Electronic Supplementary Information

For

Bi-Blatter diradicals: Conformation and substituent dependent high-spin materials

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1. NMR spectra

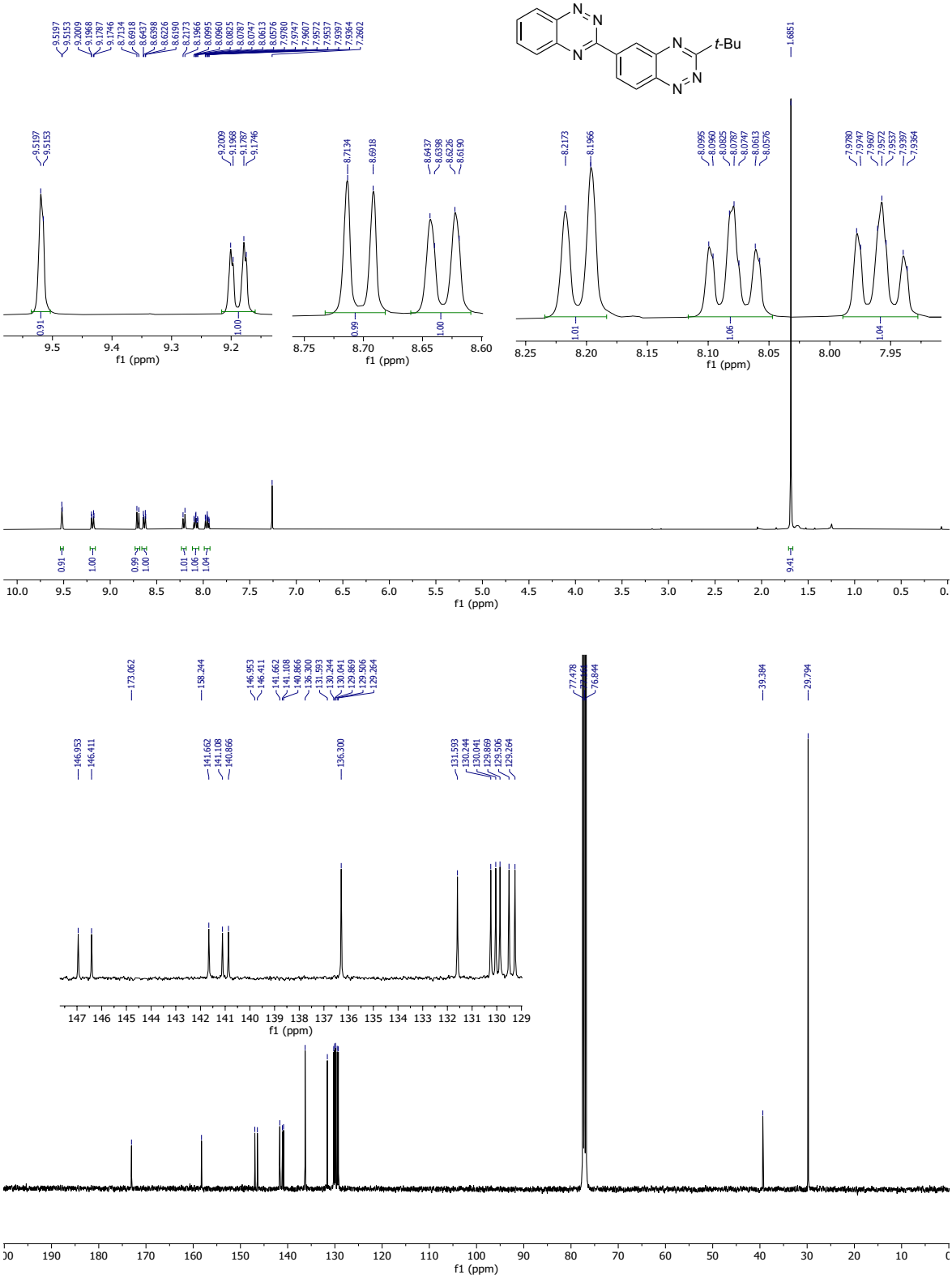


Figure S1. ^{1}H NMR (400 MHz) and $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3[3,6]** ($CDCl_3$).

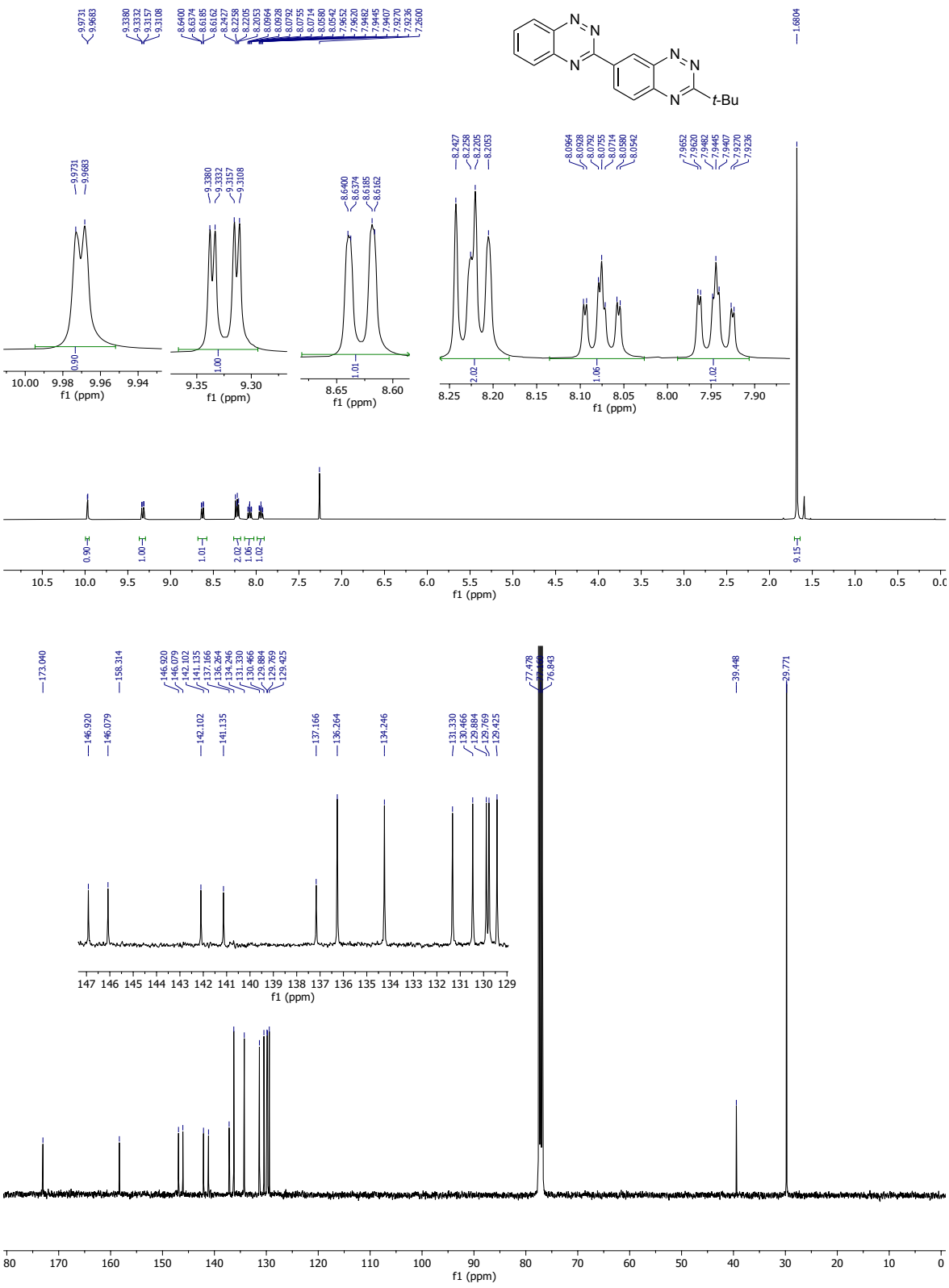
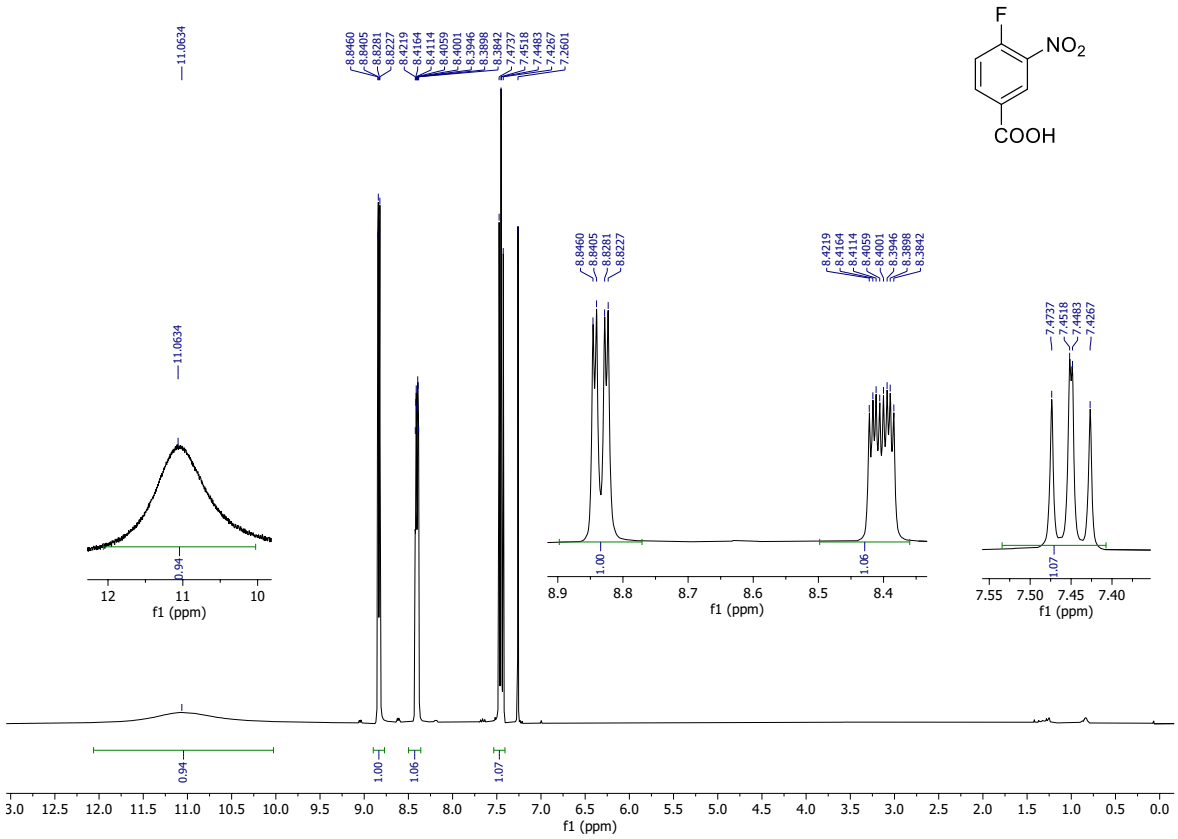


Figure S2. ^{1}H NMR (400 MHz) and $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3[3,7]** ($CDCl_3$).


F
NO2
COOH
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8.8405
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8.4219
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8.4059
8.4001
8.3946
8.3898
8.3842
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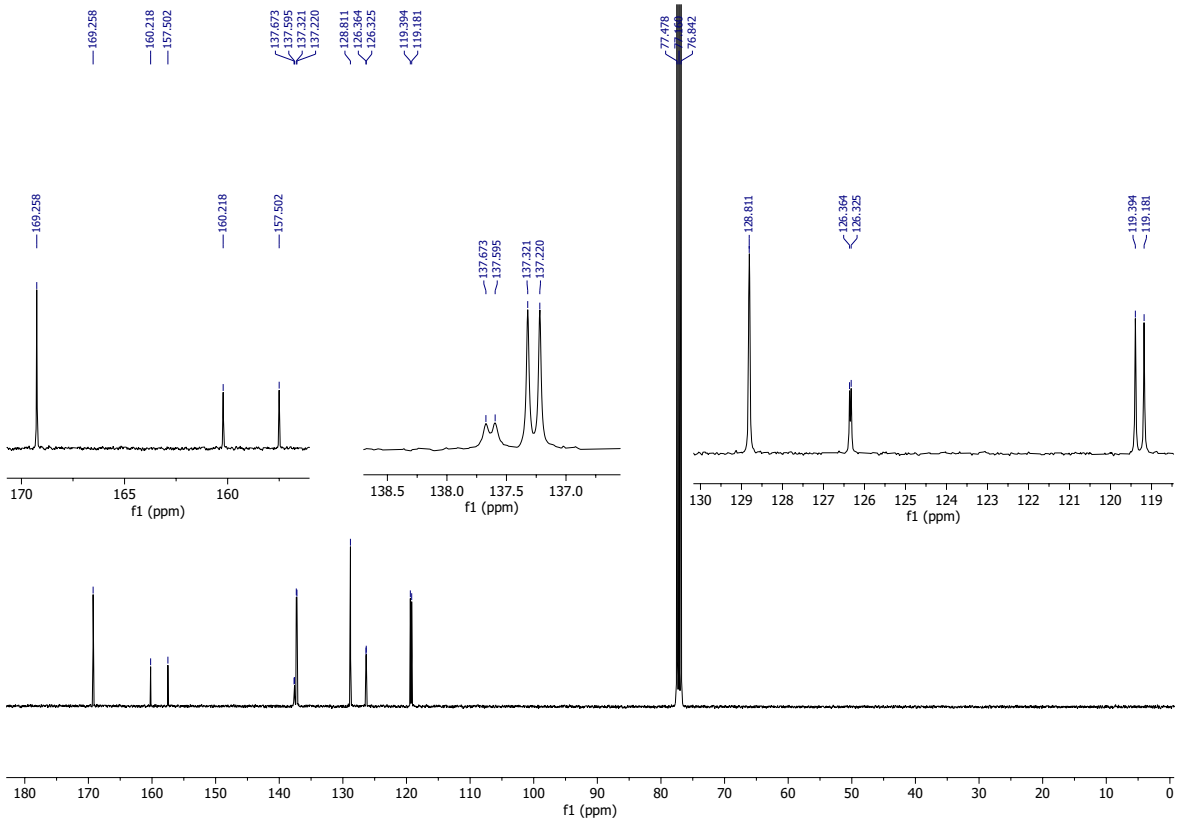
7.4518
7.4483
7.4267
7.2601
0.94
1.00
1.06
1.07
f1 (ppm)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157.502
137.673
137.595
137.321
137.220
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126.364
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77.478
76.842
f1 (ppm)

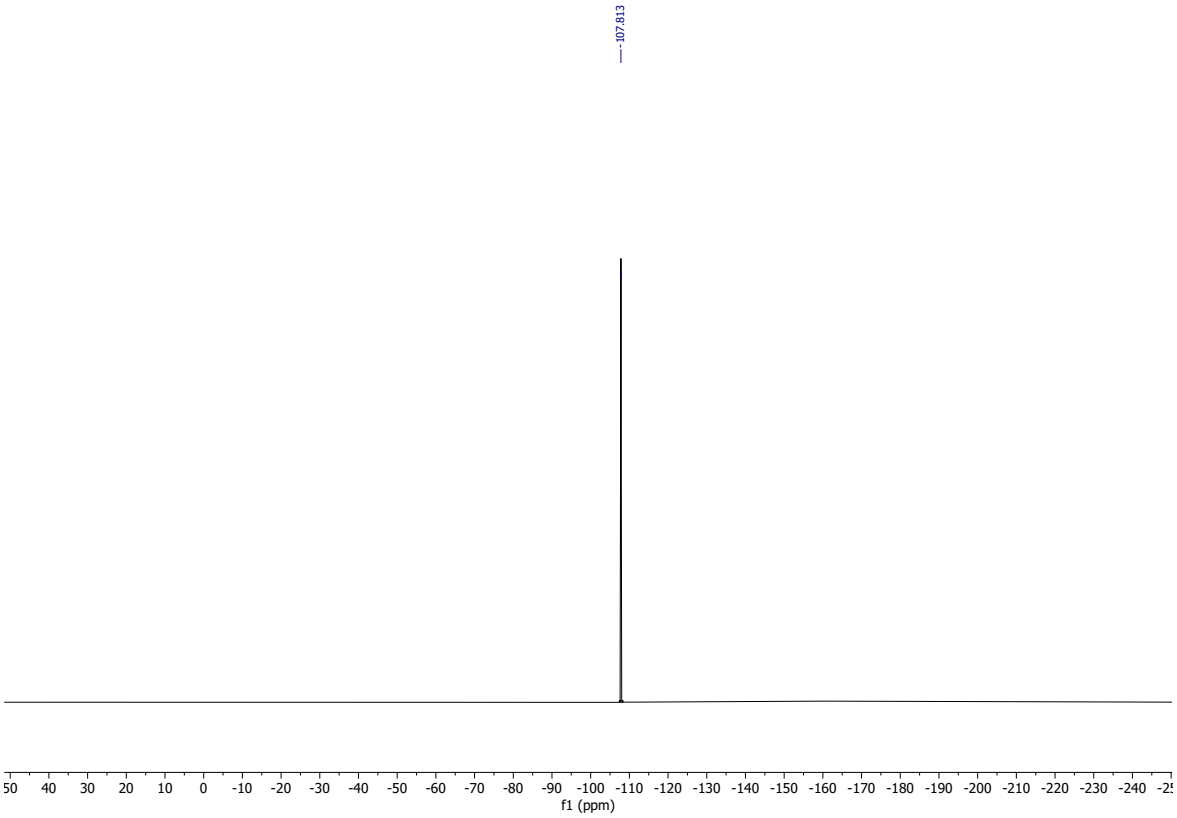


Figure S3. ^{1}H NMR (400 MHz), $^{13}C\{^{1}H\}$ NMR (100 MHz) AND ^{19}F NMR (377 MHz) spectra of **4[6]** ($CDCl_3$).

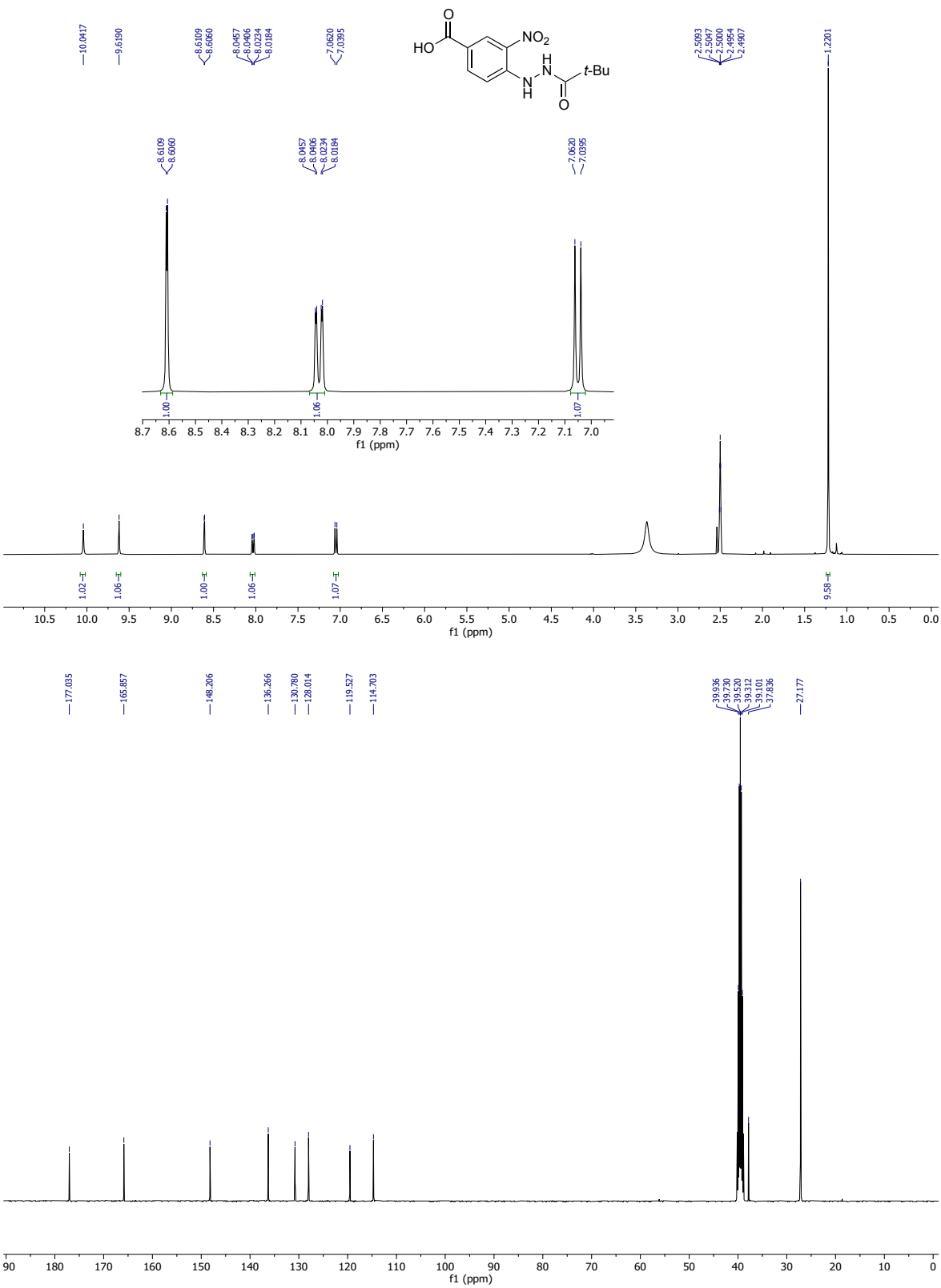


Figure S4. ^{1}H NMR (400 MHz) and $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **5[6]** (DMSO-d_6).

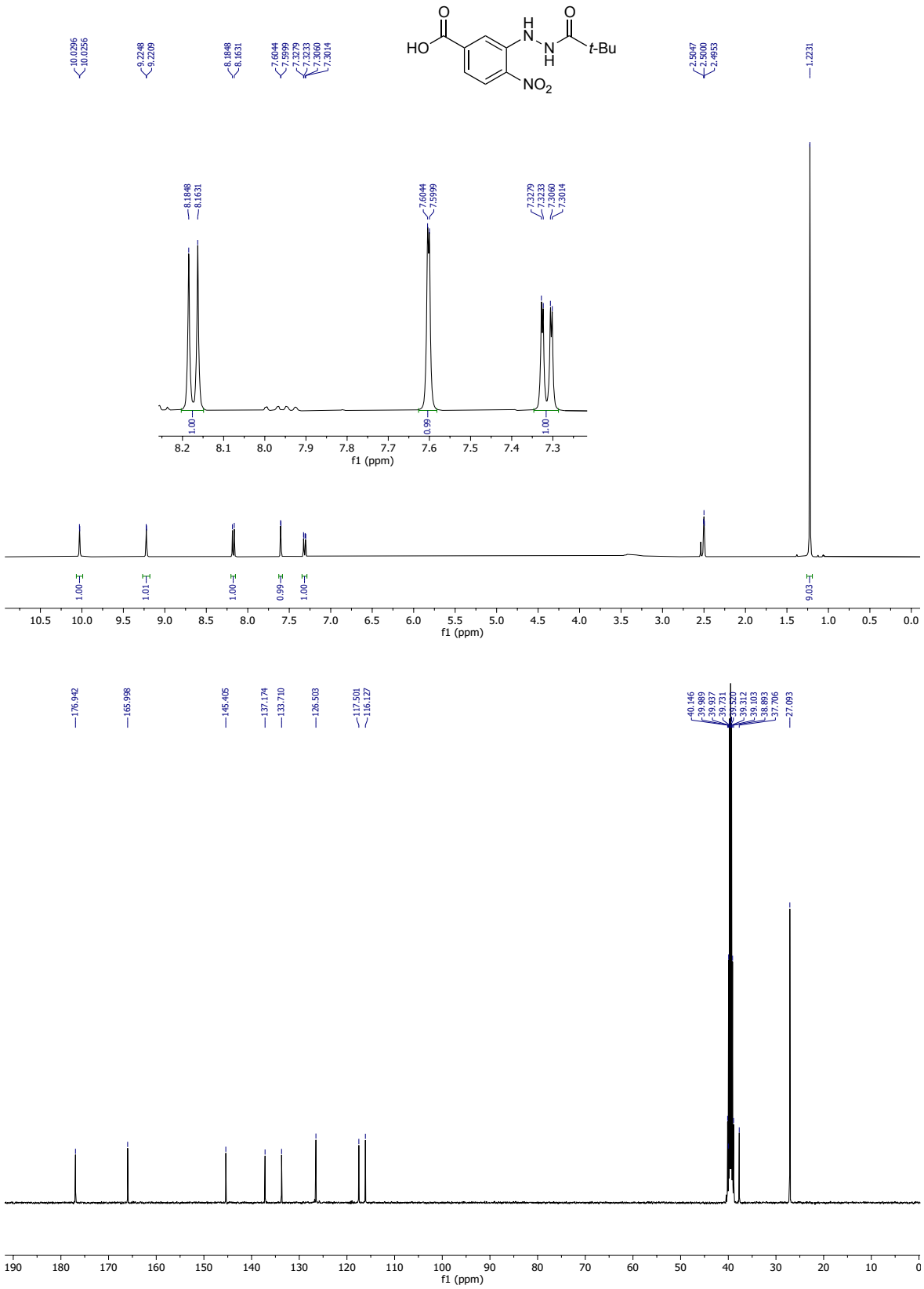


Figure S5. ^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **5[7]** (DMSO-d_6).

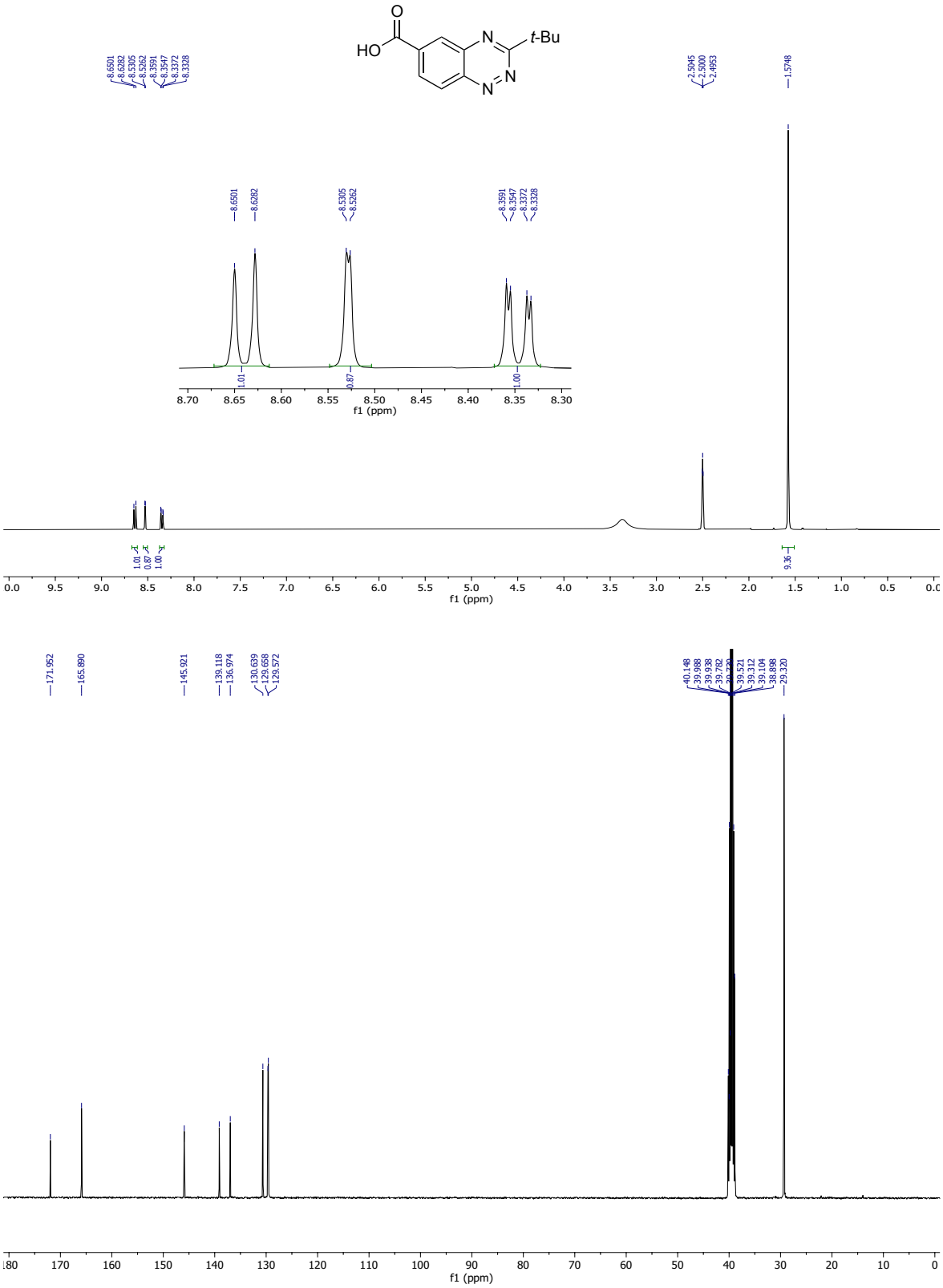


Figure S6. ^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **6[6]** (DMSO-d_6).

