	0.149670	2.741310	14.657560
H	-0.148700	3.790190	14.518990
H	1.238140	2.677360	14.521010
H	-0.067590	2.460960	15.698840
C	2.095960	-2.286340	12.156100
H	2.059900	-1.770960	11.191640
C	1.780790	-3.766030	11.889130
H	2.471790	-4.161120	11.132090
H	0.757300	-3.897470	11.514080
H	1.896480	-4.382800	12.792300
H	2.419770	1.653520	12.791950
B	0.437160	0.459030	10.187880
C	-1.168420	0.607440	10.286850
C	-1.847500	1.759700	9.855000
C	-1.961080	-0.445000	10.788640
C	-3.242450	1.854900	9.896630
C	-3.354430	-0.359360	10.838550
C	-4.003100	0.792420	10.386120
H	-1.280060	2.610850	9.474510
H	-1.481390	-1.356290	11.148110
H	-3.733880	2.763660	9.547530
H	-3.934560	-1.195270	11.230200
H	-5.090820	0.861670	10.419340
C	0.971860	-0.751480	9.234580
C	2.341480	-0.835240	8.905080
C	0.121990	-1.700170	8.642170
C	2.838720	-1.820770	8.051980
C	0.609280	-2.692580	7.783590
C	1.970280	-2.759910	7.487370
H	3.041870	-0.108410	9.322860
H	-0.948740	-1.659670	8.840670

H	3.903970	-1.851910	7.820670
H	-0.082240	-3.409290	7.339280
H	2.351860	-3.529110	6.815210

12 (Singlet state)

N	1.189998	1.736689	9.789647
N	1.137288	0.397304	11.733786
C	4.001647	5.475651	9.879940
C	2.033400	2.264053	10.739004
C	3.580861	4.374318	10.714395
C	1.272438	2.486854	8.644906
H	0.704877	2.211462	7.763853
C	2.557625	4.641522	8.001228
C	2.155922	3.560542	8.856920
C	0.048535	0.569409	13.943082
C	0.262332	-2.219405	14.247253
H	0.347218	-3.296932	14.378563
C	2.663853	3.444495	10.178557
C	3.482483	5.604244	8.518727
C	-0.222303	2.067335	13.820579
H	0.084358	2.396794	12.821747
C	4.100252	4.266617	12.034781
H	3.783182	3.434509	12.658755
C	1.996303	1.477548	11.897437
C	0.739386	-1.640177	13.069518
C	0.635697	-0.225458	12.909280
C	-0.291350	-1.450195	15.267510
H	-0.646603	-1.923552	16.182280
C	4.913419	6.399616	10.426231
H	5.251222	7.242077	9.827616
C	3.863434	6.668988	7.669729
H	4.563264	7.420078	8.027577
C	-0.392776	-0.071936	15.104470
H	-0.858257	0.524896	15.889453
C	2.462519	5.837721	5.883968
H	2.072823	5.931098	4.871102
C	3.368767	6.789422	6.382613
H	3.683165	7.623502	5.756778
C	5.403673	6.272291	11.718837
H	6.107075	7.007665	12.106319
C	4.993187	5.195245	12.527338
H	5.380479	5.096667	13.540788
C	2.989058	-2.466355	12.314352
H	3.374045	-1.438074	12.301759
H	3.521267	-3.038767	11.541473
H	3.222317	-2.906981	13.295565
C	2.067407	4.782437	6.685188
H	1.365733	4.043898	6.300179
C	-1.725092	2.382251	13.950550
H	-1.896722	3.456093	13.787000
H	-2.105405	2.132888	14.951542
H	-2.311881	1.822529	13.210475
C	0.585731	2.879336	14.850966
H	0.404896	3.955163	14.716844
H	1.666343	2.701603	14.759560
H	0.293689	2.614116	15.877562
C	1.468526	-2.501593	12.053337
H	1.305012	-2.063094	11.062516
C	0.973022	-3.953683	11.994356
H	1.435346	-4.463916	11.138807
H	-0.117537	-4.008965	11.874126
H	1.244988	-4.521258	12.896273
H	2.517460	1.640144	12.831531
B	0.535088	0.378652	10.216763
C	-1.082478	0.423366	10.278065
C	-1.815364	1.597616	10.028915
C	-1.822069	-0.727524	10.611362
C	-3.212365	1.622450	10.094378
C	-3.216681	-0.712568	10.688216
C	-3.919954	0.465715	10.425372
H	-1.288260	2.519876	9.778922
H	-1.297950	-1.663777	10.810898
H	-3.747733	2.550162	9.889028
H	-3.755290	-1.623633	10.950713
H	-5.008879	0.481160	10.479348
C	1.151295	-0.750571	9.198181
C	2.548455	-0.911643	9.090355
C	0.355459	-1.500392	8.315149
C	3.120293	-1.803436	8.183017
C	0.919155	-2.395816	7.398286
C	2.303313	-2.555006	7.331790
H	3.207634	-0.330671	9.739103

