Supporting Information

A strain-deformation nexus within pincer ligands: application to the spin states of iron(II) complexes

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Table S1. *Geometric parameters for hypothetical* $[Zn(\mathbf{L})]^{2+}$ *complexes optimised without empirical dispersion correction (B3LYP/6-31G**)*

	Zn–N(*t*) [py/pyr]	Zn–N(*c*) [py/pyr]	N(*t*)–Zn–N(*c*)	N(*t*)–Zn–N′(*t*)	θ /°	*ρ* /Å	μ_{rms} /Å
$[Zn(\mathbf{A})]^{2+}$	1.981 [py]	1.932 [py]	83.54	167.08	98	3.94	0
$[Zn(\mathbf{B})]^{1+}$	2.001† [py] 1.879 [pyr]	1.927 [py]	81.78† 86.02	167.8	96.3	3.857	0
[Zn(C)]	1.901 [pyr]	1.944 [py]	84.26	168.53	94	3.78	0
$[Zn(\mathbf{D})]^{1+}$	2.024 [py]	1.860 [pyr]	83.76	159.31	106	3.98	0.225
[Zn(E)]	2.022 [py] 1.915 [pyr]	1.884 [pyr]	82.89† 86.87	159.4	102.4	3.873	0.255

†for non-symmetric ligands $\mathbf{B}^{-}$ and $\mathbf{E}^{2-}$, the terminal Zn–N(pyridyl) distances and angles are given first and are followed by the terminal Zn–N(pyrrolide) distances.

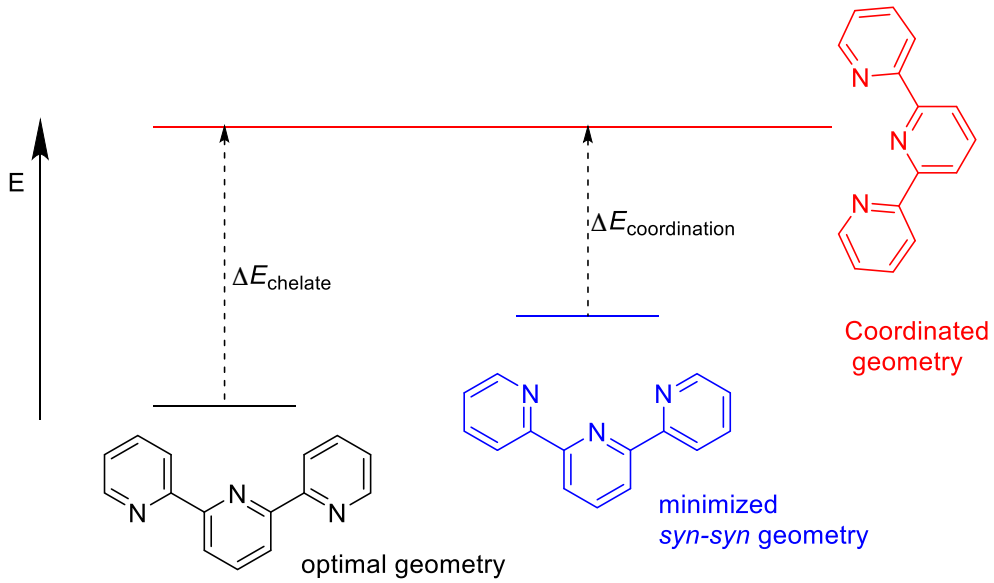


Fig. S1. *Chelate strain compared to coordination strain as defined in this work for the exemplar terpyridyl (**A**) ligand scaffold.*

Table S2. *Geometric parameters ($\rho_{L(relax)}$, $\theta_{L(relax)}$ and $\mu_{rms-L(relax)}$) and Energy ($\Delta E_{L(relax)}$) calculated (B3LYP/6-31G**) for relaxed ligand backbones (with inter-ring N-C-C-N torsions fixed at 0°).*

Entry	ligand	$\theta_{L(relax)}$ /°	$\rho_{L(relax)}$ /Å	$\mu_{rms-L(relax)}$ /Å	$\Delta E_{L(relax)}$ /E_h
1	**A**	113.3	4.514	0	–742.466
2	$\mathbf{B}^{-}$	116.4	4.766	0	–703.761
3	$\mathbf{C}^{2-}$	120.0	5.071	0	–664.943
4	$(\mathbf{C}^{2})^{2-}$	115.0	4.711	0.060	–1205.778
5	$(\mathbf{C}^{3})^{2-}$	119.6	5.004	0	–972.331
6	$\mathbf{D}^{-}$	139.3	5.322	0	–703.760
7	$(\mathbf{D}^{2})^{-}$	128.6	4.879	0.044	–971.007
8	$\mathbf{E}^{2-}$	143.7	5.625	0	–664.907

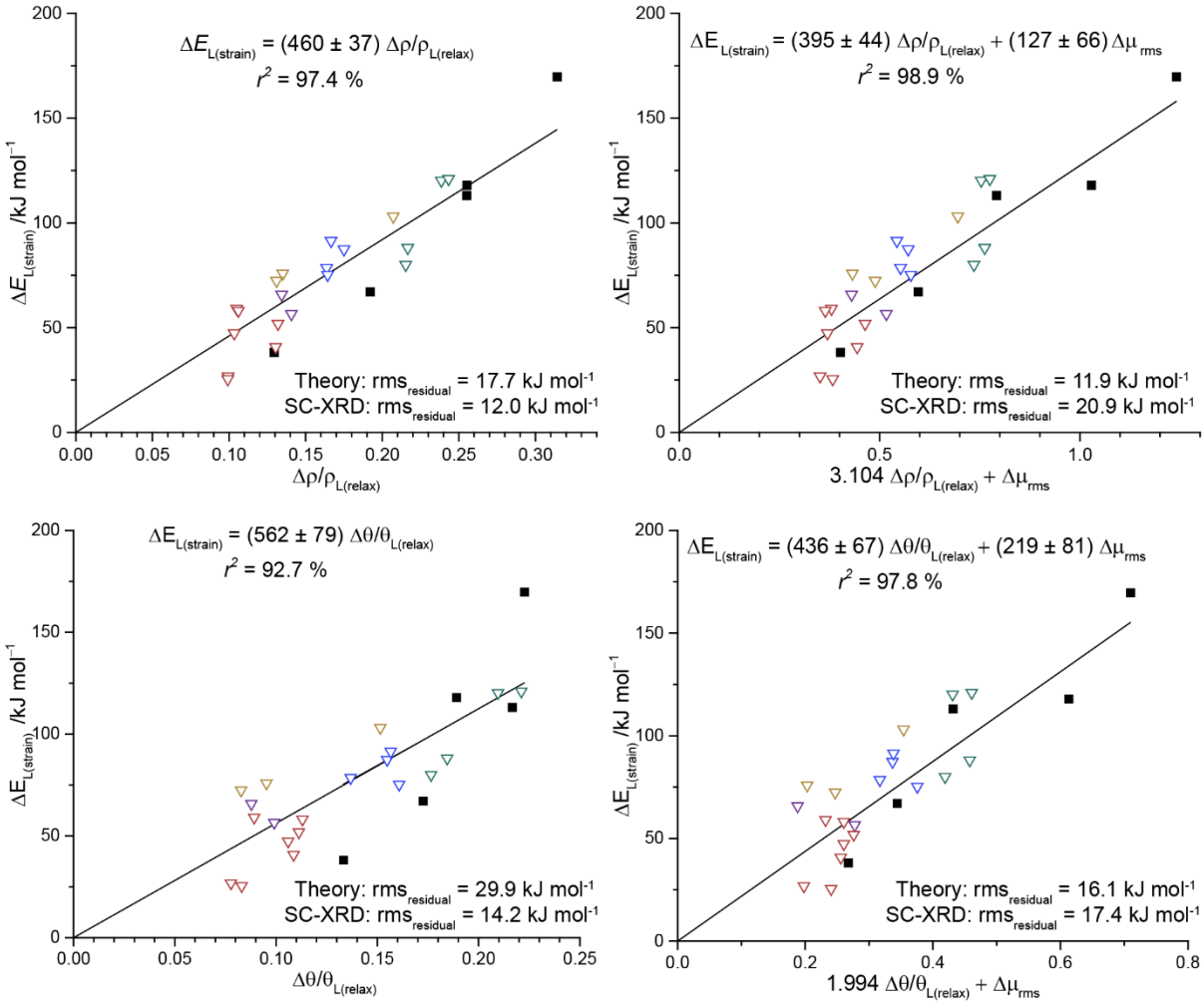
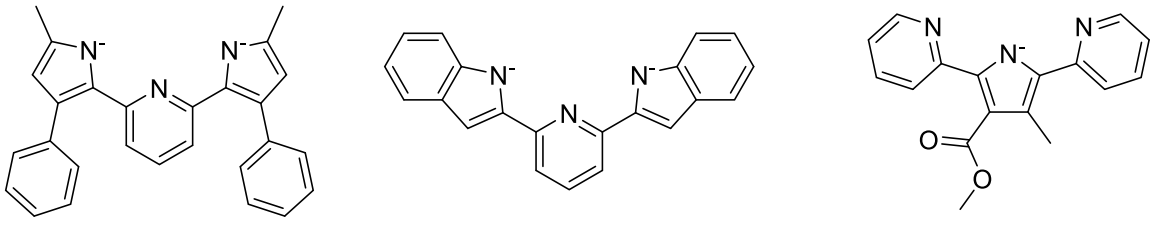


Fig. S2. *Fits of DFT-calculated ligand strain energy (B3LYP/6-31G**) for ligands (**A**–**E**$^{2-}$) in the hypothetical [Zn(**L**)]$^{z+}$ complexes against their different relative deformation parameters (data points represented as black squares, with the equation and correlation of the fit presented). DFT-calculated strain energies (empty triangles) for experimental, solid-state structures from the CSD (see Table S3) have been plotted on top of the fits as empty triangles: **A** red, (**C**^{2})$^{2-}$ purple, (**C**^{3})$^{2-}$ mustard, **D**$^{-}$ green and (**D**^{2})$^{-}$ in blue.*

Table S3. *Relative deformations ($\Delta\rho/\rho_{L(relax)}$, $\Delta\theta/\theta_{L(relax)}$ and $\Delta\mu_{rms}$) and calculated strain energies (B3LYP/6-31G**) for ligand backbones from vacuum phase [Zn(**L**)]$^{z+}$ geometries (B3LYP-GD3BJ/6-31G**) and SC-XRD structures from the CSD database (with CCDC identifier codes as listed).*

Entry	Complex (CCDC code)	ligand	θ /°	$\Delta\theta$ / $\theta_{L(relax)}$ /%	ρ /Å	$\Delta\rho$ / $\rho_{L(relax)}$ /%	$\Delta\mu_{rms}$ /Å	Strain /kJ mol^{-1}
1	[Zn(**A**)]$^{2+}$	**A**	98.1	13.3	3.929	13.0	0	38
2	[Zn(**B**)]$^{+}$	**B**$^{-}$	96.3	17.3	3.850	19.2	0	67
3	[Zn(**C**)]	**C**$^{2-}$	94.0	21.7	3.777	25.5	0	113
4	[Zn(**D**)]$^{+}$	**D**$^{-}$	105.0	18.9	3.963	25.5	0.236	118
5	[Zn(**E**)]	**E**$^{2-}$	101.9	22.2	3.858	31.4	0.266	170
6	[Fe(**A**)$_2$] 2[ClO$_4$] (DANMOU)[1]	**A**	100.9(6)	10.9	3.925(9)	13.0	0.039	41
7	[Fe(**A**)$_2$] 2[ClO$_4$] (DANMOU)[1]	**A**	100.6(6)	11.1	3.918(8)	13.2	0.054	52
8	[Ru(**A**)$_2$] 2[ClO$_4$] (BENHUZ)[2]	**A**	104.4(3)	7.8	4.065(4)	9.9	0.043	27
9	[Ru(**A**)$_2$] 2[ClO$_4$] (BENHUZ)[2]	**A**	103.8(2)	8.3	4.066(4)	9.9	0.075	25
10	[Ru(**D**^{z})(**A**)] (LOGKUP)[3]	**A**	103.1(7)	8.9	4.04(1)	10.5	0.054	59
11	[Os(**A**)$_2$] 2[ClO$_4$] (GOGDOV)[4]	**A**	101.2(9)	10.6	4.047(11)	10.3	0.049	47
12	[Os(**A**)$_2$] 2[ClO$_4$] (GOGDOV)[4]	**A**	100.4(9)	11.3	4.035(11)	10.6	0.035	58
13	[Zr(**C**^{2})$_2$] (YAHBIV)[5]	(**C**^{2})$^{2-}$	104.9(4)	8.8	4.078(4)	13.4	0.073	66
14	[Zr(**C**^{2})$_2$] (YAHBIV)[5]	(**C**^{2})$^{2-}$	103.6(4)	9.9	4.048(4)	14.1	0.140	57
15	[Pb(**C**^{3})(Ph)$_2$] (ALILUC)[6]	(**C**^{3})$^{2-}$	108.2(6)	9.5	4.328(8)	13.5	0.013	76
16	[Pb(**C**^{3})(Ph)$_2$] (ALILUC)[6]	(**C**^{3})$^{2-}$	109.7(4)	8.3	4.348(8)	13.1	0.082	72
17	[Pd(**C**^{3})(py)] (XOVFIX)[7]	(**C**^{3})$^{2-}$	101.5(3)	15.1	3.967(5)	20.7	0.052	103
18	[Pd(**D**)Cl] (TELPUX)[8]	**D**$^{-}$	110.1(7)	21.0	4.052(8)	23.9	0.013	120
19	[Pd(**D**^{2})Cl] (LOGKOJ)[3]	(**D**^{2})$^{-}$	108.68(18)	15.5	4.025(3)	17.5	0.016	87
20	[Pt(**D**)Cl] (TELQEI)[8]	**D**$^{-}$	108.5(5)	22.1	4.027(5)	24.3	0.020	121
21	[Cu(**D**)Cl] (KANXIJ)[9]	**D**$^{-}$	114.7(3)	17.7	4.176(4)	21.5	0.072	80
22	[Ru(**D**)(COD)Cl] (AYOSUE)[10]	**D**$^{-}$	113.6(2)	18.4	4.169(3)	21.7	0.090	88
23	[Ru(**D**^{2})(**A**)] (LOGKUP)[3]	(**D**^{2})$^{-}$	111.0(7)	13.7	4.08(1)	16.4	0.088	79
24	[Ru(**D**^{2})$_2$] (LOGLEA)[3]	(**D**^{2})$^{-}$	109.3(4)	15.7	4.066(6)	16.7	0.070	91
25	[Ru(**D**^{2})$_2$] (LOGLEA)[3]	(**D**^{2})$^{-}$	109.6(4)	16.1	4.077(5)	16.4	0.112	75



(**C**^{2})$^{2-}$ (**C**^{3})$^{2-}$ (**D**^{2})$^{-}$

Fig. S3. *The structures of the derivatives of **C**$^{2-}$ and **D**$^{-}$ in Table S3.*

Table S4. *Relative deformations ($\Delta\rho/\rho_{L(relax)}$, $\Delta\theta/\theta_{L(relax)}$ and $\Delta\mu_{rms}$) and calculated strain energies (B3LYP/6-31G**) for alternate ligand backbones from SC-XRD structures from the CSD database (with CCDC identifier codes as listed). The residual error is defined as the difference remaining when the calculated value is subtracted from the predicted value.*

Entry	Complex (CCDC code)	Donors Ring size	θ /°	$\Delta\theta$ / $\theta_{L(relax)}$ /%	ρ /Å	$\Delta\rho$ / $\rho_{L(relax)}$ /%	$\Delta\mu_{rms}$ /Å	Strain /kJ mol^{-1}	Residual /kJ mol^{-1}
1	[Pt(Pz_2Ph)(NN)] (KEPSUV)[11]	N-C-N 5-6-5	100.2(5)	19.3	3.976(7)	21.9	0.046	114	–13
2	[Pd(Im_2Py)Br]Br (WOXFEU)[12]	C-N-C 5-6-5	101.3(4)	11.1	4.006(7)	14.5	0.013	69	–2
3	[Cr(Im_2Py)Cl_3] (YOKGUB)[13]	C-N-C 5-6-5	103.3(3)	9.4	4.067(5)	13.2	0.018	59	2
4	[Au(Ph_2Py)(C≡CR)] (CEXYIP)[14]	C-N-C 6-6-6	103.4(5)	12.0	4.080(8)	16.9	0.019	90	–12
5	[Pd(NNN)(Me)]BAr'_4 (PUHKOS)[15]	N-N-N 6-6-6 (fused)	106.4(3)	10.1	4.134(6)	12.5	0.027	46	12
6	LS [Fe(pybox)$_2$] 2[PF_6] (IZAFOG)[16]	5-6-5	96.3(5)	16.8	3.956(6)	21.7	0.036	92	5
7	HS [Fe(pybox)$_2$] 2[PF_6] (IZAFOG01)[16]	5-6-5	101.4(3)	12.4	4.205(4)	16.2	0.054	52	23
8	[Ir(PNP)H_3] (XAMQUZ)[17]	P-N-P 6	115.5(7)	2.2	4.474(4)	4.3	0.169	46	–26
9	[Cu(SNS)Cl]$_2$[Cu_2Cl_6] (ACAROM)[18]	S-N-S 6	109.2(2)	2.5	4.5122(11)	2.8	0.166	–17	30

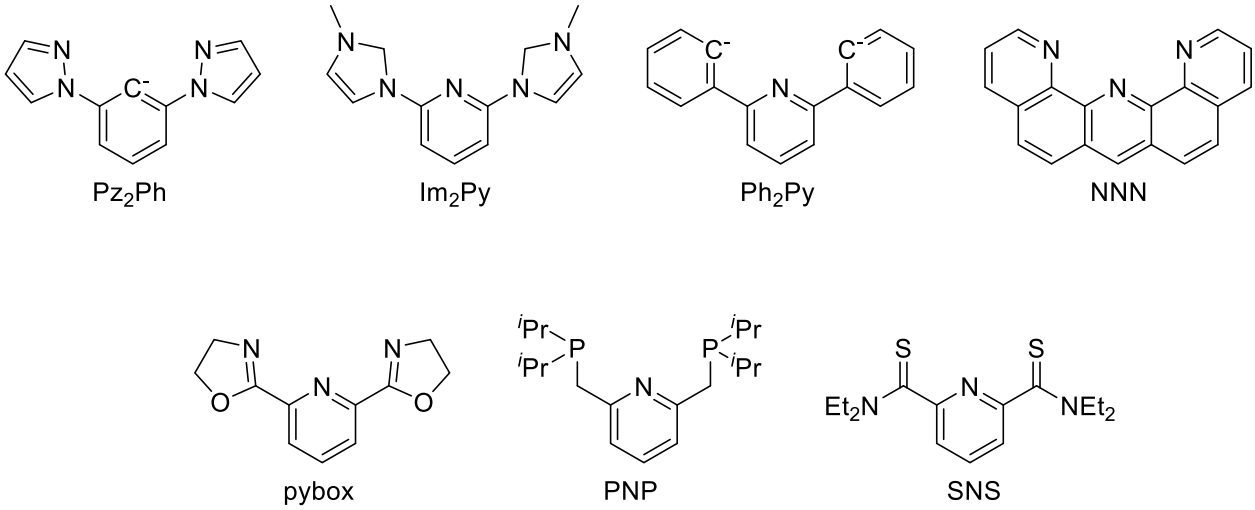


Fig. S4. *The structures of the pincer ligands in Table S4.*

Table S5. *Metric parameters ($\rho_{L(coord)}$ and Fe–N bond distances measured directly from solid state structure; $\rho_{L(relax)}$ from B3LYP/6-31G** optimised geometry) and predicted strain energies for alternate ligand backbones from SC-XRD structures of iron(II) complexes from the CSD database (with CCDC identifier codes as listed). Predicted strain was calculated according to equation 2. The structure of each ligand is represented in Figure 7.*