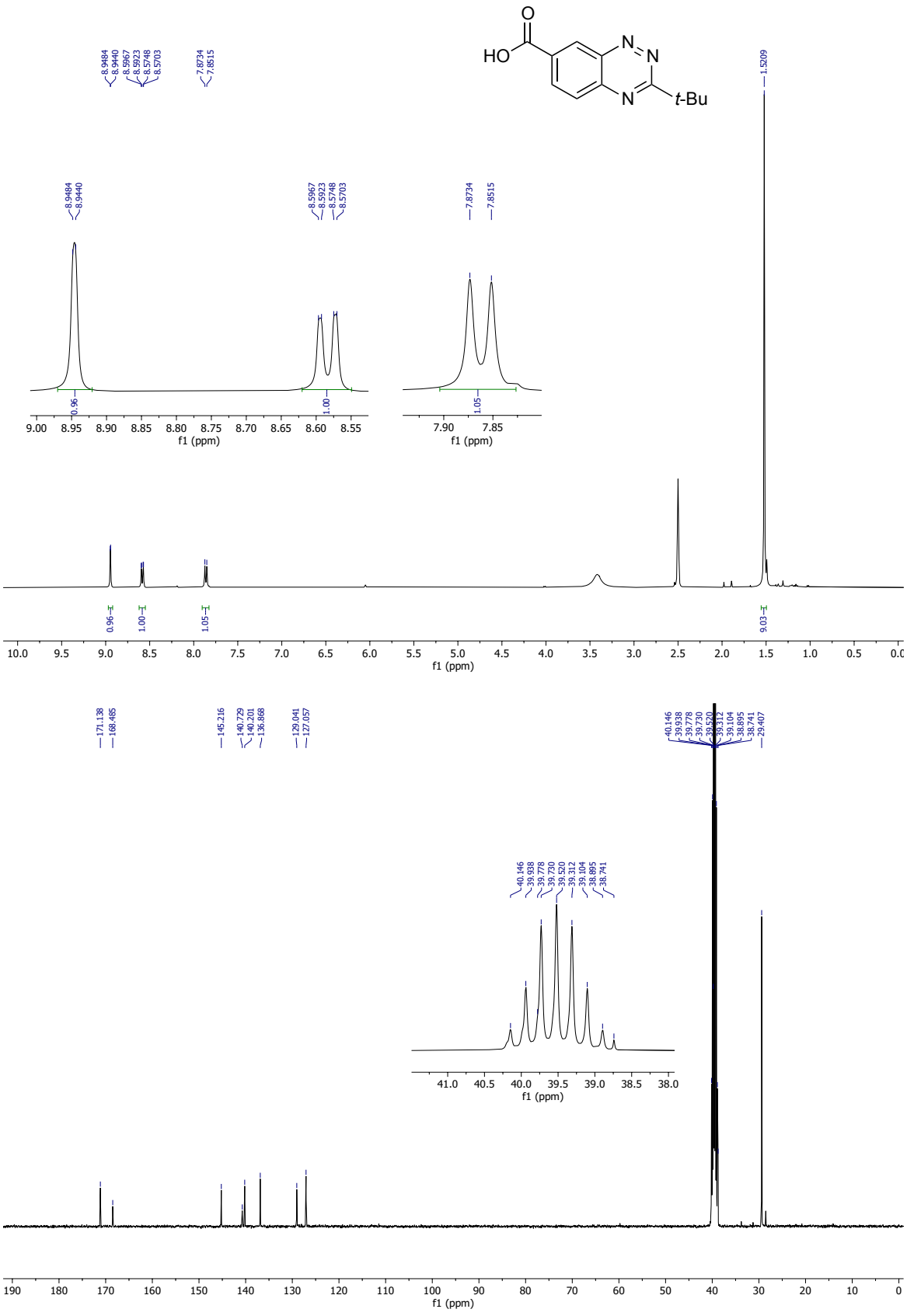


Figure S7. ^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **6[7]** (DMSO-d_6).

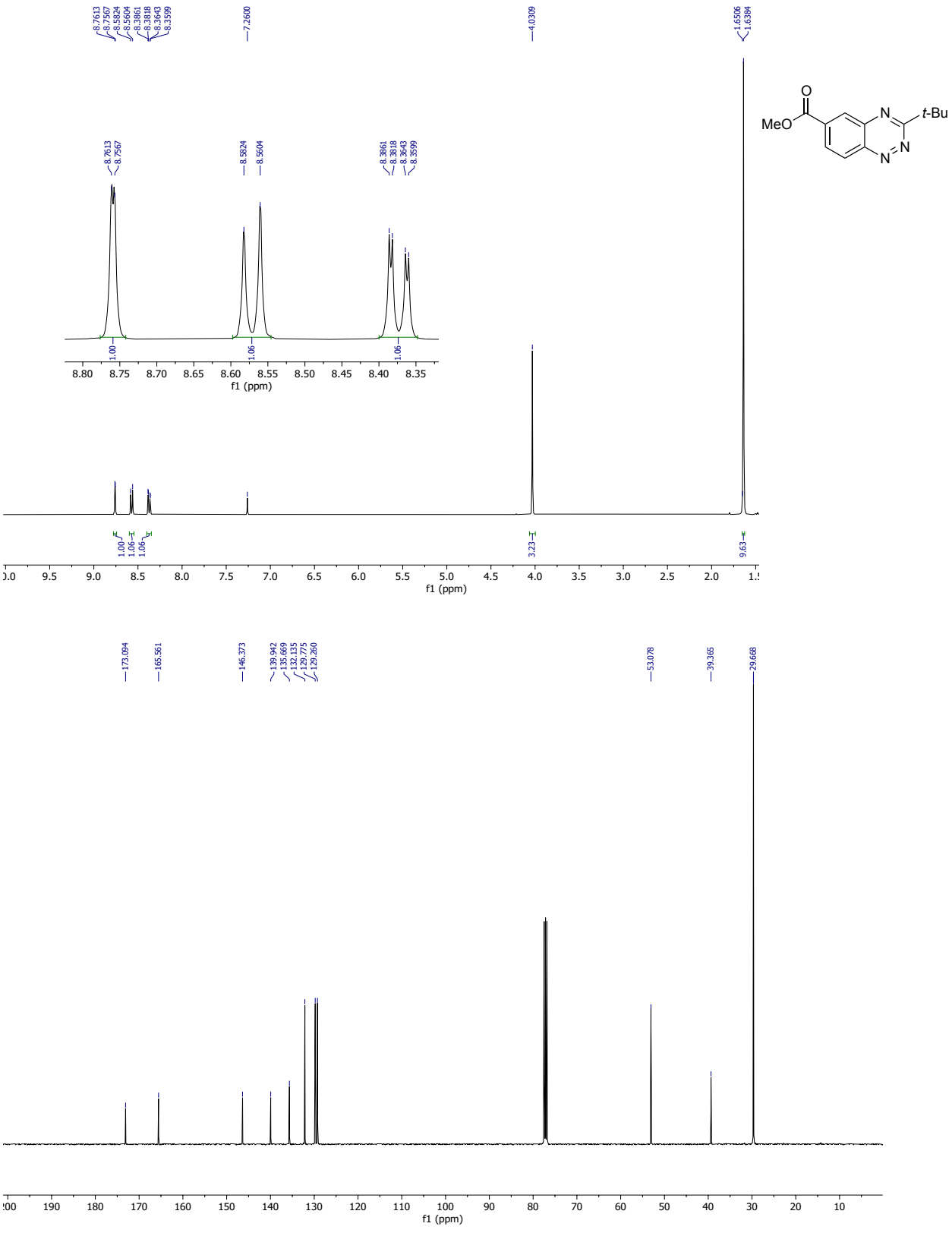


Figure S8. ^{1}H NMR (400 MHz) and $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **7[6]** ($CDCl_3$).

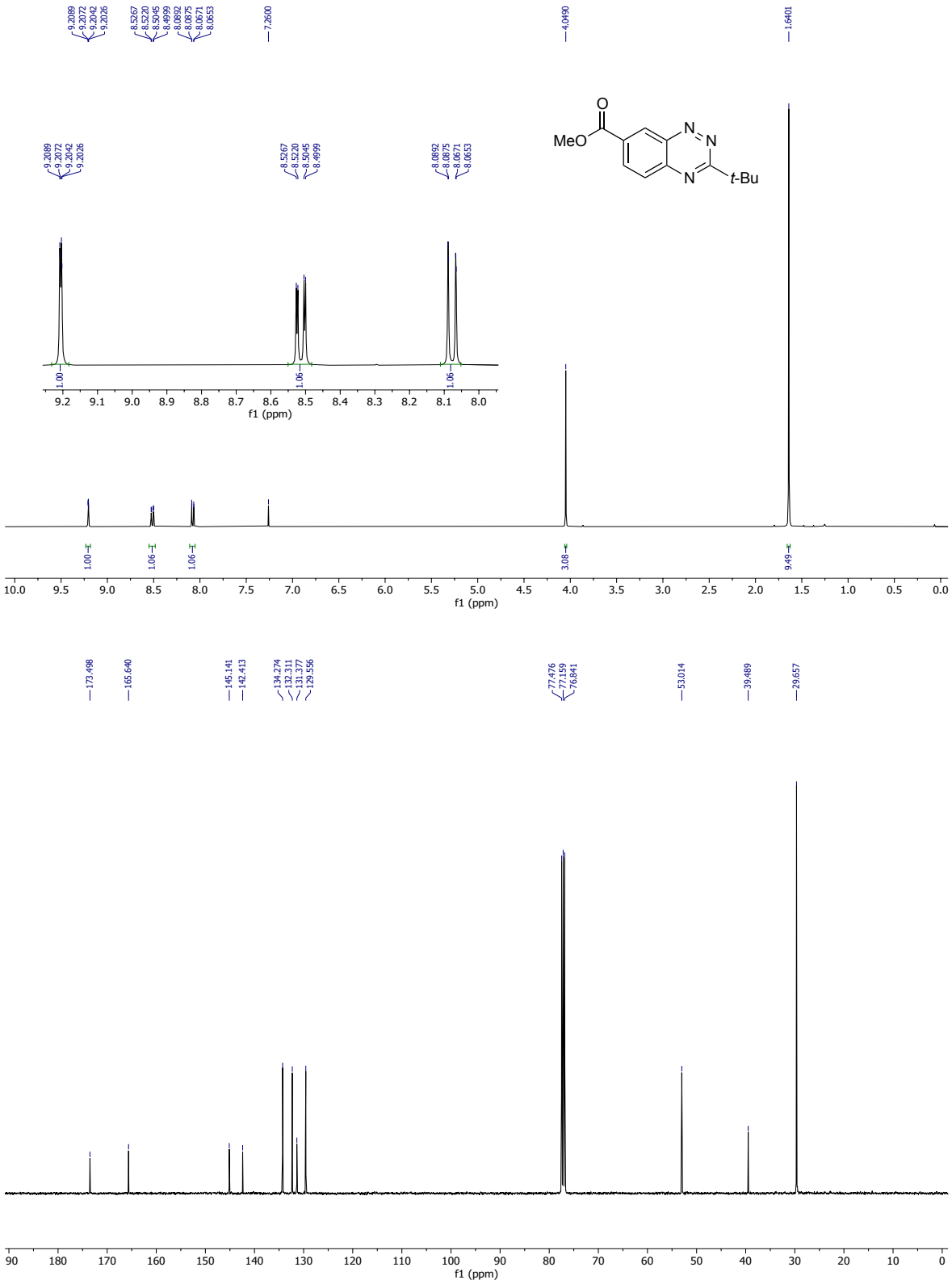


Figure S9. ^{1}H NMR (400 MHz) and $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **7[7]** ($CDCl_3$).

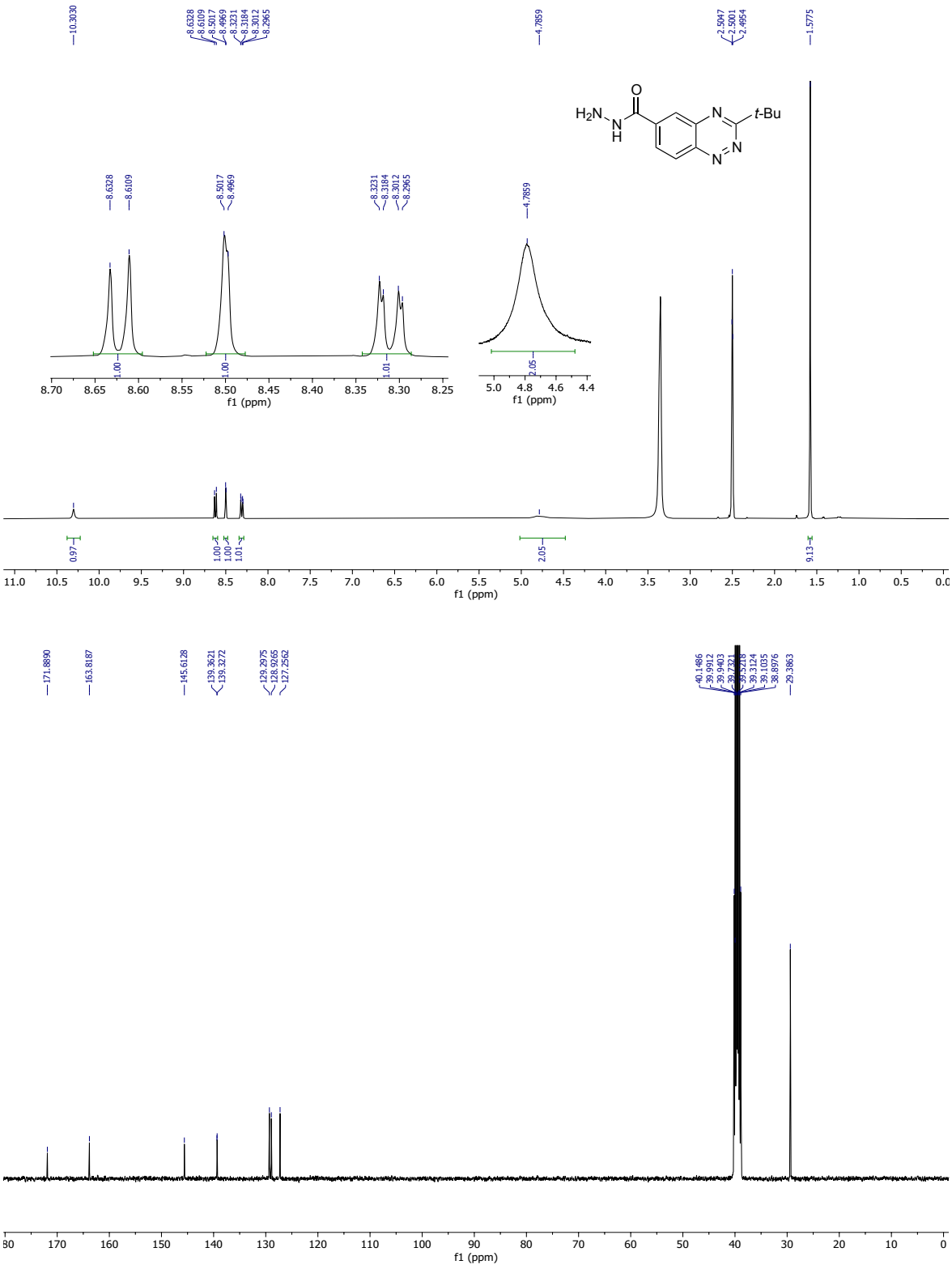


Figure S10. ^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **8[6]** (DMSO-d_6).

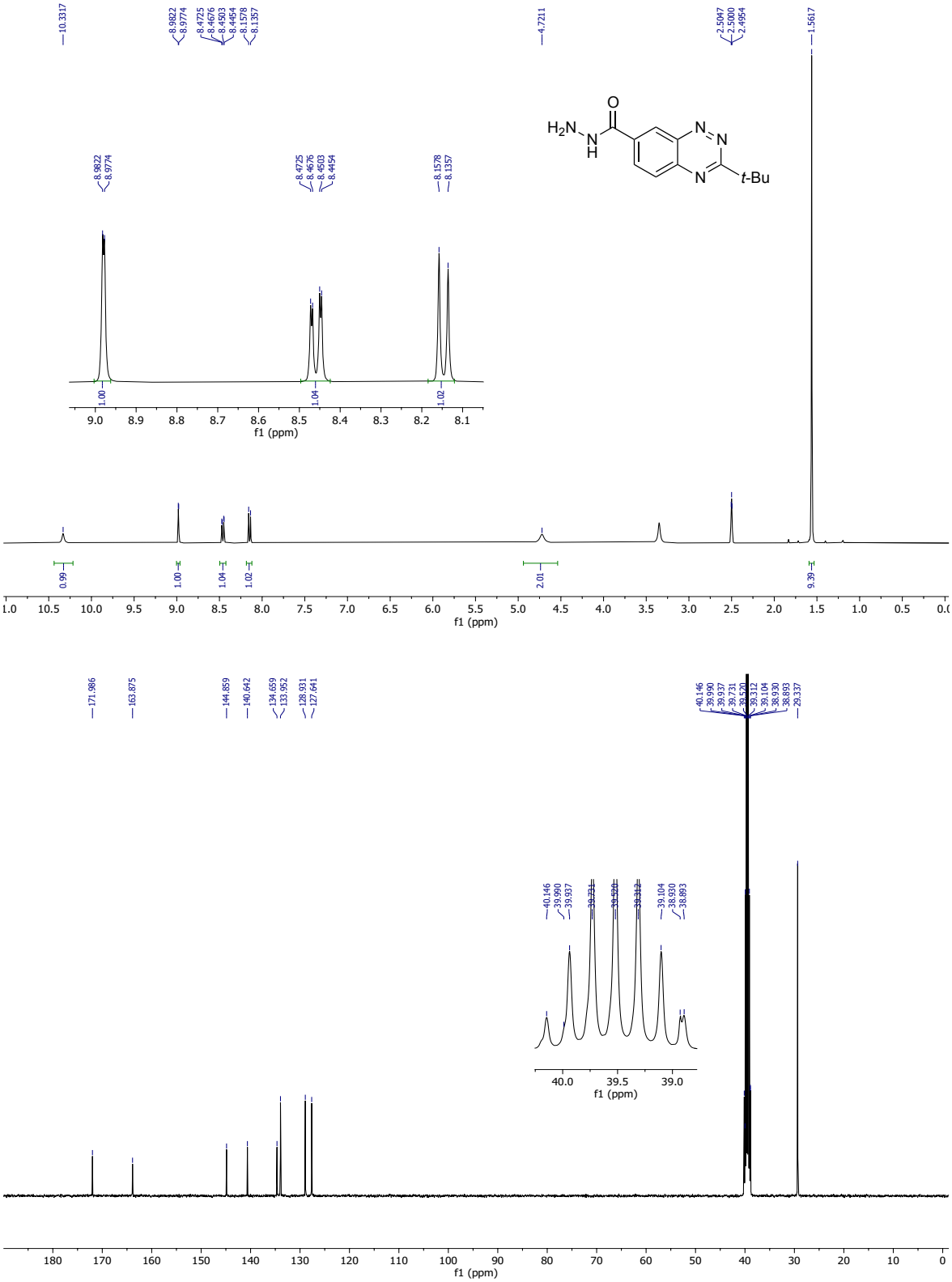


Figure S11. ^{1}H NMR (400 MHz) and ^{13}C{^{1}H} NMR (100 MHz) spectra of **8[7]** (DMSO-d_6).

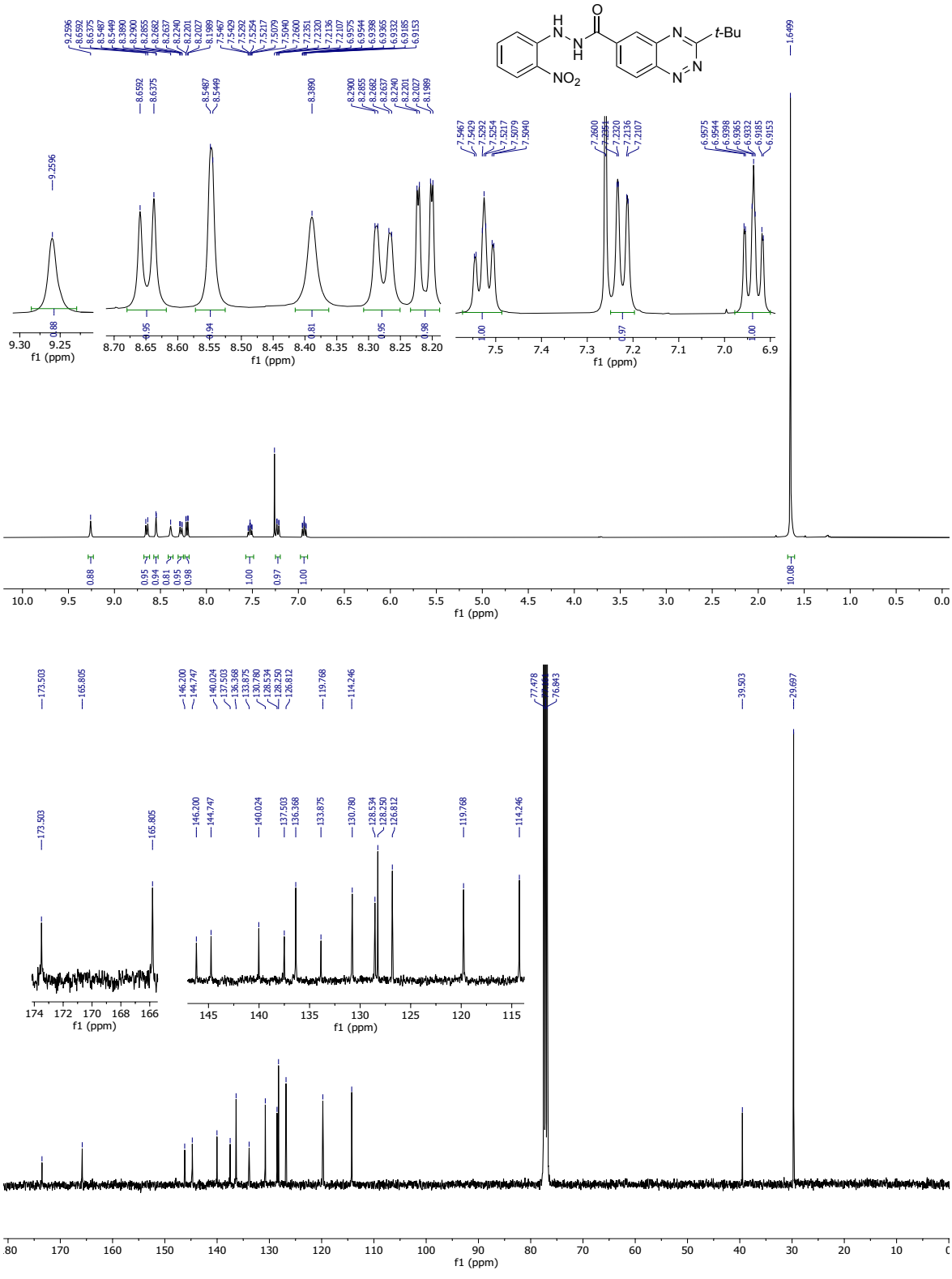


Figure S12. ^{1}H NMR (400 MHz) and $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **9[6]** ($CDCl_3$).

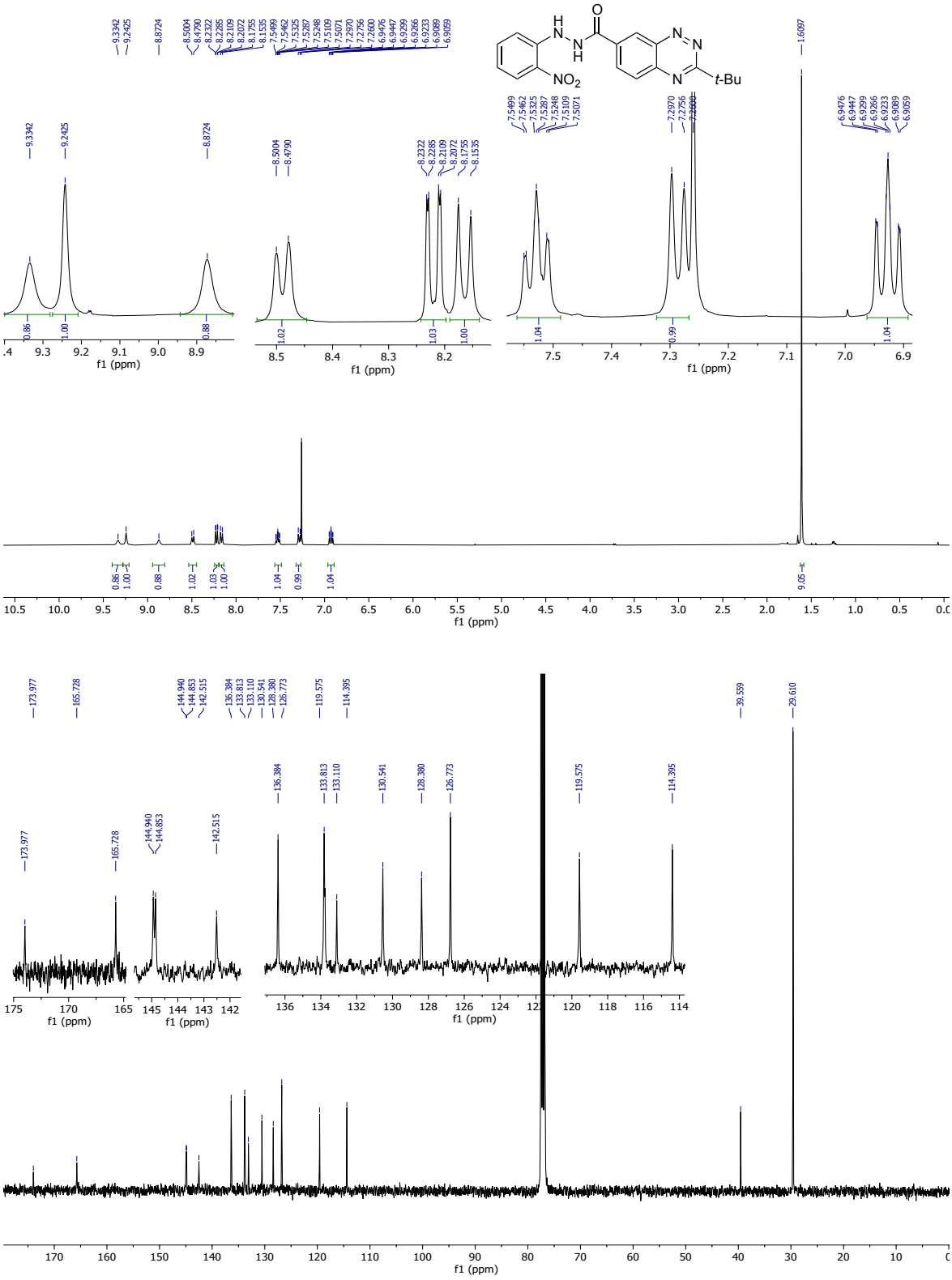


Figure S13. ^{1}H NMR (400 MHz) and $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **9[7]** ($CDCl_3$).

2. IR spectra

IR spectra of diradicals **1[3,n]** were obtained for polycrystalline samples using ATR-FTIR setup Nicolet 6700 and results are shown in Figures S14 and S15.