H	-0.728751	-1.385539	8.341482
H	4.204703	-1.907609	8.132292
H	0.271357	-2.965667	6.731232
H	2.745127	-3.249741	6.616747

12 (TD-DFT optimized geometry – Singlet)

N	1.172754	1.829808	9.856464
N	1.173091	0.458427	11.778848
C	4.101417	5.477840	9.784429
C	2.072144	2.354160	10.775517
C	3.671846	4.409544	10.656928
C	1.212315	2.574494	8.643582
H	0.588908	2.286931	7.796836
C	2.547374	4.681148	7.936800
C	2.117891	3.597510	8.815109
C	-0.142951	0.400508	13.908409
C	0.604844	-2.289959	14.304959
H	0.900787	-3.331130	14.467057
C	2.691186	3.473793	10.185551
C	3.526968	5.611988	8.411168
C	-0.582351	1.867897	13.732273
H	-0.232755	2.207940	12.746048
C	4.237080	4.302931	11.965987
H	3.903253	3.487463	12.614993
C	2.053488	1.524353	11.974810
C	1.071675	-1.615873	13.163776
C	0.686388	-0.263707	12.959993
C	-0.213397	-1.648373	15.237558
H	-0.565489	-2.186947	16.123742
C	5.072221	6.374050	10.273611
H	5.424100	7.194392	9.641734
C	3.924630	6.649680	7.541353
H	4.670035	7.380551	7.867982
C	-0.575351	-0.313153	15.039016
H	-1.214244	0.188302	15.772527
C	2.429214	5.863270	5.793735
H	2.007117	5.959695	4.787601
C	3.386969	6.777444	6.251833
H	3.720897	7.596734	5.605647
C	5.611991	6.248558	11.561507
H	6.365234	6.967316	11.904287
C	5.192445	5.207485	12.412086
H	5.617324	5.112775	13.417179
C	3.353345	-2.710959	12.896833
H	3.839103	-1.817708	13.309880
H	4.039355	-3.178483	12.178613
H	3.176762	-3.418926	13.716394
C	2.014872	4.824310	6.632974
H	1.266533	4.103884	6.284781
C	-2.126960	2.006451	13.761915
H	-2.409500	3.049806	13.571294
H	-2.530636	1.714706	14.739151
H	-2.584305	1.375390	12.989933
C	0.064851	2.774526	14.814329
H	-0.232098	3.819511	14.656231
H	1.159710	2.714844	14.772129
H	-0.258354	2.472090	15.818427
C	2.023565	-2.333691	12.190939
H	2.254799	-1.626968	11.380478
C	1.360023	-3.585901	11.561861
H	2.049793	-4.056248	10.849296
H	0.446191	-3.307049	11.022265
H	1.100720	-4.323610	12.331684
H	2.489423	1.745948	12.947745
B	0.518161	0.490643	10.335858
C	-1.094374	0.537275	10.382142
C	-1.839376	1.651477	9.942835
C	-1.824584	-0.567792	10.873738
C	-3.240182	1.665200	9.987184
C	-3.224081	-0.561172	10.927859
C	-3.939637	0.557257	10.480008
H	-1.316148	2.533830	9.559655
H	-1.286812	-1.454240	11.227794
H	-3.788443	2.547013	9.637824
H	-3.759536	-1.433539	11.318273
H	-5.034051	0.564722	10.516632
C	1.105471	-0.630183	9.301067
C	2.503238	-0.739767	9.094495
C	0.275933	-1.477887	8.535493
C	3.045657	-1.677581	8.208408
C	0.810097	-2.418749	7.645661