Entry	Complex (CCDC code)	Ring Sizes	Spin State:	$\rho_{L(coord)}$ /Å	$\rho_{L(relax)}$ /Å	Fe–N_t /Å	Fe–N_c /Å	Fe–N_{av} /Å	Strain Predicted /kJ mol^{-1}
1	[Fe(**A**)$_2$] 2[ClO_4] (DANMOU)[1]	6-6-6	LS	3.925(9)	4.514	1.990(6)	1.890(6)	1.956(6)	60
2	[Fe(**A**)$_2$] 2[ClO_4] (DANMOU)[1]	6-6-6	LS	3.918(8)	4.514	1.986(6)	1.891(6)	1.954(6)	61
3	[Fe(thiaz$_2$Py)$_2$] 2[ClO_4] (DIXDIX)[19]	5-6-5	LS	3.899(4)	4.655	1.973(3)	1.903(3)	1.950(3)	75
4	[Fe(thiaz$_2$Py)$_2$] 2[ClO_4] (DIXDIX)[19]	5-6-5	LS	3.897(4)	4.655	1.974(3)	1.910(3)	1.952(3)	75
5	[Fe(bpyt^{Ph})$_2$] 2[BF_4] (BUKDUH)[20]	6-6-6	LS	3.911(2)	4.774	1.986(2)	1.864(1)	1.945(2)	83
6	[Fe(bpyt^{Ph})$_2$] 2[BF_4] (BUKDUH)[20]	6-6-6	LS	3.907(2)	4.774	1.984(2)	1.870(1)	1.946(2)	84
7	[Fe(phen-bi)$_2$] (DOMQIH)[21]	6-6-5 (fused)	LS	3.946(4)	4.922	2.002(3)	1.891(3)	1.965(3)	91
8	[Fe(phen-bi)$_2$] (DOMQIH)[21]	6-6-5 (fused)	LS	3.931(4)	4.922	1.995(2)	1.892(2)	1.960(2)	93
9	[Fe(bpzp^{F})$_2$] 2[BF_4] (EKAKIM01)[22]	5-6-5	LS	3.89(1)	4.559	1.974(8)	1.904(7)	1.951(8)	78
10	[Fe(bpzp^{F})$_2$] 2[BF_4] (EKAKIM01)[22]	5-6-5	LS	3.90(1)	4.559	1.981(8)	1.903(7)	1.955(8)	66
11	[Fe(bpzp^{F})$_2$] 2[BF_4] (EKAKIM)[22]	5-6-5	HS	4.150(5)	4.559	2.165(4)	2.113(4)	2.147(4)	41
12	[Fe(bpzp^{F})$_2$] 2[BF_4] (EKAKIM)[22]	5-6-5	HS	4.198(5)	4.559	2.189(4)	2.126(4)	2.168(4)	36
13	[Fe(bpz^{Me}p)$_2$] 2[BF_4] (AFANEB01)[23]	5-6-5	LS	3.929(4)	4.561	1.997(3)	1.891(2)	1.962(3)	64
14	[Fe(bpz^{Me}p)$_2$] 2[BF_4] (AFANEB01)[23]	5-6-5	LS	3.931(4)	4.561	1.992(3)	1.891(3)	1.958(3)	64
15	[Fe(bpz^{Me}p)$_2$] 2[BF_4] (AFANEB01)[23]	5-6-5	HS	4.160(4)	4.561	2.158(3)	2.084(3)	2.133(3)	40
16	[Fe(bpz^{Me}p)$_2$] 2[BF_4] (AFANEB01)[23]	5-6-5	HS	4.146(4)	4.561	2.150(3)	2.079(3)	2.126(3)	42
17	[Fe(bpz^{Me}p)$_2$] 2[BF_4] (AFANEB01)[23]	5-6-5	HS	4.182(5)	4.561	2.189(3)	2.125(3)	2.167(3)	38
18	[Fe(bpz^{Me}p)$_2$] 2[BF_4] (AFANEB01)[23]	5-6-5	HS	4.197(4)	4.561	2.188(3)	2.131(2)	2.169(3)	37
19	[Fe(bpyt^{SAc})$_2$] 2[BF_4] (BUKDIV)[20]	6-6-6	LS	3.931(4)	4.772	1.998(3)	1.870(3)	1.955(3)	81
20	[Fe(bpyt^{SAc})$_2$] 2[BF_4] (BUKDIV)[20]	6-6-6	LS	3.930(5)	4.772	1.998(4)	1.867(3)	1.954(4)	81
21	[Fe(phen-tetrazolide)$_2$] (QIDJET01)[24]	6-6-5 (fused)	LS	3.938(2)	4.992	2.0017(15)	1.9064(14)	1.9699(15)	97
22	[Fe(phen-tetrazolide)$_2$] (QIDJET)[24]	6-6-5 (fused)	HS	4.259(3)	4.992	2.2163(19)	2.1204(18)	2.1843(19)	68
23	[Fe(pybox)$_2$] 2[PF_6] (IZAFOG)[16]	5-6-5	LS	3.927(6)	5.018	2.000(4)	1.935(5)	1.978(5)	100
24	[Fe(pybox)$_2$] 2[PF_6] (IZAFOG)[16]	5-6-5	LS	3.956(6)	5.018	2.016(5)	1.938(5)	1.990(5)	97
25	[Fe(pybox)$_2$] 2[PF_6] (IZAFOG01)[16]	5-6-5	HS	4.205(4)	5.018	2.186(3)	2.117(3)	2.163(3)	75
26	[Fe(pybox)$_2$] 2[PF_6] (IZAFOG01)[16]	5-6-5	HS	4.224(5)	5.018	2.195(3)	2.108(3)	2.166(3)	73
27	[Fe(bpzp^{NMe2})$_2$] 2[BF_4] (EKAJUX)[22]	5-6-5	HS	4.207(3)	4.565	2.200(2)	2.112(2)	2.170(2)	36
28	[Fe(bpzp^{NMe2})$_2$] 2[BF_4] (EKAJUX)[22]	5-6-5	HS	4.162(3)	4.565	2.184(2)	2.113(2)	2.160(2)	41
29	[Fe(bpzt^{NMe2})$_2$] 2[BF_4] (FEDRUE)[25]	5-6-5	HS	4.257(4)	4.795	2.244(3)	2.108(3)	2.199(3)	52
30	[Fe(**D**^{3})$_2$] (UCIGUJ)[26]	6-5-6	HS	4.375(11)	4.918	2.286(8)	2.016(8)	2.196(8)	51
31	[Fe(**D**^{3})$_2$] (UCIGUJ)[26]	6-5-6	HS	4.331(10)	4.918	2.265(7)	2.038(7)	2.189(7)	55
32	[Fe(Py$_2$thiaz)$_2$] 2[BF_4] (PUBCAQ)[27]	6-5-6	HS	4.35(2)	5.064	2.283(15)	2.047(6)	2.204(15)	65
33	[Fe(bppz)$_2$] 2[BF_4] (ZAJGOG)[28]	6-5-6	HS	4.349(8)	5.075	2.308(6)	2.020(8)	2.212(8)	66

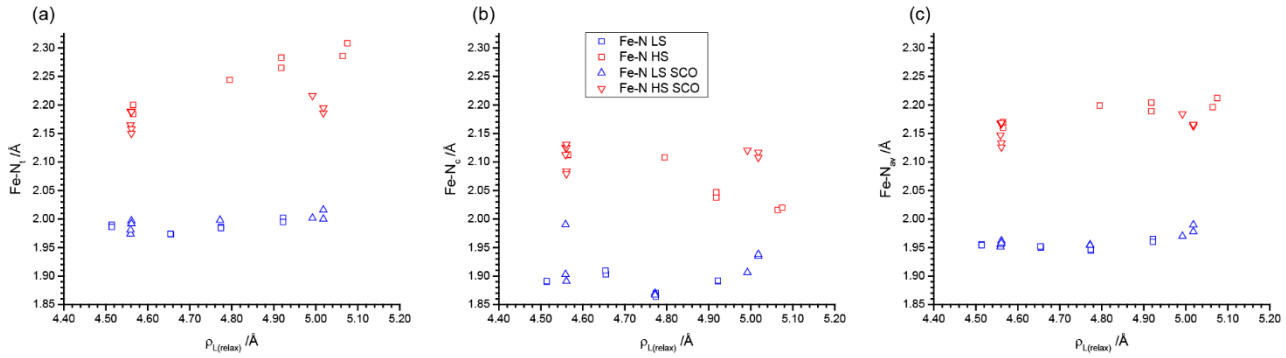


Fig. S5. *Plots of selected Fe-N distances from homoleptic $[Fe^{II}(L)_2]^{z+}$ complexes selected from the CSD (see Table S4) against the calculated (B3LYP/6-31G**) terminal N…N donor separations for the relaxed (unbound) ligands ($\rho_{L(relax)}$). (a) mean Fe–$N_{terminal}$ distances; (b) mean Fe–$N_{central}$ distances; (c) mean all Fe–N distances. Red symbols represent HS iron(II) complexes, while blue symbols are LS configurations. SCO inactive complexes are represented by squares, and those with SCO activity are indicated by triangles.*

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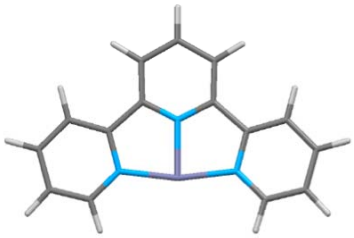
DFT Calculation output files

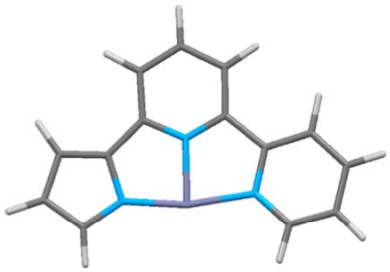
A. Hypothetical zinc complexes

$[Zn^{II}L]^{z+}$ (B3LYP-GD3BJ/6-31G Table 1):**



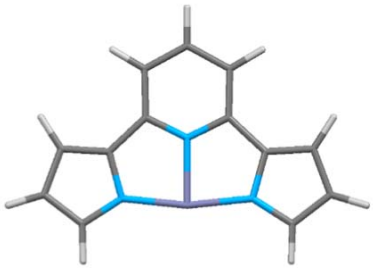
[Zn(**A**)]$^{2+}$: ΔE = –2521.22908487 E_h

C	1.18813	-1.35739	-0.00007
C	1.22577	-2.75262	-0.00000
C	-0.00001	-3.43319	0.00006
C	-1.22578	-2.75260	0.00007
N	0.00000	-0.75258	-0.00011
C	-1.18814	-1.35738	-0.00003
C	-2.31516	-0.37965	-0.00003
C	-3.65122	-0.75412	0.00013
C	-4.64733	0.22733	0.00013
C	-4.28193	1.57050	-0.00003
C	-2.92958	1.89501	-0.00020
N	-1.96464	0.95354	-0.00020
C	2.31515	-0.37966	-0.00007
C	3.65121	-0.75413	-0.00018
C	4.64731	0.22733	-0.00009
C	4.28191	1.57050	0.00012
C	2.92955	1.89500	0.00023
N	1.96462	0.95352	0.00015
H	-2.60447	2.92922	-0.00032
H	-5.02300	2.36115	-0.00003
H	-5.69325	-0.06061	0.00026
H	-3.91994	-1.80361	0.00025
H	-2.15638	-3.30655	0.00015
H	-0.00002	-4.51809	0.00013
H	2.15635	-3.30658	0.00003
H	3.91994	-1.80362	-0.00032
H	5.02298	2.36115	0.00020
H	5.69323	-0.06061	-0.00017
H	2.60444	2.92921	0.00041
Zn	0.00003	1.18027	0.00001



[Zn(**B**)]$^{+}$: ΔE = –2482.52321816 E_h

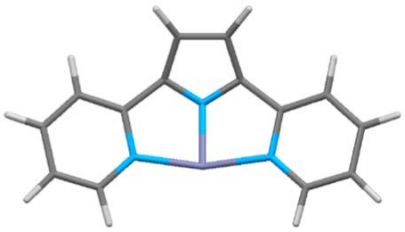
C	2.48976	0.21802	-0.00030
N	2.07432	-1.12514	-0.00047
C	-2.06897	0.43932	0.00005
C	-3.39318	0.86140	0.00013
C	-4.41929	-0.07775	0.00018
C	-4.10326	-1.43353	0.00013
C	-2.76656	-1.80018	0.00006
N	-1.76937	-0.89909	0.00003
H	-3.61649	1.92159	0.00015
H	-5.45456	0.24706	0.00023
H	-4.87213	-2.19701	0.00014
H	-2.47526	-2.84520	0.00002
C	3.20016	-1.88940	-0.00001
C	4.32974	-1.08133	0.00089
H	3.14050	-2.96917	-0.00010
C	3.88128	0.25225	0.00001
H	5.35551	-1.42094	0.00163
H	4.49712	1.14139	0.00009
C	-0.91160	1.37177	-0.00002
C	-0.89326	2.75743	0.00016
C	0.37739	3.37102	0.00007
C	1.55716	2.64090	-0.00013
C	1.47055	1.23244	-0.00020
N	0.23685	0.70332	-0.00021
H	-1.79419	3.35829	0.00037
H	0.43115	4.45506	0.00016
H	2.51894	3.13997	-0.00022
Zn	0.19924	-1.22530	-0.00013



[Zn(**C**)]: ΔE = –2444.02493861 E_h

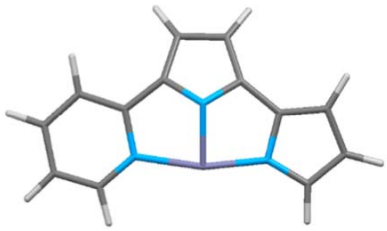
C	-1.19819	-1.27993	-0.00000
C	-1.22915	-2.67990	0.00000
C	0.00000	-3.34741	0.00000
C	1.22915	-2.67990	0.00000
C	1.19819	-1.27993	-0.00000

N	0.00000	-0.68853	-0.00000
H	-2.16431	-3.22718	0.00000
H	0.00000	-4.43408	0.00000
H	2.16431	-3.22718	0.00000
N	-1.88868	1.06309	0.00000
C	-3.03787	1.79213	0.00000
C	-4.14209	0.95153	0.00000
C	-3.64747	-0.37083	0.00000
C	-2.26188	-0.28839	0.00000
H	-3.00780	2.87363	0.00000
H	-5.17920	1.25782	0.00000
H	-4.23005	-1.28246	-0.00000
N	1.88868	1.06309	0.00000
C	2.26188	-0.28839	0.00000
C	3.64747	-0.37083	0.00000
C	4.14209	0.95153	0.00000
C	3.03787	1.79213	0.00000
H	4.23005	-1.28246	0.00000
H	5.17920	1.25782	0.00000
H	3.00780	2.87363	0.00000
Zn	0.00000	1.25720	-0.00000



[Zn(**D**)]$^{+}$: ΔG = -2482.80597731 E_h

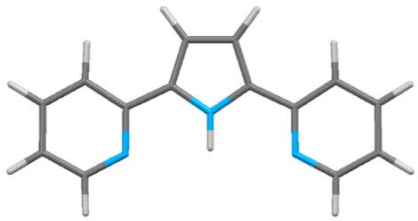
N	0.00000	0.76578	0.63249
C	-1.11021	1.44551	0.26315
C	-0.70597	2.70290	-0.24119
C	0.70598	2.70290	-0.24119
C	1.11021	1.44551	0.26315
C	-2.26760	0.57459	0.09118
C	-3.58943	1.01168	-0.03965
C	-4.60922	0.09315	-0.24526
C	-4.30842	-1.27184	-0.31614
C	-2.98685	-1.66299	-0.19146
N	-1.98130	-0.78110	-0.01073
H	-3.79613	2.07236	0.04110
H	-5.63525	0.43263	-0.33925
H	-5.07960	-2.01628	-0.47050
H	-2.70503	-2.70830	-0.25474
C	2.26760	0.57459	0.09118
C	3.58943	1.01168	-0.03965
C	4.60922	0.09315	-0.24526
C	4.30842	-1.27184	-0.31614
C	2.98685	-1.66299	-0.19146
N	1.98130	-0.78110	-0.01073
H	3.79613	2.07236	0.04110
H	5.63525	0.43263	-0.33925
H	5.07960	-2.01628	-0.47050
H	2.70503	-2.70830	-0.25474
H	1.34191	3.48894	-0.62365
H	-1.34191	3.48894	-0.62365
Zn	0.00000	-1.05598	0.23897



[Zn(**E**)]: ΔE = –2444.26367302 E_h

N	-0.25272	0.76668	-0.68769
C	-1.35113	1.40484	-0.22872
C	-0.93806	2.67433	0.26326
C	0.46576	2.70374	0.19259
C	0.87894	1.45714	-0.35257
C	-2.47307	0.48921	-0.03233
N	-2.12295	-0.87590	0.10270
C	2.00414	0.59738	-0.13287
C	3.33112	1.03435	0.08062
C	4.34084	0.12625	0.31058
C	4.05243	-1.25369	0.33011
C	2.74452	-1.64470	0.13916
N	1.73051	-0.77434	-0.06395
H	3.53100	2.09897	0.03701
H	5.35844	0.47211	0.46307
H	4.82418	-1.99459	0.49789
H	2.46780	-2.69414	0.16581
H	1.10532	3.49354	0.56519
H	-1.57375	3.43809	0.68977
Zn	-0.25223	-1.06966	-0.24325
C	-3.28218	-1.57122	0.32537
C	-4.35807	-0.69966	0.35660
H	-3.26673	-2.64271	0.47164
C	-3.84275	0.60597	0.13640
H	-5.39178	-0.96817	0.52654
H	-4.40644	1.52807	0.09394

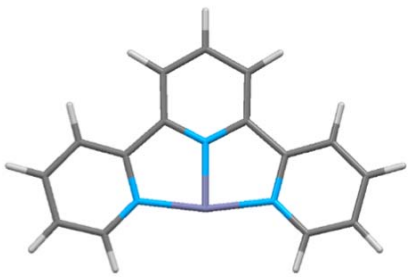
HD (B3LYP-GD3BJ/6-31G**)



H**D**: ΔE = –704.459140840 E_h

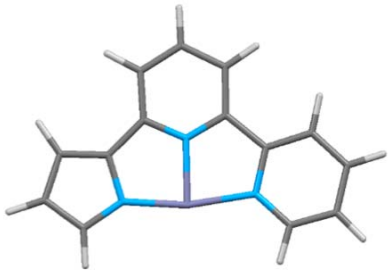
N	0.00000	0.00074	0.00000
C	-1.12529	0.77744	-0.00000
C	-0.70488	2.11019	-0.00000
C	0.70488	2.11019	-0.00000
C	1.12529	0.77744	-0.00000
C	-2.44082	0.15767	-0.00000
C	-3.62323	0.91767	0.00000
C	-4.84427	0.25731	0.00000
C	-4.86279	-1.13886	0.00000
C	-3.63947	-1.80828	-0.00000
N	-2.45515	-1.19268	-0.00000
H	-3.57453	2.00083	0.00001
H	-5.77131	0.82266	0.00001
H	-5.79467	-1.69342	0.00000
H	-3.60906	-2.89619	-0.00000
C	2.44082	0.15767	-0.00000
C	3.62323	0.91767	0.00000
C	4.84427	0.25731	0.00000
C	4.86279	-1.13886	0.00000
C	3.63947	-1.80828	0.00000
N	2.45515	-1.19268	-0.00000
H	3.57453	2.00083	0.00000
H	5.77131	0.82266	0.00001
H	5.79467	-1.69342	0.00000
H	3.60906	-2.89619	-0.00000
H	0.00000	-1.00994	0.00000
H	1.34780	2.97839	-0.00000
H	-1.34780	2.97839	-0.00000

$[Zn^{II}L]^{z+}$ (B3LYP/6-31G** Table S1):



$[Zn(\mathbf{A})]^{2+}$: ΔE = -2521.15367696 E_h

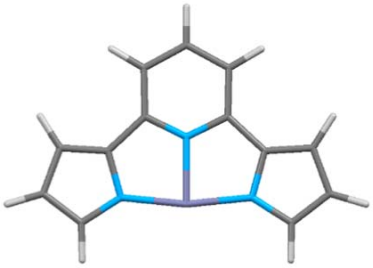
C	1.18889	-1.35780	-0.00005
C	1.22624	-2.75423	0.00004
C	0.00000	-3.43451	0.00008
C	-1.22624	-2.75423	0.00005
N	0.00000	-0.75339	-0.00011
C	-1.18889	-1.35780	-0.00004
C	-2.31834	-0.37813	-0.00003
C	-3.65572	-0.75305	-0.00004
C	-4.65278	0.22800	-0.00001
C	-4.28822	1.57173	0.00002
C	-2.93538	1.89632	0.00002
N	-1.96876	0.95542	-0.00001
C	2.31834	-0.37813	-0.00005
C	3.65572	-0.75305	-0.00005
C	4.65278	0.22800	-0.00001
C	4.28822	1.57173	0.00004
C	2.93538	1.89632	0.00003
N	1.96876	0.95542	-0.00001
H	-2.61171	2.93145	0.00005
H	-5.02962	2.36259	0.00005
H	-5.69885	-0.06093	-0.00001
H	-3.92589	-1.80258	-0.00006
H	-2.15618	-3.31009	0.00011
H	0.00000	-4.51985	0.00015
H	2.15618	-3.31009	0.00010
H	3.92589	-1.80258	-0.00009
H	5.02962	2.36259	0.00007
H	5.69885	-0.06093	-0.00001
H	2.61171	2.93145	0.00007
Zn	-0.00000	1.17833	0.00001