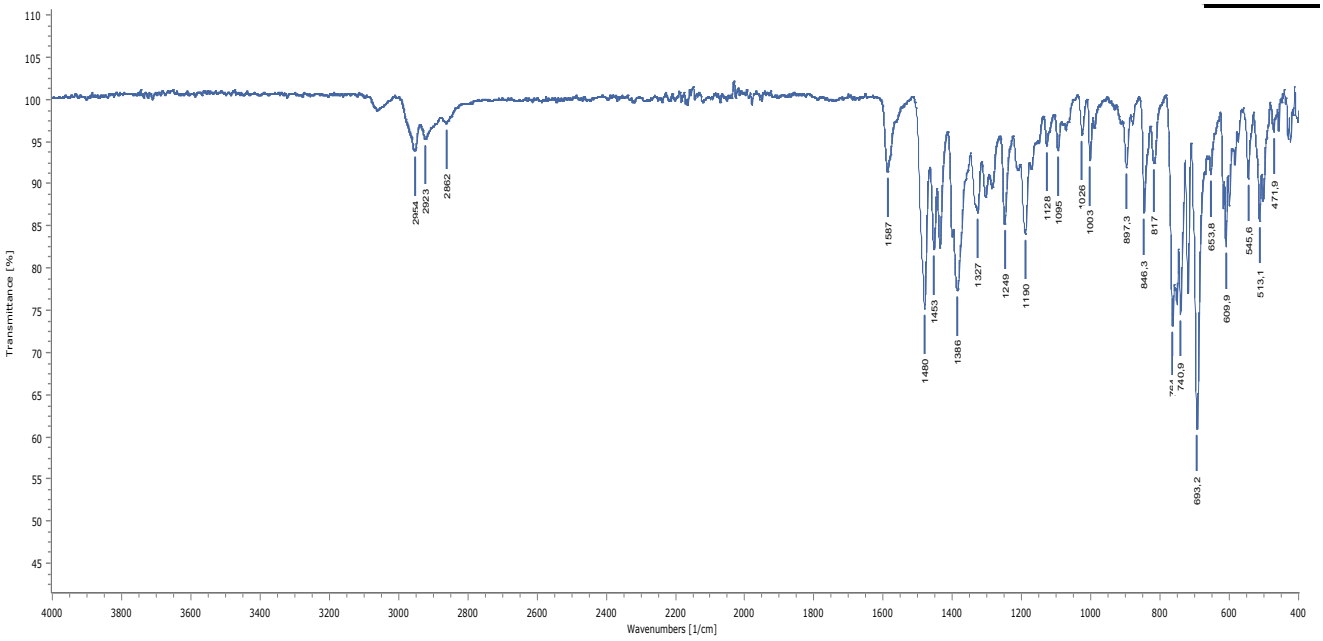


Figure S14. ATR-IR spectra for **1[3,6]**.

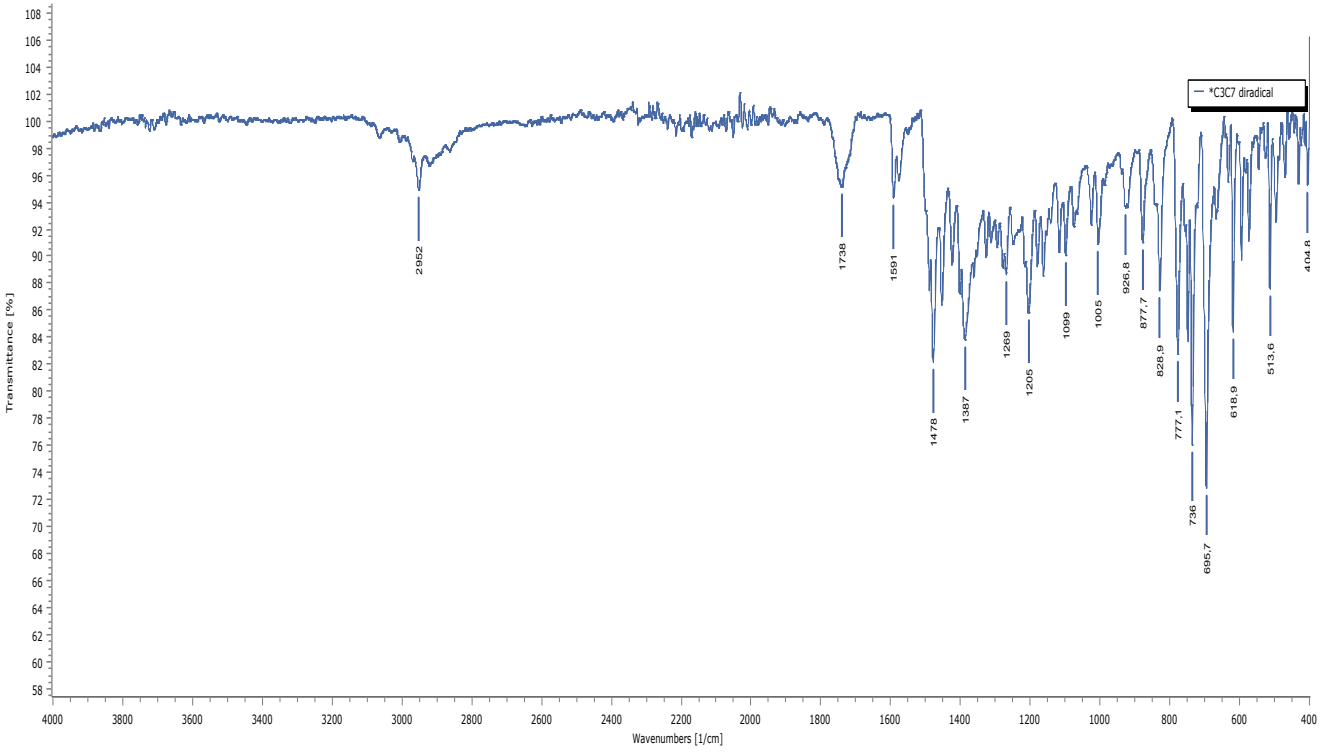


Figure S15. ATR-IR spectra for **1[3,7]**.

3. XRD data collection and refinement

Data Collection

Crystals of diradicals **1[3,6]** and **1[3,7]** were grown by slow evaporation of CH_2Cl_2/MeCN solutions at ambient temperature.

Single-crystal X-ray diffraction measurements for **1[3,6]** and **1[3,7]** were performed with XtaLAB Synergy, Pilatus 300 K diffractometer. All measurements were conducted at 100.0(1) K using Cu$K\alpha$ radiation (λ = 1.54184 Å). The data were integrated using CrysAlisPro program. Intensities for absorption were corrected using SCALE3 ABSPACK scaling algorithm implemented in CrysAlisPro program.[7]

Structure solution and refinement

Both structures **1[3,6]** and **1[3,7]** were solved with the ShelXT structure solution program[8] using Intrinsic Phasing and refined by the full-matrix least-squares minimization on F^2 with the ShelXL refinement package.[9] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were generated geometrically and refined isotropically using the riding model. Asymmetric unit of **1[3,6]** contains three water molecules and two of them are disordered over two positions each. Occupancy factors for two sites of water molecules defined by O1 and O2 atoms are 0.553(5):0.447(5) and 0.537(5):0.463(5), respectively. The oxygen atom O2b of one disordered water molecule was refined isotropically. Crystals of **1[3,7]** are twinned. The measured one was refined as a merohedral twin with scales 0.907(2):0.093(2). The twin law was applied by the instruction TWIN 1 0 0 0 -1 0 1 0 1.

The crystal data and structure refinement descriptors for **1[3,6]** and **1[3,7]** are presented in Table S1. Their molecular structures are shown in Figures S16 and S17 unit cell packing diagrams in Figures S18 and S19, and partial packing in Figures S20 and S21. Table S2 contains a list of close nonbonding intermolecular distances in both crystal structures.

CCDC 232867 and 232868 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures"

Table S1. Crystal data and refinement details for diradicals **1[3,n]**.

Compound	**1[3,6]**	**1[3,7]**
CCDC	2328268	2328267
Empirical formula	$C_{60}H_{58}N_{12}O_3$	$C_{30}H_{26}N_6$
Formula weight	995.18	470.57
Crystal system	Triclinic	Monoclinic
Space group	$P\bar{1}$	$P21/c$
a/Å	6.72380(10)	10.4665(12)
b/Å	17.1497(4)	6.8859(6)
c/Å	22.8862(5)	32.972(3)
α/°	100.979(2)	90
β/°	95.399(3)	98.817(11)
γ/°	92.002(4)	90
Volume/Å^3	2575.46(9)	2348.2(4)
Z	2	4
Goodness-of-fit	1.039	1.071
R_{int}	0.0666	0.1086
Final R indexes [I>=2δ (I)]	R_1=0.0582, wR_2=0.1555	R_1=0.1039, wR_2=0.2937
Final R indexes [all data]	R_1=0.0733, wR_2= 0.1655	R_1=0.1574, wR_2=0.3399
Largest diff. peak/hole /eÅ^{-3}	0.54/0.32	0.38/-0.39

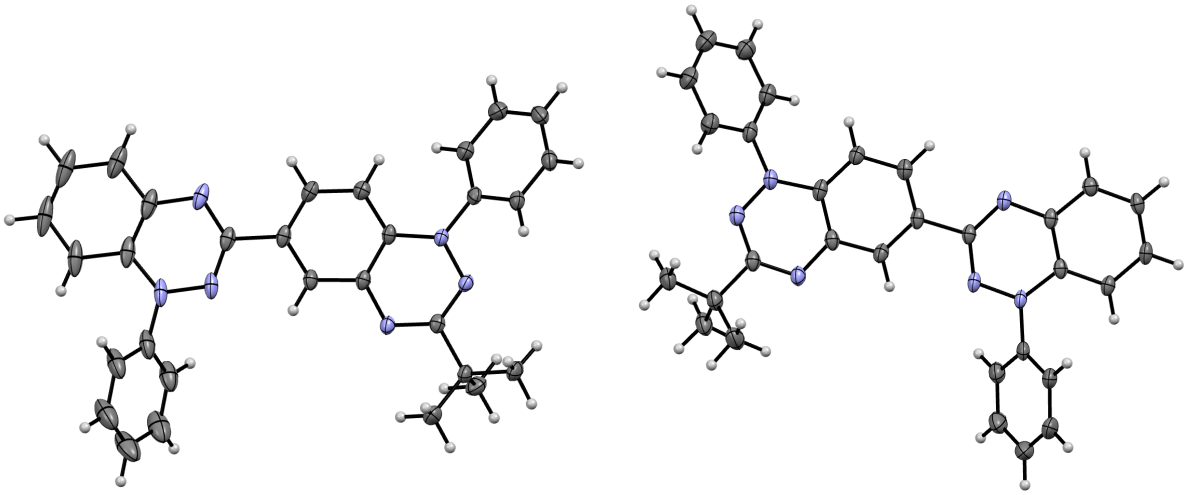


Figure S16. Atomic displacement ellipsoid diagram for two unique molecules of diradical **1[3,6]**. Ellipsoids are drawn at 50% probability level. Color code: carbon, dark gray; blue, nitrogen.

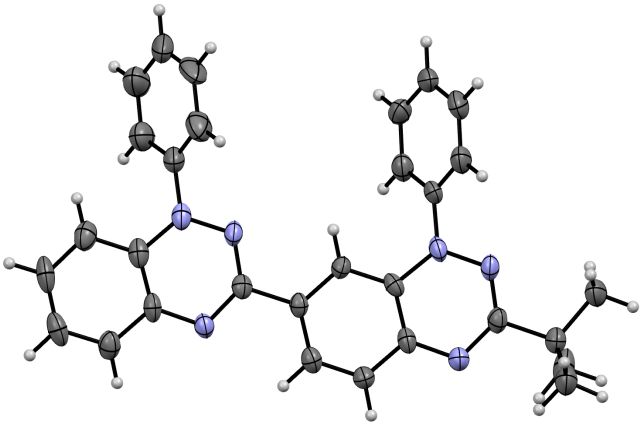


Figure S17. Atomic displacement ellipsoid diagram for diradical **1[3,7]**. Ellipsoids are drawn at 50% probability level. Color code: carbon, dark gray; blue, nitrogen.

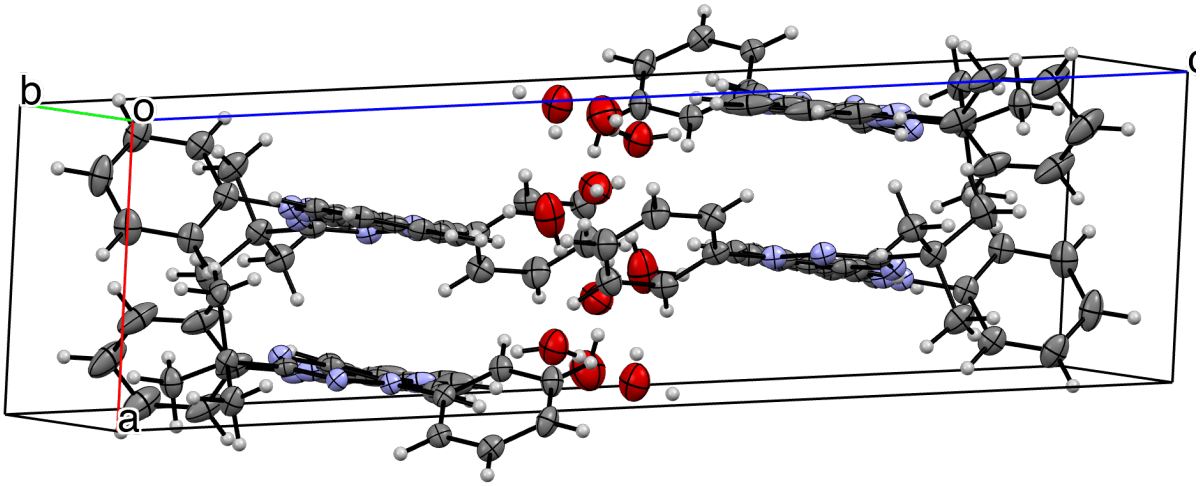


Figure S18. Unit cell packing diagram for **1[3,6]**. Ellipsoids are drawn at 50% probability level. The diagram contains disordered sites of water molecules. Color code: carbon, dark gray; blue, nitrogen; red, oxygen.

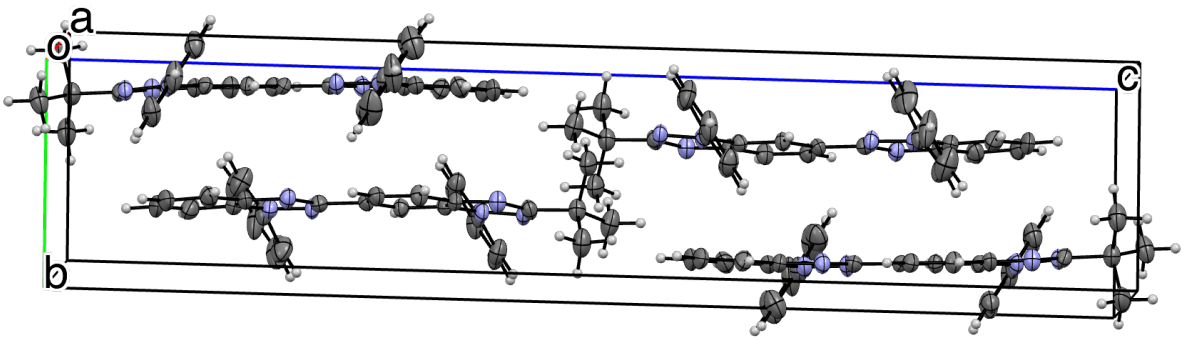


Figure S19. Unit cell packing diagram for **1[3,7]**. Ellipsoids are drawn at 50% probability level. Color code: carbon, dark gray; blue, nitrogen.

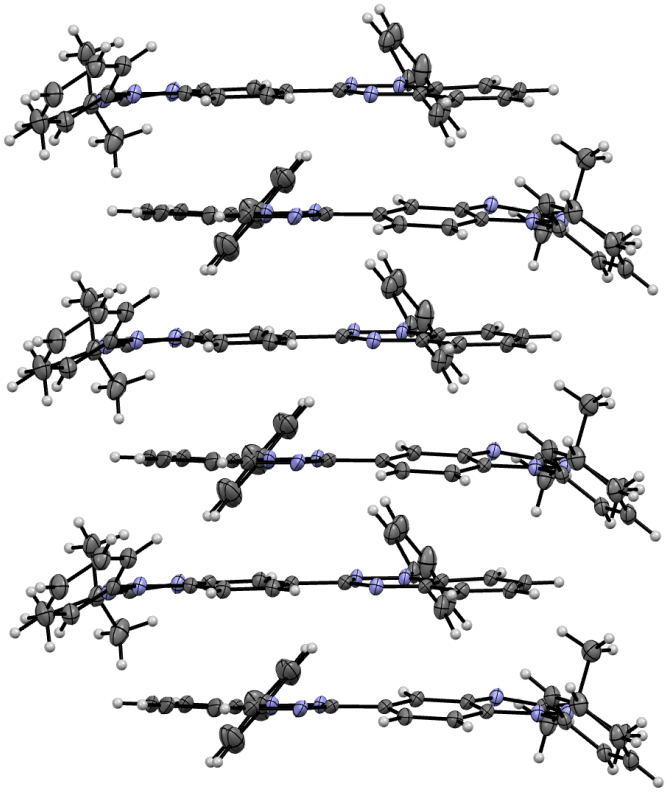


Figure S20. Partial packing diagram for **1[3,6]**. Ellipsoids are drawn at 50% probability level. Color code: carbon, dark gray; blue, nitrogen.

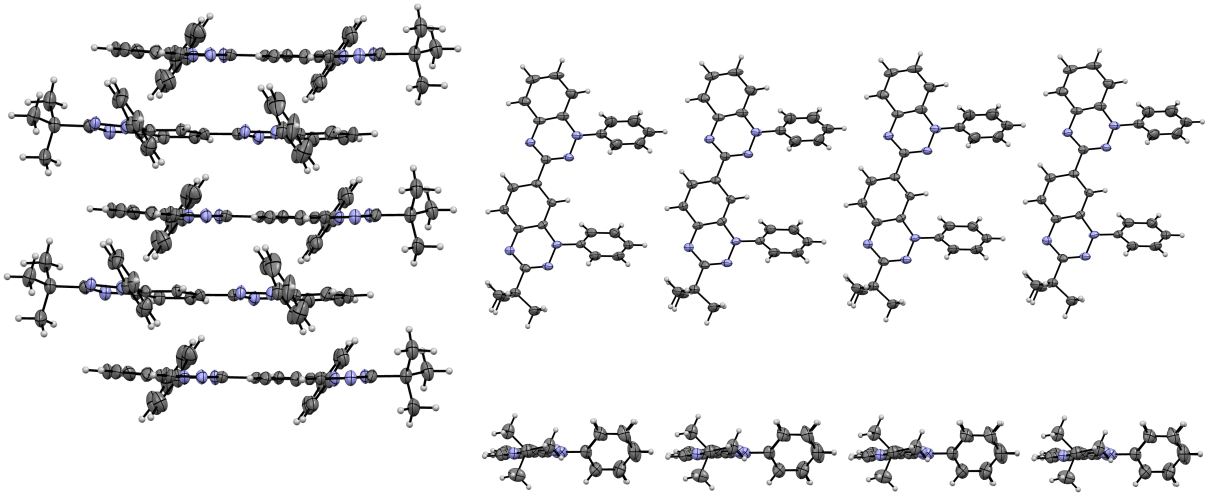


Figure S21. Partial packing diagrams for **1[3,7]**; left: the stack, right: two views of the sheet. Ellipsoids are drawn at 50% probability level. Color code: carbon, dark gray; blue, nitrogen.

Table S2. Selected close contacts in the solid-state structures of **1[3,n]** with the threshold of -0.07 Å.

Contact X···Y	$d_{X...Y}$ /Å	d_{X-Y} –VdW /Å
1[3,6], in the unique pair:		
C(5)···C(8a')	3.296	-0.104
C(5)···C(8')	3.239	-0.161
N(4)···H(C_{ortho}')	2.699	-0.081
between the dimers in the stack:		
C(5')···C(8)	3.231	-0.169
N(4)···H(C_{ortho}')	2.468	-0.282
C(6')···C_{ortho}	3.316	-0.081
1[3,7] in the stack:		
C(8a')···C(5)	3.323	-0.077
in the sheet:		
N(4)···H(C_{para})	2.600	-0.150
N(4')···H(C_{para}')	2.650	-0.100

4. Electronic absorption spectroscopy

Electronic absorption spectra of diradicals **1[3,n]** were recorded on a Jasco V770 spectrophotometer in spectroscopic grade CH_2Cl_2 at concentrations in a range of 2–8×10^{-5} mol·L^{-1} and the measurements were recorded immediately after. The measured UV-vis spectra were fitted to the Beer–Lambert law (A = εcl), the molar absorption coefficient (ε) was derived from the linear plots. Results are shown in Figures S22 and S23.

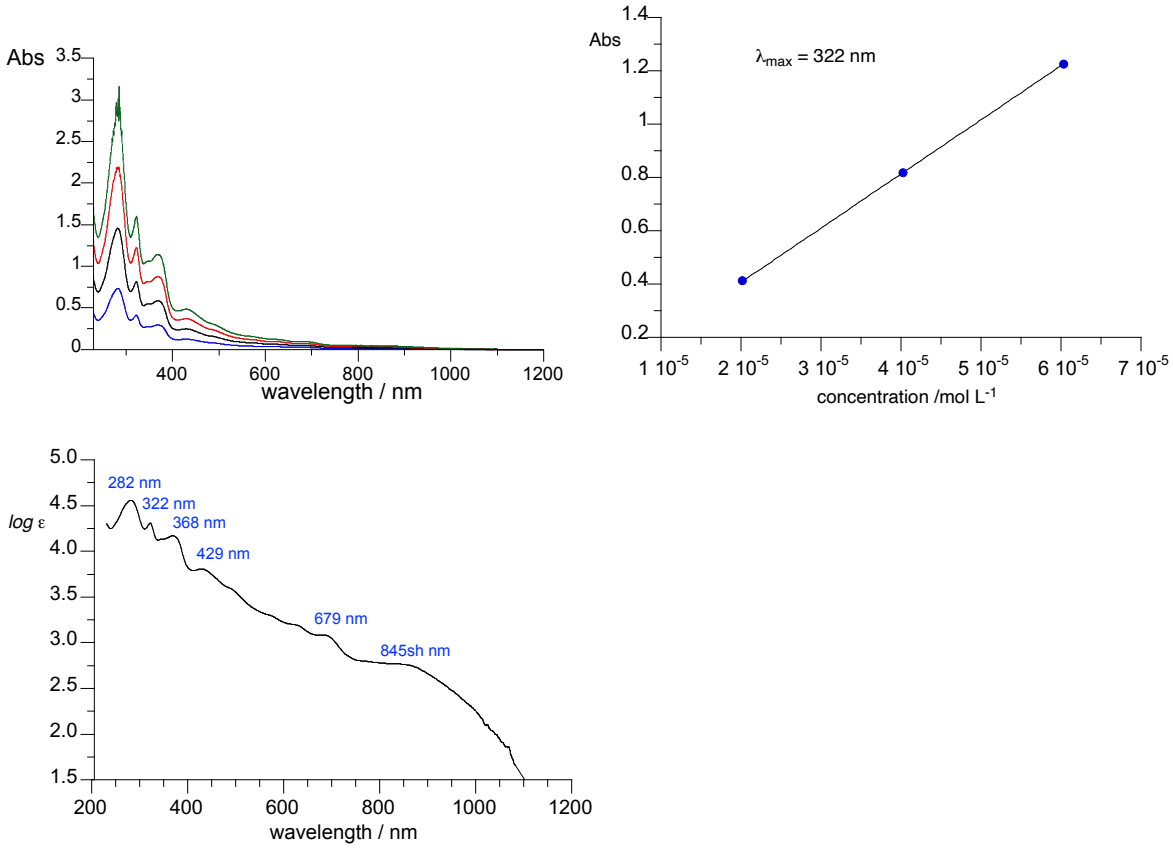
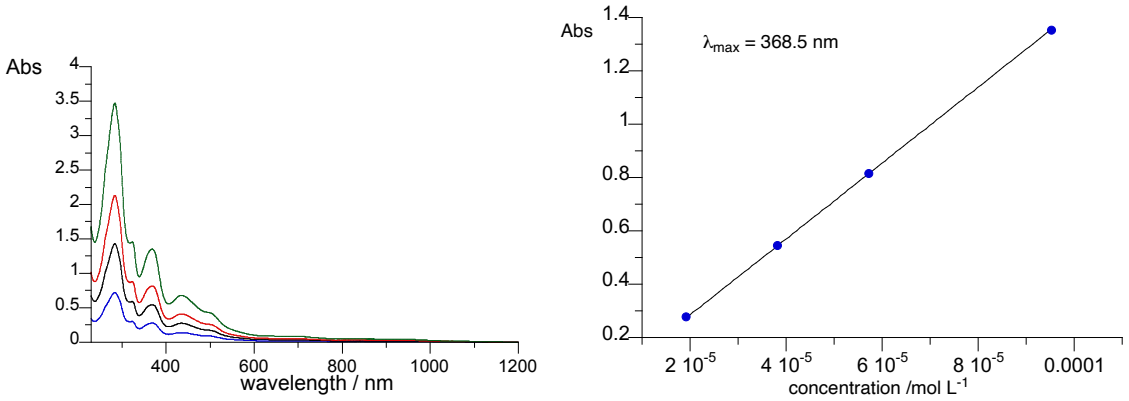


Figure S22. Clockwise: electronic absorption spectra of diradical **1[3,6]** in CH_2Cl_2 for four different concentrations, determination of molar extinction coefficient ε at λ = 322.0 nm (best fit function: ε = 20311(28)×conc, r^2 = 0.9999), and molar extinction log (ε) plot.



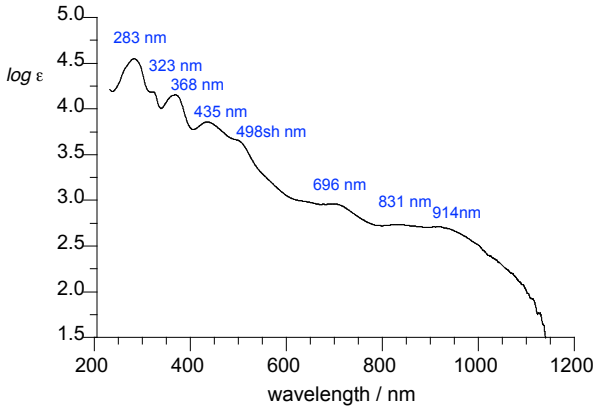


Figure S23. Clockwise: electronic absorption spectra of diradical **1[3,7]** in CH_2Cl_2 for four different concentrations, determination of molar extinction coefficient ε at λ = 368.5 nm (best fit function: ε = 7554.5(62)×conc, r^2 = 0.999), and molar extinction log (ε) plot.

5. Electrochemical results

Electrochemical characterization of diradicals **1[3,n]** was conducted using a Metrohm Autolab PGSTAT 128N potentiostat/galvanostat instrument. Diradical **1[3,n]** was dissolved in dry, spectroscopic grade CH_2Cl_2 (concentration 1.5 mM) in the presence of $[n\text{-}Bu_4N]^+[PF_6]^-$ as an electrolyte (concentration 100 mM) and the resulting solution was degassed by purging with Ar gas for 20 min. A three-electrode electrochemical cell was used with glassy carbon disk as the working electrode (ϕ 2 mm, alumina polished), Pt wire as the counter electrode and Ag/AgCl wire as the pseudoreference electrode. All samples were measured without internal reference once and afterwards with $FcMe_{10}$ as the internal reference couple with a scan rate of 50 mV s^{-1} (CV) or 5 mV s^{-1} (DPV) at *ca.* 20 °C. The oxidation potential for the $FcMe_{10}/FcMe_{10}^+$couple was established at -0.556 V in CH_2Cl_2 *vs* Fc/Fc^+, by comparison with the oxidation potential for the Fc/Fc^+ couple (0.0 V).

Cyclic voltammetry (CV) measurements were started from 0.0 V in the oxidative direction, while differential pulse voltammetry (DPV) measurements were conducted starting from -1.6 V in the oxidative direction (blue line) and starting from 0.9 V in the reductive direction (black line). Cyclic voltammetry (CV) and Differential pulse voltammetry (DPV) plots are shown in Figures S24 and S25 and numerical results are shown in Table S3.