C	2.198571	-2.524102	7.479761
H	3.180544	-0.076972	9.645775
H	-0.811137	-1.405659	8.648218
H	4.131381	-1.745144	8.078487
H	0.140892	-3.073893	7.076777
H	2.617315	-3.256018	6.780396

13 (Ground state)

N	-0.738297	-1.404384	0.130323
N	-2.684572	-0.054668	0.111533
C	3.310160	0.925750	-0.081699
C	-0.406099	-0.055686	0.040464
C	1.904477	1.183155	-0.068438
C	0.384203	-2.132486	0.164428
H	0.351548	-3.213103	0.240979
C	2.912425	-1.545718	0.076074
C	1.502792	-1.263234	0.088508
C	-4.194109	1.649509	-0.808519
C	-6.339616	0.469038	0.521221
H	-7.173727	-0.000547	1.041313
C	1.010589	0.062424	0.014462
C	3.818838	-0.448476	-0.011478
H	-3.372144	2.080547	-1.378717
C	1.443087	2.516275	-0.133232
H	0.371931	2.708003	-0.118279
C	-1.584787	0.692206	0.018465
C	-5.068428	-0.090697	0.631961
C	-3.979344	0.503951	-0.021958
C	-6.546872	1.621651	-0.239291
H	-7.543129	2.054047	-0.323234
C	4.178458	2.036643	-0.162344
H	5.254055	1.879066	-0.174244
C	5.201000	-0.739119	-0.025852
H	5.923736	0.070382	-0.092563
C	-5.467078	2.206290	-0.905645
H	-5.618750	3.089651	-1.524862
C	4.773860	-3.112553	0.130743
H	5.143528	-4.135602	0.186086
C	5.674268	-2.039319	0.043117
H	6.747198	-2.226316	0.029543
C	3.703784	3.336283	-0.226050
H	4.405567	4.167030	-0.286002
C	2.321972	3.581112	-0.210993
H	1.944411	4.601669	-0.258387
C	3.413303	-2.863076	0.146696
H	2.712398	-3.693775	0.215397
H	-4.904664	-0.973643	1.244565
H	-1.648139	1.774356	-0.055516
B	-2.296355	-1.631097	0.225165
C	-2.864498	-2.430789	-1.061233
C	-2.143115	-2.484559	-2.268377
C	-4.120727	-3.066136	-1.043308
C	-2.641759	-3.140703	-3.397245
C	-4.630158	-3.722779	-2.166314
C	-3.890358	-3.763528	-3.350147
H	-1.164083	-2.006386	-2.334045
H	-4.712822	-3.059042	-0.127216
H	-2.053030	-3.164503	-4.314885
H	-5.606304	-4.206099	-2.115610
H	-4.283611	-4.277166	-4.227957
C	-2.650184	-2.250793	1.680719
C	-2.770268	-3.641621	1.857537
C	-2.737323	-1.452408	2.836116
C	-2.977665	-4.207132	3.119346
C	-2.949439	-2.005996	4.100779
C	-3.072163	-3.389869	4.247172
H	-2.706923	-4.297636	0.988040
H	-2.641351	-0.368391	2.749892
H	-3.069236	-5.289107	3.219594
H	-3.017005	-1.356310	4.973876
H	-3.238834	-3.826581	5.232185

13 (Singlet state)

N	-0.763333	-1.362444	0.117606
N	-2.695811	-0.012593	0.068008
C	3.332181	0.883974	-0.159795
C	-0.410204	-0.034054	-0.032578
C	1.917875	1.150332	-0.196259
C	0.361601	-2.116510	0.208564
H	0.304207	-3.189917	0.343709
C	2.895233	-1.571447	0.146709
C	1.494359	-1.275885	0.101798