$[Zn(\mathbf{B})]^{+}$: ΔE = –2482.45250784 E_h

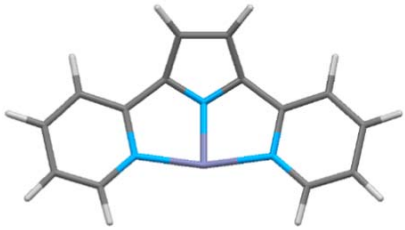
C	2.49177	0.21430	-0.00028
N	2.07786	-1.12779	-0.00046
C	-2.07210	0.43813	0.00006
C	-3.39751	0.86079	0.00013
C	-4.42471	-0.07775	0.00015
C	-4.10965	-1.43397	0.00010
C	-2.77246	-1.80072	0.00005
N	-1.77350	-0.90060	0.00003
H	-3.62216	1.92111	0.00015
H	-5.46003	0.24821	0.00020
H	-4.87885	-2.19765	0.00010
H	-2.48284	-2.84667	0.00002
C	3.20512	-1.88899	-0.00004
C	4.33379	-1.08061	0.00088
H	3.14865	-2.96937	-0.00013

C	3.88382	0.25119	-0.00002
H	5.36000	-1.41986	0.00161
H	4.49983	1.14064	0.00004
C	-0.91215	1.37220	-0.00000
C	-0.89255	2.75889	0.00015
C	0.37905	3.37132	0.00006
C	1.55878	2.64076	-0.00014
C	1.47147	1.23099	-0.00018
N	0.23669	0.70349	-0.00017
H	-1.79228	3.36227	0.00034
H	0.43356	4.45575	0.00013
H	2.52022	3.14134	-0.00024
Zn	0.20102	-1.22336	-0.00012



[Zn(**C**)]: ΔE = –2443.96053656 E_h

C	-1.19907	-1.27930	-0.00000
C	-1.22971	-2.68053	0.00000
C	0.00000	-3.34765	0.00000
C	1.22971	-2.68053	0.00000
C	1.19907	-1.27930	-0.00000
N	0.00000	-0.68879	-0.00000
H	-2.16401	-3.23007	0.00000
H	0.00000	-4.43476	0.00000
H	2.16401	-3.23007	0.00000
N	-1.89137	1.06518	0.00000
C	-3.04168	1.79143	0.00000
C	-4.14532	0.95105	0.00000
C	-3.64985	-0.36964	0.00000
C	-2.26385	-0.28508	0.00000
H	-3.01453	2.87345	0.00000
H	-5.18270	1.25746	0.00000
H	-4.23293	-1.28137	-0.00000
N	1.89137	1.06518	0.00000
C	2.26385	-0.28508	0.00000
C	3.64985	-0.36964	0.00000
C	4.14532	0.95105	0.00000
C	3.04168	1.79143	0.00000
H	4.23293	-1.28137	-0.00000
H	5.18270	1.25746	0.00000
H	3.01453	2.87345	0.00000
Zn	0.00000	1.25520	-0.00000



[Zn(**D**)]$^+$: ΔE = –2482.73721109 E_h

N	0.00000	0.75952	0.60872
C	-1.10864	1.44223	0.24828
C	-0.70543	2.70686	-0.23814
C	0.70543	2.70686	-0.23813
C	1.10864	1.44223	0.24828
C	-2.27226	0.57333	0.08710
C	-3.59594	1.01371	-0.02734
C	-4.62105	0.09760	-0.21990
C	-4.32470	-1.26844	-0.29441
C	-3.00199	-1.66251	-0.18516
N	-1.99080	-0.78351	-0.01647
H	-3.80104	2.07492	0.05582
H	-5.64759	0.44015	-0.30101
H	-5.09952	-2.01158	-0.43920
H	-2.72495	-2.70942	-0.25105
C	2.27226	0.57333	0.08710
C	3.59594	1.01371	-0.02733
C	4.62105	0.09759	-0.21990
C	4.32470	-1.26844	-0.29441
C	3.00199	-1.66251	-0.18516
N	1.99080	-0.78351	-0.01647
H	3.80104	2.07492	0.05582
H	5.64759	0.44015	-0.30101
H	5.09951	-2.01158	-0.43920
H	2.72495	-2.70942	-0.25105
H	1.34034	3.50026	-0.60798
H	-1.34034	3.50026	-0.60798
Zn	0.00000	-1.05898	0.22037

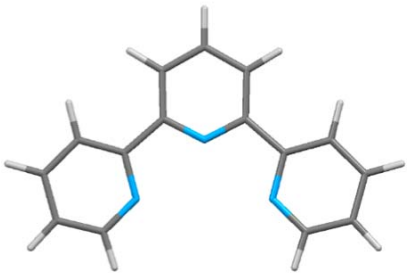
[Zn(**E**)]: ΔE = –2444.17220333 E_h

N	-0.25068	0.76152	-0.66846
C	-1.34994	1.40148	-0.22043
C	-0.94111	2.67728	0.25826
C	0.46218	2.70749	0.19230
C	0.87731	1.45457	-0.33589

C	-2.47663	0.48573	-0.03268
N	-2.13142	-0.87887	0.10457
C	2.00869	0.59670	-0.12602
C	3.33900	1.03559	0.07063
C	4.35347	0.12876	0.28786
C	4.06733	-1.25177	0.31163
C	2.75691	-1.64433	0.13637
N	1.73791	-0.77598	-0.05471
H	3.53906	2.10044	0.02368
H	5.37277	0.47657	0.42681
H	4.84208	-1.99219	0.46992
H	2.48357	-2.69507	0.16604
H	1.09846	3.50459	0.55591
H	-1.57853	3.44715	0.67199
Zn	-0.25492	-1.07061	-0.22842
C	-3.29579	-1.56959	0.31323
C	-4.36947	-0.69569	0.33292
H	-3.28714	-2.64174	0.45870
C	-3.84825	0.60760	0.11985
H	-5.40597	-0.96232	0.49060
H	-4.40953	1.53130	0.07107

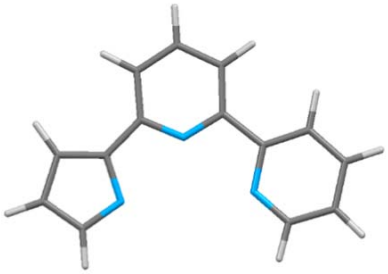
B. Calculations of $\Delta E_{L(strain)}$ (B3LYP/6-31G**)

Strained ligand geometries from theoretical $[Zn^{II}L]^{z+}$ *(Table S3 1-5)*



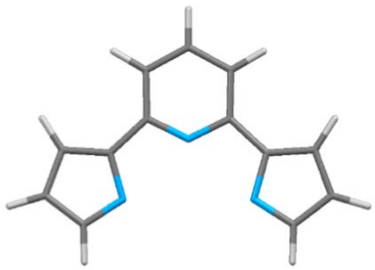
A: $\Delta E_{L(coord)}$ = –742.466359709 E_h

C	-1.18811	1.06716	-0.00009
C	-1.22581	2.46236	0.00001
C	-0.00001	3.14296	0.00011
C	1.22579	2.46237	0.00011
N	-0.00001	0.46236	-0.00009
C	1.18809	1.06717	0.00001
C	2.31519	0.08937	0.00001
C	3.65119	0.46387	0.00011
C	4.64729	-0.51753	0.00011
C	4.28190	-1.86073	0.00001
C	2.92960	-2.18523	-0.00019
N	1.96460	-1.24373	-0.00019
C	-2.31511	0.08946	-0.00009
C	-3.65121	0.46386	-0.00019
C	-4.64731	-0.51755	-0.00009
C	-4.28190	-1.86075	0.00011
C	-2.92960	-2.18524	0.00021
N	-1.96460	-1.24374	0.00011
H	2.60450	-3.21943	-0.00029
H	5.02300	-2.65132	0.00001
H	5.69320	-0.22962	0.00031
H	3.91989	1.51337	0.00031
H	2.15639	3.01637	0.00011
H	-0.00002	4.22786	0.00011
H	-2.15641	3.01636	0.00001
H	-3.91991	1.51335	-0.00029
H	-5.02300	-2.65135	0.00021
H	-5.69320	-0.22965	-0.00019
H	-2.60440	-3.21944	0.00041



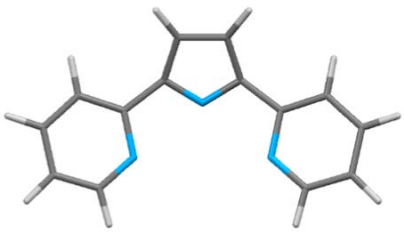
B^{-}: $\Delta E_{L(coord)}$ = –703.7611521 E_h

C	2.53982	-0.14257	-0.00034
N	2.10274	-1.47881	-0.00054
C	-2.01482	0.15213	0.00006
C	-3.33205	0.59551	0.00006
C	-4.37315	-0.32704	0.00016
C	-4.07903	-1.68765	0.00006
C	-2.74841	-2.07584	0.00006
N	-1.73682	-1.19092	-0.00004
H	-3.53824	1.65917	0.00006
H	-5.40308	0.01450	0.00016
H	-4.86003	-2.43867	0.00006
H	-2.47398	-3.12539	-0.00004
C	3.21618	-2.26114	-0.00004
C	4.35855	-1.47134	0.00086
H	3.13910	-3.33984	-0.00014
C	3.93169	-0.13069	-0.00004
H	5.37875	-1.82742	0.00156
H	4.56174	0.74837	0.00006
C	-0.84255	1.06587	-0.00004
C	-0.80193	2.45099	0.00016
C	0.47849	3.04405	0.00006
C	1.64637	2.29504	-0.00014
C	1.53700	0.88811	-0.00024
N	0.29493	0.37896	-0.00024
H	-1.69304	3.06633	0.00036
H	0.54975	4.12714	0.00016
H	2.61599	2.77858	-0.00024



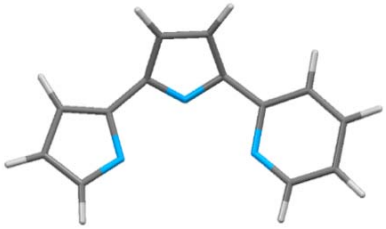
C^{2-}: $\Delta E_{L(coord)}$ = –664.9434942 E_h

C	0.00000	1.19820	0.93068
C	0.00000	1.22920	2.33068
C	0.00000	0.00000	2.99818
C	0.00000	-1.22920	2.33068
C	0.00000	-1.19820	0.93068
N	0.00000	0.00000	0.33928
H	0.00000	2.16430	2.87798
H	0.00000	0.00000	4.08488
H	0.00000	-2.16430	2.87798
N	0.00000	1.88870	-1.41232
C	0.00000	3.03790	-2.14132
C	0.00000	4.14210	-1.30072
C	0.00000	3.64750	0.02158
C	0.00000	2.26190	-0.06082
H	0.00000	3.00780	-3.22282
H	0.00000	5.17920	-1.60702
H	0.00000	4.23000	0.93328
N	0.00000	-1.88870	-1.41232
C	0.00000	-2.26190	-0.06082
C	0.00000	-3.64750	0.02158
C	0.00000	-4.14210	-1.30072
C	0.00000	-3.03790	-2.14132
H	0.00000	-4.23000	0.93328
H	0.00000	-5.17920	-1.60702
H	0.00000	-3.00780	-3.22282



D^{-}: $\Delta E_{L(coord)}$ = –703.7600816 E_h

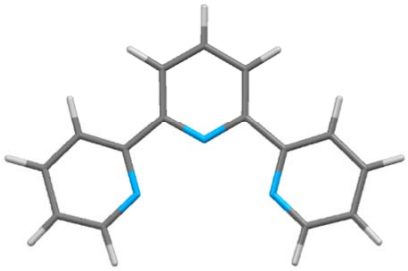
N	-0.51822	0.67429	0.00000
C	-1.18231	0.27762	1.11020
C	-2.41812	-0.27758	0.70600
C	-2.41812	-0.27758	-0.70600
C	-1.18231	0.27762	-1.11020
C	-0.30513	0.14123	2.26760
C	-0.73654	-0.00736	3.58940
C	0.18968	-0.17538	4.60920
C	1.55633	-0.19053	4.30840
C	1.94213	-0.05010	2.98690
N	1.05360	0.09463	1.98130
H	-1.79965	0.03017	3.79610
H	-0.14571	-0.28313	5.63520
H	2.30650	-0.31448	5.07960
H	2.98914	-0.07067	2.70500
C	-0.30513	0.14123	-2.26760
C	-0.73654	-0.00736	-3.58940
C	0.18968	-0.17538	-4.60920
C	1.55633	-0.19053	-4.30840
C	1.94213	-0.05010	-2.98690
N	1.05360	0.09463	-1.98130
H	-1.79965	0.03017	-3.79610
H	-0.14571	-0.28313	-5.63520
H	2.30650	-0.31448	-5.07960
H	2.98914	-0.07067	-2.70500
H	-3.18789	-0.69177	-1.34190
H	-3.18789	-0.69177	1.34190



E^{2-}: $\Delta E_{L(coord)}$ = –664.906998324 E_h

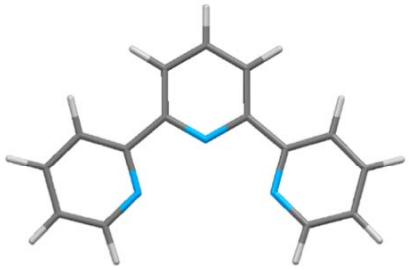
N	0.32835	0.49941	0.73341
C	1.43810	1.09749	0.24855
C	1.04694	2.34885	-0.30404
C	-0.35648	2.40404	-0.23948
C	-0.79107	1.19130	0.36241
C	2.54566	0.15579	0.09921
N	2.17379	-1.20836	0.02745
C	-1.92945	0.34034	0.17967
C	-3.24866	0.78790	-0.05859
C	-4.27231	-0.11363	-0.24896
C	-4.00620	-1.49746	-0.20252
C	-2.70529	-1.89994	0.01094
N	-1.67788	-1.03730	0.17622
H	-3.43144	1.85654	-0.06582
H	-5.28379	0.24086	-0.42096
H	-4.78944	-2.23299	-0.33783
H	-2.44552	-2.95373	0.03469
H	-0.98217	3.18555	-0.65098
H	1.69590	3.08143	-0.76390
C	3.32227	-1.93187	-0.15841
C	4.41219	-1.08016	-0.22701
H	3.28983	-3.00868	-0.25406
C	3.91750	0.24255	-0.07023
H	5.44185	-1.37290	-0.38063
H	4.49582	1.15648	-0.06931

Strained Py-Pyr^{-} ligand geometries from SC-XRD structures (Table S3 6-25; Table S5 1 & 2).



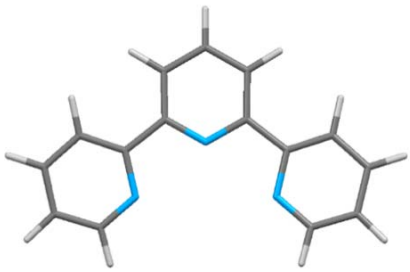
DANMOU: $\Delta E_{L(coord)}$ = –742.46535110 E_h

N	1.95217	-1.21702	-0.06774
C	2.30794	0.08667	-0.00708
C	3.62973	0.48461	0.05514
C	4.63338	-0.47676	0.08026
C	4.26800	-1.82316	-0.01622
C	2.92857	-2.14658	-0.06223
N	0.00568	0.35241	-0.01331
C	1.19000	1.00391	0.00092
C	1.22028	2.40775	0.00474
C	0.01340	3.07827	-0.01429
C	-1.18750	2.39234	-0.00377
C	-1.17355	1.02828	-0.00586
N	-1.97238	-1.20712	-0.02364
C	-2.31195	0.08100	-0.03919
C	-3.63620	0.48771	-0.02181
C	-4.64597	-0.47611	0.01025
C	-4.28557	-1.79726	0.06434
C	-2.93366	-2.12464	0.03641
H	3.89034	1.53725	0.11419
H	5.67779	-0.18695	0.14130
H	5.02525	-2.60224	-0.01706
H	2.59774	-3.18201	-0.11443
H	2.15342	2.96269	0.00274
H	0.00568	4.16475	-0.02280
H	-2.11874	2.95291	-0.00842
H	-3.89596	1.54195	-0.04138
H	-5.68977	-0.17627	0.01691
H	-5.03542	-2.58220	0.11329
H	-2.60993	-3.16395	0.05893



DANMOU: $\Delta E_{L(coord)}$ = –742.46112876 E_h

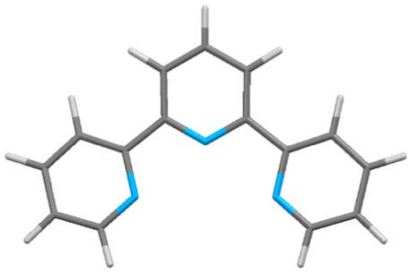
N	-1.96184	-1.20330	-0.09174
C	-2.30920	0.09597	-0.01279
C	-3.63760	0.48665	0.11073
C	-4.60906	-0.50098	0.10329
C	-4.26136	-1.80351	-0.01264
C	-2.92956	-2.14438	-0.10275
N	0.00668	0.35859	-0.02428
C	-1.19173	1.02774	-0.01017
C	-1.18525	2.40174	-0.01214
C	-0.01017	3.07906	-0.02352
C	1.18383	2.40113	-0.01038
C	1.17874	1.01791	-0.02411
N	1.95565	-1.21287	-0.01244
C	2.30629	0.08438	-0.02033
C	3.64577	0.48924	-0.02858
C	4.63647	-0.47494	0.03460
C	4.26234	-1.81324	0.06475
C	2.92055	-2.14852	0.04357
H	-3.91402	1.53213	0.20409
H	-5.65575	-0.22049	0.19175
H	-5.02303	-2.57959	-0.02391
H	-2.59646	-3.17666	-0.17970
H	-2.11999	2.95915	-0.01697
H	-0.01012	4.16528	-0.02784
H	2.11606	2.96071	-0.00580
H	3.90654	1.54300	-0.05645
H	5.68509	-0.19320	0.04586
H	5.01888	-2.59226	0.11369
H	2.58905	-3.18444	0.05730



BENHUZ: $\Delta E_{L(coord)}$ = –742.47067189 E_h

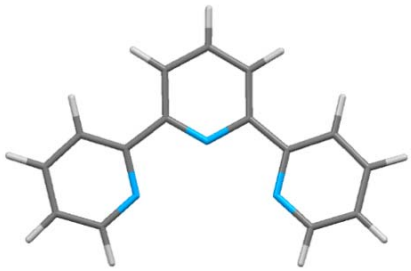
N	2.03023	-1.27151	-0.01719
N	-2.03475	-1.26029	-0.07684
C	-3.04642	-2.14257	-0.07808
H	-2.76427	-3.19178	-0.14037

C	3.04781	-2.15426	0.06007
H	2.76616	-3.20448	0.09281
C	-1.17902	0.98124	-0.00956
C	-2.34513	0.08571	-0.01266
C	2.33631	0.07014	-0.02921
C	-3.66338	0.51715	0.05317
H	-3.89368	1.57737	0.10521
C	4.37652	-1.75683	0.06788
H	5.16944	-2.49801	0.11847
C	3.65135	0.51413	-0.03489
H	3.87863	1.57523	-0.06639
C	0.01325	3.05676	0.00761
H	0.01776	4.14308	0.01953
C	-1.19636	2.37962	0.00420
H	-2.12734	2.93824	0.01139
C	-4.37358	-1.75844	0.00230
H	-5.15792	-2.51076	0.01058
C	4.67693	-0.40759	-0.00095
H	5.71137	-0.07606	-0.01057
C	-4.69279	-0.41202	0.08223
H	-5.72676	-0.08808	0.15004
N	0.00247	0.31933	-0.01766
C	1.18014	0.97542	-0.02179
C	1.21303	2.36887	-0.00749
H	2.14907	2.91858	-0.00589



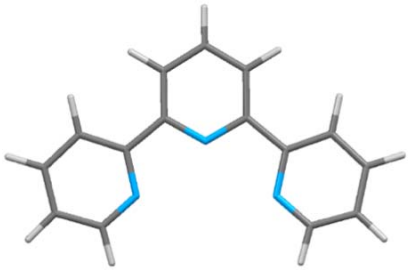
BENHUZ: $\Delta E_{L(coord)}$ = –742.47116739 E_h

C	1.18078	0.98264	-0.03031
C	3.04449	-2.14472	-0.13992
H	2.76267	-3.18958	-0.25266
C	3.64452	0.50494	0.14832
H	3.87007	1.55998	0.27083
C	-3.66481	0.51361	0.00320
H	-3.89790	1.57423	-0.00924
C	-1.19824	2.37943	-0.02942
H	-2.12843	2.93936	-0.02358
N	0.00064	0.32518	-0.03900
C	-1.17915	0.98622	-0.02924
C	4.37044	-1.76129	-0.00002
H	5.16108	-2.50645	-0.00514
C	-3.03736	-2.14797	0.04834
H	-2.74913	-3.19714	0.06196
C	4.66415	-0.42145	0.15783
H	5.69358	-0.09776	0.28429
C	-2.34052	0.07900	-0.02148
C	-4.36715	-1.76357	0.08260
H	-5.15142	-2.51411	0.13273
C	-4.68539	-0.41606	0.04437
H	-5.72227	-0.09331	0.06007
C	0.01221	3.05729	-0.03096
H	0.01147	4.14393	-0.03414
C	1.21580	2.37847	-0.03589
H	2.15099	2.92929	-0.04439
N	-2.03041	-1.26063	-0.02423
N	2.03373	-1.25772	-0.13275
C	2.33549	0.07408	-0.01223