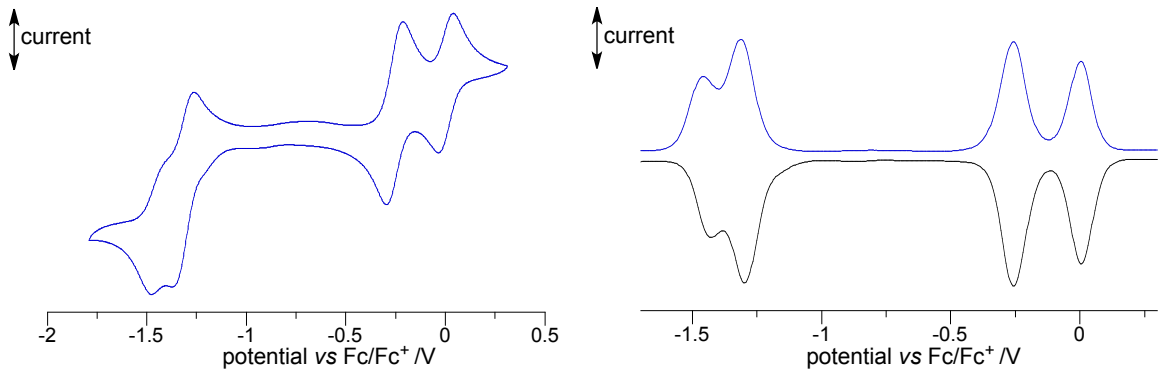


Figure S24. Cyclic voltammogram (CV, left) and differential pulse voltammogram (DPV, right) for **1[3,6]** in CH_2Cl_2 referenced to the Fc/Fc^+ couple.

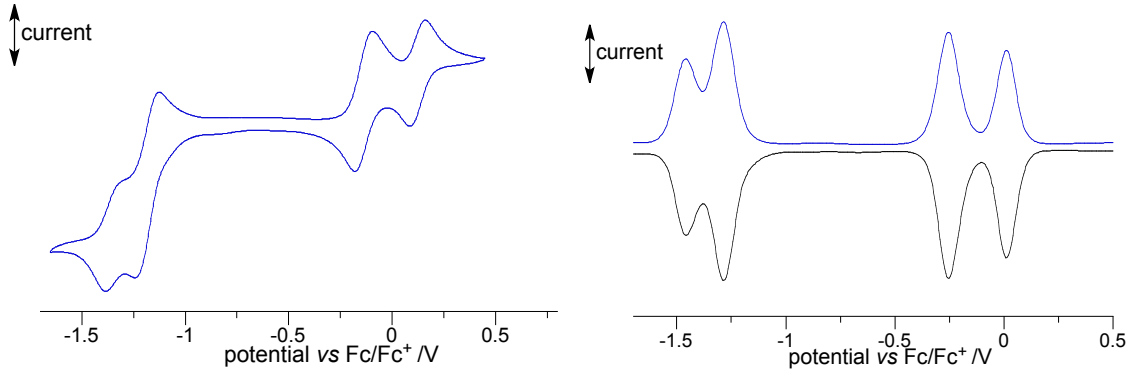


Figure S25. Cyclic voltammogram (CV, left) and differential pulse voltammogram (DPV, right) for **1[3,7]** in CH_2Cl_2 referenced to the Fc/Fc^+ couple.

Table S3. Electrochemical properties of diradicals **1[3,n]**.[a]

diradical	$E_{1/2}^{2-/-}$ /V	$E_{1/2}^{-/0}$ /V	ΔE_{red} /V	$E_{1/2}^{+/0}$ /V	$E_{1/2}^{+/2+}$ /V	ΔE_{ox} /V	ΔE_{cell} (1)[b] /V	ΔE_{cell} (2)[b] /V
1[3,6]	-1.44	-1.31	0.13	-0.26	0.01	0.27	1.05	1.43
1[3,7]	-1.46	-1.29	0.16	-0.25	0.01	0.26	1.04	1.45

[a] Data from DPV measurements. Measured in CH_2Cl_2 $[n\text{-}Bu_4N]^+[PF_6]^-$ (100 mM), *ca.* 20 °C, 5 mVs^{-1} (DPV), glassy carbon electrode. Potentials referenced to Fc/Fc^+). [b] $\Delta E_{cell}(1) = E_{1/2}^{+/0} - E_{1/2}^{-/0}$; $\Delta E_{cell}(2) = E_{1/2}^{+/2+} - E_{1/2}^{2-/-}$.

6. Details of VT EPR spectroscopy and data analysis

a) sample preparation

A solution of polystyrene (200.0 mg, d = 1.04 g cm^{-3}) in dry and distilled CH_2Cl_2 (4 mL) was degassed in vacuum and diradical **1[3,n]** (0.470 mg, 9.98×10^{-4} mmol) was added and

mixed till a homogenous mixture was formed. The resulting mixture was degassed in vacuum till complete evaporation of the solvent and formation of a fragile polystyrene film. The film was then dried for 1 h, divided into smaller pieces, placed in an EPR tube and tightly packed using a glass rod. The EPR tube containing the sample was blown with argon gas, tightly closed, and variable temperature measurement was performed.

b) measurement

Variable temperature EPR spectra for diradicals **1[3,n]** were recorded on an X-band EMX-Nano EPR spectrometer equipped with a frequency counter and nitrogen flow temperature control (120 K to ~334 K) in degassed solid polystyrene (PS) solutions (5.2 mM) at 120 K exhibit patterns with randomly oriented triplets contaminated with signal from the doublet impurity (the middle singlet). The optimum microwave power for the measurement was determined from the linear portion of the plot of signal intensity (double integral, DI, of the spectrum) *vs* square root of microwave power (Figures S26 and S27) at 120 K and ambient temperature. Half-field transition $|\Delta m_s| = 2$ was observed in both diradicals at low temperature for lower signal attenuation (Figure S28).

Variable-temperature EPR spectra for diradicals **1[3,n]** were recorded in a range 120–334 K typically every 5 K and attenuation of 22 dB. At each temperature spectra were recorded three times and averaged and selected plots are shown in Figure S28.

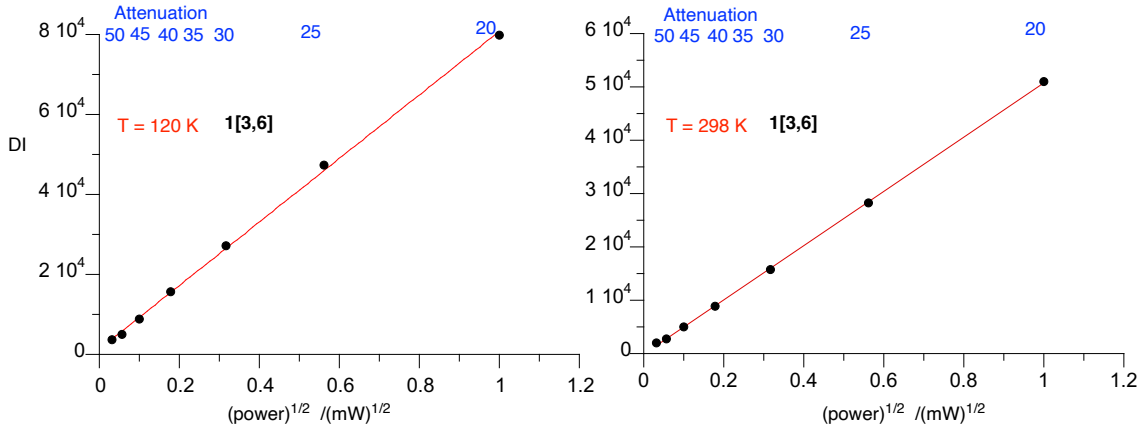


Figure S26. EPR double integrated signal intensity (DI) versus the square root of microwave power for 5.2 mM diradical **1[3,6]** in polystyrene at 120 K (left) and 298 K (right). Best fit lines: $DI_{120} = 1315+79469\times(\text{power})^{1/2}$, $r^2 = 0.9992$; $DI_{298} = -61.6+50768\times(\text{power})^{1/2}$, $r^2 = 0.9998$.

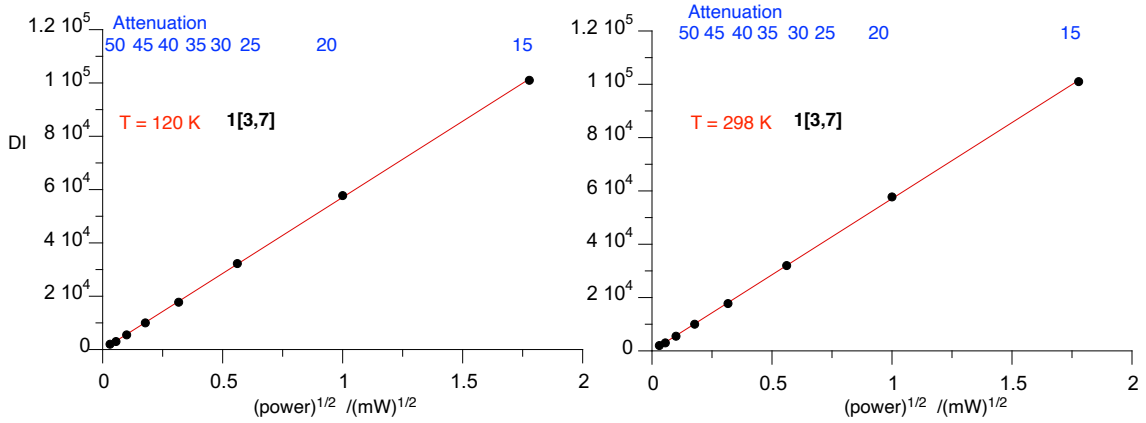


Figure S27. EPR double integrated signal intensity (DI) versus the square root of microwave power for 5.2 mM diradical **1[3,7]** in polystyrene at 120 K (left) and 298 K (right). Best fit lines: DI_{120} = -5.2+57038×(power)$^{1/2}$, r^2 = 0.9999; DI_{298} = -82.1+57101×(power)$^{1/2}$, r^2 = 0.9999.

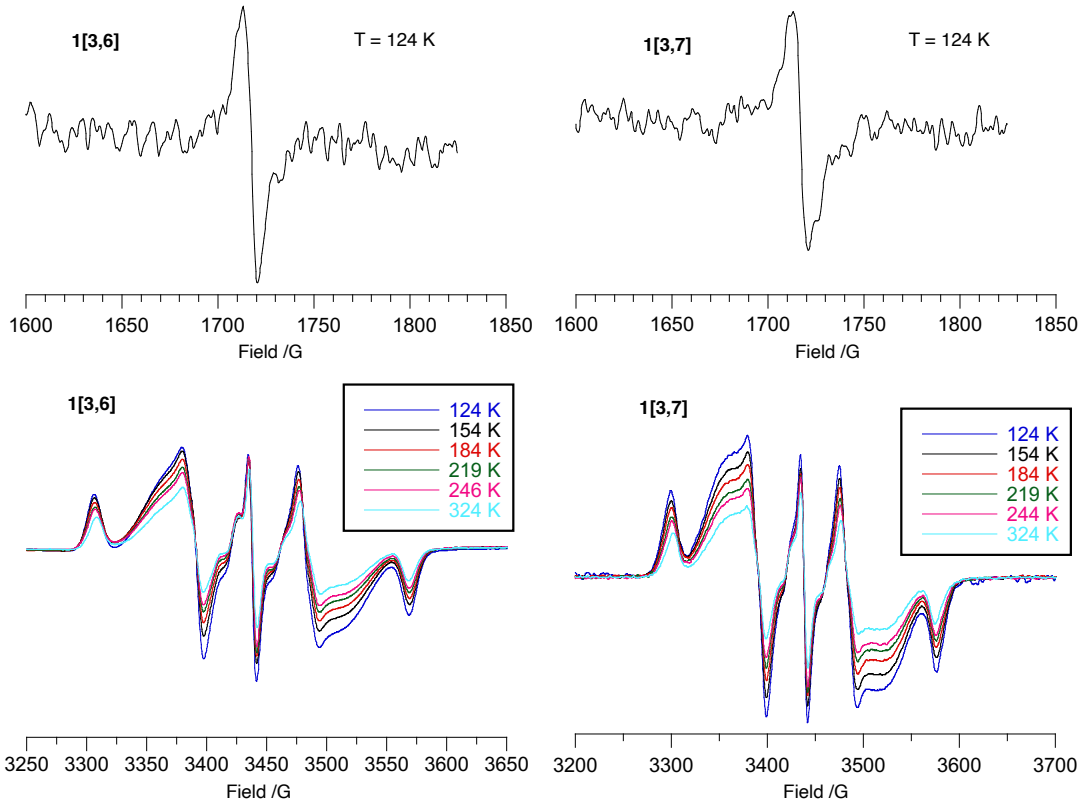


Figure S28. Half-field transitions (top) and variable temperature spectra (bottom) recorded for 5.2 mM diradical **1[3,6]** (left) and **1[3,7]** (right) in polystyrene at 22 dB in the temperature range 124–324 K.

c) spectra analysis and simulation

EPR spectra were double integrated and the resulting DI intensities were normalized for the intensity at the lowest temperature. The resulting DI_{rel} values are shown in Tables S4 and S5.

Table S4. Double integral and normalized data for **1[3,6]**.

Temp /K	DI	DI/DI_{120}	DI_{rel}•T	Temp /K	DI	DI/DI_{120}	DI_{rel}•T
120	58640	1.0000	120.40	229	41730	0.71163	163.18
124	55900	0.95327	118.49	234	40730	0.69458	162.53
130	55430	0.94526	122.60	240	39700	0.67701	162.14
134	55840	0.95225	127.70	246	39720	0.67735	166.29
139	56030	0.95549	132.91	249	38490	0.65638	163.57
144	55760	0.95089	137.02	254	38150	0.65058	165.31
149	55110	0.93980	140.12	259	37310	0.63626	165.04
154	54390	0.92752	143.12	264	36890	0.62909	166.14
159	53450	0.91149	145.11	269	36220	0.61767	166.34
164	52430	0.89410	146.72	274	35640	0.60778	166.71
169	51460	0.87756	148.57	279	34910	0.59533	166.16
174	50620	0.86323	150.38	284	34500	0.58834	167.26
179	49860	0.85027	152.45	289	33810	0.57657	166.69
184	48970	0.83510	153.74	294	33180	0.56583	166.52
189	48180	0.82162	155.37	299	32690	0.55747	166.85
194	47290	0.80645	156.53	304	32440	0.55321	168.34
199	46480	0.79263	157.89	309	32040	0.54638	169.00
204	45620	0.77797	158.94	314	31570	0.53837	169.10
209	44910	0.76586	160.29	319	30790	0.52507	167.55
214	44100	0.75205	161.09	324	30320	0.51705	167.58
219	43270	0.73789	161.67	329	29860	0.51705	167.58
224	42460	0.72408	162.48	334	29220	0.50921	167.58

Table S5. Double integral and normalized data for **1[3,7]**.

Temp /K	DI	DI/DI_{120}	DI_{rel}•T	Temp /K	DI	DI/DI_{120}	DI_{rel}•T
120	56130	1	119.90	224	36900	0.6574	147.46
124	55710	0.99252	123.37	229	36080	0.64279	147.33
130	54220	0.96597	125.09	234	35570	0.63371	148.48
135	53310	0.94976	127.74	239	34840	0.6207	148.53
139	52210	0.93016	129.66	244	34130	0.60805	148.49
144	51330	0.91448	132.05	249	33390	0.59487	148.30
149	50190	0.89417	133.59	254	32890	0.58596	149.01
154	49070	0.87422	134.89	259	32040	0.57082	147.96
159	48030	0.85569	136.31	264	31690	0.56458	149.16
164	46800	0.83378	136.91	269	30990	0.55211	148.63
169	45840	0.81668	138.18	274	30620	0.54552	149.64
174	45060	0.80278	139.92	279	29620	0.5277	147.33
179	43940	0.78283	140.36	284	29410	0.52396	148.91
184	43020	0.76644	141.25	289	28810	0.51327	148.44
189	42340	0.75432	142.79	294	28200	0.50241	147.81
194	41380	0.73722	143.24	299	27680	0.49314	147.55
199	40680	0.72475	144.44	304	27070	0.48227	146.71
204	39900	0.71085	145.23				
209	39280	0.6998	146.47				

The $DI_{rel}T(T)$ data was modeled using χ_{tot}T, which is a sum of paramagnetic contributions from *syn* and *anti* conformers scaled by mole fraction x at the equilibrium (eq S1). Paramagnetic behavior of each conformer is described by a modified Bleaney-Bowers[10] formalism (eq S2) and based on Heisenberg Hamiltonian for two spin 1/2 system,

$\hat{H} = -2J\hat{S}_1 \cdot \hat{S}_2$.

$$\chi_{tot}T = x_{anti} \bullet \chi_{anti}T + x_{syn} \bullet \chi_{syn}T \qquad \text{(eq. S1)}$$

$$\chi \bullet T = \frac{Ng^2\mu_B^2}{k}\left(\frac{2}{3+e^{-\frac{2J}{kT}}}\right)(1-\rho) + \frac{Ng^2\mu_B^2}{2k}\,\rho \qquad \text{eq S2}$$

For numeral fitting to the eq S1, a three-parameter equation S3 was used.

$$DI_{rel} \times T = m1\left(\frac{2}{3+e^{-\frac{m2}{m0}}}\right) \times x_{syn} + m1\left(\frac{2}{3+e^{-\frac{m3}{m0}}}\right) \times x_{anti} + m4 \qquad \text{eq S3}$$

For numeral fitting equation S3 the following parameters were used:

$DI_{rel} \times T$ – product of double integral and temperature determined experimentally and listed in Tables S4 and S5.
$m0 = T\ /K$
m1, *m4* – free parameters
$m2, m3 = \frac{2J}{k_B}\ /K$
x_{syn} and x_{anti} are mole fractions of conformers at thermal equilibrium at T = 298 determined by DFT (*vide infra*) and listed in Table S6.

Fitting to the four-parameter function S3 gave initial values for the parameters *m1*–*m4*. Subsequently, parameter *m3* for the antiferromagnetic component was fixed and varied in a small range to maximize the correlation parameter r^2. Results of curve fitting are shown in Figures S29 and S30 and in Table S6. A graphical comparison of the experimental and DFT-derived $\Delta E_{S\text{-}T}$ values is shown in Figure S31.

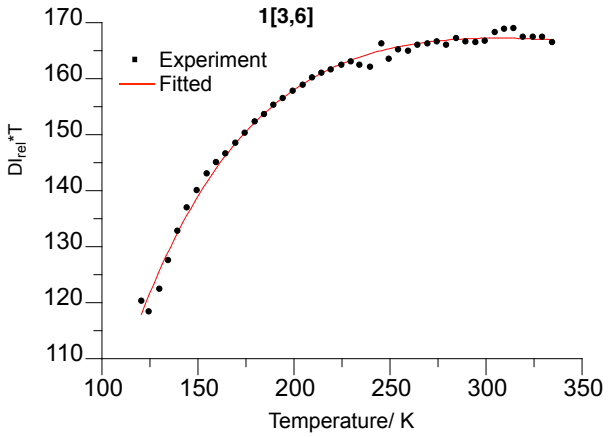


Figure S29. Determination of ΔE_{ST} for 5.2 mM diradical **1[3,6]** in polystyrene. Plot of DI_{rel}•T *vs T*, in the temperature range 120–334 K. Red line represents the best fitting function (eq. S3) with the following parameters: *m*1 = 1278(56), *m*2 = $2J/k_B$ = 515(24) K, *m*3 = $2J/k_B$ = -224, *m4* = -532(29), r^2 = 0.994.

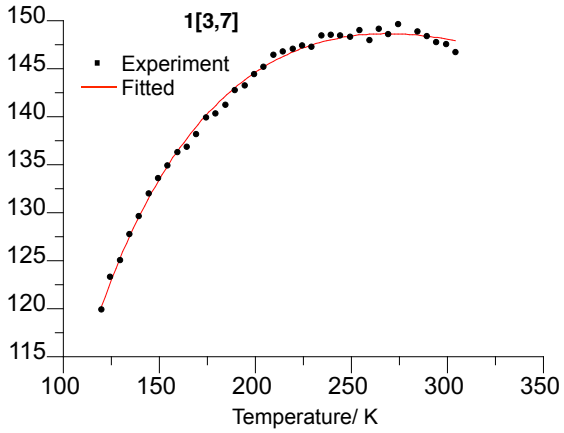


Figure S30. Determination of ΔE_{ST} for 5.2 mM diradical **1[3,7]** in polystyrene. Plot of DI_{rel}•T *vs T* in the temperature range 120–304 K. Red line represents the best fitting function (eq. S3) with the following parameters: $m1$ = 2197(43), $m2 = 2J/k_B$ = 894(13) K, $m3 = 2J/k_B$ = -51, $m4$ = -1097(24), r^2 = 0.996.

Table S6. The singlet-triplet energy gap $\Delta E_{S\text{-}T}(2J)$ for diradicals **1[3,n]** determined by fitting to the Bleaney-Bowers equation eq S3.

	x_{syn} [a]	x_{anti} [a]	$\Delta E_{S\text{-}T}$*(syn)* /kcal/mol	$\Delta E_{S\text{-}T}$*(anti)* /kcal/mol
1[3,6]	0.3425	0.6575	-0.45	1.02(5)
1[3,7]	0.50	0.50	1.78(3)	-0.10

[a] Mole fraction obtained from K_{298} calculated with DFT methods.

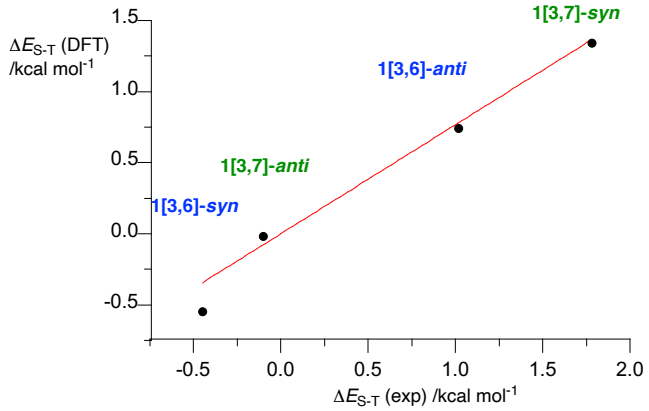


Figure S31. A correlation of experimental and DFT-derived (*vide infgra*) singlet triplet gaps for two conformers of **1[3,6]** and **1[3,7]**. Best fit line: $\Delta E_{S\text{-}T}(DFT) = 0.77(6) \times \Delta E_{S\text{-}T}(exp)$.

Simulation of triplet EPR spectra for diradicals **1[3,n]** was conducted using the *pepper* module in *EasySpin* (Matlab),[11] and results are shown in Figures S32 and S33. Assuming an isotropic *g* value, the resulting absolute values of zero-field splitting parameters (*zfp*), |*D*/*hc*| and |*E*/*hc*|, are shown in Table S7. Assuming a point dipole approximation, the mean distance between the spin centers was estimated using equation S4.

$$r = ((D/2\mathrm{g})\times 7.19\times 10^{-5})^{-1/3} \qquad \text{eq S4}$$

where *D* (in gauss) is the fitting parameter in the simulated EPR spectrum.

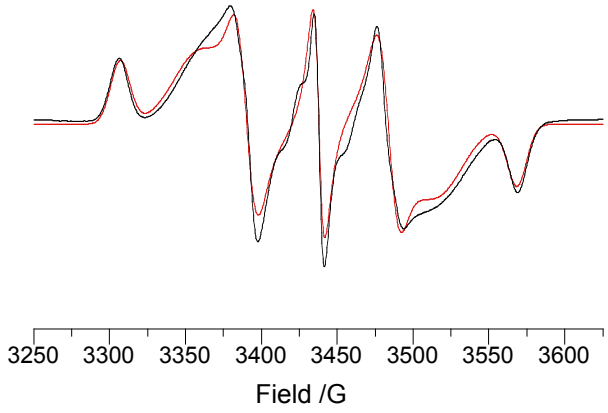


Figure S32. A complete set of fitting parameters for EPR spectrum of 5.2 mM diradical **1[3,6]** in polystyrene (124 K, ν = 9.644 GHz). Simulation $|\Delta m_S|$ = 1 region (*pepper*, *EasySpin*, rmsd = 0.0607234): Component A, weight = 1.0000, S = 1, D = 366.09 MHz, E = 32.07 MHz, g_{iso} = 2.00431; *H*-strain (MHz): H_x = 38.3555, H_y = 102.718, H_z = 41.1344; *D*-strain (MHz): D = 80.00, E = 30.00; component B, S =1/2, weight = 0.29567, g_{iso}= 2.00428, *H*-strain (MHz): H_x = 50.00, H_y = 50.00, H_z = 87.00.

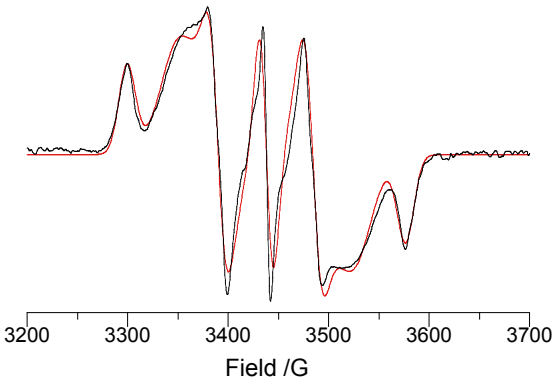


Figure S33. A complete set of fitting parameters for EPR spectrum of 5.2 mM diradical **1[3,7]** in polystyrene (124 K, ν = 9.644 GHz). Simulation $|\Delta m_S|$ = 1 region (*pepper*, *EasySpin*, rmsd = 0.0759452): Component A, weight = 1.0000, S = 1, D = 388.43 MHz, E = 39.03 MHz, g_{iso} = 2.00417, *H*-strain (MHz): H_x = 52.711 H_y = 110.397, H_z = 54.4579; *D*-strain (MHz): D = 80.00, E = 30.00; component B, S =1/2, weight = 0.216519, g_{iso} = 2.00416; *H*-strain (MHz): H_x = 50.00, H_y = 50.00, H_z = 87.00.

Table S7. Zero-field splitting parameters simulated for diradicals **1[3,n]**.

diradical	Matrix, temp/ K	$\|D/hc\|$ /cm^{-1}	$\|E/hc\|$ /cm^{-1}	g_{iso}	r [a] /Å
1[3,6]	PS, 124	1.22×10^{-2}	1.07×10^{-3}	2.0043	5.97
1[3,7]	PS, 124	1.29×10^{-2}	1.30×10^{-3}	2.0042	5.86

[a] Calculated using equation S4.

7. Computational details

a) geometry optimization

Quantum-mechanical calculations were carried out using Gaussian 09 suite of programs.[12] Geometry optimizations of the open-shell singlet and the triplet state of each diradical were undertaken at the UB3LYP/6-311G(d,p) level of theory in benzene dielectric medium (PCM model,[13] the SCRF(solvent=Benzene) keyword) using default convergence criteria and no symmetry constrains. All calculations involving the open-shell singlet (OSS) used the "guess(mix, always)" keyword (the broken symmetry, BS, approach). Limited conformational search conducted for triplet diradicals **1[3,6]** and **1[3,7]** determined their two main minima with the Ph groups in *syn* and *anti* relative orientations and the *t*-Bu group nearly eclipsing the N(2) atom. The optimized geometries of the triplet species were used as starting points for geometry optimization of the OSS species. The resulting geometries for two conformers of **1[3,6]** and **1[3,7]** in the triplet state are shown in Figures S34 and S35, while Figures S36 and S37 show spin density maps for the T and OSS sates of the two diradicals. Frequency calculations were performed to verify the nature of the stationary points and to obtain thermodynamic corrections for each species. Finally, the SCF energy of each species was obtained from single point calculations at the UB3LYP/6-311+G(d,p) level in benzene dielectric medium (the UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) method).

This protocol was used to obtained geometry optimized structures for diradicals in series **I[3,6]** and **I[3,7]**.

Also the same method (UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) in benzene dielectric medium) was used to calculate spin distribution in monoradical models.