C	-4.189998	1.910683	-0.223574
C	-6.367905	0.227359	0.279958
H	-7.214795	-0.428046	0.478586
C	1.027593	0.053518	-0.057966
C	3.818854	-0.483967	0.019139
H	-3.361193	2.578355	-0.440369
C	1.470004	2.485124	-0.370242
H	0.401292	2.683507	-0.401700
C	-1.553184	0.768735	-0.081918
C	-5.088268	-0.299974	0.290735
C	-3.958408	0.527582	0.040785
C	-6.581176	1.589843	0.019177
H	-7.590548	1.998390	0.009731
C	4.210241	1.978266	-0.300762
H	5.284638	1.813252	-0.279604
C	5.198190	-0.787491	0.076094
H	5.930525	0.010926	-0.013345
C	-5.480040	2.419176	-0.232277
H	-5.633861	3.477059	-0.443211
C	4.739267	-3.143919	0.370235
H	5.098354	-4.163151	0.506507
C	5.654233	-2.083075	0.247615
H	6.724698	-2.279352	0.289183
C	3.746959	3.274449	-0.469183
H	4.455772	4.094205	-0.575399
C	2.364495	3.528754	-0.504153
H	2.000401	4.546802	-0.637715
C	3.382992	-2.886311	0.319770
H	2.671960	-3.705180	0.417844
H	-4.932241	-1.352057	0.504458
H	-1.588795	1.842655	-0.173126
B	-2.317503	-1.581488	0.202306
C	-2.855577	-2.410612	-1.092967
C	-2.264921	-2.205975	-2.354340
C	-3.924484	-3.322222	-1.034967
C	-2.710764	-2.875268	-3.496293
C	-4.380541	-3.998570	-2.170453
C	-3.773694	-3.777654	-3.407819
H	-1.431285	-1.507274	-2.451139
H	-4.409708	-3.522530	-0.078063
H	-2.227174	-2.692748	-4.456486
H	-5.210385	-4.701012	-2.086156
H	-4.125105	-4.303899	-4.295801
C	-2.689252	-2.209717	1.652606
C	-2.565831	-3.595357	1.873436
C	-3.034880	-1.418930	2.762797
C	-2.790199	-4.164735	3.129732
C	-3.269459	-1.978228	4.021966
C	-3.149017	-3.356318	4.210735
H	-2.298082	-4.248120	1.040763
H	-3.127653	-0.337801	2.646711
H	-2.689823	-5.242386	3.263236
H	-3.543699	-1.334367	4.858174
H	-3.331101	-3.796275	5.191594

13 (TD-DFT optimized geometry – Singlet)

N	-0.780475	-1.309294	0.132030
N	-2.716241	0.046207	0.058056
C	3.371665	0.824173	-0.143442
C	-0.395268	0.018244	0.007375
C	1.960644	1.132365	-0.139547
C	0.356435	-2.156357	0.190860
H	0.241260	-3.235475	0.290546
C	2.897848	-1.662867	0.090053
C	1.473736	-1.354426	0.095774
C	-4.308096	1.946496	-0.224410
C	-6.453986	0.169269	0.084053
H	-7.290032	-0.527997	0.205228
C	1.011062	0.061182	-0.022521
C	3.840748	-0.591140	-0.027994
H	-3.484671	2.652017	-0.352000
C	1.540215	2.494097	-0.250283
H	0.468033	2.713158	-0.244636
C	-1.588484	0.852824	-0.045901
C	-5.149013	-0.315803	0.143569
C	-4.044788	0.565766	-0.010670
C	-6.704414	1.534583	-0.127296
H	-7.731296	1.909129	-0.172775
C	4.277276	1.896470	-0.258111
H	5.353528	1.702467	-0.264316
C	5.212466	-0.918857	-0.030914