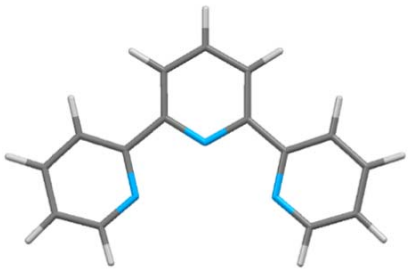
LOGKUP **A**: $\Delta E_{L(coord)}$ = –742.45838104 E_h

N	-2.00944	-1.24530	-0.01708
N	-0.00520	0.32180	0.02773
N	2.03354	-1.24373	0.02093
C	-3.02029	-2.15954	-0.08483
H	-2.71675	-3.20112	-0.14580
C	-4.34060	-1.77018	-0.06896
H	-5.12773	-2.51767	-0.13153
C	-4.66200	-0.44401	0.03018
H	-5.70751	-0.14573	0.05475
C	-3.67505	0.52692	0.09859
H	-3.92001	1.58001	0.17142
C	-2.32423	0.06850	0.04794
C	-1.22511	0.98290	0.02712
C	-1.21229	2.35665	0.02521
H	-2.14427	2.91850	0.04829
C	-0.04602	3.04532	-0.03871
H	-0.06227	4.13128	-0.05982
C	1.21549	2.37769	-0.07489
H	2.13476	2.94983	-0.13476
C	1.18029	0.99106	-0.02617
C	2.34924	0.10749	-0.01862
C	3.65967	0.51238	-0.00457
H	3.90826	1.57075	-0.00784
C	4.68514	-0.42201	-0.00217
H	5.72099	-0.09695	-0.01196
C	4.36318	-1.75578	0.01357
H	5.14538	-2.51111	0.01865
C	3.03503	-2.13776	0.05636
H	2.74211	-3.18494	0.09725



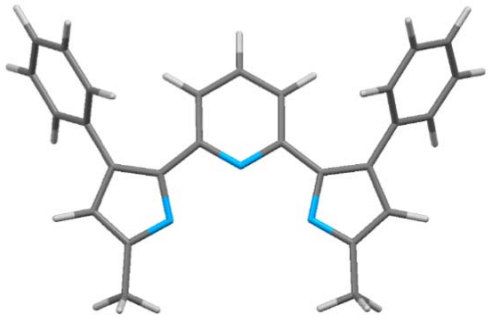
GOGDOV: $\Delta E_{L(coord)}$ = –742.46285148 E_h

N	-2.04137	-1.26546	-0.09371
N	0.00009	0.32106	-0.05275
N	2.00415	-1.26474	-0.00157
C	-3.03602	-2.13593	-0.09117
C	-4.36812	-1.76847	0.00877
C	-4.65231	-0.40861	0.10563
C	-3.64192	0.53774	0.07133
C	-2.32410	0.06754	-0.02840
C	-1.18720	1.00215	-0.00003
C	-1.16784	2.38856	-0.00640
C	0.02331	3.08627	0.01164
C	1.21583	2.34847	-0.03321
C	1.19271	0.98188	-0.02659
C	2.30187	0.07046	-0.01449
C	3.65559	0.51452	-0.01258
C	4.67052	-0.44950	0.01727
C	4.35245	-1.76148	0.06161
C	2.99517	-2.15270	0.05115
H	-2.75185	-3.18572	-0.16145
H	-5.16015	-2.51022	0.02481
H	-5.68662	-0.08484	0.19648
H	-3.86748	1.59611	0.13930
H	-2.10025	2.94948	0.01204
H	0.03964	4.17012	0.01964
H	2.15848	2.89033	-0.03219
H	3.90111	1.57044	-0.03533
H	5.70974	-0.13085	0.01481
H	5.12669	-2.52358	0.09807
H	2.71086	-3.20267	0.07287



GOGDOV: $\Delta E_{L(coord)}$ = –742.45873930 E_h

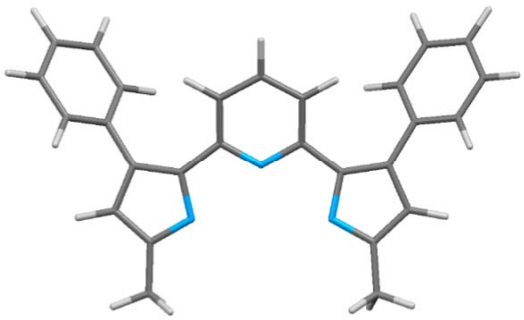
N	-2.01453	-1.27380	-0.03001
N	0.01246	0.30230	0.00647
N	2.01994	-1.25562	-0.05298
C	-3.02058	-2.13991	0.01399
C	-4.36095	-1.75346	0.06271
C	-4.65118	-0.40845	-0.00005
C	-3.64669	0.49874	-0.01666
C	-2.30145	0.05281	-0.02880
C	-1.21072	0.98114	0.00204
C	-1.22282	2.37285	0.02691
C	0.00052	3.05938	-0.01344
C	1.20371	2.37018	-0.04201
C	1.18460	1.02280	0.00299
C	2.32599	0.09254	0.00405
C	3.64290	0.51549	0.04203
C	4.66225	-0.43109	0.07041
C	4.34626	-1.77337	0.00530
C	3.02952	-2.12226	-0.06237
H	-2.74482	-3.19337	0.02030
H	-5.14761	-2.50056	0.10647
H	-5.68666	-0.07641	0.00281
H	-3.86725	1.56140	-0.03909
H	-2.14904	2.93897	0.05107
H	-0.00201	4.14504	-0.02357
H	2.13446	2.92911	-0.08207
H	3.88992	1.57218	0.08330
H	5.69833	-0.10850	0.12432
H	5.12389	-2.53161	0.01055
H	2.73753	-3.17073	-0.12101



YAHBIV: $\Delta E_{L(coord)}$ = –1205.75313190 E_h

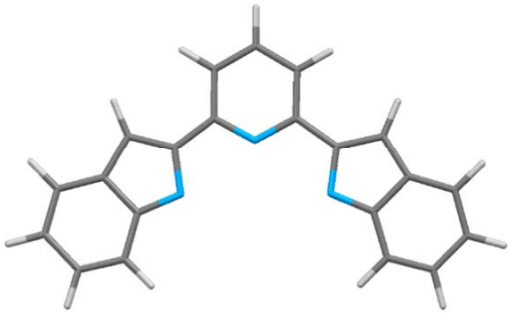
N	2.07080	2.21581	-0.01131
N	0.00912	0.70215	-0.01742
N	-2.07962	2.22103	-0.11218
C	3.31302	2.81597	0.01525
C	4.32789	1.89606	0.05878
H	5.40084	2.08118	0.04276
C	3.70690	0.61562	0.00734
C	2.34010	0.84647	0.00528
C	1.17523	0.00052	0.05991
C	1.19653	-1.37108	0.26189
H	2.13256	-1.90152	0.38588
C	0.00169	-2.04840	0.34953
H	-0.00407	-3.12444	0.52958
C	-1.19328	-1.36369	0.22909
H	-2.13277	-1.89327	0.32463
C	-1.16023	0.00348	0.03103
C	-2.32607	0.85669	-0.06918
C	-3.69741	0.61024	-0.10116
C	-4.32657	1.86585	-0.10589
H	-5.40120	2.03721	-0.15174
C	-3.32446	2.80540	-0.14162

C	4.43543	-0.66516	-0.00944
C	5.45110	-0.94320	0.90973
H	5.65940	-0.20507	1.68008
C	6.17533	-2.11759	0.85462
H	6.95997	-2.30341	1.58828
C	5.89744	-3.06478	-0.11535
H	6.46225	-3.99512	-0.15637
C	4.89807	-2.81071	-1.02005
H	4.66828	-3.54137	-1.79547
C	4.18538	-1.62930	-0.97350
H	3.40915	-1.43522	-1.70748
C	-4.41466	-0.68117	-0.04369
C	-5.36099	-0.88524	0.95555
H	-5.50227	-0.09809	1.69097
C	-6.10919	-2.05022	1.03030
H	-6.83967	-2.17280	1.83014
C	-5.91937	-3.06418	0.10722
H	-6.49545	-3.98622	0.16243
C	-4.96381	-2.88249	-0.90153
H	-4.79989	-3.66453	-1.64152
C	-4.23639	-1.70719	-0.96869
H	-3.50502	-1.56633	-1.75956
C	3.46417	4.29240	-0.03623
H	3.34719	4.70425	-1.05296
H	4.45344	4.60968	0.32323
H	2.70354	4.78917	0.57983
C	-3.51004	4.28077	-0.23837
H	-2.78391	4.81379	0.38921
H	-4.51872	4.57869	0.08086
H	-3.37069	4.66987	-1.26137



YAHBIV: $\Delta E_{L(coord)}$ = –1205.75662947 E_h

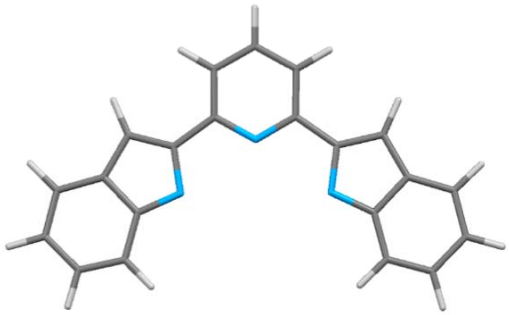
N	-2.05119	2.21845	0.06911
N	-0.00729	0.70452	-0.11802
N	2.06940	2.22634	-0.07798
C	-3.29460	2.81006	0.20934
C	-4.30155	1.88314	0.17253
H	-5.36785	2.05832	0.31279
C	-3.69118	0.60789	0.04664
C	-2.33070	0.86047	-0.04818
C	-1.17437	0.02728	-0.30077
C	-1.21370	-1.27595	-0.76306
H	-2.16011	-1.76597	-0.96071
C	-0.02457	-1.93179	-1.01223
H	-0.03236	-2.95063	-1.40149
C	1.17781	-1.28098	-0.79501
H	2.11839	-1.77099	-1.01876
C	1.14939	0.02646	-0.33168
C	2.31485	0.85948	-0.12271
C	3.66887	0.57794	-0.00728
C	4.30904	1.84078	0.06642
H	5.37519	2.00544	0.21593
C	3.31798	2.79479	0.04263
C	-4.41452	-0.67872	0.04524
C	-5.61759	-0.85230	-0.62591
H	-5.98688	-0.03539	-1.24105
C	-6.33327	-2.02979	-0.53246
H	-7.27141	-2.13050	-1.07925
C	-5.86991	-3.06828	0.23090
H	-6.43239	-3.99878	0.29990
C	-4.68713	-2.91645	0.91222
H	-4.31006	-3.72495	1.53799
C	-3.97545	-1.73174	0.83367
H	-3.05637	-1.61195	1.39758
C	4.37048	-0.72315	0.08635
C	3.90500	-1.79995	0.84566
H	2.94941	-1.70872	1.35125
C	4.64180	-2.97330	0.96344
H	4.24140	-3.79176	1.56115
C	5.86758	-3.09777	0.35621
H	6.44804	-4.01424	0.45171
C	6.35260	-2.02885	-0.38173
H	7.32313	-2.10672	-0.87290
C	5.61796	-0.87801	-0.51008
H	6.00272	-0.05272	-1.10408
C	-3.37245	4.28392	0.40587
H	-3.41978	4.58077	1.46801
H	-4.25453	4.72954	-0.07940
H	-2.47547	4.75342	-0.01144
C	3.52393	4.27175	0.14067
H	3.10434	4.80797	-0.72376
H	4.59309	4.51630	0.19669
H	3.03737	4.70473	1.02777



ALILUC: $\Delta E_{L(coord)}$ = –972.30176586 E_h

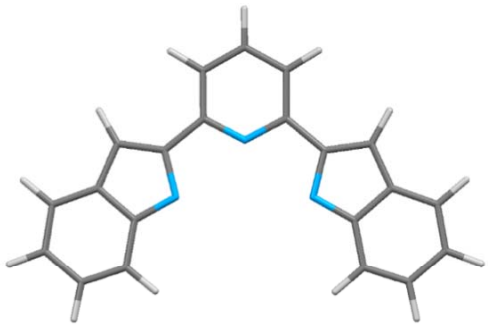
N	-2.16266	-0.53376	-0.04644
N	2.16560	-0.55340	-0.01437
N	0.02453	1.01730	-0.01686
C	-3.40593	-1.06233	-0.02425
C	-3.79721	-2.38447	-0.02336
H	-3.02877	-3.15771	-0.04808
C	-5.12624	-2.72799	0.02156
H	-5.40969	-3.78152	0.03193
C	-6.10837	-1.74790	0.05901

H	-7.16203	-2.02828	0.09395
C	-5.75449	-0.43443	0.02933
H	-6.54007	0.32797	0.04975
C	-4.41639	-0.04063	-0.00632
C	-3.67933	1.13419	-0.01900
H	-4.10705	2.13718	-0.00097
C	-2.34321	0.83517	-0.02976
C	-1.16915	1.65982	-0.02398
C	-1.19787	3.04732	-0.01974
H	-2.14750	3.57967	-0.02669
C	-0.00724	3.74270	0.02603
H	-0.01167	4.83304	0.04454
C	1.19080	3.06630	0.02192
H	2.12883	3.62001	0.05049
C	1.20346	1.65305	0.00319
C	2.34845	0.79882	0.00250
C	3.68141	1.13457	0.00257
H	4.11012	2.13406	0.01403
C	4.40114	-0.06882	0.00768
C	5.73087	-0.40366	0.02354
H	6.49781	0.37639	0.04197
C	6.10346	-1.71299	0.02131
H	7.15868	-1.98925	0.02965
C	5.12020	-2.73339	-0.01177
H	5.44206	-3.77603	-0.01502
C	3.78990	-2.42731	-0.00457
H	3.02410	-3.20145	-0.01631
C	3.41121	-1.09220	-0.00681



ALILUC: $\Delta E_{L(coord)}$ = –972.30306890 E_h

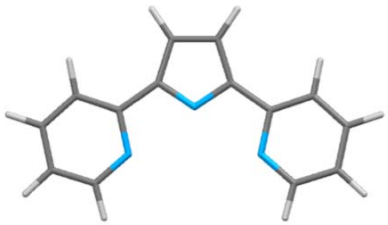
N	2.15965	-0.52560	-0.12299
N	-2.18714	-0.49950	-0.20402
N	-0.00666	1.01784	-0.07778
C	3.40775	-1.08036	-0.04978
C	3.78032	-2.43768	-0.09736
H	3.02305	-3.20950	-0.21101
C	5.11869	-2.72776	-0.00644
H	5.42784	-3.77620	-0.03760
C	6.08744	-1.76544	0.16642
H	7.13433	-2.05853	0.25581
C	5.74210	-0.43883	0.18631
H	6.51568	0.32446	0.30475
C	4.39015	-0.06476	0.06306
C	3.67374	1.14484	0.06346
H	4.10574	2.13883	0.15408
C	2.36334	0.82055	-0.04476
C	1.18461	1.66944	-0.05153
C	1.19856	3.07624	-0.04103
H	2.14449	3.61438	-0.02398
C	0.01986	3.73850	-0.03083
H	0.02381	4.83137	-0.01948
C	-1.18854	3.08044	-0.05973
H	-2.12974	3.62453	-0.06107
C	-1.16380	1.67970	-0.06594
C	-2.35852	0.85672	-0.06098
C	-3.68844	1.15970	0.12632
H	-4.12725	2.14320	0.28342
C	-4.39834	-0.05507	0.10600
C	-5.73398	-0.44229	0.23935
H	-6.51683	0.30643	0.39030
C	-6.07898	-1.76499	0.15677
H	-7.12593	-2.05527	0.26331
C	-5.10519	-2.76499	-0.01760
H	-5.41069	-3.81075	-0.06580
C	-3.79161	-2.41892	-0.16739
H	-3.01513	-3.16726	-0.31975
C	-3.42754	-1.07419	-0.09422



XOVFIX: $\Delta E_{L(coord)}$ = –972.29139833 E_h

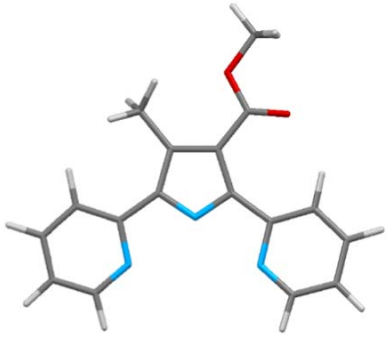
N	-1.97710	-0.41558	-0.10590
N	-0.00491	1.22577	0.01159
N	1.99014	-0.41186	-0.12285
C	-3.17109	-1.08143	-0.04806
C	-3.43737	-2.46157	-0.08720
H	-2.61384	-3.16798	-0.17078
C	-4.74094	-2.87349	-0.01835
H	-4.96769	-3.94140	-0.04534
C	-5.80945	-1.96185	0.09024
H	-6.83038	-2.34377	0.14148
C	-5.57122	-0.62472	0.12594
H	-6.40118	0.08192	0.20813
C	-4.24494	-0.15618	0.05908
C	-3.65570	1.12528	0.07221
H	-4.18836	2.07028	0.15590
C	-2.30847	0.93631	-0.02908
C	3.18267	-1.07061	-0.06594
C	3.42926	-2.46041	-0.08954
H	2.59163	-3.15031	-0.16758
C	4.72229	-2.88860	-0.00023
H	4.94267	-3.95786	-0.00755
C	5.78398	-1.98044	0.10650
H	6.80355	-2.36485	0.17712
C	5.56377	-0.63050	0.11785
H	6.40323	0.06362	0.20279
C	4.24879	-0.15785	0.03132

C	3.67385	1.12808	0.05384
H	4.21319	2.06805	0.14646
C	2.32066	0.94099	-0.02011
C	-1.19666	1.85725	-0.02834
C	-1.20483	3.24692	-0.04218
H	-2.13818	3.80877	-0.07265
C	0.00610	3.90679	-0.03509
H	0.01236	4.99843	-0.04375
C	1.21092	3.23219	-0.00909
H	2.14929	3.78673	-0.01298
C	1.19283	1.85051	-0.01564



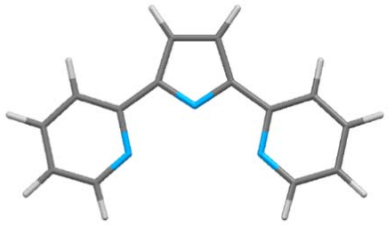
TELPUX: $\Delta E_{L(coord)}$ = –703.75923319 E_h

N	2.02588	-1.05196	0.00964
N	0.00000	0.39150	0.00000
C	3.04609	-1.93826	0.01707
C	4.37498	-1.52546	0.00261
C	4.65794	-0.18319	-0.01049
C	3.62641	0.73550	-0.01813
C	2.31577	0.29437	0.01383
C	1.11791	1.13211	0.01066
C	0.69949	2.47034	0.01429
H	2.77015	-2.99304	0.02105
H	5.17881	-2.26109	0.00719
H	5.69175	0.15893	-0.02661
H	3.83578	1.80310	-0.03207
H	1.31066	3.37289	0.01951
N	-2.02588	-1.05196	-0.00964
C	-3.04610	-1.93826	-0.01707
C	-4.37499	-1.52546	-0.00261
C	-4.65794	-0.18318	0.01048
C	-3.62641	0.73550	0.01813
C	-2.31577	0.29438	-0.01383
C	-1.11791	1.13211	-0.01066
C	-0.69949	2.47034	-0.01429
H	-2.77016	-2.99303	-0.02105
H	-5.17882	-2.26109	-0.00719
H	-5.69175	0.15894	0.02661
H	-3.83578	1.80310	0.03207
H	-1.31066	3.37289	-0.01951



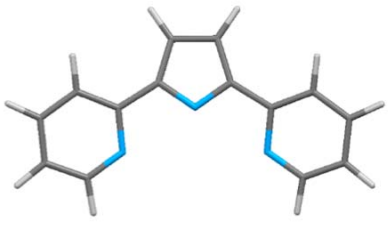
LOGKOJ: $\Delta E_{L(coord)}$ = –970.97396599 E_h

O	3.25187	-1.40912	-0.03033
O	1.97999	-3.22801	0.05623
N	0.86039	2.64704	-0.01630
N	-0.48460	0.57400	-0.03122
N	-2.89769	1.20597	0.01760
C	1.46846	3.84263	-0.01036
H	0.80806	4.71189	-0.01807
C	2.83572	3.98334	0.01602
H	3.29270	4.97209	0.02960
C	3.61374	2.84401	0.02620
H	4.69961	2.91985	0.04788
C	3.01386	1.59862	0.00016
H	3.60190	0.68934	-0.00143
C	1.62931	1.50004	-0.01923
C	0.81815	0.26463	-0.03437
C	0.89206	-1.14549	-0.02620
C	-0.44525	-1.64872	-0.03075
C	-1.27308	-0.52231	-0.01981
C	-2.68777	-0.15386	0.00323
C	-3.77423	-1.03085	0.01272
H	-3.60740	-2.10358	0.02117
C	-5.05615	-0.52588	0.01128
H	-5.91079	-1.19957	0.00877
C	-5.24575	0.83854	0.02743
H	-6.25591	1.24795	0.03402
C	-4.16262	1.67739	0.03682
H	-4.27030	2.76202	0.05578
C	2.15805	-1.90768	-0.01106
C	3.18557	-4.02145	0.06678
H	3.77172	-3.85575	-0.84202
H	2.85381	-5.05975	0.12338
H	3.81006	-3.77070	0.92904
C	-0.93308	-3.06766	-0.07192
H	-0.20093	-3.74384	-0.51753
H	-1.85604	-3.14388	-0.65840
H	-1.15992	-3.46998	0.92848