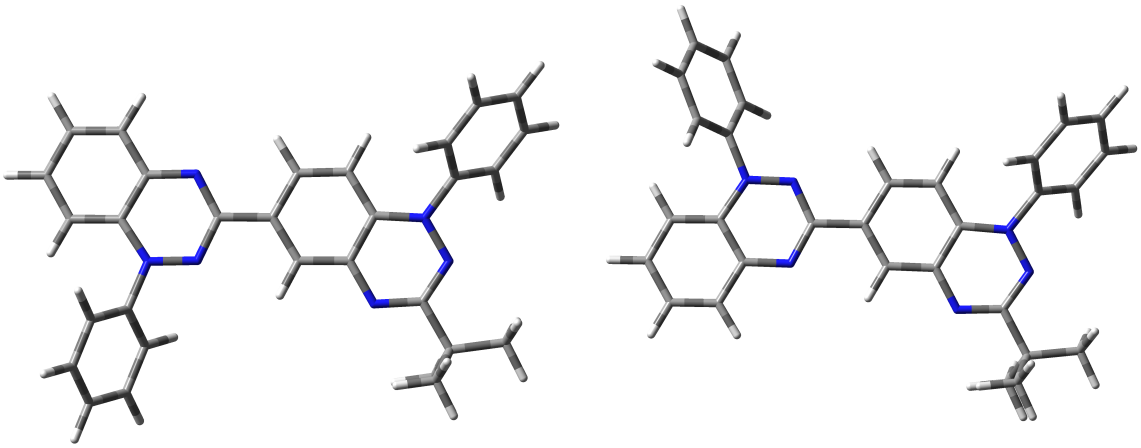


Figure S34. Optimized geometries for triplet diradical **1[3,6]-T** in the *anti* (left) and *syn* conformation (right).

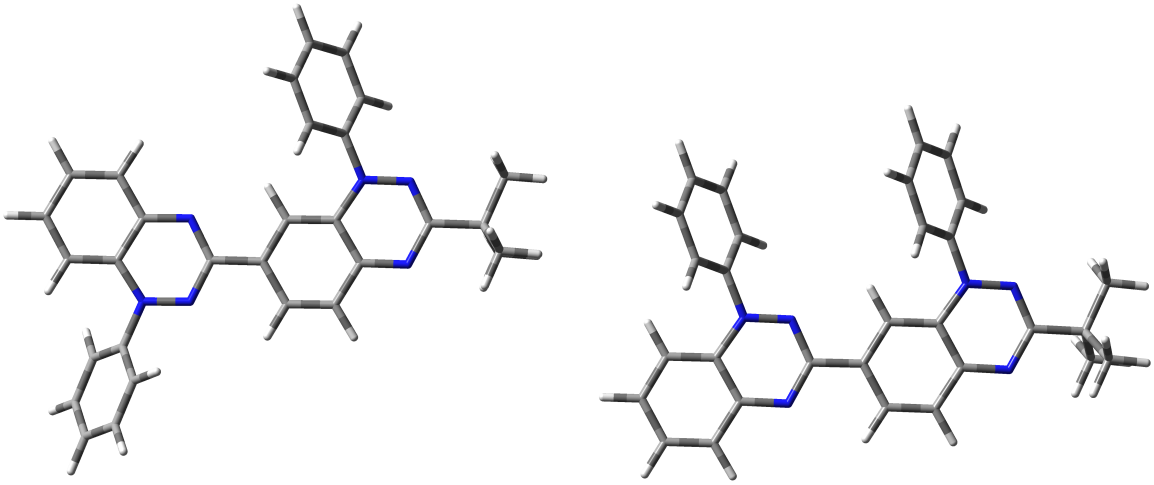


Figure S35. Optimized geometries for triplet diradical **1[3,7]-T** in the *anti* (left) and *syn* conformation (right).

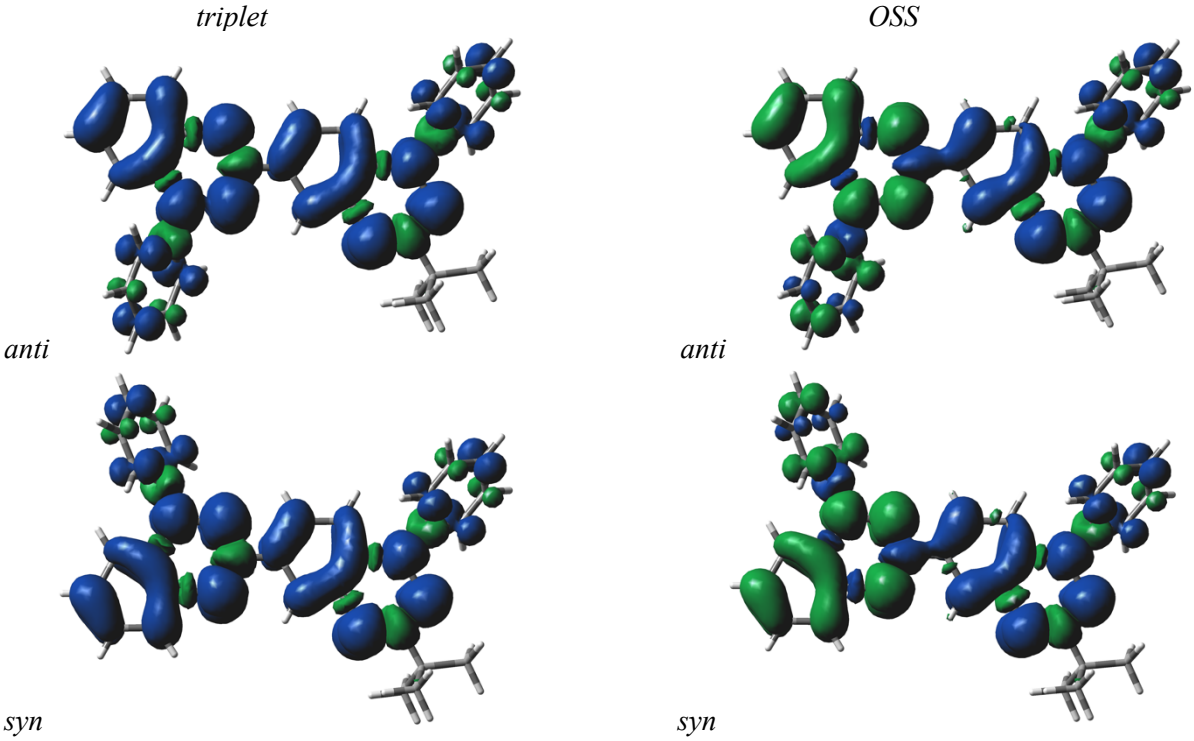


Figure S36. Spin density maps for triplet (left) and OSS (right) states of **1[3,6]** in the *anti* (top) and *syn* (bottom) conformation (top). *Density* = 0.0008.

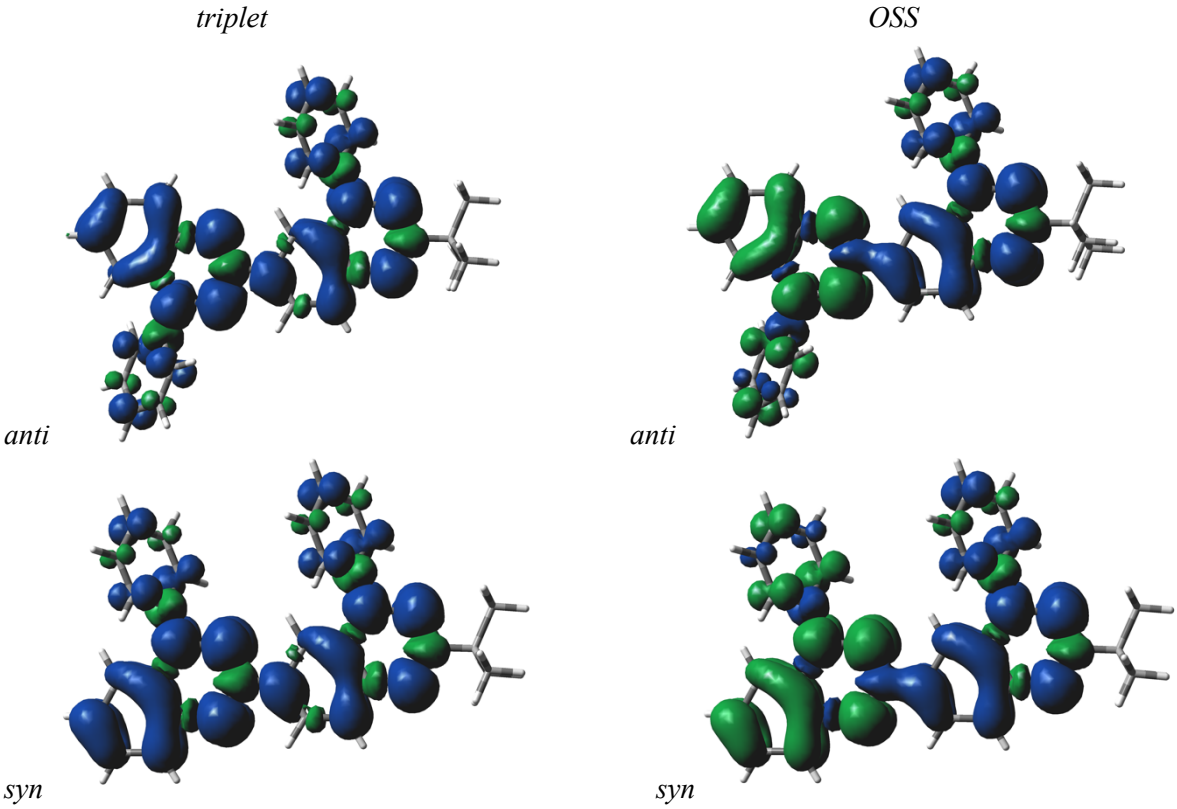


Figure S37. Spin density maps for triplet (left) and OSS (right) states of **1[3,7]** in the *anti* (top) and *syn* (bottom) conformation (top). *Density* = 0.0008.

b) intramolecular spin-spin exchange interactions

Adiabatic singlet-triplet energy gaps, $\Delta E_{S\text{-}T}$, for diradicals **1[3,n]** were calculated as a difference of E_S and E_T energies calculated using the Yamaguchi formalism[14] (eq S5) at the UB3LYP/6-311+G(d,p) level of theory and corrected for ZPE.

$$\Delta E_{S-T} = 2J = 2\frac{E_{BS}-E_T}{\langle S^2\rangle_T - \langle S^2\rangle_{BS}} \qquad \text{eq. S5}$$

where $\langle S^2\rangle$ is the total spin angular momentum before spin annihilation. Energies of the triplet (E_T) and broken symmetry singlet (E_{BS}) were obtained as E_{SCF} at the UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) level of theory in benzene dielectric medium and corrected by ZPEC. The results are shown in Table S8. The same protocol was used for calculations of $\Delta E_{S\text{-}T}$ values for derivatives **I[3,6]** and **I[3,7]** and results are shown in Tables S9 and S10.

Table S8. DFT calculated energies, thermodynamic corrections and S–T gaps for diradicals **1[3,n]**.

diradical	E_{SCF} [a] /Ha	ZPEC [b] /Ha	H corr [b] /Ha	G_{298} corr [b] /Ha	$\langle S^2\rangle$ [b]	$\Delta E_{S\text{-}T}$ [c] /cal mol^{-1}
1[3,6]						
anti-S	-1487.6728593	0.495123	0.525595	0.432475	1.0295	
anti-T	-1487.6734961	0.495172	0.525635	0.431551	2.0281	738.7
syn-S	-1487.6733490	0.495191	0.525641	0.432718	0.9980	
syn-T	-1487.6728601	0.495153	0.525624	0.431530	2.0282	-549.3
1[3,7]						
anti-S	-1487.6740744	0.495181	0.525672	0.432163	0.9899	
anti-T	-1487.6740154	0.495138	0.525649	0.430959	2.0321	-19.3
syn-S	-1487.6731960	0.495075	0.525589	0.432128	1.0247	
syn-T	-1487.6743138	0.495116	0.525618	0.431263	2.0323	1341.2

[a] Obtained at the UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) level of theory in benzene dielectric medium.
[b] Obtained at the UB3LYP/6-311G(d,p) level of theory in benzene dielectric medium. [c] Obtained using eq S5.

Table S9. DFT calculated energies, thermodynamic corrections and S–T gaps for diradicals **I[3,6]**.

diradical	E_{SCF} [a] /Ha	ZPEC [b] /Ha	H corr [b] /Ha	G_{298} corr [b] /Ha	$\langle S^2 \rangle$ [b]	$\Delta E_{S\text{-}T}$ [c] /cal mol^{-1}
X = H, Y = H, Ar = Ph						
anti-S	-1330.3703760	0.384174	0.408815	0.328250	1.0295	
anti-T	-1330.3710244	0.384220	0.408853	0.327278	2.0285	756.3
syn-S	-1330.3707825	0.384171	0.408817	0.328144	1.0001	
syn-T	-1330.3703720	0.384138	0.408805	0.326943	2.0285	-461.3
X = H, Y = CF_3, Ar = Ph						
anti-S	-1667.516041	0.388174	0.416607	0.326226	1.0293	
anti-T	-1667.516684	0.38822	0.416648	0.325219	2.0281	750.1
syn-S	-1667.516391	0.388215	0.416625	0.326587	0.9993	
syn-T	-1667.515975	0.388182	0.416614	0.325417	2.0282	-467.2
X = H, Y = NMe_2, Ar = Ph						
anti-S	-1464.388088	0.455983	0.485443	0.393863	1.0263	
anti-T	-1464.388888	0.456014	0.485477	0.392867	2.0280	963.1
syn-S	-1464.388697	0.455913	0.485457	0.393252	0.9955	
syn-T	-1464.388411	0.455909	0.485453	0.392206	2.0279	-342.1
X = CF_3, Y = NMe_2, Ar = Ph						
anti-S	-1801.537921	0.460238	0.493515	0.391498	1.0244	
anti-T	-1801.538725	0.460317	0.493579	0.390645	2.0281	907.2
syn-S	-1801.538752	0.460244	0.493519	0.391577	0.9819	
syn-T	-1801.538131	0.460176	0.4935	0.389823	2.0280	-663.2
X = H, Y = H, Ar = 2-Pyridyl						
anti-S	-1362.461515	0.360908	0.385208	0.305266	1.0322	
anti-T	-1362.461998	0.360942	0.385235	0.304307	2.0300	564.4
syn-S	-1362.461475	0.360824	0.385158	0.304762	1.0108	
syn-T	-1362.461181	0.360792	0.385146	0.303516	2.0301	-322.5
X = H, Y = H, Ar = 4-Me_2NPh						
anti-S	-1598.381057	0.52888	0.56273	0.460176	1.0274	
anti-T	-1598.381754	0.528955	0.562782	0.459345	2.0272	780.4
syn-S	-1598.381566	0.528936	0.562708	0.460823	0.9939	
syn-T	-1598.381098	0.528894	0.56269	0.459630	2.0274	-517.2

[a] Obtained at the UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) level of theory in benzene dielectric medium. [b] Obtained at the UB3LYP/6-311G(d,p) level of theory in benzene dielectric medium. [c] Obtained using eq S5.

Table S10. DFT calculated energies, thermodynamic corrections and S–T gaps for diradicals **I[3,7]**.

diradical	E_{SCF} [a] /Ha	ZPEC [b] /Ha	H corr [b] /Ha	G_{298} corr [b] /Ha	$\langle S^2 \rangle$ [b]	$\Delta E_{S\text{-}T}$ [c] /cal mol^{-1}
X = H, Y = H, Ar = Ph						
anti-S	-1330.371485	0.384166	0.408813	0.328229	0.9926	
anti-T	-1330.371416	0.384116	0.408787	0.327043	2.0323	-23
syn-S	-1330.370663	0.384163	0.408812	0.328207	1.0253	
syn-T	-1330.371782	0.384188	0.408834	0.327215	2.0327	1362.5
X = H, Y = CF_3, Ar = Ph						
anti-S	-1667.517079	0.388252	0.416682	0.326135	1.0249	
anti-T	-1667.517082	0.388204	0.416656	0.324983	2.0324	63
syn-S	-1667.516200	0.388188	0.416636	0.325915	1.0249	
syn-T	-1667.517308	0.388216	0.416656	0.325025	2.0327	1344
X = H, Y = NMe_2, Ar = Ph						
anti-S	-1464.389944	0.456124	0.485588	0.393924	0.9930	
anti-T	-1464.389623	0.456108	0.485572	0.392863	2.0279	371
syn-S	-1464.389069	0.455966	0.485515	0.393237	1.0248	
syn-T	-1464.389866	0.456038	0.485538	0.392683	2.0282	906
X = CF_3, Y = NMe_2, Ar = Ph						
anti-S	-1801.540168	0.460355	0.493585	0.391944	0.9793	
anti-T	-1801.539492	0.460309	0.493564	0.390507	2.0274	-754
syn-S	-1801.538959	0.460168	0.493541	0.390615	1.023	
syn-T	-1801.539748	0.460293	0.493595	0.390234	2.0278	829
X = H, Y = H, Ar = 2-Pyridyl						
anti-S	-1362.461858	0.360872	0.385171	0.305210	1.0043	
anti-T	-1362.462122	0.360836	0.385152	0.304067	2.0354	365
syn-S	-1362.461027	0.36085	0.385158	0.305225	1.0275	
syn-T	-1362.462099	0.360879	0.385185	0.304178	2.036	1298
X = H, Y = H, Ar = 4-Me_2NPh						
anti-S	-1598.382188	0.528702	0.562606	0.459825	0.9863	
anti-T	-1598.381909	0.528662	0.562578	0.458717	2.0299	-287.5
syn-S	-1598.381328	0.528912	0.562666	0.461045	1.0242	
syn-T	-1598.382285	0.528943	0.562688	0.460121	2.0302	1155

[a] Obtained at the UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) level of theory in benzene dielectric medium.
[b] Obtained at the UB3LYP/6-311G(d,p) level of theory in benzene dielectric medium. [c] Obtained using eq S5.

c) ratio of conformers

The ratio of conformers K_{298} = [*anti*]/[*syn*] at standard temperature (298 K) was calculated using equation S6:

$$-298 \times RlnK_{298} = (G_{298}anti - G_{298}syn) \qquad \text{eq S6}$$

The results are shown in Figure 10 in the main text.

It was assumed that the ratio K_{298} does not change upon cooling in rigid polystyrene solutions. Population of states at 298 K for each diradical was calculated using K_{298} and ratio of OSS and T states was obtained from $\Delta E_{S\text{-}T}$ (Tables S9 and S10) and the general formula S6. Results are shown in Table S11.

Table S11. Population of states at 298 K.[a]

Diradical	K_{298}	*anti*-T	*anti*-OSS	*syn*-T	*syn*-OSS
1[3,6]	1.92	0.513	0.147	0.096	0.244
1[3,7]	1.01	0.246	0.254	0.453	0.047

[a] mole fraction.

Total populations of singlet (η_{OSS}) and triplet (η_T) states for each isomer in a function of temperature was calculated with equations S7 and S8, respectively, using DFT-derived thermodynamic parameters and experimentally determined $\Delta E_{S\text{-}T}$ energies listed in Table S12.

$$\eta_{OSS}(T) = x_{anti} \times \frac{K_{ST(a)}}{K_{ST(a)}+1} + x_{syn} \times \frac{K_{ST(s)}}{K_{ST(s)}+1} = \frac{K_{a/s}}{K_{a/s}+1} \times \frac{K_{ST(a)}}{K_{ST(a)}+1} + \frac{1}{K_{a/s}+1} \times \frac{K_{ST(s)}}{K_{ST(s)}+1}$$

$$\eta_{OSS}(T) = \frac{1}{K_{a/s}+1} \times \left[\frac{K_{a/s}K_{ST(a)}}{K_{ST(a)}+1} + \frac{K_{ST(s)}}{K_{ST(s)}+1}\right] \qquad \text{eq S7}$$

$$\eta_T(T) = x_{anti} \times \frac{1}{K_{ST(a)}+1} + x_{syn} \times \frac{1}{K_{ST(s)}+1} = \frac{K_{a/s}}{K_{a/s}+1} \times \frac{1}{K_{ST(a)}+1} + \frac{1}{K_{a/s}+1} \times \frac{1}{K_{ST(s)}+1}$$

$$\eta_T(T) = \frac{1}{K_{a/s}+1} \times \left[\frac{K_{a/s}}{K_{ST(a)}+1} + \frac{1}{K_{ST(s)}+1}\right] \qquad \text{eq S8}$$

where

syn –> anti

$K_{a/s} = e^{-\frac{\Delta H_{a/s} - T\Delta S_{a/s}}{RT}}$ and $\Delta H_{a/s} = H_{anti} - H_{syn}$ and $\Delta S_{a/s} = S_{anti} - S_{syn}$ determined from DFT calculations

T –> OSS

$K_{ST} = e^{-\frac{\Delta E_{ST}}{RT}}$ and $\Delta E_{ST} = E_{OSS} - E_T$ determined from experiment

Table S12. Parameters used to determine temperature dependent population of OSS and T states.

Diradical	$\Delta H_{a/s}$ [a] /cal mol^{-1}	$\Delta S_{a/s}$ [a] cal mol^{-1}K^{-1}	$\Delta E_{S\text{-}T(a)}$ [b] /cal mol^{-1}	$\Delta E_{S\text{-}T(s)}$ [b] /cal mol^{-1}
1[3,6]	-392	-0.021	1020	-450
1[3,7]	207	0.703	-100	1780

[a] Obtained at the UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) level of theory in benzene dielectric medium.
[b] determined from the experiment.

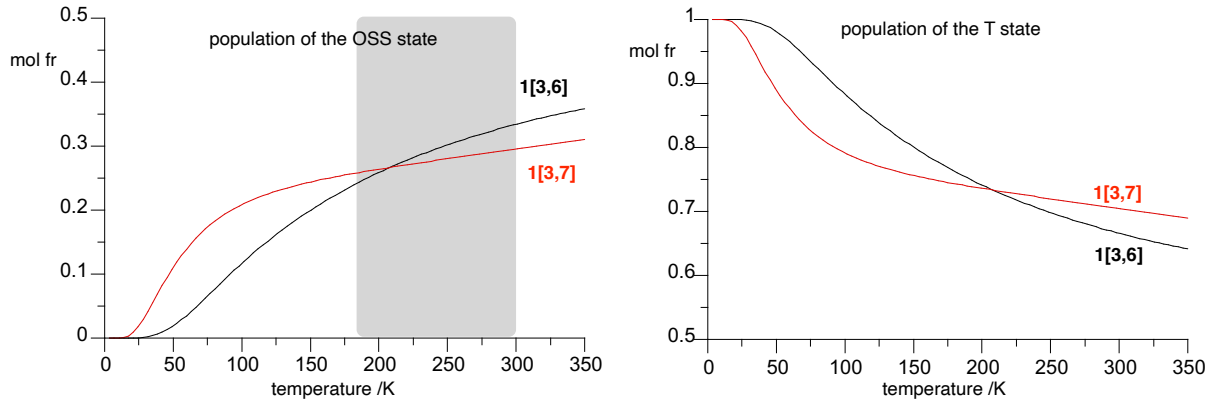


Figure S38. Profiles of the OSS mole fraction (η_{OSS}, left) and T mole fraction (η_T, left) in function of temperature using eqs S7 and S8 and data in Table S12. The shaded area is accessible by experiment.

d) activation energy for conformer interconversion

Transition states for the two isomeric diradicals were located with the QST3 keyword in both the OSS and triplet states in benzene dielectric medium using the UB3LYP/6-311G(d,p) method with default convergence limits. All species exhibited a single imaginary frequency of about -27 cm^{-1} corresponding to the rotation about the central C–C bond and essentially orthogonal orientation of the two heterocyclic rings. For all four TS geometries single point calculations were performed at the UB3LYP/6-311+G(d,p) level. Activation energies were calculated using the single point energies with thermodynamic corrections obtained at the UB3LYP/6-311G(d,p) level of theory. The resulting geometries are shown in Figure S39 and activation energies are listed in Table S13.

Table S13. DFT activation energies for conformer interconversion.[a]

	triplet			*OSS*		
Diradical	$\Delta E^{\ddagger}$ [b]	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}_{298}$	$\Delta E^{\ddagger}$ [b]	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}_{298}$
1[3,6]	5.25	4.79	6.23	5.06	4.60	6.00
1[3,7]	5.74	5.25	6.90	5.49	5.03	6.53

[a] UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) in benzene dielectric medium with thermodynamic corrections obtained at the UB3LYP/6-311G(d,p) level of theory. [b] SCF energy corrected for ZPE.

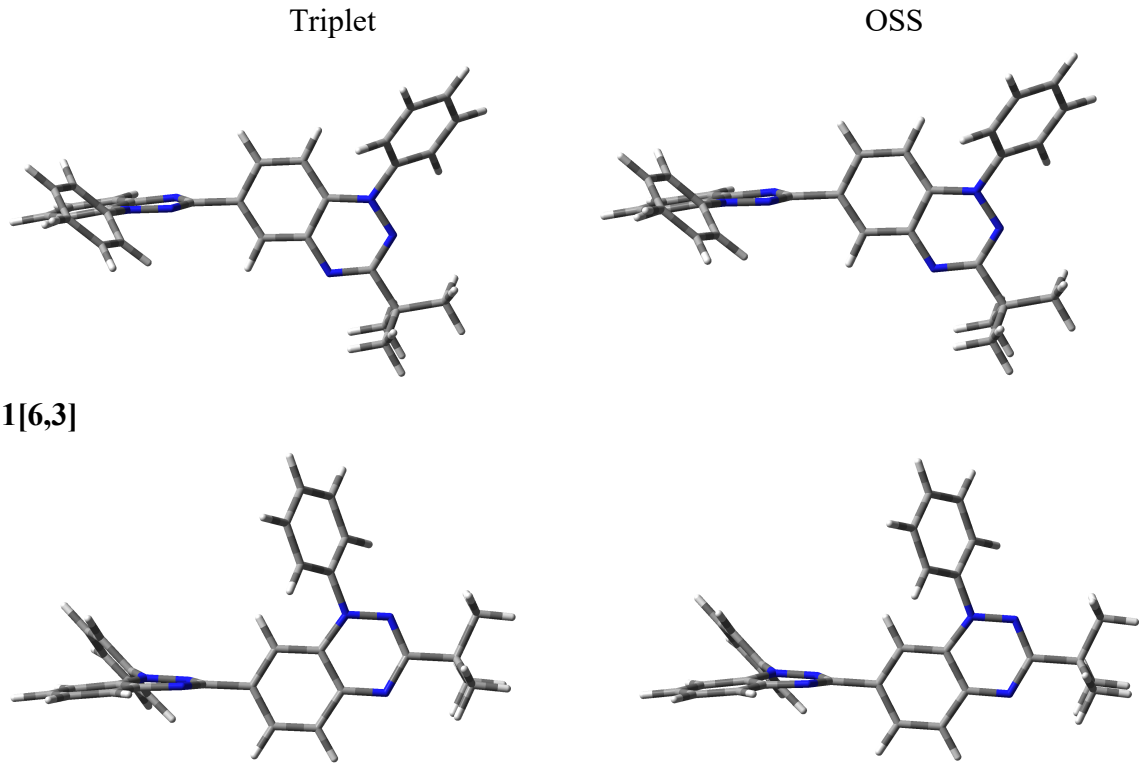


Figure S39. Optimized geometries for TS for interconversion of *syn* and *anti* conformers of diradicals **1[3,6]** (top) and **1[3,7]** (bottom) in the triplet (left) and OSS (right) states.

e) spin concentration in model monoradicals

Spin distribution in the key positions of diradicals **I[3,6]** and **I[3,7]** in two conformations was assessed as a superposition of spin density in two model monoradicals shown in Figure S40 calculated at the UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) level of theory in benzene dielectric medium.