H	5.963280	-0.128202	-0.119030
C	-5.621489	2.412263	-0.280132
H	-5.802844	3.479568	-0.447505
C	4.726433	-3.291605	0.192486
H	5.067182	-4.329161	0.276973
C	5.653496	-2.247540	0.077404
H	6.728014	-2.462025	0.071253
C	3.840270	3.225264	-0.366002
H	4.578073	4.031365	-0.453313
C	2.465153	3.525733	-0.361900
H	2.127770	4.564427	-0.445585
C	3.359354	-2.997913	0.198473
H	2.625178	-3.806297	0.287749
H	-4.962995	-1.379304	0.309283
H	-1.631390	1.931495	-0.168295
B	-2.338401	-1.487833	0.207439
C	-2.847424	-2.364300	-1.056408
C	-2.372644	-2.064103	-2.353137
C	-3.773276	-3.421254	-0.942271
C	-2.800300	-2.778383	-3.478937
C	-4.209689	-4.141159	-2.062716
C	-3.722724	-3.823151	-3.336881
H	-1.652623	-1.248465	-2.485960
H	-4.165832	-3.688788	0.044896
H	-2.413558	-2.520452	-4.470935
H	-4.934084	-4.954067	-1.941251
H	-4.060221	-4.385856	-4.213834
C	-2.663733	-2.092086	1.676317
C	-2.401177	-3.448843	1.972224
C	-3.146313	-1.287113	2.729957
C	-2.639640	-3.984241	3.243801
C	-3.393365	-1.815360	4.003854
C	-3.141463	-3.168092	4.266262
H	-2.007522	-4.105187	1.188508
H	-3.344538	-0.225539	2.548253
H	-2.433313	-5.042272	3.439203
H	-3.781316	-1.167086	4.797322
H	-3.329857	-3.582665	5.262364

14 (Ground state)

N	-0.060264	0.967328	18.309614
N	-1.535074	1.536434	16.544048
C	-2.197322	1.550769	17.768814
C	2.263973	4.811588	15.449099
H	2.800537	5.706232	15.132362
C	-3.549934	1.932953	17.549169
C	0.877596	2.476646	16.278091
C	-2.390654	1.889821	15.577644
H	-2.076175	1.950487	14.542203
C	-3.662641	2.142598	16.153578
C	1.322421	2.636664	14.952243
H	1.137784	1.842456	14.227235
C	2.313979	0.730051	18.808836
H	2.545896	1.320798	17.927145
C	1.827066	4.681700	16.769387
H	2.018975	5.477624	17.489398
C	0.360798	-0.211114	15.962210
C	1.140744	3.532673	17.169700
H	0.807042	3.458695	18.206406
C	0.972062	0.482207	19.139527
C	0.696197	-0.244715	20.311448
H	-0.329055	-0.508871	20.564450
C	-1.291803	1.199005	18.769955
H	-1.518550	1.122559	19.829386
C	2.004891	3.784600	14.539225
H	2.338176	3.874468	13.504841
C	-0.623968	-1.187050	15.718913
H	-1.659843	-0.990044	16.001271
C	1.994418	-1.746880	14.971036
H	3.023895	-1.955180	14.677728
C	0.996058	-2.695198	14.739049
H	1.239487	-3.647080	14.266267
C	-0.317860	-2.410169	15.116315
H	-1.107739	-3.141072	14.940502
C	1.676249	-0.526806	15.573260
H	2.471749	0.203110	15.729254
B	-0.005498	1.183862	16.695979
N	4.095641	-0.934552	21.628430
N	5.577364	-1.507484	23.386750
C	6.231028	-1.534404	22.157591
C	1.753958	-4.736368	24.532455
H	1.210993	-5.623452	24.859453