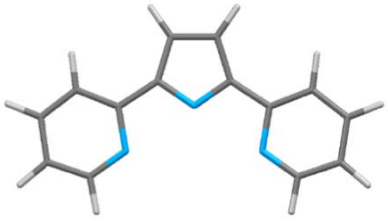
TELQEI: $\Delta E_{L(coord)}$ = –703.75892247 E_h

N	-0.00858	2.01370	-1.05785
N	0.00000	0.00000	0.41424
C	-0.02614	3.02688	-1.94056
H	-0.04841	2.74210	-2.99387
C	0.00000	4.35744	-1.54899
H	-0.01081	5.15886	-2.28578
C	0.03542	4.63594	-0.19936
H	0.06039	5.67242	0.13655
C	0.04464	3.62561	0.72507
H	0.07126	3.84969	1.78974
C	0.00835	2.29663	0.30255
C	0.00473	1.12076	1.14894
C	-0.00533	0.70013	2.49723
H	-0.00164	1.31127	3.39924
N	0.00858	-2.01370	-1.05785
C	0.02614	-3.02688	-1.94056
H	0.04841	-2.74210	-2.99387
C	0.00000	-4.35744	-1.54899
H	0.01081	-5.15886	-2.28578
C	-0.03542	-4.63594	-0.19936
H	-0.06039	-5.67242	0.13655
C	-0.04464	-3.62561	0.72507
H	-0.07126	-3.84969	1.78974
C	-0.00835	-2.29663	0.30255
C	-0.00473	-1.12076	1.14894
C	0.00533	-0.70013	2.49723
H	0.00164	-1.31127	3.39924



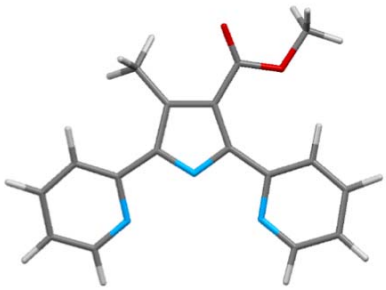
KANXIJ: $\Delta E_{L(coord)}$ = –703.77453085 E_h

N	-0.00878	0.27257	0.04975
N	-2.21241	-1.08824	0.23994
N	2.19945	-1.10471	0.16052
C	-3.30842	-1.86511	0.16077
H	-3.12627	-2.92714	0.34333
C	-4.57282	-1.42144	-0.10634
H	-5.41569	-2.10743	-0.15040
C	-4.72295	-0.06721	-0.30520
H	-5.69838	0.36623	-0.51845
C	-3.60983	0.75264	-0.23902
H	-3.73447	1.82193	-0.40951
C	-2.34025	0.26602	0.01726
C	-1.10317	1.03336	0.09893
C	-0.68554	2.37608	0.17977
H	-1.29964	3.27122	0.25694
C	0.70874	2.35891	0.17904
H	1.33739	3.24485	0.25320
C	1.10602	1.03128	0.09521
C	2.33682	0.25288	0.01449
C	3.60826	0.75566	-0.18055
H	3.73411	1.83214	-0.29408
C	4.73277	-0.05868	-0.25129
H	5.71244	0.38735	-0.41195
C	4.58040	-1.42826	-0.12152
H	5.42257	-2.11400	-0.17025
C	3.28987	-1.88285	0.08268
H	3.10078	-2.95228	0.20429



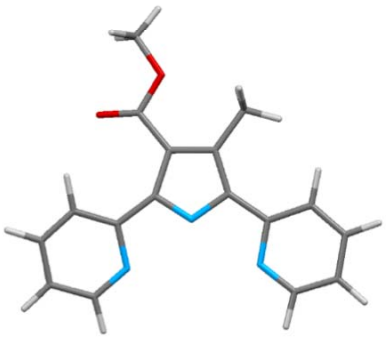
AYOSUE: $\Delta E_{L(coord)}$ = –703.77144698 E_h

N	-0.00578	0.28008	0.00637
N	2.08736	-1.10549	-0.03833
N	-2.08394	-1.11027	0.05946
C	-3.17562	-1.88527	0.05382
H	-2.97588	-2.95957	0.09883
C	-4.47877	-1.44138	0.00256
H	-5.30718	-2.14607	0.00401
C	-4.69003	-0.07757	-0.04594
H	-5.70223	0.32347	-0.08408
C	-3.61305	0.77177	-0.04544
H	-3.75359	1.84959	-0.08479
C	-2.31569	0.25832	0.00027
C	-1.11369	1.04601	0.01146
C	-0.69660	2.39581	0.00713
H	-1.31619	3.29094	0.01022
C	0.69689	2.39301	0.00705
H	1.32103	3.28476	0.00734
C	1.10258	1.04074	0.00881
C	2.31290	0.25396	-0.00793
C	3.60262	0.77304	0.02372
H	3.73787	1.85202	0.05287
C	4.69165	-0.06735	0.01798
H	5.70010	0.34309	0.04251
C	4.48902	-1.43841	-0.01615
H	5.32231	-2.13722	-0.02092
C	3.18858	-1.88770	-0.04237
H	2.98555	-2.96105	-0.06829



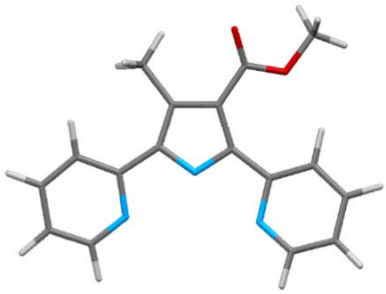
LOGKUP D: $\Delta E_{L(coord)}$ = –970.97734902 E_h

O	3.01287	-1.66032	0.33574
O	1.75323	-3.44808	-0.29772
N	0.98235	2.51268	0.04033
N	-0.52218	0.54489	-0.15009
N	-2.90359	1.28241	0.21576
C	1.69726	3.65607	0.01667
H	1.10869	4.57050	0.11452
C	3.08608	3.70731	-0.07652
H	3.63143	4.64712	-0.07254
C	3.72967	2.46938	-0.16324
H	4.81713	2.43249	-0.22556
C	3.02502	1.30831	-0.18300
H	3.54846	0.36407	-0.26596
C	1.62499	1.29128	-0.11162
C	0.75043	0.12696	-0.12186
C	0.72233	-1.28216	-0.12541
C	-0.62391	-1.72119	-0.13331
C	-1.38159	-0.48510	-0.11472
C	-2.77401	-0.08975	-0.02737
C	-3.88557	-0.89126	-0.18530
H	-3.75774	-1.94676	-0.40847
C	-5.13072	-0.35214	-0.09367
H	-6.01002	-0.98008	-0.22841
C	-5.28735	1.00626	0.18662
H	-6.27644	1.44928	0.27737
C	-4.14267	1.77503	0.32489
H	-4.21131	2.84543	0.52928
C	1.82367	-2.24669	-0.06332
C	4.11951	-2.55178	0.48399
H	4.32245	-3.09694	-0.44355
H	3.93151	-3.28624	1.27454
H	4.97446	-1.92653	0.75054
C	-1.19365	-3.08806	-0.01156
H	-1.55930	-3.47912	-0.97464
H	-2.04972	-3.09524	0.67495
H	-0.45139	-3.80558	0.34413



LOGLEA: $\Delta E_{L(coord)}$ = –970.97243597 E_h

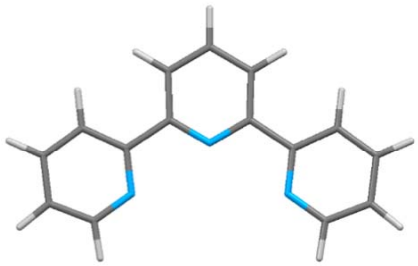
O	3.24131	1.49269	0.05724
O	1.82123	3.26318	0.03578
N	0.92856	-2.68112	0.11406
N	-0.45604	-0.62508	-0.11699
N	-2.88333	-1.26568	0.07990
C	1.59752	-3.83350	0.19199
H	0.99511	-4.72973	0.35250
C	2.99410	-3.91026	0.06731
H	3.51201	-4.86432	0.13966
C	3.68278	-2.72800	-0.14441
H	4.76717	-2.75639	-0.25234
C	3.03719	-1.54327	-0.22221
H	3.57547	-0.61380	-0.36660
C	1.65366	-1.48697	-0.07441
C	0.83416	-0.30665	-0.11052
C	0.85482	1.16219	-0.07117
C	-0.45468	1.61342	-0.07261
C	-1.27340	0.48215	-0.08301
C	-2.67770	0.09620	-0.02862
C	-3.78440	0.95550	-0.09612
H	-3.64698	2.02634	-0.20067
C	-5.05658	0.42820	-0.04333
H	-5.90686	1.10859	-0.09687
C	-5.27093	-0.91634	0.06907
H	-6.27310	-1.33623	0.11011
C	-4.15287	-1.72230	0.12056
H	-4.24870	-2.80644	0.20569
C	2.11554	1.94167	-0.00537
C	2.96250	4.11931	0.22298
H	3.47153	3.89335	1.16516
H	2.57394	5.13974	0.23884
H	3.68332	4.00095	-0.59183
C	-0.90546	3.06993	-0.03733
H	-0.55405	3.62830	-0.91231
H	-0.51561	3.59708	0.83977
H	-1.99540	3.14087	-0.01084



LOGLEA: $\Delta E_{L(coord)}$ = –970.97859669 E_h

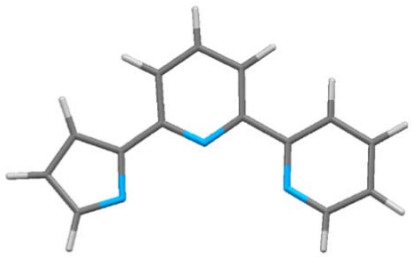
O	1.86433	-3.35547	-0.47868
O	2.98630	-1.67195	0.42784
N	0.93591	2.53665	0.10366
N	-0.52440	0.52331	0.06921
N	-2.92860	1.24206	0.21869
C	1.63271	3.66886	-0.01127
H	1.05300	4.59106	0.06889
C	3.00397	3.71316	-0.19710
H	3.51803	4.66805	-0.29181
C	3.69445	2.52082	-0.27904
H	4.77339	2.51743	-0.42516
C	3.01441	1.33080	-0.15160
H	3.53835	0.38517	-0.20530
C	1.62097	1.32343	0.00562
C	0.76038	0.15479	0.04782
C	0.74763	-1.28378	-0.05671
C	-0.59716	-1.68776	-0.08551
C	-1.35860	-0.53225	0.01179
C	-2.75245	-0.11234	0.04301
C	-3.87123	-0.94425	-0.12235
H	-3.73287	-2.01167	-0.26786
C	-5.14191	-0.39866	-0.12033
H	-6.00923	-1.04187	-0.25737
C	-5.29948	0.96373	0.05895
H	-6.29002	1.41479	0.06570
C	-4.18121	1.72924	0.22220
H	-4.25961	2.80840	0.36882
C	1.86836	-2.21371	-0.08458
C	4.12931	-2.55006	0.45869
H	3.93399	-3.41779	1.09534
H	4.94663	-1.95321	0.86789
H	4.37935	-2.90958	-0.54355
C	-1.13462	-3.10304	-0.13224
H	-1.87088	-3.27362	0.66480
H	-0.33267	-3.83551	-0.03471
H	-1.64611	-3.31044	-1.08384

Relaxed Py-Pyr$^{\cdot}$ ligand geometries *(Table S2; Table S3; Table S5 1 & 2, 29 & 30)*



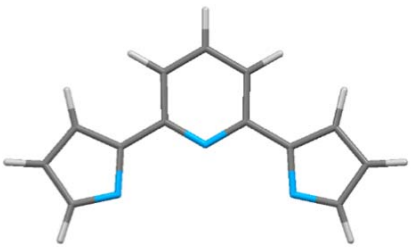
A: $\Delta E_{L(relax)}$ = –742.4808698 E_h

C	-1.15933	0.83517	0.00000
C	-1.20037	2.24041	0.00001
C	0.00000	2.94135	0.00002
C	1.20037	2.24040	0.00002
N	0.00000	0.16594	0.00000
C	1.15933	0.83517	0.00001
C	2.41348	0.00960	0.00001
C	3.69020	0.59775	0.00003
C	4.81829	-0.21801	0.00003
C	4.65119	-1.60010	0.00003
C	3.34493	-2.09437	0.00002
N	2.25683	-1.32528	0.00001
C	-2.41348	0.00960	-0.00001
C	-3.69020	0.59775	-0.00002
C	-4.81829	-0.21801	-0.00004
C	-4.65119	-1.60010	-0.00005
C	-3.34493	-2.09437	-0.00003
N	-2.25683	-1.32528	-0.00002
H	3.16647	-3.16889	0.00001
H	5.49986	-2.27653	0.00003
H	5.81077	0.22337	0.00004
H	3.81535	1.67391	0.00003
H	2.13721	2.78385	0.00002
H	0.00000	4.02743	0.00002
H	-2.13721	2.78385	0.00001
H	-3.81536	1.67391	-0.00002
H	-5.49986	-2.27653	-0.00006
H	-5.81077	0.22336	-0.00005
H	-3.16647	-3.16889	-0.00004



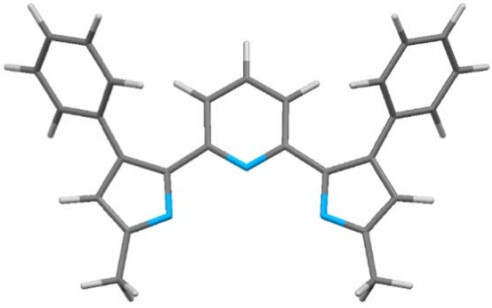
B^{-}: $\Delta E_{L(relax)}$ = –703.7867049 E_h

C	2.67577	-0.23060	0.00006
N	2.63598	-1.60880	-0.00007
C	-2.15495	0.03464	-0.00003
C	-3.38944	0.71823	-0.00007
C	-4.58045	0.00154	-0.00012
C	-4.53293	-1.39196	-0.00012
C	-3.27021	-1.98588	-0.00008
N	-2.12067	-1.31192	-0.00004
H	-3.42221	1.80087	-0.00007
H	-5.53310	0.52633	-0.00015
H	-5.43537	-1.99666	-0.00015
H	-3.17945	-3.07302	-0.00008
C	3.91701	-1.99835	-0.00007
C	4.82566	-0.90823	0.00027
H	4.17323	-3.05740	-0.00008
C	4.02532	0.23399	-0.00012
H	5.91095	-0.95282	0.00050
H	4.37318	1.26195	-0.00019
C	-0.84131	0.76575	0.00002
C	-0.81145	2.17072	0.00004
C	0.44725	2.78585	0.00007
C	1.58867	2.01274	0.00009
C	1.48868	0.58681	0.00013
N	0.25730	0.00492	0.00006
H	-1.71003	2.77627	0.00002
H	0.52214	3.87214	0.00006
H	2.56660	2.48158	0.00007



C^{2-}: $\Delta E_{L(relax)}$ = –664.9865477 E_h

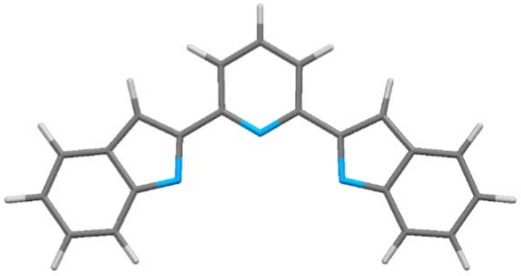
C	0.00000	1.17655	0.54554
C	0.00000	1.20268	1.96636
C	0.00000	0.00000	2.66066
C	0.00000	-1.20268	1.96636
C	0.00000	-1.17655	0.54554
N	0.00000	0.00000	-0.12740
H	0.00000	2.14839	2.49885
H	0.00000	0.00000	3.75346
H	0.00000	-2.14839	2.49885
N	0.00000	2.53570	-1.56168
C	0.00000	3.85381	-1.84350
C	0.00000	4.65930	-0.68435
C	0.00000	3.75014	0.38737
C	0.00000	2.45027	-0.19052
H	0.00000	4.19732	-2.88022
H	0.00000	5.74711	-0.62818
H	0.00000	4.00695	1.44317
N	0.00000	-2.53570	-1.56168
C	0.00000	-2.45027	-0.19052
C	0.00000	-3.75014	0.38737
C	0.00000	-4.65930	-0.68435
C	0.00000	-3.85381	-1.84350
H	0.00000	-4.00695	1.44317
H	0.00000	-5.74711	-0.62818
H	0.00000	-4.19732	-2.88022



($\mathbf{C}^{\mathbf{2}}$)$^{2-}$: $\Delta E_{L(relax)}$ = –1205.778176110 E_h

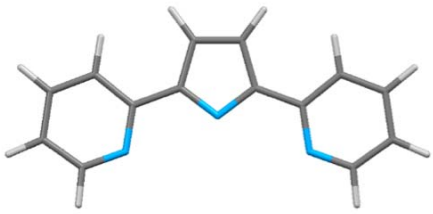
N	2.35548	2.32629	-0.12987
N	-0.00001	0.84585	0.02505
N	-2.35547	2.32633	-0.12966
C	3.62492	2.79629	-0.10682
C	4.55427	1.76625	0.04964
H	5.63808	1.84618	0.02977
C	3.80899	0.55342	0.08553
C	2.42676	0.97564	0.01251
C	1.17683	0.18326	0.09543
C	1.20392	-1.20224	0.38661
H	2.13956	-1.71887	0.54827
C	-0.00001	-1.87798	0.53605
H	-0.00003	-2.93735	0.79501
C	-1.20395	-1.20228	0.38638
H	-2.13958	-1.71900	0.54776
C	-1.17686	0.18325	0.09533
C	-2.42678	0.97564	0.01252
C	-3.80900	0.55346	0.08540
C	-4.55428	1.76627	0.04952
H	-5.63809	1.84620	0.02960
C	-3.62488	2.79633	-0.10669
C	4.49551	-0.73666	0.03717
C	5.67777	-0.94773	0.79305
H	5.99343	-0.16013	1.47162
C	6.42160	-2.12141	0.69878
H	7.31992	-2.23560	1.30542
C	6.01852	-3.15663	-0.15055

H	6.59273	-4.07833	-0.21955
C	4.85655	-2.97644	-0.90987
H	4.52777	-3.76019	-1.59122
C	4.12072	-1.79743	-0.82612
H	3.24079	-1.66890	-1.44759
C	-4.49552	-0.73664	0.03708
C	-5.67761	-0.94780	0.79318
H	-5.99315	-0.16027	1.47188
C	-6.42144	-2.12150	0.69895
H	-7.31961	-2.23577	1.30578
C	-6.01851	-3.15662	-0.15056
H	-6.59271	-4.07833	-0.21953
C	-4.85671	-2.97633	-0.91012
H	-4.52808	-3.76000	-1.59163
C	-4.12089	-1.79731	-0.82642
H	-3.24111	-1.66868	-1.44806
C	3.90314	4.26886	-0.24027
H	3.40783	4.69456	-1.12378
H	4.98041	4.46315	-0.33085
H	3.53581	4.84434	0.62337
C	-3.90308	4.26893	-0.23988
H	-3.53734	4.84411	0.62466
H	-4.98022	4.46316	-0.33221
H	-3.40627	4.69502	-1.12234



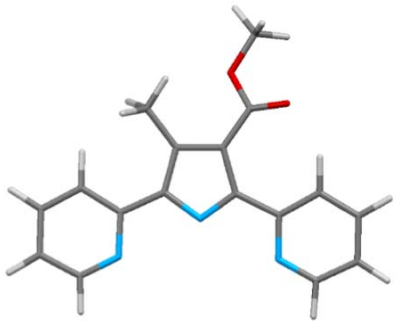
$(\mathbf{C}^{\mathbf{3}})^{2-}$: $\Delta E_{L(relax)}$ = –972.330651272 E_h