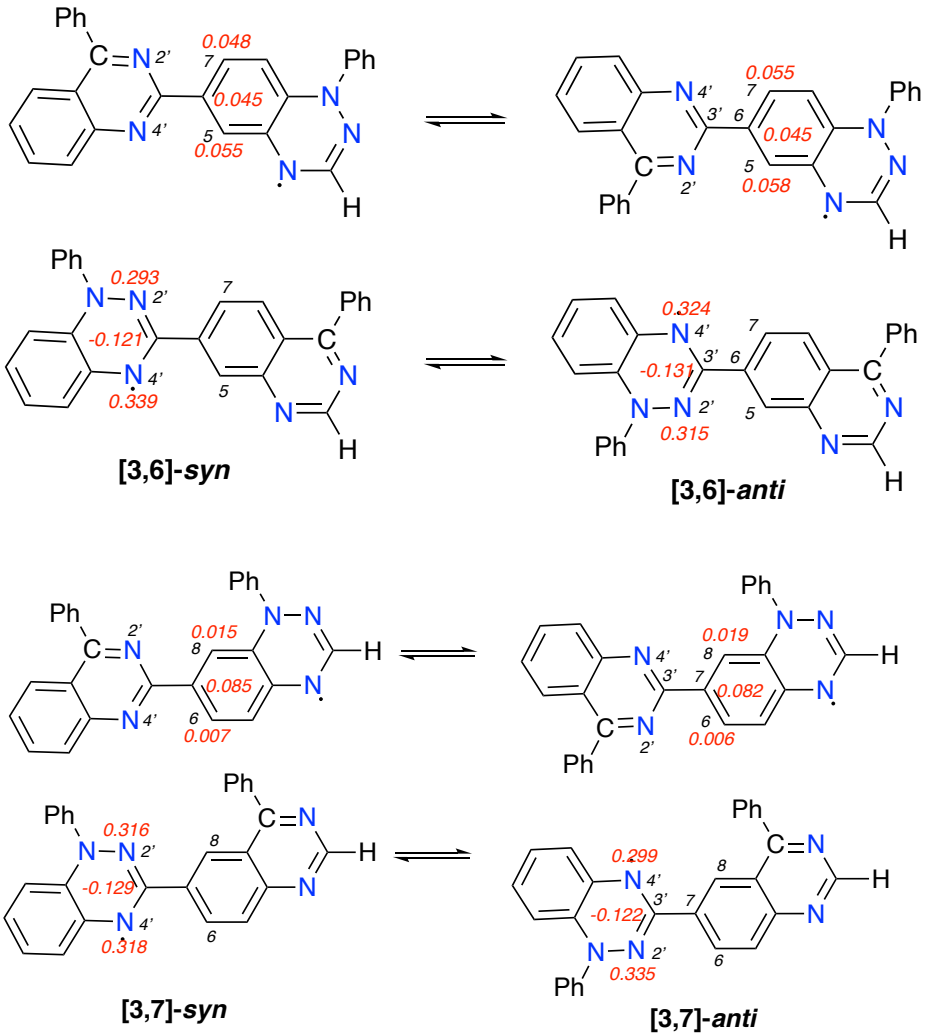


Figure S40. Spin density in key positions of two conformers in model monoradicals calculated at the UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) level of theory in benzene dielectric medium.

f) electronic excitations

Electronic excitation energies in CH_2Cl_2 dielectric medium were obtained for derivatives **1[3,n]** at the UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) level of theory using time-dependent[15] DFT method supplied in the Gaussian 09 package. Solvation models in calculations were implemented by PCM model[16] using the SCRF(solvent=CH2CL2) keyword. The lowest energy excitations with significant probability, classified as $\pi \rightarrow \pi^*$ transitions, are listed in Table S14. Energies of FMOs involved in the low energy transitions are listed in Table S15.

Table S14. Low energy electronic transitions and oscillator strength values for significant excitations in diradicals **1[3,n]**.[a]

Radical **1[3,n]**	state	$\pi \rightarrow \pi^*$ /nm (state, *f*)	$\pi \rightarrow \pi^*$ /nm (state, *f*)	$\pi \rightarrow \pi^*$ /nm (state, *f*)	$\pi \rightarrow \pi^*$ /nm (state, *f*)
1[3,6] ***anti***	T	572.9 (S2, 0.094)	478.4 (S3, 0.053)	468.3 (S4, 0.010)	432.5 (S6, 0.032)
	OSS	845.6 (S2, 0.004)	552.9 (S3, 0.022)	534.2 (S4, 0.059)	458.5 (S6, 0.035)
1[3,6] ***syn***	T	623.9 (S1, 0.033)	562.0 (S2, 0.034)	461.4 (S4, 0.039)	
	OSS	869.1 (S1, 0.076)	835.6 (S2, 0.020)	561.7 (S3, 0.019)	553.5 (S4, 0.037)
1[3,7] ***anti***	T	613.0 (S1, 0.032)	559.1 (S2, 0.15)	515.4 (S3, 0.031)	464.3 (S4, 0.055)
	OSS	908.7 (S1, 0.074)	562.6 (S3, 0.024)	537.6 (S4, 0.021)	483.8 (S5, 0.067)
1[3,7] ***syn***	T	571.4 (S2, 0.057)	493.4 (S3, 0.103)	435.5 (S6, 0.083)	435.5 (S6, 0.083)
	OSS	973.5 (S1, 0.004)	876.0 (S2, 0.004)	548.9 (S3, 0.034)	485.3 (S5, 0.045)

[a] Obtained with the UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) method in CH_2Cl_2 dielectric medium.

Table S15. Calculated energies for selected MOs.[a]

Radical **1[3,n]**	state	α-HOMO-1 β-HOMO-1 /eV	α-HOMO β-HOMO /eV	α-LUMO β-LUMO /eV	α-LUMO+1 β-LUMO+1 /eV
1[3,6] ***anti***	T	-5.059	-4.798	-1.838	-1.084
			-6.468	-2.929	-2.915
	OSS	-6.589	-4.939	-2.941	-1.708
			-4.859	-2.952	-1.702
1[3,6] ***syn***	T	-5.046	-4.789	-1.852	-1.090
			-6.433	-3.084	-2.728
	OSS	-6.612	-4.861	-2.936	-1.732
			-4.943	-2.921	-1.747
1[3,7] ***anti***	T	-5.059	-4.798	-1.838	-1.103
			-6.383	-3.120	-2.752
	OSS	-6.527	-4.949	-2.973	-1.706
			-4.852	-2.961	-1.721
1[3,7] ***syn***	T	-4.969	-4.885	-1.823	-1.095
			-6.418	-2.992	-2.897
	OSS	-6.550	-4.945	-2.994	-1.665
			-4.852	-2.963	-1.693

[a] Obtained with the UB3LYP/6-311+G(d,p) // UB3LYP/6-311G(d,p) method in CH_2Cl_2 dielectric medium.

g) partial output data for TD-DFT calculations

Excitation energies were calculated with the TD UB3LYP/6-311+G(d,p)//UB3LYP/6-311G(d,p) method in CH_2Cl_2 dielectric medium. Only the lowest energy excitations are listed along with energies of the relevant MOs.

1[3,6]-T *anti*

```
Excited State   1:  3.036-A   2.0930 eV  592.36 nm  f=0.0009  <S**2>=2.054
    124A ->126A        0.92810
    124A ->129A        0.11279
    124A ->131A       -0.11992
    125A ->126A        0.19492
    123B ->124B        0.15025
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1487.60206305
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  3.057-A   2.1643 eV  572.86 nm  f=0.0944  <S**2>=2.086
    124A ->126A       -0.19433
    125A ->126A        0.92582
    125A ->128A       -0.14779
    125A ->129A       -0.12036
    125A ->131A        0.16648

 Excited State   3:  3.125-A   2.5917 eV  478.38 nm  f=0.0526  <S**2>=2.192
    121B ->125B        0.10236
    122B ->125B        0.44594
    123B ->124B       -0.53823
    123B ->125B        0.62838

 Excited State   4:  3.070-A   2.6475 eV  468.31 nm  f=0.0103  <S**2>=2.106
    124A ->126A       -0.12746
    124A ->127A       -0.18206
    122B ->124B       -0.44373
    123B ->124B        0.60895
    123B ->125B        0.53464

Excited State   5:  3.041-A   2.7937 eV  443.80 nm  f=0.0059  <S**2>=2.062
    118B ->125B       -0.16678
    119B ->124B       -0.10358
    119B ->125B        0.22087
    120B ->125B       -0.18679
    121B ->124B       -0.35916
    121B ->125B        0.79853
    123B ->125B       -0.21161

 Excited State   6:  3.051-A   2.8664 eV  432.54 nm  f=0.0315  <S**2>=2.077
    125A ->126A        0.18713
    125A ->128A        0.81267
    125A ->131A       -0.28357
    119B ->125B       -0.17402
```

```
    122B ->125B        0.19327
    123B ->125B       -0.26426

 Excited State   7:  3.038-A   2.8985 eV  427.76 nm  f=0.0046  <S**2>=2.058
    124A ->127A        0.14168
    116B ->124B       -0.18578
    117B ->124B       -0.34900
    117B ->125B       -0.12268
    120B ->124B        0.74646
    120B ->125B        0.28724
    121B ->124B        0.23932
    122B ->124B       -0.14827
    123B ->124B       -0.16869

 Excited State   8:  3.099-A   2.9656 eV  418.07 nm  f=0.0711  <S**2>=2.150
    124A ->127A        0.91911
    120B ->124B       -0.11300
    123B ->124B        0.13898
    123B ->125B        0.10159
```

1[3,6]-T *syn*

```
Excited State   1:  3.037-A   1.9872 eV  623.91 nm  f=0.0334  <S**2>=2.056
    124A ->126A        0.24986
    124A ->131A       -0.14459
    125A ->126A        0.92518
    123B ->124B       -0.13273
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1487.60549151
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  3.062-A   2.2061 eV  562.02 nm  f=0.0335  <S**2>=2.094
    124A ->126A        0.89144
    125A ->126A       -0.25657
    125A ->129A        0.11627
    125A ->131A       -0.20704
    123B ->124B       -0.12548
    123B ->125B        0.11961

 Excited State   3:  3.097-A   2.4641 eV  503.17 nm  f=0.0009  <S**2>=2.148
    124A ->126A        0.15217
    122B ->125B        0.25735
    123B ->124B        0.90912

 Excited State   4:  3.071-A   2.6870 eV  461.42 nm  f=0.0389  <S**2>=2.108
    124A ->127A       -0.10673
    125A ->127A       -0.12224
    125A ->128A       -0.11794
    125A ->131A        0.12875
    120B ->124B        0.14862
    121B ->124B        0.21193
    121B ->125B        0.25187
    122B ->124B        0.60869
    123B ->125B        0.58310

 Excited State   5:  3.048-A   2.7845 eV  445.27 nm  f=0.0119  <S**2>=2.072
```

```
    125A ->128A        0.11081
    118B ->124B       -0.13620
    118B ->125B       -0.10900
    119B ->124B       -0.15556
    119B ->125B       -0.11617
    120B ->125B        0.16370
    121B ->124B        0.68686
    121B ->125B        0.49689
    122B ->124B       -0.11493
    122B ->125B        0.10658
    123B ->125B       -0.28335

 Excited State   6:  3.044-A   2.8616 eV  433.27 nm  f=0.0021  <S**2>=2.066
    125A ->127A        0.11913
    125A ->128A        0.20632
    115B ->124B        0.17257
    115B ->125B       -0.10309
    117B ->124B        0.28544
    117B ->125B       -0.18381
    119B ->124B        0.24735
    119B ->125B       -0.20348
    120B ->124B        0.68858
    120B ->125B       -0.36454

 Excited State   7:  3.056-A   2.8988 eV  427.71 nm  f=0.0478  <S**2>=2.085
    124A ->126A       -0.10100
    124A ->127A       -0.15290
    124A ->128A       -0.29983
    124A ->131A        0.12223
    125A ->128A        0.72775
    125A ->129A        0.12827
    125A ->131A       -0.21892
    125A ->133A       -0.10254
    117B ->124B       -0.10108
    119B ->124B       -0.16571
    120B ->125B        0.15639
    122B ->125B       -0.10427
    123B ->125B        0.32360

 Excited State   8:  3.089-A   2.9407 eV  421.62 nm  f=0.0840  <S**2>=2.136
    124A ->126A       -0.10837
    124A ->127A        0.57359
    125A ->127A        0.71779
```

1[3,6]-S *anti*

```
Excited State   1:  1.367-A   1.3389 eV  925.99 nm  f=0.0019  <S**2>=0.217
    124A ->125A       -0.53938
    124A ->126A       -0.15610
    124B ->125B        0.81616
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1487.62908966
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  1.292-A   1.4662 eV  845.64 nm  f=0.0042  <S**2>=0.167
    124A ->125A        0.80919
```

```
   124A ->126A        0.13827
   124B ->125B        0.56384

 Excited State   3:  2.255-A   2.2425 eV  552.89 nm  f=0.0215  <S**2>=1.021
   124A ->125A        0.15071
   124A ->126A       -0.63899
   124B ->126B        0.68115
   124B ->128B       -0.12608
   124B ->131B        0.12405

 Excited State   4:  2.234-A   2.3211 eV  534.17 nm  f=0.0594  <S**2>=0.997
   124A ->125A       -0.15680
   124A ->126A        0.66863
   124A ->131A       -0.11822
   124B ->126B        0.64269
   124B ->128B       -0.10727
   124B ->131B        0.11896

 Excited State   5:  2.396-A   2.6064 eV  475.69 nm  f=0.0093  <S**2>=1.185
   121A ->125A       -0.18250
   122A ->125A        0.16751
   123A ->125A        0.84719
   123B ->125B        0.30474
   124B ->128B        0.13074

 Excited State   6:  2.333-A   2.7040 eV  458.52 nm  f=0.0351  <S**2>=1.111
   121A ->125A        0.21146
   122A ->125A       -0.17515
   123A ->125A       -0.22778
   124A ->127A        0.19860
   116B ->125B       -0.11163
   121B ->125B        0.14840
   122B ->125B        0.21395
   123B ->125B        0.81577
   124B ->128B       -0.11248

 Excited State   7:  2.301-A   2.7846 eV  445.25 nm  f=0.0089  <S**2>=1.074
   119A ->125A        0.23484
   121A ->125A        0.86849
   122A ->125A       -0.11673
   123A ->125A        0.23201
   123B ->125B       -0.12382
   124B ->128B        0.19710

 Excited State   8:  2.318-A   2.8779 eV  430.82 nm  f=0.0528  <S**2>=1.093
   115A ->125A       -0.10117
   121A ->125A       -0.11185
   122A ->125A        0.17065
   123A ->125A       -0.25500
   121B ->125B        0.15283
   124B ->126B        0.19129
   124B ->128B        0.81317
   124B ->130B       -0.10599
   124B ->131B       -0.24871
```

1[3,6]-S *syn*

```
Excited State   1:  1.265-A    1.4266 eV  869.09 nm  f=0.0757  <S**2>=0.150
    124A ->125A        0.98477
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1487.62657997
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  1.325-A   1.4837 eV  835.62 nm  f=0.0195  <S**2>=0.189
    124A ->125A        0.12153
    124B ->125B        0.96785
    124B ->126B        0.18908

 Excited State   3:  2.398-A   2.2073 eV  561.71 nm  f=0.0189  <S**2>=1.187
    124A ->126A        0.84259
    124A ->131A        0.16893
    124B ->126B        0.42416

 Excited State   4:  2.102-A   2.2400 eV  553.51 nm  f=0.0373  <S**2>=0.854
    124A ->126A       -0.43079
    124A ->131A       -0.11276
    124B ->125B       -0.19803
    124B ->126B        0.82546
    124B ->131B       -0.14585

 Excited State   5:  2.367-A   2.6273 eV  471.91 nm  f=0.0365  <S**2>=1.150
    123A ->125A        0.12870
    124A ->128A        0.12425
    117B ->125B        0.10355
    121B ->125B       -0.18255
    122B ->125B       -0.24844
    123B ->125B        0.88250

 Excited State   6:  2.347-A   2.6895 eV  460.99 nm  f=0.0292  <S**2>=1.127
    121A ->125A       -0.14589
    122A ->125A        0.21927
    123A ->125A        0.88815
    123B ->125B       -0.12760
    124B ->126B        0.10052
    124B ->127B        0.19646
```

1[3,7]-T *anti*

```
Excited State   1:  3.033-A    2.0225 eV  613.02 nm  f=0.0315  <S**2>=2.050
    124A ->126A       -0.22770
    124A ->131A        0.15366
    125A ->126A        0.93467
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1487.60488970
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  3.062-A   2.2177 eV  559.07 nm  f=0.0148  <S**2>=2.094
    124A ->126A        0.86024
    125A ->126A        0.22355
    125A ->131A        0.20265
    123B ->124B       -0.30676
```

```
Excited State   3:  3.075-A   2.4058 eV  515.36 nm  f=0.0307  <S**2>=2.115
   124A ->126A        0.29109
   122B ->125B        0.21949
   123B ->124B        0.87974
   123B ->125B       -0.15760

Excited State   4:  3.066-A   2.6701 eV  464.34 nm  f=0.0547  <S**2>=2.101
   124A ->126A        0.10952
   124A ->127A        0.13695
   120B ->125B       -0.11310
   121B ->124B        0.22191
   121B ->125B       -0.11308
   122B ->124B        0.57727
   123B ->124B        0.10031
   123B ->125B        0.66312

Excited State   5:  3.046-A   2.7964 eV  443.37 nm  f=0.0079  <S**2>=2.069
   125A ->128A       -0.11219
   116B ->125B       -0.14077
   118B ->124B        0.17538
   118B ->125B       -0.17148
   120B ->125B       -0.19751
   121B ->124B        0.73924
   121B ->125B       -0.39136
   123B ->125B       -0.31039

Excited State   6:  3.076-A   2.8593 eV  433.62 nm  f=0.0576  <S**2>=2.116
   124A ->126A        0.11191
   124A ->128A        0.26418
   125A ->127A        0.28082
   125A ->128A        0.63040
   115B ->124B        0.13494
   116B ->124B        0.20041
   118B ->124B        0.10850
   120B ->124B        0.36163
   120B ->125B        0.16874
   121B ->125B       -0.26648
   122B ->124B       -0.13683
   122B ->125B       -0.12330

Excited State   7:  3.056-A   2.8684 eV  432.25 nm  f=0.0260  <S**2>=2.084
   124A ->128A       -0.21291
   125A ->127A       -0.29872
   125A ->128A       -0.44430
   115B ->124B        0.18640
   115B ->125B        0.10829
   116B ->124B        0.30153
   116B ->125B        0.12773
   118B ->124B        0.13031
   120B ->124B        0.48388
   120B ->125B        0.23901
   121B ->124B       -0.11422
   121B ->125B       -0.30300
   122B ->125B       -0.12715
   123B ->125B        0.13138
```

```
 Excited State   8:  3.095-A   2.9459 eV  420.87 nm  f=0.0989  <S**2>=2.145
    124A ->127A       -0.59764
    125A ->127A        0.62615
    125A ->128A       -0.32517
    123B ->125B        0.15700
```

1[3,7]-T syn

```
Excited State   1:  3.035-A   2.1282 eV  582.58 nm  f=0.0060  <S**2>=2.053
    124A ->126A        0.93808
    124A ->131A        0.14322
    125A ->126A        0.15274
    123B ->125B       -0.12979
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1487.60136394
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  3.048-A   2.1700 eV  571.37 nm  f=0.0566  <S**2>=2.072
    124A ->126A       -0.14619
    125A ->126A        0.92495
    125A ->128A        0.16154
    125A ->131A       -0.17057
    123B ->124B        0.12552

 Excited State   3:  3.094-A   2.5129 eV  493.39 nm  f=0.1034  <S**2>=2.142
    122B ->124B        0.17760
    122B ->125B       -0.25878
    123B ->124B        0.84570
    123B ->125B       -0.30739

 Excited State   4:  3.070-A   2.6562 eV  466.77 nm  f=0.0088  <S**2>=2.106
    124A ->126A        0.13685
    124A ->127A       -0.17803
    122B ->124B       -0.36915
    122B ->125B       -0.30796
    123B ->124B        0.24484
    123B ->125B        0.76291

 Excited State   5:  3.043-A   2.8121 eV  440.89 nm  f=0.0033  <S**2>=2.065
    117B ->124B        0.10427
    118B ->124B        0.18747
    118B ->125B       -0.12689
    119B ->124B       -0.13652
    120B ->124B       -0.13435
    120B ->125B        0.10231
    121B ->124B        0.74390
    121B ->125B       -0.48927
    121B ->126B        0.12045
    123B ->125B       -0.13839

 Excited State   6:  3.086-A   2.8467 eV  435.53 nm  f=0.0827  <S**2>=2.131
    125A ->126A       -0.19564
    125A ->128A        0.92960
    125A ->131A       -0.10137
    125A ->133A        0.11067
```

```
 Excited State   7:  3.042-A   2.8860 eV  429.60 nm  f=0.0051  <S**2>=2.063
    115B ->124B       -0.14518
    115B ->125B       -0.16958
    116B ->124B       -0.14114
    116B ->125B       -0.16220
    117B ->124B       -0.17128
    117B ->125B       -0.18167
    119B ->124B        0.12083
    119B ->125B        0.15228
    120B ->124B        0.46402
    120B ->125B        0.55909
    121B ->124B        0.17333
    121B ->125B        0.26768
    122B ->124B       -0.17881
    122B ->125B       -0.22939
    123B ->124B       -0.11041
    123B ->125B       -0.20665

 Excited State   8:  3.101-A   2.9689 eV  417.61 nm  f=0.0735  <S**2>=2.155
    124A ->127A        0.92477
    125A ->127A        0.12763
    123B ->125B        0.15761
```

1[3,7]-S *anti*

```
Excited State   1:  1.313-A   1.3645 eV  908.65 nm  f=0.0740  <S**2>=0.181
    124A ->125A       -0.49194
    124A ->126A       -0.16670
    124B ->125B        0.84416
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1487.62920700
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  1.339-A   1.4105 eV  879.02 nm  f=0.0014  <S**2>=0.198
    124A ->125A        0.83769
    124A ->126A        0.13400
    124B ->125B        0.52156

 Excited State   3:  2.378-A   2.2038 eV  562.60 nm  f=0.0235  <S**2>=1.163
    124A ->126A        0.21189
    124B ->126B        0.91959
    124B ->127B       -0.12466
    124B ->131B       -0.20814

 Excited State   4:  2.096-A   2.3064 eV  537.56 nm  f=0.0213  <S**2>=0.848
    124A ->125A       -0.22283
    124A ->126A        0.90176
    124A ->131A       -0.15528
    123B ->125B       -0.11596
    124B ->126B       -0.20375

 Excited State   5:  2.372-A   2.5630 eV  483.75 nm  f=0.0673  <S**2>=1.156
    122A ->125A        0.21216
    123A ->125A        0.92653

 Excited State   6:  2.330-A   2.6681 eV  464.68 nm  f=0.0418  <S**2>=1.108
    124A ->126A        0.10448
```

```
    124A ->127A        0.19620
    122B ->125B        0.32063
    123B ->125B        0.88030

 Excited State   7:  2.299-A   2.8091 eV  441.36 nm  f=0.0035  <S**2>=1.072
    118A ->125A       -0.10083
    119A ->125A        0.21156
    120A ->125A        0.14840
    121A ->125A        0.87055
    121A ->126A       -0.12685
    122A ->125A       -0.26653
    123A ->125A        0.15955

 Excited State   8:  2.311-A   2.8970 eV  427.97 nm  f=0.0228  <S**2>=1.085
    124A ->127A       -0.13088
    117B ->125B       -0.21594
    118B ->125B       -0.26761
    120B ->125B       -0.30648
    121B ->125B        0.55280
    122B ->125B        0.26670
    124B ->127B       -0.51955
    124B ->128B       -0.19491
```

1[3,7]-S *syn*

```
Excited State   1:  1.415-A   1.2735 eV  973.54 nm  f=0.0043  <S**2>=0.251
    124A ->125A       -0.68449
    124A ->126A        0.17625
    124B ->125B        0.69403
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1487.63170215
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  1.288-A   1.4153 eV  876.00 nm  f=0.0043  <S**2>=0.165
    124A ->125A        0.69157
    124A ->126A       -0.10580
    124B ->125B        0.70952

 Excited State   3:  2.290-A   2.2588 eV  548.89 nm  f=0.0340  <S**2>=1.061
    124A ->126A       -0.29568
    124B ->126B        0.87773
    124B ->127B        0.19078
    124B ->131B       -0.17947

 Excited State   4:  2.183-A   2.3486 eV  527.90 nm  f=0.0085  <S**2>=0.942
    123A ->125A        0.18389
    124A ->125A        0.19560
    124A ->126A        0.86954
    124A ->131A        0.14071
    123B ->125B        0.11578
    124B ->126B        0.27660

 Excited State   5:  2.369-A   2.5551 eV  485.25 nm  f=0.0446  <S**2>=1.153
    121A ->125A        0.12974
    122A ->125A        0.16640
    123A ->125A        0.88382
```

```
    124A ->126A       -0.16263
    122B ->125B       -0.11241
    123B ->125B        0.20137
    124B ->126B       -0.12256
    124B ->127B       -0.11087

 Excited State   6:  2.322-A   2.7048 eV  458.39 nm  f=0.0376  <S**2>=1.098
    121A ->125A       -0.15007
    122A ->125A       -0.11519
    123A ->125A       -0.19890
    124A ->127A        0.20398
    122B ->125B       -0.35889
    123B ->125B        0.81638
```

2

```
Excited State     1:    2.086-A          2.5287  eV    490.31  nm    f=0.0071
<S**2>=0.838
     71A -> 72A        0.85938
     71A -> 73A       -0.41366
     71A -> 74A       -0.18658
     66B -> 71B        0.11191
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -822.995565353
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State     2:    2.109-A          2.6753  eV    463.43  nm    f=0.0329
<S**2>=0.862
     71A -> 72A        0.17259
     71A -> 73A        0.11911
     67B -> 71B        0.10414
     69B -> 71B        0.27640
     70B -> 71B        0.90284

 Excited State     3:    2.053-A          2.8415  eV    436.33  nm    f=0.0035
<S**2>=0.804
     71A -> 72A       -0.11826
     71A -> 73A       -0.17571
     68B -> 71B        0.22215
     69B -> 71B        0.89879
     70B -> 71B       -0.24242

 Excited State     4:    2.104-A          2.9452  eV    420.97  nm    f=0.0798
<S**2>=0.857
     71A -> 72A        0.39498
     71A -> 73A        0.82427
     71A -> 74A        0.12203
     66B -> 71B       -0.12370
     67B -> 71B       -0.10109
     69B -> 71B        0.16308
     70B -> 71B       -0.22681

 Excited State     5:    2.116-A          3.2928  eV    376.53  nm    f=0.0054
<S**2>=0.869
     71A -> 72A        0.10237
     71A -> 73A       -0.20477
     71A -> 74A        0.92738
```

```
     71A -> 75A         0.13606
     68B -> 71B        -0.13319
```

8. Archive for DFT calculations

1[3,6]-T, *anti*

```
1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C30H26N6(3)\PKASZYNSKI\08
 -Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,No
 Angle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-tBu-1-Ph-benzo[e][1
 ,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer anti\\0,
 3\C,-0.4103196743,-1.9697230408,-0.12010716\C,0.4218029976,-0.83636597
 39,-0.0425634681\C,-1.7886633402,-1.8501585771,-0.1056318614\C,-0.1634
 879555,0.4253558755,0.023356204\C,-2.3786149298,-0.5803103579,-0.00707
 98137\C,-1.5575843843,0.5829766039,0.0253660979\N,-2.1027302656,1.8396
 724461,0.0363295048\N,-3.7471436134,-0.3586973222,0.0338368485\N,-4.28
 7788132,0.8958432681,-0.0518737198\C,-3.4329970475,1.9138941871,-0.045
 6469123\C,-4.7172106179,-1.4087325158,0.1199132424\C,-5.7625143084,-1.
 4493783922,-0.8040729415\C,-4.6435468403,-2.3534458585,1.1452628297\C,
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 \C,4.5925911567,-1.2428275764,-0.1619302446\N,2.3765754994,-2.25602378
 71,-0.0850108309\N,2.6077159909,0.119664691,-0.0081569021\N,3.96123141
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 ,1.1172342411\C,4.9922583222,3.5131077803,-0.5655775105\C,6.3014090211
 ,2.6070844525,1.2460418819\C,5.9804777045,3.6713398812,0.4053671949\C,
 4.3173008879,-3.6550565045,-0.2998724376\C,5.9732491168,-1.3961577078,
 -0.3428057655\C,5.686251688,-3.8007641213,-0.4459595211\C,6.5113852039
 ,-2.6695177309,-0.4792837994\H,-2.4062884052,-2.7342701948,-0.17728744
 9\H,0.4461209862,1.3170877954,0.0660183872\H,-5.8139890413,-0.69555195
 75,-1.5784448323\H,-3.848779268,-2.2959429377,1.8784496558\H,-7.533715
 9552,-2.4825460558,-1.4292971008\H,-5.5531353297,-4.0828778031,2.02832
 61184\H,-7.3996833537,-4.1849270184,0.3723887198\H,0.0502296486,-2.945
 10269,-0.1952322372\H,3.5580289478,2.1624123626,-1.4492368414\H,5.8734
 48764,0.5668495279,1.7869630393\H,4.7335132873,4.338626411,-1.21834760
 34\H,7.0550364377,2.7283558593,2.0154232795\H,6.4916163015,4.620988221
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 33,-0.5291468393,-0.3816345082\H,3.6508026506,-4.5088095985,-0.2944057
 075\H,7.5803655845,-2.7808637846,-0.6167805749\C,-3.6200574349,4.09408
 50693,1.1489180207\H,-2.5337248716,4.1237936038,1.2430853823\H,-3.9966
 812883,5.1202015011,1.1030524988\H,-4.0302904183,3.6230330224,2.047129
 4136\C,-5.5736104876,3.2873524613,-0.2148112372\H,-5.9098760382,2.7581
 165569,-1.1088284763\H,-6.0183956004,2.7917279876,0.6500577438\H,-5.95
 49048042,4.3116856875,-0.2601540075\C,-4.039974462,3.3210265473,-0.120
 8298643\C,-3.4645956874,4.0310274368,-1.3659590411\H,-3.8471574853,5.0
 54338558,-1.4227476686\H,-2.375194693,4.0664546424,-1.3232317728\H,-3.
 7555190051,3.5103458509,-2.2833565299\\Version=ES64L-G09RevD.01\State=
 3-A\HF=-1487.6576401\S2=2.028123\S2-1=0.\S2A=2.000459\RMSD=6.919e-09\R
 MSF=3.826e-06\Dipole=0.9839986,-0.6243977,-0.002848\Quadrupole=18.3049
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 6N6)]\\@
```