C	7.580994	-1.929757	22.369838
C	3.157272	-2.421232	23.676855
C	6.435808	-1.865309	24.349011
H	6.127715	-1.918049	25.386802
C	7.701136	-2.133786	23.765675
C	2.713945	-2.564102	25.005111
H	2.906639	-1.764104	25.721577
C	1.720502	-0.690865	21.134115
H	1.488478	-1.280706	22.016481
C	2.189165	-4.623523	23.209998
H	1.989432	-5.425244	22.498607
C	3.703198	0.263469	23.969290
C	2.883893	-3.484220	22.796606
H	3.216130	-3.423493	21.758554
C	3.062416	-0.444991	20.802022
C	3.338322	0.283384	19.631149
H	4.363846	0.547298	19.378860
C	5.321831	-1.179372	21.160814
H	5.541447	-1.110273	20.099329
C	2.023185	-3.702279	25.431234
H	1.691561	-3.778983	26.467207
C	4.700262	1.228642	24.205147
H	5.733309	1.016970	23.923066
C	2.089658	1.825725	24.951793
H	1.063086	2.048757	25.244451
C	3.099999	2.762994	25.176876
H	2.868866	3.720851	25.643718
C	4.409925	2.459273	24.800256
H	5.208970	3.181465	24.970652
C	2.392079	0.597959	24.357177
H	1.587427	-0.122912	24.206092
B	4.050388	-1.140407	23.243578
C	-4.677261	2.110223	18.420465
C	-5.922796	2.504018	17.840533
C	-4.594393	1.910844	19.816080
C	-7.024180	2.674169	18.708030
C	-5.693596	2.086395	20.636483
C	-6.920419	2.471747	20.074289
H	-3.643436	1.614086	20.254006
H	-7.987488	2.973038	18.302365
H	-5.607327	1.927607	21.710517
H	-7.792853	2.613076	20.710720
C	-4.904670	2.540130	15.548498
C	-5.026920	2.754412	14.159036
C	-6.038324	2.721022	16.394380
C	-6.231904	3.137754	13.598113
C	-7.252785	3.112413	15.788523
C	-7.353933	3.317577	14.422199
H	-4.154392	2.615699	13.522236
H	-6.308811	3.299809	12.523773
H	-8.139520	3.260836	16.399865
H	-8.306579	3.619906	13.989341
C	8.942980	-2.541767	24.364150
C	9.072518	-2.750583	25.753773
C	10.068640	-2.739318	23.511367
C	10.277129	-3.144251	26.308310
C	11.282976	-3.140842	24.110812
C	11.391405	-3.340260	25.477430
H	8.205965	-2.599307	26.395846
H	10.359699	-3.301897	27.382891
H	12.163774	-3.301944	23.494134
H	12.343737	-3.650656	25.905217
C	8.700149	-2.124022	21.491632
C	9.945281	-2.528678	22.064917
C	8.609597	-1.931290	20.095557
C	11.038452	-2.716044	21.190611
C	9.700866	-2.123845	19.268391
C	10.927230	-2.520010	19.824029
H	7.658928	-1.626277	19.662696
H	12.001131	-3.023713	21.591128
H	9.608702	-1.970083	18.194117
H	11.793414	-2.674865	19.182201

14 (Singlet state)

N	-0.091622	0.861829	18.332998
N	-1.538027	1.502742	16.564662
C	-2.221671	1.482645	17.776094
C	2.343294	4.708140	15.544140
H	2.901237	5.595375	15.243797
C	-3.572794	1.886843	17.541150
C	0.897769	2.391872	16.329569
C	-2.374466	1.901904	15.592004