N	-2.50191	-0.78646	0.00023
N	-0.00000	0.64684	0.00014
N	2.50191	-0.78647	0.00022
C	-3.82623	-1.08365	0.00006
C	-4.43782	-2.35468	0.00040
H	-3.81138	-3.24530	0.00075
C	-5.82551	-2.45109	0.00031
H	-6.30101	-3.43229	0.00057
C	-6.63640	-1.28769	-0.00007
H	-7.72209	-1.39222	-0.00014
C	-6.06427	-0.01987	-0.00035
H	-6.70363	0.86525	-0.00064
C	-4.65834	0.11088	-0.00034
C	-3.73652	1.17831	-0.00054
H	-3.97892	2.23476	-0.00125
C	-2.44988	0.57736	-0.00011
C	3.82622	-1.08366	-0.00001
C	4.43782	-2.35468	-0.00006
H	3.81140	-3.24531	0.00011
C	5.82551	-2.45108	-0.00030
H	6.30103	-3.43227	-0.00037
C	6.63641	-1.28768	-0.00040
H	7.72210	-1.39221	-0.00056
C	6.06427	-0.01986	-0.00020
H	6.70362	0.86527	-0.00019
C	4.65834	0.11088	-0.00006
C	3.73652	1.17831	0.00040
H	3.97891	2.23476	-0.00138
C	2.44987	0.57735	0.00032
C	-1.16956	1.32263	-0.00016
C	-1.19950	2.73678	-0.00042
H	-2.14598	3.26543	-0.00101
C	0.00001	3.43618	0.00019
H	0.00000	4.52668	0.00036
C	1.19950	2.73678	0.00070
H	2.14599	3.26541	0.00169
C	1.16955	1.32262	0.00028



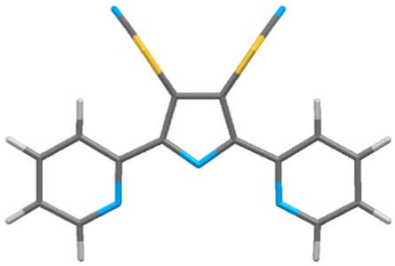
$\mathbf{D}^{-}$: $\Delta E_{L(relax)}$ = –703.8050017 E_h

N	0.00000	0.25022	0.00000
C	0.00000	-0.56692	1.08348
C	0.00000	-1.94494	0.69244
C	0.00000	-1.94494	-0.69244
C	0.00000	-0.56692	-1.08348
C	0.00000	-0.06105	2.44736
C	-0.00000	-0.95349	3.55474
C	-0.00000	-0.46227	4.84902
C	0.00000	0.92236	5.05629
C	0.00000	1.72798	3.91638
N	0.00000	1.28211	2.66122
H	-0.00000	-2.02394	3.37949
H	-0.00000	-1.14960	5.69342
H	0.00000	1.35689	6.05205
H	0.00000	2.81530	4.02740
C	0.00000	-0.06105	-2.44736
C	-0.00000	-0.95349	-3.55474
C	-0.00000	-0.46227	-4.84902
C	0.00000	0.92236	-5.05629
C	0.00000	1.72798	-3.91638
N	0.00000	1.28211	-2.66122
H	-0.00000	-2.02394	-3.37949
H	-0.00000	-1.14960	-5.69342
H	0.00000	1.35689	-6.05205
H	0.00000	2.81530	-4.02740
H	0.00000	-2.81915	-1.33446
H	0.00000	-2.81915	1.33446



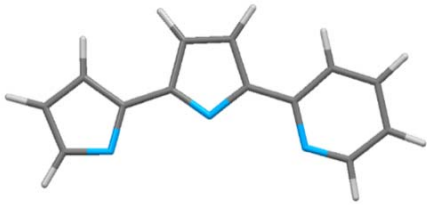
$(\mathbf{D}^{2})^{2-}$: $\Delta E_{L(relax)}$ = –971.007250295 E_h

O	2.82920	-1.99356	-0.62927
O	1.30920	-3.22844	0.46768
N	1.70626	2.64536	0.08192
N	-0.41645	0.99136	-0.03572
N	-3.07578	1.67848	0.00296
C	2.71961	3.50311	0.15420
H	2.44025	4.55606	0.23997
C	4.06896	3.14484	0.12920
H	4.85140	3.89611	0.19717
C	4.35222	1.78475	0.00561
H	5.38190	1.43355	-0.03108
C	3.31102	0.86822	-0.08039
H	3.51664	-0.18456	-0.20918
C	1.97132	1.31794	-0.03019
C	0.79259	0.42384	-0.09351
C	0.66542	-1.02847	-0.11450
C	-0.73442	-1.28375	-0.08902
C	-1.34918	-0.00507	-0.03730
C	-2.77103	0.35273	-0.01674
C	-3.82055	-0.60241	0.02937
H	-3.60060	-1.65896	0.05706
C	-5.14525	-0.18755	0.05782
H	-5.94211	-0.92828	0.09067
C	-5.44053	1.17620	0.05332
H	-6.46118	1.54764	0.07519
C	-4.35136	2.05075	0.03221
H	-4.52555	3.12937	0.04401
C	1.69976	-2.04843	-0.14875
C	2.26909	-4.27698	0.40509
H	2.52339	-4.53318	-0.62889
H	1.80692	-5.13399	0.90156
H	3.19572	-4.00052	0.91856
C	-1.40778	-2.62348	-0.23639
H	-0.68788	-3.40539	-0.47121
H	-2.15803	-2.60660	-1.03675
H	-1.92556	-2.93904	0.68148



$(\mathbf{D}^{3})^{2-}$: $\Delta E_{L(relax)}$ = –1684.665547790 E_h

S	1.67885	2.21762	-0.88976
S	-1.67903	2.21755	-0.88937
N	2.45874	-2.49098	0.21028
N	-0.00007	-1.31180	-0.00633
N	-2.45899	-2.49079	0.21017
N	2.57233	3.45567	1.55360
N	-2.57115	3.45597	1.55431
C	3.63521	-3.10242	0.32728
H	3.59109	-4.17315	0.53434
C	4.87289	-2.46856	0.20552
H	5.79967	-3.02457	0.31395
C	4.85914	-1.09871	-0.05360
H	5.78764	-0.54169	-0.15420
C	3.64194	-0.43996	-0.17767
H	3.62487	0.62240	-0.37494
C	2.43565	-1.16241	-0.04613
C	1.10028	-0.54136	-0.16004
C	0.71101	0.80096	-0.42677
C	-0.71096	0.80104	-0.42674
C	-1.10037	-0.54124	-0.16011
C	-2.43580	-1.16223	-0.04626
C	-3.64204	-0.43970	-0.17773
H	-3.62490	0.62268	-0.37494
C	-4.85928	-1.09834	-0.05368
H	-5.78775	-0.54124	-0.15425
C	-4.87315	-2.46821	0.20543
H	-5.79998	-3.02415	0.31385
C	-3.63551	-3.10215	0.32716
H	-3.59147	-4.17288	0.53421
C	2.16867	2.92352	0.59587
C	-2.16806	2.92369	0.59642

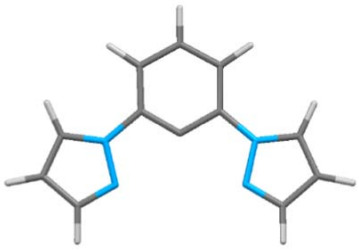


$\mathbf{E}^{2-}$: $\Delta E_{L(relax)}$ = –664.9069983 E_h

N	0.30762	-0.38111	0.00000
C	1.40862	0.39232	0.00000

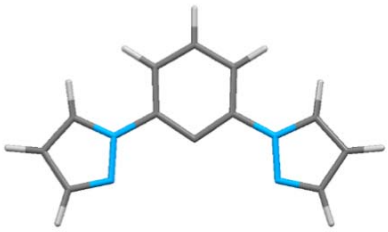
C	1.04483	1.79272	0.00000
C	-0.33537	1.84285	0.00000
C	-0.78160	0.47621	0.00000
C	2.79813	-0.08413	0.00000
N	3.16427	-1.40919	0.00000
C	-2.14184	0.04936	0.00000
C	-3.22405	1.00233	0.00000
C	-4.53807	0.59068	0.00000
C	-4.84105	-0.78871	0.00000
C	-3.73870	-1.65139	0.00000
N	-2.45986	-1.29728	0.00000
H	-2.99161	2.06317	0.00000
H	-5.33865	1.33333	0.00000
H	-5.86174	-1.16514	0.00000
H	-3.92019	-2.73440	-0.00000
H	-0.94703	2.74187	0.00000
H	1.72801	2.63726	0.00000
C	4.51922	-1.41064	0.00000
C	5.06510	-0.11259	0.00000
H	5.07089	-2.35476	0.00000
C	3.94697	0.74889	0.00000
H	6.11860	0.16795	0.00000
H	3.96437	1.83627	-0.00000

Strain within pincer ligand geometries from SC-XRD structures (Table S4; Table S5 23–26)



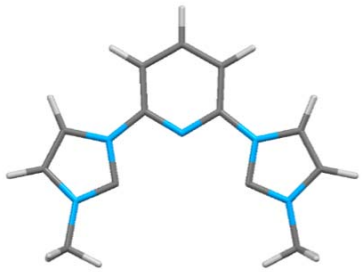
KEPSUV: $\Delta E_{L(coord)}$ = –681.57708049 E_h

N	-1.99473	-1.39905	-0.08869
N	-2.29861	-0.05695	0.00632
C	-3.63523	0.08410	0.09243
H	-4.09260	1.06072	0.18024
C	-4.19769	-1.14068	0.03981
H	-5.26099	-1.35143	0.08924
C	-3.13321	-2.05703	-0.07191
H	-3.14435	-3.13736	-0.13845
C	0.01133	0.15909	-0.02128
C	-1.21155	0.84643	-0.00671
C	-1.22687	2.23174	0.01953
H	-2.13618	2.84450	0.05451
C	0.01100	2.88778	0.00227
H	0.01464	3.97811	0.01286
C	1.24069	2.22136	-0.03499
H	2.15734	2.82308	-0.05384
C	1.19971	0.84312	-0.03672
N	1.98029	-1.41327	0.01016
N	2.29091	-0.07464	-0.03033
C	3.62618	0.09583	-0.02065
H	4.07165	1.08078	-0.04665
C	4.20381	-1.14800	0.04937
H	5.26763	-1.35763	0.07532
C	3.13350	-2.05621	0.06271
H	3.14791	-3.13853	0.10141



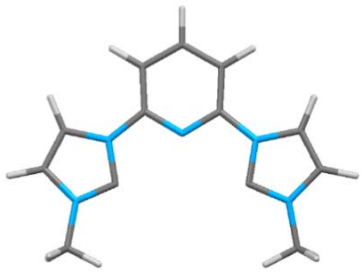
KEPSUV: $\Delta E_{L(relax)}$ = –681.620400283 E_h

N	-2.54625	-1.52464	0.00047
N	-2.46242	-0.17512	0.00019
C	-3.70389	0.39329	-0.00046
H	-3.84566	1.46137	-0.00093
C	-4.63662	-0.62769	-0.00056
H	-5.71384	-0.53077	-0.00090
C	-3.85052	-1.79808	0.00003
H	-4.17521	-2.83189	0.00016
C	-0.00002	-0.26489	0.00026
C	-1.16093	0.51373	0.00007
C	-1.20656	1.91859	0.00005
H	-2.13298	2.49086	0.00010
C	0.00004	2.61742	0.00017
H	0.00007	3.70550	0.00025
C	1.20661	1.91853	0.00026
H	2.13306	2.49077	0.00056
C	1.16094	0.51369	0.00015
N	2.54624	-1.52468	0.00042
N	2.46239	-0.17516	0.00024
C	3.70386	0.39328	-0.00044
H	3.84560	1.46136	-0.00077
C	4.63660	-0.62768	-0.00055
H	5.71382	-0.53072	-0.00101
C	3.85052	-1.79808	-0.00010
H	4.17522	-2.83189	-0.00001



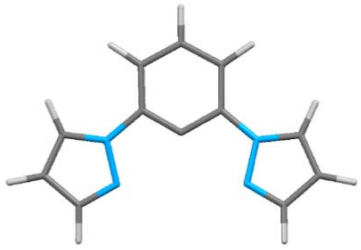
WOXFEU: $\Delta E_{L(coord)}$ = –776.83661624 E_h

C	1.99662	-0.99519	0.00616
N	3.21098	-1.53591	-0.02121
C	3.51661	-2.96734	0.00942
H	4.11618	-3.24910	-0.86139
H	2.56486	-3.49768	-0.00968
H	4.06357	-3.22241	0.92217
C	4.19617	-0.55337	-0.01725
H	5.25437	-0.77802	-0.03436
C	3.59974	0.62917	0.00270
H	4.02838	1.61982	0.00744
N	2.23543	0.36774	0.02176
C	1.15256	1.25363	0.01554
N	0.00681	0.60068	0.00772
C	-1.16370	1.25866	0.00134
C	-1.20677	2.63077	-0.01112
H	-2.13673	3.19051	-0.02433
C	0.01146	3.29708	-0.00406
H	0.01800	4.38328	-0.01200
C	1.20971	2.61508	0.00700
H	2.14910	3.15924	0.01087
N	-2.25246	0.36454	-0.01401
C	-2.00950	-1.00103	-0.02559
N	-3.23053	-1.53346	-0.00628
C	-3.49835	-2.97092	0.00293
H	-4.08340	-3.26046	-0.87557
H	-4.04457	-3.25536	0.90769
H	-2.52976	-3.46890	-0.01650
C	-4.20679	-0.54770	0.01640
H	-5.26579	-0.76830	0.03198
C	-3.60446	0.62773	0.00060
H	-3.88560	1.64282	0.01325



YOKGUB: $\Delta E_{L(coord)}$ = –776.84060739 E_h

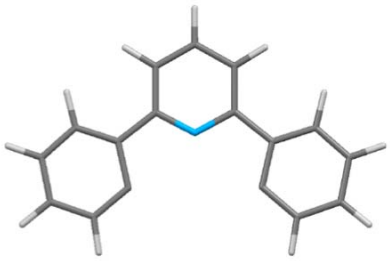
N	-0.00000	0.55420	0.00000
N	-2.25104	0.35814	-0.00720
N	-3.25009	-1.51652	0.00792
C	-1.15087	1.22904	-0.00861
C	-1.21152	2.60304	-0.01926
C	0.00000	3.27629	0.00000
C	-2.03355	-0.98808	0.02073
C	-3.61654	0.64057	-0.04592
C	-4.22495	-0.52829	-0.03529
C	-3.51850	-2.94952	0.07173
H	-2.14950	3.14740	-0.03226
H	0.00000	4.36292	0.00000
H	-4.02900	1.63732	-0.07862
H	-5.28509	-0.74250	-0.05506
H	-4.07488	-3.19904	0.98090
H	-4.09442	-3.27572	-0.80025
H	-2.55072	-3.44929	0.08349
N	2.25105	0.35814	0.00720
N	3.25008	-1.51652	-0.00792
C	1.15088	1.22904	0.00861
C	1.21154	2.60304	0.01927
C	2.03354	-0.98808	-0.02073
C	3.61654	0.64057	0.04591
C	4.22496	-0.52831	0.03528
C	3.51849	-2.94953	-0.07172
H	2.14952	3.14740	0.03226
H	4.02900	1.63732	0.07862
H	5.28509	-0.74252	0.05505
H	4.07485	-3.19905	-0.98090
H	4.09440	-3.27573	0.80025
H	2.55070	-3.44930	-0.08348



WOXFEU/YOKGUB: $\Delta E_{L(relax)}$ = –776.8629151 E_h

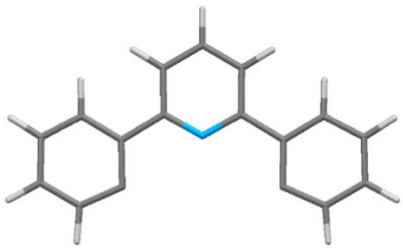
N	0.00000	0.34678	0.00000
N	-2.33824	0.24581	0.00014
N	-3.68054	-1.40854	-0.00018
C	-1.14541	1.02055	0.00015
C	-1.20572	2.42273	0.00037
C	0.00000	3.11427	0.00000
C	-2.34343	-1.14564	-0.00001
C	-3.63321	0.78652	0.00029
C	-4.48021	-0.26564	0.00018
C	-4.19942	-2.76639	-0.00037
H	-2.14221	2.96380	0.00093
H	0.00000	4.20018	0.00000
H	-3.85459	1.84022	0.00020
H	-5.55977	-0.29298	-0.00000
H	-4.80917	-2.95179	0.89016
H	-4.80886	-2.95176	-0.89126
H	-3.34169	-3.43778	-0.00027

N	2.33824	0.24581	-0.00014
N	3.68054	-1.40854	0.00018
C	1.14541	1.02055	-0.00015
C	1.20572	2.42273	-0.00037
C	2.34343	-1.14564	0.00001
C	3.63321	0.78652	-0.00029
C	4.48021	-0.26564	-0.00018
C	4.19942	-2.76639	0.00037
H	2.14221	2.96380	-0.00093
H	3.85459	1.84022	-0.00020
H	5.55977	-0.29298	0.00000
H	4.80917	-2.95179	-0.89016
H	4.80886	-2.95176	0.89126
H	3.34169	-3.43778	0.00027



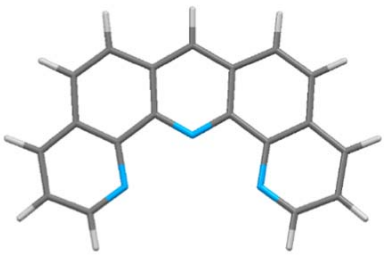
CEXYIP: $\Delta E_{L(coord)}$ = –708.93490374 E_h

N	0.01205	0.33341	0.00825
C	3.11010	-2.23048	-0.02297
H	2.95210	-3.32366	-0.04387
C	2.04140	-1.34990	-0.01069
C	-1.20545	0.98861	-0.00779
C	-2.35562	0.06880	-0.02714
C	-2.03818	-1.32130	-0.01259
C	2.35295	0.07161	0.02164
C	4.69614	-0.41800	0.01689
H	5.73077	-0.06570	0.01907
C	0.01113	3.04624	-0.01019
H	0.01630	4.13885	-0.02258
C	-1.19893	2.37567	-0.03461
H	-2.12883	2.94556	-0.06385
C	4.42842	-1.76962	-0.02619
H	5.28497	-2.46732	-0.04673
C	-3.11186	-2.23217	0.01179
H	-2.94193	-3.32097	0.02966
C	-4.44297	-1.76964	0.02409
H	-5.29943	-2.46670	0.04013
C	-3.67435	0.49132	-0.00082
H	-3.93680	1.56169	0.00394
C	1.20861	0.96243	0.02277
C	3.66012	0.49961	0.02443
H	3.92650	1.56791	0.05038
C	1.20813	2.36815	0.01665
H	2.14223	2.93159	0.03250
C	-4.70493	-0.41117	0.00266
H	-5.73843	-0.05600	0.01610



CEXYIP: $\Delta E_{L(relax)}$ = –708.969073512 E_h

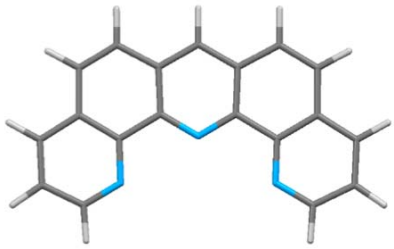
N	0.00001	0.03231	-0.00015
C	3.75213	-2.10673	0.00010
H	3.83848	-3.20741	0.00022
C	2.45331	-1.52985	0.00016
C	-1.18056	0.69097	-0.00004
C	-2.47943	-0.09706	-0.00023
C	-2.45335	-1.52984	-0.00053
C	2.47944	-0.09707	0.00000
C	4.93323	-0.00916	0.00015
H	5.85518	0.57583	0.00035
C	-0.00003	2.80433	0.00001
H	-0.00001	3.89639	0.00007
C	-1.19985	2.10851	0.00050
H	-2.13039	2.66352	0.00128
C	4.96488	-1.40841	-0.00010
H	5.93021	-1.93201	-0.00039
C	-3.75211	-2.10673	-0.00018
H	-3.83849	-3.20744	-0.00075
C	-4.96488	-1.40840	0.00058
H	-5.93027	-1.93201	0.00122
C	-3.69546	0.63487	-0.00037
H	-3.72120	1.72689	-0.00117
C	1.18061	0.69100	-0.00016
C	3.69549	0.63487	0.00035
H	3.72117	1.72687	0.00097
C	1.19984	2.10850	-0.00053
H	2.13033	2.66358	-0.00120
C	-4.93323	-0.00917	0.00029
H	-5.85518	0.57584	0.00031



PUHKOS: $\Delta E_{L(coord)}$ = –894.93190061 E_h

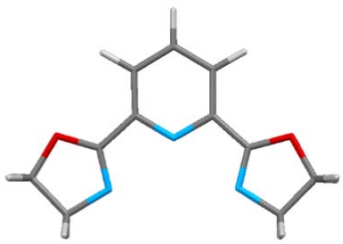
N	-2.06758	-1.77121	-0.03249
N	-0.00011	-0.19752	-0.01889
N	2.06632	-1.76749	-0.04207
C	-3.13420	-2.54922	-0.01614