1[3,6]-T, *syn*

```
1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C30H26N6(3)\PKASZYNSKI\08
```

-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,No
Angle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-tBu-1-Ph-benzo[e][1
,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer syn\\0,3
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,-0.01576246\C,-1.3015739988,1.4231323445,0.0895848475\C,-0.4998060583
,-1.2509444978,-0.0851359856\C,-2.2717896998,0.413040258,-0.0132277619
\C,-1.870944599,-0.9509090991,-0.0708545258\N,-2.7915177526,-1.9657864
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296062,-0.3695428585,0.051314116\C,-4.0731552378,-1.6086021298,0.01807
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9591927,0.8369838803\C,-3.8482249943,2.8511923483,-1.0911034513\C,-5.8
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0102076,-0.0348125801\C,3.5656798329,-2.1839201896,-0.1226422411\C,4.5
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0257\C,5.5522796295,3.3669182235,1.143779754\C,6.714114562,2.621782491
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3\C,5.3265045709,-3.8550594998,-0.0834459136\C,6.2840574311,-2.8476902
994,0.092212241\H,-1.599829305,2.4582012564,0.1779377631\H,-0.20288122
34,-2.288712536,-0.1411335821\H,-5.4997830957,1.5802817841,1.590835263
2\H,-3.1100934088,2.5630580801,-1.8289545616\H,-6.5630689178,3.8238080
813,1.4939999854\H,-4.1575189352,4.8019422726,-1.9257354887\H,-5.88551
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,-1.6862047565\H,5.4096255923,4.0967493115,1.9322598842\H,7.4685747053
,2.7756950639,-1.5969082917\H,7.1672403741,4.4456481808,0.2145147479\H
,5.6351160853,-4.8927361422,-0.1295957678\H,6.6520176956,-0.7435706269
,0.2936390118\H,3.2196133672,-4.2827026296,-0.2977591309\H,7.331555908
1,-3.1061960233,0.1922121261\C,-5.0024620109,-3.5516846289,-1.23218426
68\H,-3.990356258,-3.9317844073,-1.3783538407\H,-5.6943425819,-4.39865
92237,-1.2046674198\H,-5.2639550746,-2.9290068602,-2.0929297089\C,-6.5
354558544,-2.2212100675,0.2542355593\H,-6.6460276028,-1.6533497079,1.1
806085622\H,-6.8264529358,-1.5683959185,-0.5705135703\H,-7.2284363278,
-3.0670041598,0.2869903658\C,-5.1013902803,-2.7457099993,0.0823607329\
C,-4.7421430669,-3.6613479065,1.2726171746\H,-5.4324566737,-4.50905644
9,1.3145790686\H,-3.7249250316,-4.0422963148,1.1749168842\H,-4.8156612
969,-3.1190003926,2.2201506985\\Version=ES64L-G09RevD.01\State=3-A\HF=
-1487.6570143\S2=2.028181\S2-1=0.\S2A=2.000461\RMSD=5.998e-09\RMSF=4.4
41e-06\Dipole=1.5625061,1.8226954,0.0983654\Quadrupole=14.2618782,-0.3
285983,-13.9332799,-5.803,-3.7941502,0.201144\PG=C01 [X(C30H26N6)]\\@

1[3,6]-T,TS

1\1\GINC-LOCALHOST\FTS\UB3LYP\6-311G(d,p)\C30H26N6(3)\PIOTR\25-Jun-202
4\0\\#P UB3LYP/6-311G(d,p) Opt=QST3 SCF=Direct Geom=(NoDistance,NoAngl
e) fcheck #P freq SCRF=(solvent=Benzene)\\3-(3-tBu-1-Ph-benzo[e][1,2,4
]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer anti\\0,3\C,-
0.4149849912,-1.9945834084,-0.0780848108\C,0.4150421444,-0.863460937,-
0.0276172677\C,-1.7958683372,-1.8662010989,-0.0641525424\C,-0.15461464
71,0.398906446,0.0096600844\C,-2.375793686,-0.5921677006,0.0101042573\
C,-1.5518333412,0.5671961642,0.0143700342\N,-2.0846873681,1.8264459022
,-0.0029469261\N,-3.74827309,-0.3597906464,0.0508115222\N,-4.275934818
8,0.8960369831,-0.0759015353\C,-3.415792725,1.9075723435,-0.0937723557
\C,-4.7258589934,-1.3965924187,0.1751028496\C,-5.7958477208,-1.4362955

177,-0.7210537622\C,-4.638809353,-2.3299502467,1.2105917244\C,-6.76785
74499,-2.4224176228,-0.5881353897\C,-5.6144557261,-3.315789532,1.33157
3042\C,-6.6787478464,-3.3675801613,0.4332501717\C,1.9044758645,-1.0215
432437,-0.0439066765\C,3.8774699322,-1.0982333871,-1.1990988063\C,4.59
5298691,-1.1762307929,0.0271119485\N,2.504956948,-1.0533596971,-1.2311
507808\N,2.4617637613,-1.1289635477,1.1591729633\N,3.8205355898,-1.281
9917162,1.1838744608\C,4.3613973764,-1.4924742433,2.4911624995\C,3.940
8190946,-0.6727619109,3.5406705972\C,5.2576244034,-2.5375990708,2.7279
662812\C,4.435603269,-0.889646687,4.8223058097\C,5.7499477445,-2.74243
68087,4.0139662652\C,5.3448365174,-1.9191435753,5.0629951797\C,4.60361
77309,-1.0312422486,-2.4015518255\C,5.995836144,-1.1143959739,0.027490
5348\C,5.9876249548,-1.0071512481,-2.3944376236\C,6.6809406823,-1.0348
936594,-1.1776416602\H,-2.4188790702,-2.7479322945,-0.1154889711\H,0.4
554257196,1.293698746,0.0209741484\H,-5.8577527292,-0.6921515957,-1.50
38016106\H,-3.8262623902,-2.2730936409,1.9239569648\H,-7.5956188793,-2
.4533967343,-1.2871298094\H,-5.5474762973,-4.0353655101,2.1392872336\H
,-7.4377183175,-4.1346866803,0.5328741566\H,0.0271971281,-2.9820061283
,-0.1336681539\H,3.2252234991,0.1139562871,3.3426670642\H,5.5504823944
,-3.1948664984,1.9190442121\H,4.110551177,-0.2499251419,5.6345239206\H
,6.440808272,-3.5573388983,4.1963112699\H,5.728434388,-2.0840113145,6.
0629994805\H,6.534488014,-0.9520625064,-3.3282357248\H,6.5414432698,-1
.122166647,0.9603892801\H,4.0355930626,-0.9826323698,-3.3223748043\H,7
.7634967656,-0.9890819213,-1.1688668195\C,-3.6019193642,4.1153080592,1
.0480174489\H,-2.5165302105,4.141798906,1.1537596042\H,-3.9723044051,5
.1420773216,0.9750035791\H,-4.0247266733,3.6665498789,1.9518110768\C,-
5.5444778896,3.2891325106,-0.3195314095\H,-5.8727801593,2.7404356824,-
1.204701769\H,-6.0019259477,2.816367194,0.5514958758\H,-5.9197735044,4
.3140207512,-0.3933467792\C,-4.0120334431,3.3163631427,-0.2089864588\C
,-3.4180587031,3.9944465132,-1.4631172847\H,-3.792935646,5.0187282519,
-1.5469800006\H,-2.328960585,4.0238253228,-1.4096652398\H,-3.702330289
7,3.4552334661,-2.371775213\\Version=ES64L-G16RevC.01\State=3-A\HF=-14
87.6471338\S2=2.027604\S2-1=0.\S2A=2.000457\RMSD=4.895e-09\RMSF=3.268e
-06\Dipole=0.9780137,-1.4064093,0.8188553\Quadrupole=17.4717633,-10.93
2948,-6.5388153,3.772887,7.1460384,-2.4139495\PG=C01 [X(C30H26N6)]\\

1[3,6]-S, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C30H26N6\PKASZYNSKI\08-Ja
n-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAng
le) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-tBu-
1-Ph-benzo[e][1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazinyl, conf
ormer anti\\0,1\C,-0.4109178082,-1.9734449046,-0.1283669063\C,0.421090
4181,-0.8411300334,-0.0447531358\C,-1.7901136632,-1.8522507813,-0.1135
035524\C,-0.1627266101,0.4198421231,0.0271248322\C,-2.3790780374,-0.58
37544955,-0.0083720848\C,-1.558310456,0.5784624138,0.0289264326\N,-2.0
991867272,1.8357274521,0.0421149615\N,-3.7502787769,-0.359626721,0.034
0476103\N,-4.2856527856,0.8964548123,-0.0556323898\C,-3.4303426588,1.9
126563742,-0.0461443982\C,-4.72217813,-1.4064338641,0.1219019381\C,-5.
7785627705,-1.4360484933,-0.7902890744\C,-4.6406264766,-2.3608966914,1
.1380213356\C,-6.742772597,-2.4341035546,-0.6929854679\C,-5.6082715417
,-3.3582013121,1.2237183508\C,-6.6588878048,-3.4003111689,0.3089436427
\C,1.8989167562,-1.0123722154,-0.0518448325\C,3.7388094853,-2.37994495
59,-0.1723915202\C,4.5940602951,-1.24238119,-0.1631440461\N,2.37871836
08,-2.2569594988,-0.0864473326\N,2.6077024158,0.1179507519,-0.00956988
62\N,3.9621931052,-0.0089862264,0.0021886734\C,4.667062455,1.230839013
4,0.1339840021\C,4.329969426,2.2976173964,-0.7006047096\C,5.6452906766
,1.3845049787,1.1182938938\C,4.9879819866,3.5149641599,-0.5578803805\C
,6.3009446546,2.6057282203,1.2493665561\C,5.9775061913,3.6718166386,0.

4119827285\C,4.3202285829,-3.6550204813,-0.3019010161\C,5.9750684641,-
1.3949689913,-0.3445980663\C,5.689161262,-3.79977499,-0.4483380559\C,6
.5136246952,-2.6678099038,-0.4815999115\H,-2.4080316019,-2.7358268054,
-0.189599006\H,0.4471056698,1.3112349704,0.0740179002\H,-5.8364143176,
-0.6754516817,-1.5575015691\H,-3.8379538273,-2.3125666642,1.8631477672
\H,-7.5602407417,-2.4575928947,-1.4042783952\H,-5.5458795513,-4.094840
2785,2.0162492594\H,-7.4116357572,-4.176631444,0.380594881\H,0.0485699
937,-2.9489184239,-0.208071812\H,3.5538975452,2.1649784442,-1.44284219
8\H,5.8762331849,0.5636668146,1.7856640304\H,4.7272708252,4.341901702,
-1.2080650359\H,7.0555271627,2.7258632563,2.0179854558\H,6.4876606699,
4.6217913941,0.5199546706\H,6.1222859658,-4.7878587014,-0.5499196384\H
,6.6187662384,-0.5275924031,-0.3835190925\H,3.6542413904,-4.5091637461
,-0.2965826721\H,7.5826042474,-2.7785624734,-0.6195985641\C,-3.6173614
364,4.0935036324,1.1469067909\H,-2.5313946429,4.1204968542,1.246134085
2\H,-3.9910279706,5.1205947071,1.0989056207\H,-4.032989305,3.623857293
1,2.0433600509\C,-5.5666761912,3.2908950347,-0.2253523298\H,-5.9001496
036,2.7625959326,-1.1209912585\H,-6.0164340303,2.7961875195,0.63746908
41\H,-5.9454615985,4.3160775645,-0.272292412\C,-4.0334544983,3.3210811
639,-0.1245339383\C,-3.4508330613,4.0294123772,-1.367273314\H,-3.83040
04389,5.0537275959,-1.425831652\H,-2.3615182897,4.0620553414,-1.319905
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.654e-09\RMSF=2.327e-06\Dipole=1.0376292,-0.5868247,-0.0045588\Quadrup
ole=18.3141868,-3.0964146,-15.2177723,13.7348022,3.7524887,-2.7643323\
PG=C01 [X(C30H26N6)]\\@

1[3,6]-S, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C30H26N6\PKASZYNSKI\09-Ja
n-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAng
le) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-tBu-
1-Ph-benzo[e][1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2,4]triazi nyl, conf
ormer syn\\0,1\C,0.0457019926,1.0894180245,0.0854257491\C,0.4637323327
,-0.2518954922,-0.016249558\C,-1.2984676054,1.4207799065,0.0914332218\
C,-0.4974900909,-1.2538880149,-0.0884428766\C,-2.2689764687,0.41287821
44,-0.0132682356\C,-1.8698358974,-0.9527283747,-0.0733378127\N,-2.7883
360829,-1.9655451949,-0.091404903\N,-3.6383149803,0.645733756,-0.03468
17468\N,-4.5513109916,-0.3707317932,0.0495017991\C,-4.0722535827,-1.60
83933895,0.0153711204\C,-4.2219712307,1.951328561,-0.0895714153\C,-5.2
093735439,2.2952297036,0.8355403712\C,-3.8440210164,2.853593633,-1.086
2896245\C,-5.8043525282,3.5509635228,0.7709569257\C,-4.4422937158,4.10
96617617,-1.1389419442\C,-5.4202585289,4.4633746372,-0.2111357879\C,1.
9064859358,-0.6066827373,-0.0348203693\C,3.5688558042,-2.1871434975,-0
.1192776377\C,4.5545223492,-1.1698765969,0.0162460318\N,2.2332277713,-
1.893335534,-0.1698066204\N,2.746133975,0.4259372349,0.074723589\N,4.0
73542917,0.1417838236,0.0402731535\C,4.9242463858,1.2936867782,0.09075
89725\C,4.7387735261,2.2336419904,1.1054351148\C,5.8971036052,1.493310
5936,-0.8899939625\C,5.5418855036,3.3690555451,1.1439842706\C,6.698563
5122,2.6308143571,-0.8397961304\C,6.5258927905,3.5688634637,0.17642779
31\C,3.9947421334,-3.5270715025,-0.1772107995\C,5.9079150906,-1.506011
0142,0.1460885279\C,5.337421283,-3.8505513597,-0.0780290625\C,6.291767
9751,-2.8402368406,0.09452134\H,-1.5955751752,2.4560844499,0.180933904
\H,-0.2005051825,-2.2914807151,-0.1467819348\H,-5.5038778448,1.5745233
867,1.5866461446\H,-3.1030404556,2.5681686611,-1.8223124724\H,-6.56833
38019,3.8173794251,1.4921177062\H,-4.151589928,4.8064029616,-1.9165481
792\H,-5.8858068364,5.4408861159,-0.2577726904\H,0.7912500445,1.868992
0078,0.1591462578\H,3.967840556,2.0685228738,1.8468027461\H,6.01279213
47,0.7748430404,-1.6919234175\H,5.4000915915,4.0970314657,1.9343115728

\H,7.4498215563,2.7883330528,-1.6048791597\H,7.1499261619,4.4542125929
,0.2104278061\H,5.6494654904,-4.8873469089,-0.1224758303\H,6.650072738
7,-0.7335385907,0.2910467714\H,3.2320572851,-4.2877077465,-0.289648206
5\H,7.3403390712,-3.0944064176,0.1937655652\C,-4.9985047289,-3.5531632
477,-1.2343136393\H,-3.9858616535,-3.9319859867,-1.3801316696\H,-5.689
0633509,-4.4011736057,-1.2062292403\H,-5.260844647,-2.9315201024,-2.09
55398751\C,-6.5334390815,-2.2229386483,0.2505220059\H,-6.6449077134,-1
.6547599685,1.1765948079\H,-6.8244175729,-1.5706943995,-0.5747111092\H
,-7.2258557039,-3.0691673304,0.2832311823\C,-5.0989437393,-2.746418961
5,0.0796741267\C,-4.7392454703,-3.6609173595,1.2707395165\H,-5.4287001
162,-4.5092923393,1.3128502145\H,-3.7216442085,-4.0410975606,1.1737997
383\H,-4.8137890388,-3.1180583098,2.2178888643\\Version=ES64L-G09RevD.
01\State=1-A\HF=-1487.6574391\S2=0.997985\S2-1=0.\S2A=0.222815\RMSD=8.
561e-09\RMSF=3.835e-06\Dipole=1.5281455,1.8507439,0.1010633\Quadrupole
=14.3590741,-0.4459325,-13.9131416,-5.0816663,-3.807983,0.1863334\PG=C
01 [X(C30H26N6)]\\@

1[3,6]-S,TS

1\1\GINC-LOCALHOST\FTS\UB3LYP\6-311G(d,p)\C30H26N6\PIOTR\27-Jun-2024\0
\\#P UB3LYP/6-311G(d,p) Opt=QST3 SCF=Direct Geom=(NoDistance,NoAngle)
fcheck #P freq SCRF=(solvent=Benzene) guess(mix,always)\\3-(3-tBu-1-Ph
-benzo[e][1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazinyl, conforme
r anti\\0,1\C,-0.4011951134,-1.9729778226,-0.0769638875\C,0.4216118366
,-0.8367942879,-0.0292693044\C,-1.7832606175,-1.8527337303,-0.06210100
41\C,-0.1549369939,0.4222473207,0.0058922487\C,-2.3706296744,-0.582511
2324,0.0101957778\C,-1.5536155339,0.5822849747,0.0111711402\N,-2.09329
19073,1.8375252492,-0.009424654\N,-3.744724592,-0.3574976636,0.0523626
229\N,-4.2792599816,0.8948706418,-0.0783282136\C,-3.4255536649,1.91101
88561,-0.1002039027\C,-4.7162815815,-1.3993050786,0.1809943273\C,-5.78
80495747,-1.446882873,-0.7126630015\C,-4.621734928,-2.3301426132,1.218
143098\C,-6.7541171092,-2.4382974833,-0.5757121071\C,-5.5914405611,-3.
3212936295,1.3431569869\C,-6.6573747266,-3.3809811165,0.4472436884\C,1
.9114655522,-0.9875199766,-0.0437351749\C,3.8870639203,-1.0636491884,-
1.1946861994\C,4.6008514456,-1.1684607209,0.0318121995\N,2.5150702441,
-1.0019445562,-1.229435144\N,2.465001942,-1.1112491344,1.1598239869\N,
3.822334594,-1.2757680231,1.185864411\C,4.3582595044,-1.5028232011,2.4
926231872\C,3.9490884133,-0.6828346419,3.5463143337\C,5.2378858927,-2.
5629737534,2.7241660439\C,4.438863476,-0.9147684152,4.8272386498\C,5.7
255135832,-2.7829147559,4.0095179191\C,5.3318331983,-1.9595878629,5.06
28317055\C,4.6166657291,-0.9889063266,-2.3944811113\C,6.0021939643,-1.
1277037477,0.035693391\C,6.0008977784,-0.9839490298,-2.3843798123\C,6.
6909707421,-1.0400576612,-1.1667953288\H,-2.4009085424,-2.7383701775,-
0.110773542\H,0.4498481701,1.3205922882,0.0148050904\H,-5.8559462029,-
0.7046324292,-1.4967063633\H,-3.8079373707,-2.2673568192,1.9295745048\
H,-7.5832175203,-2.4753293754,-1.2728269045\H,-5.5185839615,-4.0388774
166,2.1521371464\H,-7.4116766011,-4.1522730179,0.5499638459\H,0.047005
8503,-2.9577831221,-0.1303175446\H,3.2459392609,0.1159886595,3.3520899
615\H,5.5214963321,-3.219854571,1.9116274839\H,4.1227331779,-0.2749216
407,5.6428660181\H,6.4035538231,-3.6093810898,4.1878848529\H,5.7116139
322,-2.1361812966,6.062294162\H,6.5505059416,-0.9222862869,-3.31614723
38\H,6.545725966,-1.1569875748,0.9693438145\H,4.0513155838,-0.91940287
31,-3.3156068883\H,7.7740522652,-1.0098554604,-1.1551075931\C,-3.61635
97961,4.125605626,1.027885295\H,-2.5305889996,4.1579361434,1.127736974
7\H,-3.9920458879,5.1500549321,0.9496597662\H,-4.03231243,3.681152033,
1.9369716778\C,-5.5619147999,3.2805597972,-0.3238051582\H,-5.892093731
9,2.7248876487,-1.2038715795\H,-6.0124090963,2.8107981301,0.5524880352

\H,-5.9427500503,4.3030901666,-0.4017678077\C,-4.0291262844,3.31605747
18,-0.221387001\C,-3.4448993307,3.9883987417,-1.4832355131\H,-3.824956
5926,5.0103497487,-1.5720361825\H,-2.355672294,4.023362031,-1.43571375
36\H,-3.7313861277,3.4417261067,-2.3867189064\\Version=ES64L-G16RevC.0
1\State=1-A\HF=-1487.6472665\S2=1.021853\S2-1=0.\S2A=0.223122\RMSD=6.2
23e-09\RMSF=2.249e-06\Dipole=0.9867092,-1.4234749,0.828478\Quadrupole=
17.2650282,-10.7481157,-6.5169124,3.5136037,7.176995,-2.4986117\PG=C01
[X(C30H26N6)]\\@

1[3,7]-T, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C30H26N6(3)\PIOTR\09-Jan-20
24\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle)
fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-tBu-1-Ph-benzo[e][1,2,4]tr
iazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer anti\\0,3\C,-1.6
642498446,0.0271974155,-0.0365420362\C,-2.9942504791,1.8949361167,-0.1
798931122\C,-4.1586116241,1.0841556884,-0.0645830469\C,-0.3143169908,-
0.5848813275,0.0342933533\C,-0.150963176,-1.9816955459,0.1460916837\C,
0.8134677515,0.2366755514,-0.0138148569\C,1.1090761405,-2.5379252716,0
.1859615529\C,2.0921012081,-0.3186365522,0.06176026\C,2.2658602348,-1.
7314371612,0.1276572642\N,3.4978664784,-2.3074903062,0.1071790143\N,3.
2698442905,0.4316127452,0.048919592\N,4.4979872966,-0.1546185225,-0.08
03707052\C,4.5407415751,-1.4777223272,-0.0445448403\C,3.3066169489,1.8
595018496,0.1145829193\C,4.0927900965,2.5633144648,-0.8005227503\C,2.6
073518017,2.5423729399,1.1126946433\C,4.1642508215,3.9501351358,-0.723
1225607\C,2.6820425053,3.9308392816,1.1778663631\C,3.4567081146,4.6392
179176,0.2612073643\N,-3.9389031621,-0.2930412931,-0.0274028961\N,-2.6
888045463,-0.8261529172,0.0521688356\N,-1.7391690677,1.3519484005,-0.1
911913234\C,-5.4245078459,1.6766896688,0.0349694982\C,-3.1535207229,3.
2915534524,-0.2554184294\C,-4.4102980558,3.8674321134,-0.188354662\C,-
5.5435202444,3.0587982145,-0.030946004\C,-4.9930575432,-1.2625443661,-
0.0046308926\C,-5.001438208,-2.2360853431,0.9955744669\C,-5.9730675787
,-1.261683373,-0.9990090673\C,-6.0037085019,-3.2008825458,1.0059922929
\C,-6.9747113287,-2.2285997785,-0.9763244832\C,-6.9947508937,-3.197903
1944,0.0249910515\H,-1.0297051632,-2.6108869989,0.1834359281\H,0.67042
31583,1.3019936247,-0.1108695352\H,1.2529622422,-3.6097793798,0.245303
8751\H,4.6433823236,2.0168938959,-1.5543539477\H,2.0245516235,1.992259
798,1.8402686175\H,4.7723263742,4.4935057886,-1.4371396634\H,2.1416303
596,4.4566172996,1.9564107518\H,3.5137464381,5.7199956184,0.3172884779
\H,-4.5174668495,4.9441861533,-0.2453342124\H,-2.2565799985,3.89051735
36,-0.3543228794\H,-6.3042159732,1.0629865613,0.1679209297\H,-4.222436
7145,-2.2309447926,1.7465819329\H,-5.9403105523,-0.5233588304,-1.79038
20472\H,-6.0111255387,-3.9547586925,1.7845826519\H,-7.7315176629,-2.23
07189034,-1.7520484801\H,-7.7739147754,-3.950961992,0.0367475984\H,-6.
5257999525,3.5097640001,0.0451987216\C,5.9226957249,-2.1300396692,-0.1
67986218\C,5.9033625444,-3.081742772,-1.3844506726\H,5.1140636859,-3.8
275707874,-1.2813097334\H,5.733037725,-2.5276874047,-2.3124916749\H,6.
8641183897,-3.5976898553,-1.470537596\C,6.18385726,-2.9473532926,1.116
8827883\H,7.1421187986,-3.4693056243,1.0390875678\H,6.22428342,-2.2945
768783,1.9938985525\H,5.3959143164,-3.685199572,1.2742456328\C,7.03921
0096,-1.0903690915,-0.3488101797\H,7.0845443532,-0.3994559642,0.494913
9797\H,8.0019512349,-1.603723197,-0.4274725872\H,6.8927186623,-0.49793
45256,-1.2543630674\\Version=ES64L-G09RevD.01\State=3-A\HF=-1487.65830
49\S2=2.032052\S2-1=0.\S2A=2.000589\RMSD=8.142e-09\RMSF=4.040e-06\Dipo
le=-2.1243175,0.8539275,0.0702331\Quadrupole=10.8462782,0.9242821,-11.
7705603,9.2819886,-1.264287,-1.5220372\PG=C01 [X(C30H26N6)]\\@

1[3,7]-T, *syn*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C30H26N6(3)\PIOTR\07-Jan-20
24\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle)
fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-tBu-1-Ph-benzo[e][1,2,4]tr
iazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer syn\\0,3\C,1.661
5902934,-1.4807700554,-0.0735959273\C,3.7216677406,-2.4961463955,-0.02
76168181\C,4.3524765501,-1.2287570422,0.1170453066\C,0.1828728839,-1.5
79365839,-0.1247884973\C,-0.4292709304,-2.844914846,-0.2279856515\C,-0
.6138558533,-0.432539083,-0.0672022925\C,-1.8026767411,-2.9602376663,-
0.2470406053\C,-2.004304473,-0.5407601266,-0.1195350887\C,-2.631454807
9,-1.8209978396,-0.1752515714\N,-3.9831265047,-1.9617945259,-0.1353542
037\N,-2.8724891679,0.5514538295,-0.0933503709\N,-4.2235107119,0.39977
9993,0.0484890017\C,-4.6967095783,-0.8366342868,0.0197708918\C,-2.4405
85141,1.9138544433,-0.1524632464\C,-2.9255205764,2.8229215072,0.790247
769\C,-1.584388053,2.3430654279,-1.1690836321\C,-2.5401265515,4.157539
5082,0.7208722889\C,-1.2011455353,3.6801262642,-1.2264247811\C,-1.6745
350627,4.5902188661,-0.28305788\N,3.5065447042,-0.1193539726,0.0659804
31\N,2.1525302978,-0.2416100953,0.0332220618\N,2.3640897061,-2.6141947
389,-0.1500626658\C,5.7349206005,-1.1470138636,0.3279332928\C,4.526441
7825,-3.6507431142,-0.0148435152\C,5.89629171,-3.5600529782,0.16320064
55\C,6.4972651215,-2.3081302259,0.3458749445\C,3.9739530002,1.23414583
42,0.1036814922\C,3.4463600183,2.1103026458,1.0533211286\C,4.911151036
9,1.6828592942,-0.8287936261\C,3.8718278145,3.4346348181,1.0768462296\
C,5.3338332491,3.009075294,-0.7935005147\C,4.8187980414,3.8869146716,0
.1586933524\H,0.202962586,-3.7205907379,-0.2793764941\H,-0.1368109756,
0.5318906684,0.0165561039\H,-2.2891243442,-3.9262786102,-0.3023038661\
H,-3.6032311991,2.4766448198,1.559017206\H,-1.234632861,1.6416095703,-
1.9157715999\H,-2.9157853289,4.8602671891,1.4556779262\H,-0.5396393228
,4.0104164522,-2.0187404779\H,-1.3757680772,5.6307468006,-0.333542158\
H,6.5024028367,-4.4582049878,0.1735210555\H,4.0295079699,-4.6054020238
,-0.1356505103\H,6.2069143338,-0.1869862158,0.4824123245\H,2.706879878
8,1.7484349554,1.7555225653\H,5.2916019419,1.0057623896,-1.5833866572\
H,3.4636311231,4.1131557147,1.8167961949\H,6.0573707254,3.3575495438,-
1.5212791183\H,5.148455088,4.9190168093,0.1808398623\H,7.5662303212,-2
.2373908096,0.5081082399\C,-6.2148488247,-1.001212203,0.1564500004\C,-
6.497600477,-1.9012419184,1.3795309633\H,-5.9936672767,-2.8634463135,1
.2785734946\H,-6.1509994315,-1.4273552304,2.3028973622\H,-7.5732488089
,-2.0770776393,1.4732434198\C,-6.7401665541,-1.6934733308,-1.121066725
4\H,-7.8162048036,-1.8703411648,-1.0338475743\H,-6.5705631329,-1.06808
41288,-2.0025880473\H,-6.2407161965,-2.6504714551,-1.2783241095\C,-6.9
28577361,0.3473593148,0.3370536585\H,-6.7506916862,1.0122078263,-0.510
1076942\H,-8.0057960782,0.1775261476,0.4228577341\H,-6.5905249277,0.86
21338646,1.2387749726\\Version=ES64L-G09RevD.01\State=3-A\HF=-1487.658
5223\S2=2.032287\S2-1=0.\S2A=2.000595\RMSD=5.918e-09\RMSF=3.113e-06\Di
pole=2.1155299,1.724286,0.1138155\Quadrupole=5.5286268,3.1859579,-8.71
45847,0.7727569,-4.2321988,1.1232801\PG=C01 [X(C30H26N6)]\\@