H	-2.039797	1.994011	14.565501	C	1.783049	-0.333010	21.297307
C	-3.654692	2.151432	16.152192	H	1.601054	-0.612375	22.329741
C	1.180410	2.662606	14.976026	C	1.972823	-4.457952	23.075400
H	0.844612	1.962847	14.208765	H	1.629353	-5.169506	22.324151
C	2.249058	0.321066	18.621820	C	3.732606	0.297290	23.967603
H	2.431159	0.600387	17.589443	C	2.685536	-3.322131	22.680760
C	2.071625	4.468169	16.892214	H	2.886107	-3.177825	21.617776
H	2.414461	5.170601	17.652325	C	3.103743	-0.437238	20.779618
C	0.302103	-0.272822	15.941474	C	3.296498	-0.093065	19.406953
C	1.354779	3.329894	17.272115	H	4.287029	-0.125392	18.961915
H	1.150241	3.174728	18.332775	C	5.392348	-1.095639	21.127403
C	0.928882	0.428232	19.140268	H	5.646067	-1.007653	20.080206
C	0.735531	0.080691	20.512070	C	2.160073	-3.764581	25.375586
H	-0.255011	0.112674	20.957091	H	1.960976	-3.929546	26.434956
C	-1.357783	1.094383	18.795674	C	4.690897	1.328738	23.995447
H	-1.613211	0.996202	19.841533	H	5.661352	1.174765	23.519213
C	1.889871	3.800522	14.584018	C	2.244589	1.776052	25.236375
H	2.092524	3.976691	13.527121	H	1.283025	1.939252	25.724152
C	-0.659034	-1.301131	15.900090	C	3.213984	2.780251	25.247724
H	-1.629789	-1.149921	16.376589	H	3.015730	3.732023	25.741299
C	1.788057	-1.741087	14.658111	C	4.442106	2.551757	24.622126
H	2.750044	-1.901427	14.170237	H	5.209060	3.326858	24.624435
C	0.815781	-2.742241	14.633386	C	2.505498	0.556969	24.603915
H	1.012144	-3.688777	14.129096	H	1.734939	-0.215877	24.620652
C	-0.412750	-2.517442	15.259508	B	4.056683	-1.099188	23.205626
H	-1.181917	-3.290191	15.246877	C	-4.705359	2.043800	18.399188
C	1.529516	-0.528668	15.304161	C	-5.937394	2.486608	17.816416
H	2.302437	0.241973	15.297852	C	-4.652675	1.778873	19.787516
B	-0.019430	1.115608	16.719155	C	-7.050673	2.637457	18.670772
N	4.125821	-0.863137	21.589104	C	-5.764700	1.938029	20.593168
N	5.576539	-1.480550	23.362276	C	-6.975046	2.371630	20.028658
C	6.258718	-1.470661	22.149873	H	-3.716696	1.441597	20.227295
C	1.706034	-4.683813	24.426872	H	-8.001405	2.971260	18.262588
H	1.151275	-5.569067	24.738646	H	-5.702245	1.727751	21.660091
C	7.611431	-1.868038	22.387425	H	-7.855943	2.499480	20.656049
C	3.143486	-2.373030	23.611601	C	-4.874021	2.598393	15.544510
C	6.415365	-1.866885	24.338028	C	-4.967872	2.875881	14.162520
H	6.082123	-1.949693	25.365792	C	-6.020383	2.769010	16.380834
C	7.695654	-2.118350	23.778911	C	-6.152932	3.311899	13.600492
C	2.865644	-2.629435	24.968904	C	-7.213897	3.215876	15.771509
H	3.201947	-1.920313	25.727312	C	-7.285340	3.482844	14.414326

H	-4.087557	2.744514	13.535116
H	-6.208192	3.523106	12.533409
H	-8.107439	3.359643	16.373868
H	-8.222674	3.826832	13.979160
C	8.916833	-2.555985	24.389665
C	9.012705	-2.820347	25.774083
C	10.062727	-2.731811	23.553801
C	10.199243	-3.248666	26.338900
C	11.257661	-3.170955	24.165929
C	11.331071	-3.425138	25.525450
H	8.132728	-2.685103	26.401150
H	10.256054	-3.449740	27.407860
H	12.150707	-3.319083	23.563897
H	12.269357	-3.763943	25.962601
C	8.743932	-2.028916	21.530001
C	9.977828	-2.462426	22.115828
C	8.689565	-1.776115	20.139477
C	11.091161	-2.616745	21.262163
C	9.801630	-1.938605	19.334531
C	11.013794	-2.363122	19.902035
H	7.752188	-1.445853	19.697353
H	12.043438	-2.943086	21.672774
H	9.737847	-1.737803	18.265858
H	11.894825	-2.493119	19.275273

14 (TD-DFT optimized geometry – Singlet)