C	-4.43945	-2.05408	0.03336
C	-4.66261	-0.69900	0.03854
C	-3.55664	0.17734	0.00318
C	-2.29174	-0.41105	-0.02051
C	-3.64503	1.61577	0.00426
C	-2.54785	2.41022	0.01800
C	-1.14212	0.44165	-0.01359
C	-1.21825	1.84990	0.00329
C	-0.00082	2.54484	-0.00494
C	1.21756	1.85377	-0.01213
C	1.15539	0.44717	-0.01669
C	2.53812	2.41523	-0.01794
C	3.63529	1.61976	-0.00158
C	2.29576	-0.41397	-0.02287
C	3.56202	0.17358	0.01551
C	4.65703	-0.69457	0.05802
C	4.44141	-2.04756	0.04432
C	3.13983	-2.55943	-0.02271
H	-2.95349	-3.62324	-0.03344
H	-5.27679	-2.74632	0.05996
H	-5.67320	-0.29935	0.06970
H	-4.63469	2.06624	0.01279
H	-2.66290	3.49156	0.02829
H	-0.00132	3.63286	0.00038
H	2.65605	3.49625	-0.02841
H	4.62340	2.07428	0.00364
H	5.66802	-0.29606	0.09940
H	5.28467	-2.73280	0.07519
H	2.95766	-3.63184	-0.04957



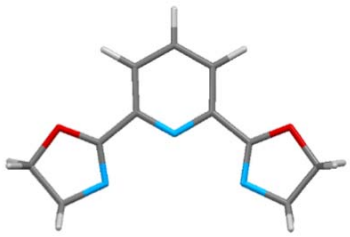
PUHKOS: $\Delta E_{L(relax)}$ = –894.949534156 E_h

N	-2.36240	-1.82461	0.00000
N	-0.00003	-0.39947	-0.00007
N	2.36240	-1.82458	0.00002
C	-3.50578	-2.49308	0.00007
C	-4.77544	-1.88408	-0.00004
C	-4.83737	-0.50527	0.00001
C	-3.64160	0.24282	0.00005
C	-2.41184	-0.47552	-0.00005
C	-3.64409	1.68127	0.00010
C	-2.48180	2.38369	0.00004
C	-1.15330	0.27499	-0.00010
C	-1.21213	1.70976	-0.00005
C	-0.00002	2.40282	-0.00004
C	1.21214	1.70968	-0.00005
C	1.15337	0.27503	-0.00012
C	2.48176	2.38367	0.00003
C	3.64409	1.68128	0.00004
C	2.41181	-0.47555	-0.00007
C	3.64165	0.24285	0.00002
C	4.83735	-0.50525	0.00001
C	4.77541	-1.88410	0.00001
C	3.50582	-2.49310	0.00015
H	-3.42579	-3.57937	-0.00002
H	-5.67480	-2.49168	-0.00018
H	-5.79225	0.01420	-0.00002
H	-4.60157	2.19560	0.00029
H	-2.48996	3.47046	0.00007
H	0.00006	3.49065	0.00002
H	2.48989	3.47044	0.00012
H	4.60156	2.19566	0.00013
H	5.79228	0.01413	-0.00009
H	5.67483	-2.49162	-0.00009
H	3.42575	-3.57936	0.00001



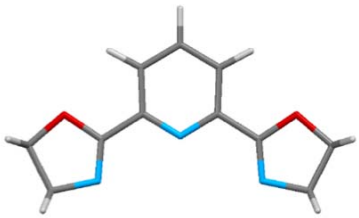
IZAFOG: $\Delta E_{L(coord)}$ = –740.44345037 E_h

O	-3.59281	0.27248	0.07071
O	3.57001	0.28435	-0.01659
N	-1.97746	-1.31525	-0.05939
N	-0.00246	0.21733	-0.01912
N	1.97837	-1.35306	-0.02134
C	-3.25521	-2.11168	-0.04274
H	-3.25354	-2.77748	0.82596
H	-3.31048	-2.72601	-0.94646
C	-4.32224	-1.02981	0.02229
H	-4.97038	-0.98459	-0.85718
H	-4.94785	-1.06422	0.91806
C	-2.28410	-0.07067	0.01661
C	-1.19580	0.89733	0.00866
C	-1.20001	2.30928	0.02805
H	-2.14643	2.84220	0.06234
C	-0.00121	3.01342	-0.00326
H	0.00841	4.09723	0.00264
C	1.20819	2.28309	-0.04396
H	2.15928	2.80737	-0.06672
C	1.17226	0.90972	-0.03609
C	2.28011	-0.08824	-0.02952
C	4.34347	-0.99718	0.06909
H	4.90625	-0.95818	1.00491
H	5.03848	-0.99764	-0.77334
C	3.26701	-2.11910	0.02082
H	3.35000	-2.75082	-0.86931
H	3.28474	-2.76255	0.90545



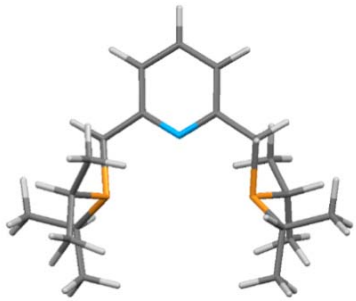
IZAFOG01: $\Delta E_{L(coord)}$ = –740.45869954 E_h

O	3.53488	0.33372	-0.10781
O	-3.54011	0.35113	-0.02824
N	2.09405	-1.38814	0.03569
N	-0.00541	0.13721	-0.03324
N	-2.11081	-1.37686	0.01241
C	3.43617	-2.01306	0.07349
H	3.54218	-2.71444	-0.76151
H	3.54548	-2.58922	0.99863
C	4.41099	-0.83358	-0.01251
H	5.03870	-0.70315	0.87362
H	5.04917	-0.83909	-0.90026
C	2.29359	-0.13869	-0.04267
C	1.15671	0.79455	-0.03320
C	1.20581	2.18635	0.00311
H	2.15403	2.71340	0.00050
C	0.00436	2.85592	0.07454
H	0.00688	3.94202	0.12482
C	-1.18117	2.19268	0.06312
H	-2.12619	2.72546	0.10740
C	-1.15872	0.80236	-0.00052
C	-2.29745	-0.12793	-0.01230
C	-4.39027	-0.84703	-0.09248
H	-4.89309	-0.82516	-1.06515
H	-5.14874	-0.74350	0.68802
C	-3.45571	-2.00126	0.07683
H	-3.56233	-2.51347	1.04067
H	-3.55505	-2.75892	-0.70682



IZAFOG/IZAFOG01: $\Delta E_{L(relax)}$ = –740.4786437 E_h

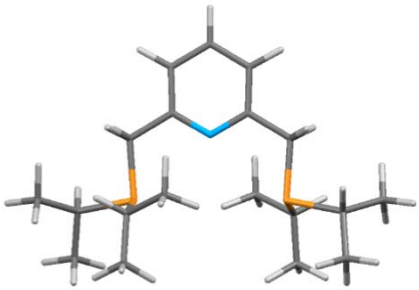
O	3.54960	0.51332	0.00047
O	-3.54960	0.51332	-0.00005
N	2.50903	-1.51311	0.00012
N	0.00000	-0.14654	0.00009
N	-2.50904	-1.51310	-0.00009
C	3.94657	-1.81113	0.00101
H	4.19904	-2.41302	-0.87912
H	4.19833	-2.40920	0.88401
C	4.64934	-0.42759	-0.00171
H	5.25998	-0.24258	0.88688
H	5.25511	-0.24409	-0.89402
C	2.40275	-0.24465	0.00018
C	1.14557	0.54320	0.00017
C	1.19933	1.94586	0.00019
H	2.15715	2.45074	0.00024
C	0.00001	2.65120	0.00017
H	0.00001	3.73696	0.00017
C	-1.19931	1.94586	0.00010
H	-2.15714	2.45075	0.00009
C	-1.14556	0.54320	0.00005
C	-2.40275	-0.24465	-0.00004
C	-4.64935	-0.42759	-0.00025
H	-5.25737	-0.24336	-0.89084
H	-5.25771	-0.24333	0.89010
C	-3.94657	-1.81113	-0.00012
H	-4.19871	-2.41102	0.88151
H	-4.19868	-2.41117	-0.88165



XAMQUZ: $\Delta E_{L(coord)}$ = –1482.59857081 E_h

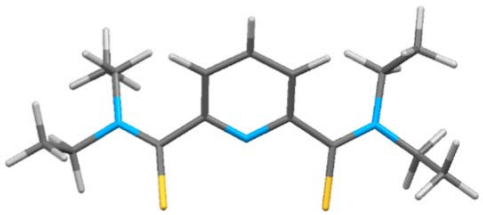
P	2.23414	-0.49677	0.11905
N	-0.00001	1.36674	0.00046
C	2.33945	1.25681	0.73270
C	1.12614	2.06420	0.32336
C	1.14920	3.45986	0.33096
C	-0.00006	4.15998	-0.00031
C	3.16165	-1.44444	1.39040
C	2.96471	-2.95027	1.26661
C	4.63685	-1.07451	1.52001
C	3.29460	-0.42204	-1.39405
C	3.36680	-1.78696	-2.08050
C	2.76483	0.64702	-2.34528
H	3.34781	-3.45842	2.15983
H	2.35612	1.20352	1.83084
H	-0.00010	5.24659	-0.00053
H	2.06226	3.98612	0.59598
H	4.78107	0.00028	1.67180
H	3.49953	-3.36767	0.40808
H	3.26075	1.77818	0.44462
H	2.65417	-1.13572	2.31743
H	4.32206	-0.13011	-1.12449
H	5.19987	-1.35939	0.62431
H	5.10924	-1.58905	2.36757
H	1.90743	-3.20862	1.15531
H	3.89271	-2.52869	-1.47420

H	1.72276	0.45367	-2.62396
H	2.36521	-2.17822	-2.29158
H	3.35858	0.66121	-3.26748
H	3.90294	-1.70826	-3.03436
H	2.80835	1.65118	-1.91495
P	-2.23404	-0.49691	-0.11857
C	-2.33900	1.25633	-0.73325
C	-1.12597	2.06399	-0.32357
C	-1.14909	3.45964	-0.33195
C	-3.16069	-1.44531	-1.38999
C	-2.96377	-2.95106	-1.26525
C	-4.63581	-1.07549	-1.52076
C	-3.29548	-0.42137	1.39381
C	-3.36808	-1.78592	2.08095
C	-2.76635	0.64822	2.34479
H	-3.34627	-3.45971	-2.15844
H	-2.35497	1.20244	-1.83138
H	-2.06209	3.98573	-0.59752
H	-4.77997	-0.00080	-1.67324
H	-3.49913	-3.36802	-0.40685
H	-3.26050	1.77783	-0.44605
H	-2.65262	-1.13708	-2.31686
H	-4.32277	-0.12963	1.12343
H	-5.19941	-1.35990	-0.62528
H	-5.10764	-1.59052	-2.36835
H	-1.90656	-3.20931	-1.15312
H	-3.89358	-2.52800	1.47472
H	-1.72445	0.45505	2.62425
H	-2.36662	-2.17704	2.29290
H	-3.36070	0.66290	3.26661
H	-3.90485	-1.70672	3.03443
H	-2.80962	1.65215	1.91388



XAMQUZ: $\Delta E_{L(relax)}$ = –1482.615905080 E_h

P	2.32535	-0.51511	0.22588
N	-0.00001	1.47505	-0.00000
C	2.45542	1.36783	0.18995
C	1.15729	2.14866	0.07189
C	1.19743	3.54968	0.06413
C	-0.00001	4.25574	0.00001
C	4.05039	-0.84844	0.97228
C	4.14813	-2.28334	1.51819
C	5.27356	-0.49289	0.11535
C	2.54848	-0.91350	-1.61481
C	2.64519	-2.43240	-1.83033
C	1.39245	-0.33575	-2.44744
H	5.06673	-2.40891	2.10443
H	2.93694	1.65669	1.13326
H	-0.00002	5.34229	0.00002
H	2.14969	4.06930	0.11579
H	5.24280	0.53956	-0.24721
H	4.17321	-3.02672	0.71507
H	3.14184	1.69737	-0.60189
H	4.04849	-0.18098	1.84629
H	3.48367	-0.45077	-1.95783
H	5.35936	-1.15003	-0.75645
H	6.19635	-0.60852	0.69753
H	3.29814	-2.52341	2.16369
H	3.52129	-2.87059	-1.34416
H	0.42374	-0.70180	-2.09414
H	1.75618	-2.94166	-1.44252
H	1.51103	-0.62994	-3.49793
H	2.71721	-2.65920	-2.90090
H	1.36296	0.75641	-2.41174
P	-2.32537	-0.51511	-0.22590
C	-2.45544	1.36783	-0.18996
C	-1.15731	2.14866	-0.07189
C	-1.19745	3.54968	-0.06412
C	-4.05042	-0.84845	-0.97225
C	-4.14818	-2.28334	-1.51816
C	-5.27357	-0.49290	-0.11527
C	-2.54843	-0.91351	1.61478
C	-2.64513	-2.43242	1.83030
C	-1.39237	-0.33576	2.44739
H	-5.06679	-2.40891	-2.10437
H	-2.93697	1.65669	-1.13326
H	-2.14972	4.06930	-0.11577
H	-5.24280	0.53954	0.24729
H	-4.17324	-3.02672	-0.71505
H	-3.14186	1.69735	0.60189
H	-4.04855	-0.18098	-1.84625
H	-3.48361	-0.45079	1.95785
H	-5.35933	-1.15005	0.75652
H	-6.19638	-0.60854	-0.69743
H	-3.29821	-2.52341	-2.16370
H	-3.52124	-2.87061	1.34416
H	-0.42367	-0.70181	2.09405
H	-1.75613	-2.94167	1.44246
H	-1.51092	-0.62996	3.49787
H	-2.71711	-2.65923	2.90088
H	-1.36289	0.75639	2.41168

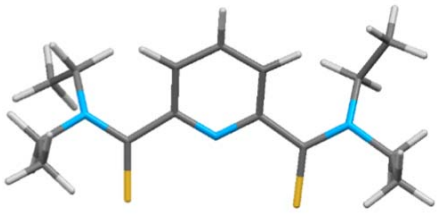


ACAROM: $\Delta E_{L(coord)}$ = –1546.08474654 E_h

S	2.12981	2.16371	0.36921
S	-2.31785	2.14241	-0.39013
N	-0.04717	0.29053	-0.04998
N	3.47900	-0.09968	0.50235

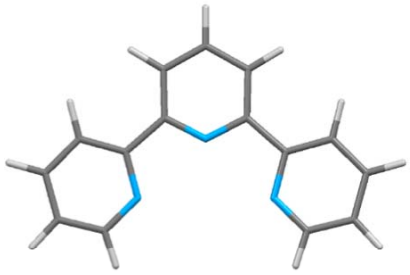
N	-3.54517	-0.13670	0.23792
C	1.14954	-0.30141	-0.27638
C	1.21835	-1.47516	-1.01320
H	2.16763	-1.90951	-1.29877
C	0.05438	-2.06918	-1.44841
H	0.10067	-2.96968	-2.05444
C	-1.16835	-1.50296	-1.14673
H	-2.08222	-1.95261	-1.52047
C	-1.18892	-0.32160	-0.42326
C	2.32825	0.47413	0.20951
C	3.69306	-1.54574	0.74170
H	2.72968	-2.05133	0.75559
H	4.10944	-1.64554	1.75186
C	4.63799	-2.17452	-0.26655
H	4.28645	-2.04213	-1.29404
H	4.73162	-3.24890	-0.07419
H	5.64006	-1.74293	-0.20330
C	4.66335	0.73398	0.80110
H	5.34740	0.11143	1.38678
H	4.33704	1.57058	1.42101
C	5.34793	1.23615	-0.45341
H	5.69907	0.41625	-1.08602
H	6.21481	1.84789	-0.18119
H	4.66749	1.86239	-1.03418
C	-2.43549	0.45449	-0.14762
C	-3.64086	-1.53779	0.72440
H	-2.72325	-2.06241	0.47782
H	-4.45547	-2.03146	0.18052
C	-3.86508	-1.61445	2.21336
H	-3.05169	-1.12276	2.75541
H	-3.89444	-2.66340	2.52820
H	-4.80551	-1.15629	2.52984
C	-4.82723	0.62424	0.27906
H	-4.57621	1.67176	0.43714
H	-5.39315	0.26867	1.14378
C	-5.60252	0.42452	-0.98737
H	-5.04779	0.81586	-1.84521
H	-6.55674	0.95990	-0.93563
H	-5.82922	-0.63088	-1.17510
H	-2.22883	1.98857	-0.92502
C	-0.10346	2.23733	-1.03569
H	-0.15988	3.18136	-1.56969
C	1.12891	1.65396	-0.77090
H	2.03938	2.11962	-1.12457
C	1.15949	0.40462	-0.11734
C	-2.37750	-0.53907	0.25428
C	-3.88094	1.33858	0.86162
H	-2.93202	1.77076	1.17783
H	-4.41619	1.07671	1.78641
C	-4.69726	2.36492	0.07554
H	-4.18441	2.68659	-0.83582
H	-4.87199	3.24896	0.69733
H	-5.67374	1.97072	-0.21935
C	-4.81098	-0.79143	0.04364
H	-5.67882	-0.15433	0.22948
H	-4.77037	-1.54548	0.83769
C	-4.95658	-1.45779	-1.32298
H	-5.02472	-0.70898	-2.11802
H	-5.86690	-2.06563	-1.34237
H	-4.10990	-2.11446	-1.53297
C	2.45270	-0.37399	0.01873
C	3.87247	1.55683	0.61429
H	2.92833	2.06496	0.80382
H	4.50073	2.24072	0.03136
C	4.53247	1.23988	1.96225
H	3.91112	0.55615	2.54747
H	4.65810	2.16548	2.53384
H	5.51922	0.78483	1.84243
C	4.84401	-0.38319	-0.57228
H	5.05601	-1.16273	0.16801
H	5.65988	0.34526	-0.53634
C	4.77033	-0.98551	-1.97456
H	3.97646	-1.73185	-2.04422
H	5.71774	-1.47911	-2.21363
H	4.58731	-0.20883	-2.72333

Relaxed ligand geometries from iron(II) complexes (Table S5)



ACAROM: $\Delta E_{L(relax)}$ = –1546.078130720 E_h

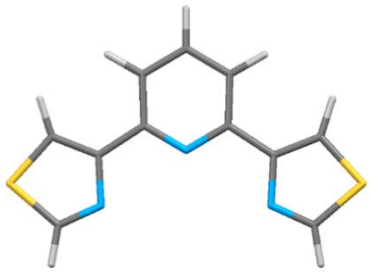
S	-2.18860	-2.11583	0.74110
S	2.44617	-1.96300	0.49479
N	0.03055	-0.25065	0.16342
N	-3.61652	0.07424	0.13134
N	3.61561	0.35106	-0.21227
C	-1.16118	0.32764	-0.01430
C	-1.26664	1.57545	-0.65929



DANMOU: $\Delta E_{L(coord)}$ = –742.480870195 E_h

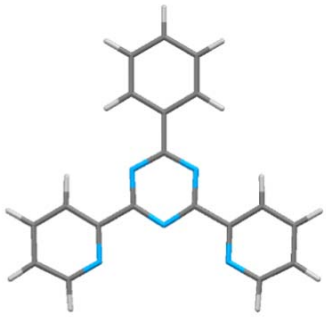
C	-1.18811	1.06716	-0.00009
C	-1.22581	2.46236	0.00001
C	-0.00001	3.14296	0.00011
C	1.22579	2.46237	0.00011

N	-0.00001	0.46236	-0.00009
C	1.18809	1.06717	0.00001
C	2.31519	0.08937	0.00001
C	3.65119	0.46387	0.00011
C	4.64729	-0.51753	0.00011
C	4.28190	-1.86073	0.00001
C	2.92960	-2.18523	-0.00019
N	1.96460	-1.24373	-0.00019
C	-2.31511	0.08946	-0.00009
C	-3.65121	0.46386	-0.00019
C	-4.64731	-0.51755	-0.00009
C	-4.28190	-1.86075	0.00011
C	-2.92960	-2.18524	0.00021
N	-1.96460	-1.24374	0.00011
H	2.60450	-3.21943	-0.00029
H	5.02300	-2.65132	0.00001
H	5.69320	-0.22962	0.00031
H	3.91989	1.51337	0.00031
H	2.15639	3.01637	0.00011
H	-0.00002	4.22786	0.00011
H	-2.15641	3.01636	0.00001
H	-3.91991	1.51335	-0.00029
H	-5.02300	-2.65135	0.00021
H	-5.69320	-0.22965	-0.00019
H	-2.60440	-3.21944	0.00041



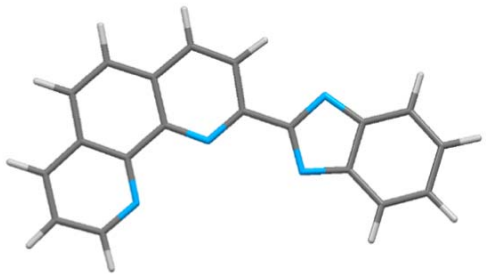
DIXDIX: $\Delta E_{L(relax)}$ = –1384.004886870 E_h

N	2.32735	-1.38155	0.00012
C	3.50590	-1.91469	-0.00008
S	4.84194	-0.77775	0.00007
C	3.68234	0.50170	0.00017
C	2.40109	0.00000	-0.00016
N	-0.00001	0.12937	-0.00000
C	1.15610	0.80694	-0.00022
C	1.19991	2.21118	-0.00012
C	0.00003	2.91295	0.00001
C	-1.19988	2.21119	0.00003
C	-1.15614	0.80697	0.00016
C	-2.40108	0.00006	0.00001
C	-3.68236	0.50153	-0.00013
S	-4.84210	-0.77764	0.00021
C	-3.50559	-1.91494	-0.00016
N	-2.32730	-1.38161	-0.00028
H	3.69358	-2.98176	-0.00003
H	4.00904	1.53062	0.00029
H	2.14381	2.74457	-0.00015
H	0.00003	3.99894	-0.00009
H	-2.14375	2.74460	-0.00002
H	-4.00889	1.53059	-0.00016
H	-3.69351	-2.98200	-0.00029



BUKDUH: $\Delta E_{L(relax)}$ = –1005.64335514 E_h

N	-2.38855	2.75721	0.00005
N	-0.00080	1.40692	-0.00002
N	2.38545	2.75987	-0.00001
N	-1.18307	-0.65370	-0.00009
N	1.18380	-0.65238	-0.00006
C	-3.54593	3.41898	0.00010
H	-3.47375	4.50526	0.00021
C	-4.79753	2.79638	0.00010
H	-5.70636	3.38988	0.00021
C	-4.83900	1.40394	-0.00002
H	-5.78792	0.87571	-0.00004
C	-3.63940	0.69737	-0.00010
H	-3.61450	-0.38482	-0.00018
C	-2.43511	1.41581	-0.00008
C	-1.12826	0.68724	-0.00012
C	0.00071	-1.28527	-0.00006
C	1.12748	0.68851	-0.00005
C	2.43351	1.41853	-0.00004
C	3.63861	0.70143	-0.00006
H	3.61490	-0.38079	-0.00013
C	4.83741	1.40933	0.00002
H	5.78692	0.88217	0.00004
C	4.79439	2.80173	0.00009
H	5.70257	3.39622	0.00021
C	3.54210	3.42293	0.00003
H	3.46870	4.50913	0.00005
C	0.00156	-2.76872	-0.00000
C	-1.20851	-3.47973	0.00005
H	-2.14004	-2.92639	0.00007
C	-1.20584	-4.87210	0.00008
H	-2.14746	-5.41315	0.00013
C	0.00314	-5.57161	0.00006
H	0.00375	-6.65781	0.00006
C	1.21132	-4.87074	0.00003
H	2.15355	-5.41072	0.00005
C	1.21243	-3.47836	0.00000
H	2.14333	-2.92398	-0.00001

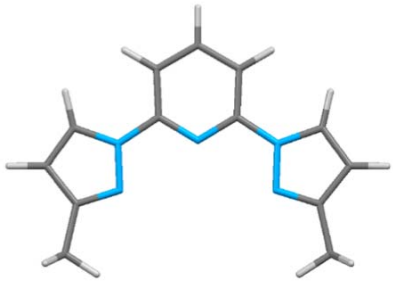


DOMQIH: $\Delta E_{L(relax)}$ = –949.749856724 E_h

N	-2.63577	1.87796	-0.00009
N	-0.54626	0.06046	-0.00031
N	2.20069	0.96380	-0.00028
N	2.86288	-1.26907	-0.00000
C	-3.63900	2.73865	0.00003
H	-3.36582	3.79440	-0.00006
C	-4.99925	2.36800	0.00019
H	-5.77654	3.12698	0.00035
C	-5.30350	1.02315	0.00024
H	-6.33642	0.68079	0.00035
C	-4.26265	0.06800	0.00010
C	-2.91606	0.55341	0.00000
C	-4.52501	-1.33874	0.00009
H	-5.55821	-1.67814	0.00010
C	-3.49138	-2.23031	0.00003
H	-3.68839	-3.30089	-0.00001
C	-2.13233	-1.79503	-0.00001
C	-1.80933	-0.40442	-0.00011
C	-1.04395	-2.70411	0.00005
H	-1.24570	-3.77400	0.00017
C	0.23914	-2.22782	-0.00002
H	1.10935	-2.87304	0.00010
C	0.46722	-0.81520	-0.00036
C	1.85331	-0.34664	-0.00035
C	3.97130	-0.48364	0.00001
C	3.55975	0.89937	-0.00016
C	5.34110	-0.81904	0.00030
H	5.65264	-1.86162	0.00053
C	6.27210	0.21053	0.00035
H	7.33526	-0.02418	0.00053
C	5.86816	1.57121	0.00015
H	6.63132	2.34764	0.00018
C	4.52622	1.92613	-0.00008
H	4.21673	2.96888	-0.00024

EKAKIM/EKAKIM01: $\Delta E_{L(relax)}$ = –797.5346654 E_h

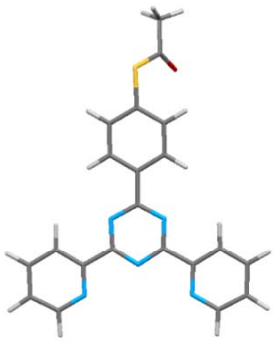
N	0.00001	-0.33520	0.00019
C	1.14158	0.34483	0.00015
C	1.21443	1.74510	0.00017
H	2.13746	2.30686	0.00019
C	0.00003	2.41235	0.00007
C	-1.21442	1.74505	0.00008
H	-2.13739	2.30694	-0.00015
C	-1.14164	0.34485	0.00019
N	2.33043	-0.42240	0.00016
N	2.27957	-1.78401	0.00020
C	3.54630	-2.16565	-0.00000
H	3.78094	-3.22175	0.00005
C	4.44218	-1.06438	-0.00040
H	5.52170	-1.07729	-0.00061
C	3.62708	0.03845	-0.00026
H	3.86861	1.08874	-0.00040
N	-2.33042	-0.42242	0.00012
N	-2.27955	-1.78403	0.00005
C	-3.54629	-2.16566	0.00016
H	-3.78095	-3.22175	0.00052
C	-4.44217	-1.06439	-0.00023
H	-5.52168	-1.07732	-0.00061
C	-3.62706	0.03843	-0.00049
H	-3.86858	1.08874	-0.00052
F	-0.00006	3.75436	-0.00001



AFANEB/AFANEB01: $\Delta E_{L(relax)}$ = –776.951804 E_h

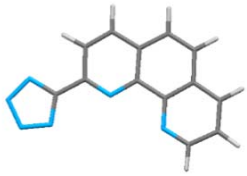
N	-2.28064	1.05715	-0.00001
N	-2.32968	-0.30574	-0.00008
C	-3.87996	2.91346	-0.00001
H	-2.96019	3.50139	0.00026
H	-4.46891	3.18707	0.88252
H	-4.46841	3.18712	-0.88285
C	-3.54581	1.45379	0.00004
C	-4.43786	0.34150	0.00010
H	-5.51805	0.35465	0.00002
C	-3.62652	-0.76235	0.00022
H	-3.87140	-1.81213	0.00044
N	0.00002	-0.39665	-0.00011
C	-1.14203	-1.07588	-0.00013
C	-1.20657	-2.47763	-0.00009
H	-2.14600	-3.01408	-0.00013
C	-0.00006	-3.16848	-0.00004
H	-0.00006	-4.25410	0.00001
C	1.20650	-2.47767	-0.00002
H	2.14589	-3.01421	0.00000
C	1.14208	-1.07594	-0.00005

N	2.32970	-0.30579	-0.00005
N	2.28066	1.05711	-0.00011
C	3.62656	-0.76236	0.00013
H	3.87146	-1.81213	0.00026
C	4.43788	0.34152	0.00023
H	5.51807	0.35469	0.00024
C	3.54583	1.45379	-0.00004
C	3.87992	2.91348	-0.00004
H	2.96014	3.50138	-0.00105
H	4.46948	3.18695	-0.88220
H	4.46773	3.18732	0.88317



BUKDIV: $\Delta E_{L(relax)}$ = –1556.48288288 E_h

N	-4.47983	-2.10823	0.19198
N	-2.91226	0.13697	0.03698
N	-4.02990	2.64146	0.08329
N	-0.97930	-1.23827	-0.08789
N	-0.75633	1.11809	-0.14266
C	-5.24720	-3.19574	0.26786
H	-6.31849	-3.01857	0.34626
C	-4.74865	-4.50169	0.25129
H	-5.42450	-5.34854	0.31639
C	-3.37060	-4.67804	0.14955
H	-2.93691	-5.67357	0.13284
C	-2.55471	-3.55276	0.06935
H	-1.47826	-3.63331	-0.01108
C	-3.15287	-2.28471	0.09422
C	-2.30554	-1.05469	0.01016
C	-0.24190	-0.12027	-0.16206
C	-2.09300	1.19136	-0.04171
C	-2.69384	2.56102	-0.01717
C	-1.86802	3.69158	-0.09603
H	-0.79588	3.56487	-0.17454
C	-2.45759	4.95257	-0.06968
H	-1.84454	5.84704	-0.12869
C	-3.84379	5.04299	0.03397
H	-4.34816	6.00381	0.05836
C	-4.57885	3.85609	0.10710
H	-5.66398	3.88717	0.18915
C	1.23034	-0.26218	-0.27271
C	1.82331	-1.53307	-0.28683
H	1.19072	-2.40929	-0.21133
C	3.20442	-1.66617	-0.38345
H	3.65849	-2.65179	-0.37783
C	4.01388	-0.52735	-0.48439
C	3.43008	0.74597	-0.48171
H	4.05214	1.62886	-0.56143
C	2.05023	0.87276	-0.36669
H	1.59019	1.85354	-0.35791
S	5.77564	-0.75537	-0.68766
O	5.82601	1.01823	1.33846
C	6.48051	0.29479	0.63070
C	7.98287	0.13076	0.73846
H	8.19678	-0.62165	1.50537
H	8.41942	1.07980	1.05680
H	8.43348	-0.19777	-0.20084

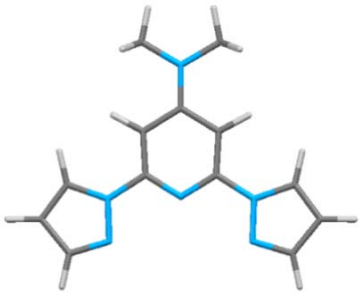


QIDJET: $\Delta E_{L(relax)}$ = –828.145023125 E_h

N	-1.76874	-1.78697	0.00006
N	0.57405	-0.31305	0.00004
N	3.21985	-1.60726	-0.00002
N	4.54399	-1.72566	0.00003
N	5.11261	-0.50452	-0.00002
N	4.16283	0.42199	-0.00012
C	-2.89200	-2.48348	0.00004
H	-2.78405	-3.56860	0.00008
C	-4.17932	-1.90830	-0.00004
H	-5.06374	-2.53916	-0.00009
C	-4.27389	-0.53283	-0.00007
H	-5.24211	-0.03619	-0.00024
C	-3.09874	0.25129	-0.00003
C	-3.14187	1.68176	0.00000
H	-4.11062	2.17592	0.00000
C	-1.98387	2.40380	0.00001
H	-2.01379	3.49189	0.00004
C	-0.70782	1.76413	0.00002
C	0.50746	2.49515	0.00002
H	0.47307	3.58324	-0.00001
C	1.70212	1.82814	0.00003
H	2.65842	2.33782	0.00005
C	1.70982	0.39611	0.00004
C	-0.60298	0.34129	0.00001
C	-1.84309	-0.43507	0.00003
C	2.99929	-0.27476	0.00001

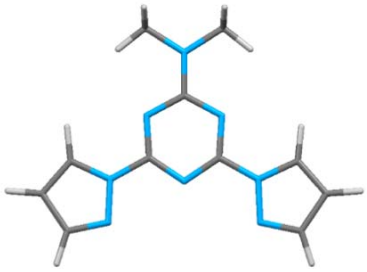
IZAFOG/IZAFOG01: $\Delta E_{L(relax)}$ = -740.47864374 E_h

O	3.54960	0.51332	0.00047
O	-3.54960	0.51332	-0.00005
N	2.50903	-1.51311	0.00012
N	0.00000	-0.14654	0.00009
N	-2.50904	-1.51310	-0.00009
C	3.94657	-1.81113	0.00101
H	4.19904	-2.41302	-0.87912
H	4.19833	-2.40920	0.88401
C	4.64934	-0.42759	-0.00171
H	5.25998	-0.24258	0.88688
H	5.25511	-0.24409	-0.89402
C	2.40275	-0.24465	0.00018
C	1.14557	0.54320	0.00017
C	1.19933	1.94586	0.00019
H	2.15715	2.45074	0.00024
C	0.00001	2.65120	0.00017
H	0.00001	3.73696	0.00017
C	-1.19931	1.94586	0.00010
H	-2.15714	2.45075	0.00009
C	-1.14556	0.54320	0.00005
C	-2.40275	-0.24465	-0.00004
C	-4.64935	-0.42759	-0.00025
H	-5.25737	-0.24336	-0.89084
H	-5.25771	-0.24333	0.89010
C	-3.94657	-1.81113	-0.00012
H	-4.19871	-2.41102	0.88151
H	-4.19868	-2.41117	-0.88165



EKAJUX: $\Delta E_{L(relax)}$ = –832.281429214 E_h

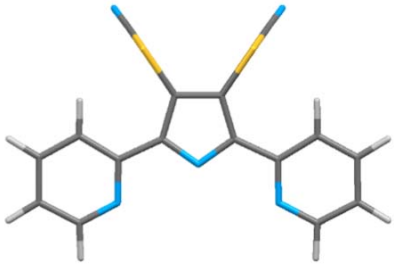
N	-0.00003	-0.92542	-0.00039
C	-1.13119	-0.22851	-0.00069
C	-1.20548	1.16442	-0.00130
H	-2.15687	1.67210	-0.00138
C	0.00002	1.89800	-0.00195
C	1.20550	1.16437	-0.00121
H	2.15690	1.67205	-0.00099
C	1.13117	-0.22855	-0.00067
N	-2.33024	-0.99552	-0.00016
N	-2.28238	-2.35535	0.00060
C	-3.55021	-2.73776	0.00089
H	-3.78447	-3.79403	0.00152
C	-4.44381	-1.63696	0.00030
H	-5.52352	-1.64708	0.00028
C	-3.62470	-0.53504	-0.00043
H	-3.86673	0.51497	-0.00093
N	2.33018	-0.99560	-0.00010
N	2.28226	-2.35544	0.00068
C	3.55007	-2.73789	0.00088
H	3.78430	-3.79417	0.00146
C	4.44373	-1.63713	0.00026
H	5.52344	-1.64732	0.00015
C	3.62467	-0.53518	-0.00034
H	3.86672	0.51482	-0.00088
N	0.00009	3.27309	-0.00339
C	-1.25728	4.00303	0.00231
H	-1.86513	3.77567	-0.88339
H	-1.05020	5.07319	-0.00077
H	-1.85666	3.77861	0.89468
C	1.25754	4.00287	0.00201
H	1.85686	3.77887	0.89453
H	1.05059	5.07306	-0.00175
H	1.86539	3.77494	-0.88353



FEDRUE: $\Delta E_{L(relax)}$ = –864.400166097 E_h

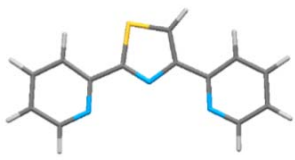
N	0.00002	-1.00950	-0.00000
C	1.10660	-0.26828	0.00001
N	1.19246	1.05983	0.00004
C	-0.00001	1.69574	0.00007
N	-1.19248	1.05981	0.00006
C	-1.10659	-0.26830	0.00004
N	2.33496	-0.94822	-0.00001
N	2.39772	-2.31167	-0.00005
C	3.69213	-2.57712	-0.00002
H	4.02107	-3.60800	-0.00004
C	4.48956	-1.39769	0.00003
H	5.56640	-1.31991	0.00001
C	3.58465	-0.36987	0.00003
H	3.69592	0.70110	0.00011
N	-2.33493	-0.94826	-0.00001
N	-2.39767	-2.31171	-0.00010
C	-3.69207	-2.57718	-0.00004
H	-4.02100	-3.60807	-0.00003
C	-4.48952	-1.39776	0.00011
H	-5.56636	-1.32001	0.00021
C	-3.58463	-0.36993	-0.00003
H	-3.69590	0.70104	-0.00002
N	-0.00004	3.05406	0.00010
C	1.23160	3.82785	-0.00005
H	1.27451	4.46995	0.88850
H	1.27416	4.47012	-0.88848
H	2.08549	3.15605	-0.00027
C	-1.23172	3.82779	-0.00009
H	-2.08557	3.15594	0.00004
H	-1.27448	4.46976	-0.88872

H	-1.27451	4.47014	0.88826



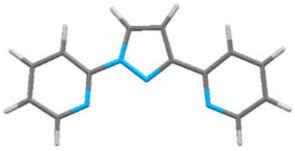
UCIGUJ: $\Delta E_{L(relax)}$ = –1684.66554780 E_h

S	1.67885	2.21762	-0.88976
S	-1.67903	2.21755	-0.88937
N	2.45874	-2.49098	0.21028
N	-0.00007	-1.31180	-0.00633
N	-2.45899	-2.49079	0.21017
N	2.57233	3.45567	1.55360
N	-2.57115	3.45597	1.55431
C	3.63521	-3.10242	0.32728
H	3.59109	-4.17315	0.53434
C	4.87289	-2.46856	0.20552
H	5.79967	-3.02457	0.31395
C	4.85914	-1.09871	-0.05360
H	5.78764	-0.54169	-0.15420
C	3.64194	-0.43996	-0.17767
H	3.62487	0.62240	-0.37494
C	2.43565	-1.16241	-0.04613
C	1.10028	-0.54136	-0.16004
C	0.71101	0.80096	-0.42677
C	-0.71096	0.80104	-0.42674
C	-1.10037	-0.54124	-0.16011
C	-2.43580	-1.16223	-0.04626
C	-3.64204	-0.43970	-0.17773
H	-3.62490	0.62268	-0.37494
C	-4.85928	-1.09834	-0.05368
H	-5.78775	-0.54124	-0.15425
C	-4.87315	-2.46821	0.20543
H	-5.79998	-3.02415	0.31385
C	-3.63551	-3.10215	0.32716
H	-3.59147	-4.17288	0.53421
C	2.16867	2.92352	0.59587
C	-2.16806	2.92369	0.59642



PUBCAQ: $\Delta E_{L(relax)}$ = –1063.246660590 E_h

N	-2.58823	-1.36279	-0.00024
N	2.47550	-1.47529	-0.00012
C	-3.79365	-1.93638	0.00002
C	-4.99544	-1.22775	0.00032
C	-4.92835	0.16502	0.00027
C	-3.68098	0.77852	0.00001
C	-2.52418	-0.02082	-0.00017
C	-1.16953	0.58355	-0.00023
C	-0.89605	1.93343	0.00009
C	1.05030	0.45369	-0.00030
H	-3.79900	-3.02527	-0.00005
H	-5.94635	-1.75046	0.00042
H	-5.83327	0.76570	0.00039
H	-3.61017	1.86081	-0.00022
H	-1.58314	2.76645	0.00098
N	-0.05614	-0.22539	-0.00035
S	0.80281	2.21570	-0.00001
C	4.88157	-1.32047	0.00025
C	4.80784	0.07074	0.00025
C	3.55552	0.67704	0.00006
C	2.40819	-0.13295	-0.00018
C	3.68353	-2.03939	0.00006
H	3.47465	1.75947	0.00008
H	5.70893	0.67666	0.00041
H	5.83538	-1.83772	0.00038
H	3.69747	-3.12799	0.00008



ZAJGOG: $\Delta E_{L(relax)}$ = –720.396353421 E_h

N	0.00753	-0.19577	0.00003
N	-2.57289	-1.25629	0.00009
C	-2.42538	0.08103	0.00003
N	1.08592	0.62329	-0.00003
C	-0.64558	1.98520	0.00012
C	0.72276	1.94953	0.00016
C	-1.04903	0.61566	0.00000
H	1.44325	2.75096	0.00013
C	2.40278	0.08765	-0.00004
N	2.50179	-1.23862	0.00000
C	3.72696	-1.77135	0.00001
C	4.90135	-1.02099	0.00004
C	4.78036	0.36869	-0.00008
C	3.51516	0.94458	-0.00015
H	3.40873	2.02207	-0.00028
H	5.66138	1.00334	-0.00012
H	5.87078	-1.50720	0.00018
H	3.76597	-2.85890	0.00008
H	-1.26118	2.87167	0.00027
C	-3.52826	0.95163	-0.00004

C	-4.81330	0.41811	-0.00011
C	-4.96737	-0.96661	-0.00009
C	-3.81148	-1.75064	0.00007
H	-3.88755	-2.83707	0.00009
H	-5.94910	-1.42907	-0.00023
H	-5.67881	1.07446	-0.00021
H	-3.38363	2.02645	-0.00004