N	-0.129809	0.902248	18.335413
N	-1.559652	1.539782	16.560929
C	-2.279704	1.537859	17.789390
C	2.390250	4.711623	15.613359
H	2.974937	5.590798	15.322701
C	-3.635599	1.928446	17.514827
C	0.877030	2.420723	16.370347
C	-2.410433	1.913454	15.558147
H	-2.068702	1.986045	14.520486
C	-3.702694	2.160112	16.111425
C	1.060143	2.772285	15.014352
H	0.611289	2.149920	14.232341
C	2.215161	0.230503	18.588529
H	2.350595	0.403254	17.517260
C	2.216433	4.392335	16.965045
H	2.664079	5.025322	17.739103
C	0.285827	-0.234189	15.979621
C	1.466271	3.266744	17.331964
H	1.340915	3.046127	18.397077
C	0.922650	0.457948	19.163931
C	0.764173	0.223753	20.570192
H	-0.203733	0.382950	21.051478
C	-1.409953	1.149962	18.823118
H	-1.661365	1.040033	19.880597
C	1.804110	3.896612	14.636304
H	1.928406	4.138561	13.575082
C	-0.608441	-1.323818	16.068999
H	-1.529966	-1.216433	16.652601
C	1.718984	-1.644451	14.568821
H	2.635375	-1.762055	13.980074
C	0.813923	-2.707330	14.673249
H	1.016883	-3.658333	14.169321
C	-0.355000	-2.542429	15.428078
H	-1.070482	-3.367363	15.516207
C	1.454202	-0.429074	15.214911
H	2.173467	0.391221	15.114833
B	-0.043742	1.150390	16.746567
N	4.169530	-0.878213	21.592665
N	5.598981	-1.516563	23.367164
C	6.319774	-1.512258	22.139144
C	1.652359	-4.695051	24.306557
H	1.068577	-5.575452	24.595316
C	7.675968	-1.901575	22.414047
C	3.163265	-2.400985	23.554507
C	6.449606	-1.890444	24.370003
H	6.107348	-1.964702	25.407371
C	7.742488	-2.134892	23.817201
C	2.980423	-2.755613	24.909746
H	3.428573	-2.134448	25.693114
C	1.824448	-0.206974	21.339408
H	1.689004	-0.379791	22.410667
C	1.825900	-4.372698	22.955567
H	1.378937	-5.004490	22.180140
C	3.750690	0.253948	23.950198
C	2.574913	-3.245550	22.591075

H	2.700047	-3.022554	21.526435
C	3.117022	-0.434187	20.764057
C	3.275476	-0.200086	19.357772
H	4.243338	-0.359431	18.876451
C	5.450218	-1.123992	21.105394
H	5.702188	-1.012267	20.048238
C	2.237602	-3.881506	25.285370
H	2.113498	-4.125830	26.346070
C	4.643075	1.345279	23.862927
H	5.564897	1.240530	23.279314
C	2.314764	1.659214	25.363187
H	1.398043	1.774179	25.951942
C	3.217992	2.723846	25.260827
H	3.013279	3.673609	25.766383
C	4.387362	2.562312	24.505952
H	5.101419	3.388649	24.419430
C	2.581815	0.445448	24.715015
H	1.863972	-0.376284	24.813474
B	4.082701	-1.128830	23.181071
C	-4.792885	2.096873	18.364123
C	-6.029443	2.508386	17.752596
C	-4.748549	1.872500	19.769092
C	-7.161931	2.672916	18.594507
C	-5.876425	2.043971	20.557415
C	-7.092984	2.447627	19.964210
H	-3.805427	1.560944	20.226017
H	-8.115602	2.984927	18.160551
H	-5.826027	1.867627	21.637519
H	-7.984619	2.583630	20.585516
C	-4.937201	2.573965	15.471191
C	-5.020544	2.807466	14.071797
C	-6.101586	2.748257	16.293511
C	-6.214349	3.202816	13.485586
C	-7.305887	3.154173	15.656314
C	-7.364953	3.377010	14.286157
H	-4.124936	2.670895	13.457570
H	-6.266681	3.379962	12.405705
H	-8.211343	3.296340	16.252159
H	-8.307994	3.689147	13.824663
C	8.977093	-2.548079	24.457677
C	9.059858	-2.783198	25.856834
C	10.142177	-2.720002	23.635851
C	10.253766	-3.177880	26.443286
C	11.346563	-3.125300	24.273282
C	11.405055	-3.349754	25.643200
H	8.163719	-2.648420	26.470682
H	10.305650	-3.356292	27.522980
H	12.252544	-3.265685	23.677814
H	12.348179	-3.661363	26.104881
C	8.833966	-2.067597	21.565248
C	10.070635	-2.478420	22.177019
C	8.790222	-1.841547	20.160528
C	11.203824	-2.640595	21.335591
C	9.918775	-2.010730	19.372680
C	11.135444	-2.413698	19.966125
H	7.847012	-1.530534	19.703413
H	12.157595	-2.952030	21.769741
H	9.868824	-1.833115	18.292764
H	12.027612	-2.547901	19.345194