1[3,7]-T,TS

1\1\GINC-LOCALHOST\FTS\UB3LYP\6-311G(d,p)\C30H26N6(3)\PIOTR\25-Jun-202
4\0\\#P UB3LYP/6-311G(d,p) Opt=QST3 SCF=Direct Geom=(NoDistance,NoAngl
e) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-tBu-1-Ph-benzo[e][1,2,4
]triazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer syn\\0,3\C,1.
665910125,-1.4916459558,-0.0929002779\C,3.6750513485,-1.3315538799,-1.
1761576014\C,4.3567404256,-1.4252825208,0.0694011642\C,0.1727596822,-1
.6018870362,-0.138679204\C,-0.4365076532,-2.8585562487,-0.2845916326\C
,-0.6075811289,-0.4549977431,-0.0499542211\C,-1.8143612872,-2.96584630
13,-0.3120842491\C,-2.0036219077,-0.5517217064,-0.1174948385\C,-2.6324
744519,-1.8243182788,-0.2123724281\N,-3.9918617594,-1.9582217934,-0.18

21917926\N,-2.8624093021,0.5446884508,-0.0661110059\N,-4.2154334044,0.
3987383337,0.0731165456\C,-4.6954743221,-0.8368350314,0.007733837\C,-2
.4202865127,1.9042832082,-0.1042486768\C,-2.8995016932,2.8039880905,0.
8502560067\C,-1.5585083836,2.3404421291,-1.1135634426\C,-2.5007869924,
4.1356327146,0.8015369766\C,-1.1620691075,3.6745237563,-1.1498880154\C
,-1.6282131742,4.5748133437,-0.1935679111\N,3.5499934615,-1.4459330216
,1.2087514391\N,2.1892240711,-1.5563701187,1.1283438981\N,2.303266812,
-1.3331388885,-1.2507039134\C,5.7549345218,-1.5229839736,0.1004875564\
C,4.4356984532,-1.2698364186,-2.3573374092\C,5.8179510222,-1.331771087
5,-2.3154220729\C,6.4743763048,-1.4718152625,-1.0859883724\C,4.0563804
178,-1.4167825729,2.5464196107\C,3.5887140029,-2.3536043703,3.47031075
65\C,4.9662895065,-0.4322260551,2.9387913299\C,4.0498564067,-2.3141935
596,4.7818695498\C,5.4247327734,-0.4052191307,4.2530613388\C,4.9723675
398,-1.3458806892,5.176559955\H,0.1801508615,-3.7459065551,-0.36483888
64\H,-0.1322949693,0.5077864618,0.073479528\H,-2.3069128125,-3.9265382
827,-0.3980236887\H,-3.5824020798,2.4523373114,1.6119175302\H,-1.21566
0332,1.647250083,-1.8712704216\H,-2.8713131305,4.8309555937,1.54587454
34\H,-0.4973140454,4.0108321882,-1.9370258542\H,-1.31921932,5.61298784
07,-0.2275114135\H,6.3915567043,-1.2864852251,-3.2335646146\H,3.895325
0519,-1.1893872162,-3.2924954869\H,6.2718528311,-1.6441029713,1.041842
3036\H,2.8629771298,-3.0907834152,3.1540875216\H,5.2959695325,0.315904
2757,2.2290410608\H,3.6878717382,-3.0441432006,5.4964975655\H,6.126272
0577,0.3630007226,4.5567520583\H,5.3294848221,-1.319178469,6.199327829
3\H,7.5548351195,-1.54671633,-1.0532742803\C,-6.2154948023,-0.99434476
32,0.1415536498\C,-6.5031890366,-1.9328137521,1.3339895168\H,-6.010542
7535,-2.8962791606,1.1965262566\H,-6.1466634295,-1.4956297739,2.271560
1874\H,-7.580319887,-2.0996115958,1.4271659729\C,-6.7476369592,-1.6395
805207,-1.1573829296\H,-7.8256899677,-1.8069910989,-1.0764141841\H,-6.
5700177886,-0.9888133618,-2.01870832\H,-6.2584573553,-2.596678215,-1.3
43879057\C,-6.9195121274,0.3524302785,0.369250849\H,-6.7355269102,1.04
61844959,-0.4529869645\H,-7.998120253,0.1876693384,0.4477155061\H,-6.5
797733829,0.8323037351,1.2895113126\\Version=ES64L-G16RevC.01\State=3-
A\HF=-1487.6473026\S2=2.028271\S2-1=0.\S2A=2.000483\RMSD=8.610e-09\RMS
F=9.512e-07\Dipole=2.275267,0.7892489,0.8296776\Quadrupole=4.1056032,-
1.9021232,-2.20348,-2.4694,1.981612,-2.4402673\PG=C01 [X(C30H26N6)]\\@

1[3,7]-S, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C30H26N6\PIOTR\09-Jan-2024\
0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fch
eck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-tBu-1-Ph-be
nzo[e][1,2,4]triazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer a
nti\\0,1\C,1.6627377094,0.0362372277,0.042400668\C,2.9974630927,1.8995
910794,0.1746395027\C,4.1588826036,1.08522986,0.0593669758\C,0.3144848
547,-0.5820477916,-0.0267600465\C,0.1535987418,-1.9784838914,-0.131570
5284\C,-0.8122137479,0.2396812252,0.0167785824\C,-1.1074844653,-2.5359
081695,-0.1707671913\C,-2.0917449227,-0.3175411425,-0.0568551225\C,-2.
2634694649,-1.7309063823,-0.1183870214\N,-3.498359611,-2.3061215098,-0
.1008005022\N,-3.2671556442,0.4317494637,-0.0459676411\N,-4.497309194,
-0.151665535,0.0756930576\C,-4.5397878679,-1.4766255595,0.0419178518\C
,-3.3018775859,1.860754349,-0.1090351817\C,-4.0771370121,2.5637498124,
0.8155270386\C,-2.6115332477,2.5430413019,-1.113265332\C,-4.1461809862
,3.9509071538,0.7415174425\C,-2.6839848828,3.9318050595,-1.1753541706\
C,-3.4474789567,4.6398972543,-0.2491815416\N,3.9322004947,-0.294066882
7,0.0280938585\N,2.683617503,-0.8198294222,-0.042478414\N,1.7400010462
,1.3610022648,0.1907231139\C,5.4272170425,1.6692042926,-0.0468937582\C
,3.1650479555,3.2952180642,0.2445290907\C,4.4252890077,3.8642755231,0.
1711865617\C,5.5546482154,3.0513367788,0.0132166641\C,4.9834759681,-1.

2676251318,0.0051577736\C,4.9870486993,-2.2417815784,-0.9942456427\C,5
.9643700958,-1.2685488156,0.9985027165\C,5.9857687979,-3.2102831008,-1
.0046207429\C,6.9620972815,-2.2394742938,0.9760396879\C,6.9774733288,-
3.2098961945,-0.0243274438\H,1.0326557983,-2.6072443257,-0.164686956\H
,-0.6688898007,1.3053235414,0.1100969373\H,-1.2502089816,-3.6081359884
,-0.2261173602\H,-4.6210885962,2.0169244869,1.5739278759\H,-2.03715461
1,1.9925065051,-1.8472329158\H,-4.7454426196,4.4944960965,1.4627429961
\H,-2.1505488372,4.4579840221,-1.9583844303\H,-3.5027271471,5.72089641
94,-0.3027321041\H,4.537059134,4.9408823177,0.2239811458\H,2.272115184
8,3.9000710666,0.3439573751\H,6.3028691407,1.0496894304,-0.1801218593\
H,4.2076397183,-2.2342129158,-1.7448608331\H,5.9352696265,-0.528695903
9,1.7885616643\H,5.9898731501,-3.964866693,-1.7825197277\H,7.719721030
6,-2.2435810318,1.7509299089\H,7.7538596907,-3.9658096366,-0.035991922
7\H,6.538786021,3.4972207143,-0.0674707659\C,-5.9238067518,-2.12656717
69,0.1575040234\C,-5.913857856,-3.0753190197,1.3763347424\H,-5.1243225
073,-3.8218205174,1.2804084913\H,-5.7496249311,-2.5191666732,2.3042264
947\H,-6.8756279885,-3.5902602782,1.4568869714\C,-6.1772867015,-2.9465
407782,-1.1271954458\H,-7.1372955127,-3.4660992061,-1.0551586617\H,-6.
2097789915,-2.2959404301,-2.0061648357\H,-5.3898055523,-3.6864591034,-
1.2768471235\C,-7.0402935139,-1.0850907163,0.3282540185\H,-7.079532591
2,-0.3963608486,-0.5175531656\H,-8.0040578303,-1.5972629877,0.40203230
58\H,-6.8990850231,-0.4903916787,1.2331438509\\Version=ES64L-G09RevD.0
1\State=1-A\HF=-1487.6582675\S2=0.989866\S2-1=0.\S2A=0.188161\RMSD=4.2
20e-09\RMSF=7.507e-06\Dipole=2.0988976,0.81837,-0.0782579\Quadrupole=1
0.9688773,0.7904494,-11.7593267,-10.1287063,-1.310458,1.4958924\PG=C01
[X(C30H26N6)]\\@

1[3,7]-S, *syn*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C30H26N6\PIOTR\08-Jan-2024\
0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fch
eck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-tBu-1-Ph-be
nzo[e][1,2,4]triazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer s
yn\\0,1\C,1.6642096539,-1.4832959947,-0.0750424482\C,3.7245894438,-2.4
948100922,-0.0377791153\C,4.3534495115,-1.2272128695,0.115134814\C,0.1
812977999,-1.5837774573,-0.1245192966\C,-0.4306246955,-2.848485497,-0.
2230708274\C,-0.6134765082,-0.4372257777,-0.0698523902\C,-1.805435328,
-2.9624675128,-0.2399315319\C,-2.0055277216,-0.5451316912,-0.121023494
7\C,-2.6320716291,-1.8235132781,-0.1719967258\N,-3.9878694493,-1.96233
71511,-0.1302025023\N,-2.8709213573,0.5492260355,-0.0958288821\N,-4.22
14763113,0.4007345633,0.0506530199\C,-4.6967055439,-0.8377813467,0.025
0095408\C,-2.4365576455,1.9103687561,-0.1634787366\C,-2.9189258707,2.8
257643654,0.7744944943\C,-1.581171555,2.3321968025,-1.1839343325\C,-2.
5311226978,4.1591697702,0.6969434246\C,-1.1956464344,3.6682314686,-1.2
49463906\C,-1.6660626534,4.5845082532,-0.3106485296\N,3.5051943368,-0.
1195373393,0.0709767211\N,2.1515760997,-0.2448512702,0.0391102078\N,2.
3670707465,-2.6139311434,-0.1604212202\C,5.7359015698,-1.1437389454,0.
3268162774\C,4.5319768119,-3.6475027045,-0.0332968139\C,5.9017068169,-
3.554863802,0.1451098278\C,6.5005889983,-2.3031389021,0.3366329337\C,3
.9694508608,1.2348300728,0.1149620304\C,3.4377685701,2.1058646233,1.06
70693092\C,4.9073880321,1.6893660377,-0.8139827027\C,3.8602081204,3.43
10020274,1.0967936957\C,5.3266299734,3.0164659628,-0.7726327333\C,4.80
77735708,3.88920244,0.182180881\H,0.2006552931,-3.7249671357,-0.272525
692\H,-0.1362147114,0.5273256971,0.0117550775\H,-2.2922864296,-3.92857
47522,-0.2908813782\H,-3.5962886415,2.4850022706,1.5459934784\H,-1.234
3788741,1.626026284,-1.9275495285\H,-2.904502185,4.8668137375,1.428178
0855\H,-0.5348517202,3.9928488278,-2.0447043081\H,-1.3655708403,5.6242
040655,-0.3675483186\H,6.5096341984,-4.4518630432,0.1489830099\H,4.037

3342672,-4.6024987527,-0.1605501284\H,6.2056315406,-0.1837414012,0.488
2306257\H,2.6977887125,1.7393577693,1.7662997054\H,5.2908629901,1.0162
772307,-1.5705961185\H,3.4490850926,4.1055457297,1.8387431584\H,6.0505
958405,3.3696266933,-1.4977084278\H,5.1349342242,4.921978152,0.2091011
889\H,7.5693953961,-2.2315831807,0.499393052\C,-6.215473357,-0.9970580
07,0.165625588\C,-6.4981320718,-1.8949591761,1.3902347203\H,-5.9975083
548,-2.8588129449,1.2887842917\H,-6.1475491354,-1.4214111148,2.3122825
528\H,-7.5741347568,-2.0670643044,1.4869178826\C,-6.7459080432,-1.6889
206666,-1.1099673365\H,-7.8224026161,-1.8618314996,-1.0203228924\H,-6.
5759045564,-1.0651712668,-1.9925817223\H,-6.2499935498,-2.6477648543,-
1.267062484\C,-6.9249467026,0.353780375,0.3465889183\H,-6.7474828738,1
.0172454322,-0.5017248644\H,-8.0024114113,0.1869452594,0.435380552\H,-
6.5832252401,0.8686161724,1.2468903243\\Version=ES64L-G09RevD.01\State
=1-A\HF=-1487.6573857\S2=1.024715\S2-1=0.\S2A=0.204724\RMSD=3.822e-09\
RMSF=3.573e-06\Dipole=2.1545697,1.7691466,0.1159457\Quadrupole=5.45351
82,3.1737501,-8.6272683,0.7615543,-4.1952745,1.1046087\PG=C01 [X(C30H2
6N6)]\\@

1[3,7]-S, TS

1\1\GINC-GAUSIANDELL\FTS\UB3LYP\6-311G(d,p)\C30H26N6\PKASZYNSKI\28-Jun
-2024\0\\#P UB3LYP/6-311G(d,p) Opt=QST3 SCF=Direct Geom=(NoDistance,No
Angle) fcheck freq #P SCRF=(solvent=Benzene) guess(mix,always)\\3-(3-t
Bu-1-Ph-benzo[e][1,2,4]triazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, c
onformer syn\\0,1\C,1.6699337019,-1.4540188574,-0.0825428656\C,3.67904
54559,-1.302037013,-1.1661185012\C,4.3605114492,-1.4262371159,0.076879
843\C,0.1776538846,-1.5704524283,-0.1305346085\C,-0.423450917,-2.83198
58341,-0.2660156323\C,-0.6089398672,-0.427289419,-0.0520224788\C,-1.80
09235974,-2.9479853147,-0.2915212182\C,-2.0047224979,-0.5331763297,-0.
1177840842\C,-2.6255639358,-1.8110218694,-0.2009676424\N,-3.9844141906
,-1.9523067193,-0.1678589989\N,-2.8698331571,0.557578613,-0.0756609311
\N,-4.2220900581,0.4055065719,0.0654747937\C,-4.6943831211,-0.83393642
54,0.0123094288\C,-2.4358904661,1.9196489616,-0.1262512503\C,-2.919794
6306,2.8243038121,0.8210183575\C,-1.5780058423,2.3523884269,-1.1402639
669\C,-2.5302439283,4.1581628819,0.7602210036\C,-1.1909646342,3.688862
7006,-1.188890143\C,-1.6619803417,4.5943927123,-0.2399348882\N,3.55528
03788,-1.4444309619,1.2173000136\N,2.1929993572,-1.5365944193,1.137437
3668\N,2.3072692281,-1.280084338,-1.2382069643\C,5.7566149215,-1.55143
62897,0.1042335159\C,4.4392750876,-1.2357934566,-2.3473332804\C,5.8202
490349,-1.3229835919,-2.3083420146\C,6.4754930627,-1.4948053703,-1.082
2636773\C,4.0645460982,-1.4346362853,2.5539281571\C,3.5830789701,-2.36
99601924,3.4722745025\C,4.9928510063,-0.4692521322,2.9512464728\C,4.04
87607514,-2.34873585,4.7827118714\C,5.4556100179,-0.4604939748,4.26413
00933\C,4.9894741891,-1.4000531954,5.1819657964\H,0.1988389876,-3.7160
63915,-0.3380092651\H,-0.1391097323,0.5392885378,0.0623409499\H,-2.287
7397936,-3.9123958768,-0.3682084204\H,-3.5994385051,2.4746327626,1.586
4899932\H,-1.2307338465,1.6546494774,-1.8917795705\H,-2.9043276186,4.8
574212833,1.4990527251\H,-0.5293614689,4.0226225653,-1.9797754067\H,-1
.3598863448,5.6342504222,-0.2835101007\H,6.393463465,-1.2734947579,-3.
2265202396\H,3.8992899527,-1.1319602279,-3.2804046978\H,6.2722837017,-
1.6968102647,1.0428912627\H,2.843396366,-3.0917623118,3.1528766025\H,5
.3337642865,0.278334054,2.2462788329\H,3.6758676823,-3.0775777244,5.49
2858344\H,6.1716390596,0.29284587,4.5713325051\H,5.3501519648,-1.38737
89515,6.2037619352\H,7.5544177829,-1.5903042275,-1.0523937823\C,-6.213
2713628,-0.9997807509,0.1491723289\C,-6.4933710152,-1.9312771825,1.349
0190502\H,-5.9934256343,-2.8920104436,1.2187870713\H,-6.1399989537,-1.
484333524,2.2832063944\H,-7.5691583612,-2.1054567009,1.444000737\C,-6.
742650512,-1.6577699481,-1.1443343569\H,-7.8193015097,-1.8328961125,-1

.0604055423\H,-6.5710054116,-1.0113872333,-2.0101284487\H,-6.246382183
,-2.6122008465,-1.3253340817\C,-6.9260331531,0.343898106,0.3679763794\
H,-6.7490127343,1.0324941021,-0.4600729195\H,-8.0032604021,0.172157401
,0.4505649333\H,-6.587699816,0.833275922,1.2837487068\\Version=ES64L-G
09RevD.01\State=1-A\HF=-1487.647362\S2=1.018685\S2-1=0.\S2A=0.21722\RM
SD=6.631e-09\RMSF=4.321e-06\Dipole=2.2547268,0.7736672,0.8105826\Quadr
upole=4.1215405,-1.8452461,-2.2762944,-2.8395767,1.9818965,-2.6194369\
PG=C01 [X(C30H26N6)]\\

I[3,6]H,H,Ph -T, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C26H18N6(3)\PKASZYNSKI\10
-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,No
Angle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benzo[e][1,2
,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer anti\\0,3\
C,-0.4063132409,-1.9725764043,-0.1186899662\C,0.4283732324,-0.84211944
59,-0.0483806571\C,-1.7852073206,-1.8501161876,-0.1037881721\C,-0.1553
092367,0.4212371006,0.0099126436\C,-2.3738449877,-0.5798250378,-0.0101
647989\C,-1.5468806568,0.5808316462,0.0139689796\N,-2.0869527885,1.847
1423106,0.0148388748\N,-3.7472374504,-0.3622175358,0.0329608699\N,-4.2
854124904,0.8929236708,-0.0557493516\C,-3.4101443629,1.8916547275,-0.0
576483003\C,-4.7188359528,-1.410151692,0.1214215346\C,-5.7832350402,-1
.4251811849,-0.7815905186\C,-4.6336883022,-2.3724421982,1.1296372848\C
,-6.7521504668,-2.4183452481,-0.6843581589\C,-5.6064603853,-3.36492181
74,1.214900462\C,-6.6646488334,-3.3936443867,0.3084372143\C,1.90333846
59,-1.0162581962,-0.0542316381\C,3.7442918294,-2.3839964229,-0.1610363
149\C,4.5989787048,-1.2460799622,-0.1550829268\N,2.3835080441,-2.26195
54779,-0.0819785758\N,2.6122629841,0.1143881359,-0.0161345323\N,3.9658
249905,-0.0108761304,-0.0012096908\C,4.6684036101,1.2307731618,0.12710
79734\C,4.3256906422,2.295287276,-0.7081201173\C,5.6471869268,1.389658
3786,1.1101541633\C,4.9783204426,3.51564165,-0.5672396194\C,6.29737967
12,2.6140113848,1.2394029801\C,5.968079906,3.6779157356,0.4014946896\C
,4.3274127826,-3.6594848152,-0.27855794\C,5.9807923958,-1.3990327373,-
0.3272390615\C,5.6974186404,-3.804543359,-0.4147267851\C,6.521405016,-
2.6725638173,-0.4511107124\H,-2.4031555731,-2.7342232275,-0.1706872002
\H,0.4550475284,1.3126319909,0.044855839\H,-5.8446591935,-0.6555172574
,-1.5394032327\H,-3.8263551314,-2.3329653546,1.8500034462\H,-7.5761442
262,-2.4309516346,-1.388275565\H,-5.5419874255,-4.1079130487,2.0012532
396\H,-7.4210641956,-4.1663293411,0.3804172376\H,0.0515594299,-2.94968
99916,-0.1882954321\H,3.5493245629,2.1589632079,-1.4493068307\H,5.8820
229655,0.5706048599,1.778240131\H,4.7130378645,4.3408122794,-1.2177927
206\H,7.0521951393,2.738278493,2.0070972674\H,6.4739851265,4.630303918
2,0.5080819075\H,6.1314997998,-4.7931888941,-0.5060774036\H,6.62390616
7,-0.5313025812,-0.3684043903\H,3.6623555301,-4.5142924815,-0.27112163
92\H,7.5912811657,-2.7834713332,-0.5815642724\H,-3.8740764636,2.872190
3349,-0.1155119533\\Version=ES64L-G09RevD.01\State=3-A\HF=-1330.353946
5\S2=2.028462\S2-1=0.\S2A=2.000469\RMSD=8.277e-09\RMSF=7.530e-06\Dipol
e=1.0699092,-0.7889636,-0.0008506\Quadrupole=17.7657702,-3.7593318,-14
.0064384,16.5853748,3.8524548,-2.9184308\PG=C01 [X(C26H18N6)]\\@

I[3,6]H,H,Ph -T, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C26H18N6(3)\PKASZYNSKI\10
-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,No
Angle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benzo[e][1,2
,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer syn\\0,3\C
,0.0432551022,1.0911327655,0.0589585142\C,0.46472588,-0.2489061134,-0.
0375553807\C,-1.3005766095,1.4213540892,0.07130439\C,-0.4980681384,-1.
252230219,-0.0958204652\C,-2.2714504952,0.4117795509,-0.0202967741\C,-

1.8667796855,-0.9524266862,-0.0736370361\N,-2.788705804,-1.975667046,-0.0736436425\N,-3.6422051677,0.6531357731,-0.0318742791\N,-4.5565153698,-0.3609977287,0.0612637221\C,-4.0525869222,-1.5896097422,0.0321016856\C,-4.2217597873,1.9610904792,-0.0822740928\C,-5.1968169673,2.3068877847,0.8549726934\C,-3.8569954385,2.8601023574,-1.0865592746\C,-5.7923828749,3.5623860869,0.7952399681\C,-4.4560098339,4.1161146493,-1.1341885451\C,-5.4213286794,4.4722183012,-0.1941957671\C,1.9088645421,-0.6001058376,-0.0602149665\C,3.5646165861,-2.1877228811,-0.1475147266\C,4.5538480697,-1.1756666777,0.0040241882\N,2.2315804134,-1.8864147037,-0.2076467179\N,2.7521548732,0.428608415,0.0603493854\N,4.0814876694,0.1372809378,0.025613647\C,4.9366067937,1.284740149,0.0820823854\C,4.7332624518,2.2373386818,1.0818601107\C,5.932237023,1.4695989942,-0.8790389475\C,5.5410021401,3.3691790679,1.1259659361\C,6.7384058784,2.6034551539,-0.822833466\C,6.5475685613,3.5536482794,0.1787595855\C,3.9817513837,-3.53069997,-0.2075387864\C,5.9032149714,-1.5228409543,0.151675305\C,5.320218962,-3.8636285756,-0.0916471337\C,6.2779580866,-2.859231589,0.0996461929\H,-1.5976370402,2.4568426472,0.157650675\H,-0.202319544,-2.2906439644,-0.1473852745\H,-5.4841004079,1.5865709339,1.6093729997\H,-3.1275923858,2.5723615545,-1.8332745938\H,-6.5472012042,3.8303895582,1.5253702676\H,-4.175907441,4.8105157834,-1.917750947\H,-5.8874220141,5.4496215592,-0.2373179743\H,0.7877729129,1.8725786387,0.1252472743\H,3.9449564555,2.0841946299,1.8071812553\H,6.0617585871,0.7423963028,-1.6708201269\H,5.3854559244,4.1065307014,1.9049101193\H,7.5074251531,2.7487348473,-1.5725050499\H,7.1752488041,4.4362113524,0.2170805304\H,5.6266057876,-4.9019980708,-0.1364828839\H,6.6487267153,-0.7567475853,0.3113806913\H,3.2151256658,-4.2853446666,-0.3329574048\H,7.3232836659,-3.1208028908,0.2132934892\H,-4.8084805991,-2.3674051626,0.0933178755\\Version=ES64L-G09RevD.01\State=3-A\HF=-1330.353264\S2=2.02854\S2-1=0.\S2A=2.000471\RMSD=4.710e-09\RMSF=8.424e-06\Dipole=1.6868207,1.9630953,0.1239642\Quadrupole=12.1649445,-1.1319931,-11.0329514,-11.5338954,-4.0611088,0.0528627\PG=C01 [X(C26H18N6)]\\@

I[3,6]H,H,Ph -S, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C26H18N6\PKASZYNSKI\10-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benzo[e][1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer anti\\0,1\C,-0.4046842802,-1.977017285,-0.1291127038\C,0.4294076219,-0.8471248224,-0.0539989986\C,-1.7844443664,-1.8533276219,-0.1151554969\C,-0.153271587,0.4154542902,0.007252157\C,-2.3725406887,-0.5843916175,-0.0174176995\C,-1.5463369707,0.5756165176,0.0098476178\N,-2.08263365,1.8422413489,0.0101058518\N,-3.7488777939,-0.3647754377,0.0264274335\N,-4.2820869624,0.8914428538,-0.0687184271\C,-3.4067562866,1.8887001383,-0.0690997536\C,-4.7219832283,-1.4094863408,0.1197313505\C,-5.7994545565,-1.4142176597,-0.7683086563\C,-4.6268809924,-2.3807005419,1.1190061322\C,-6.7706413071,-2.404479776,-0.6650668546\C,-5.601998108,-3.3702298372,1.2099849766\C,-6.6731284461,-3.3881149712,0.3185220743\C,1.9071396984,-1.0186170967,-0.0573305121\C,3.7487116808,-2.3843172919,-0.1591193365\C,4.6023802438,-1.245419349,-0.153671906\N,2.3876823128,-2.2629825473,-0.0819704195\N,2.6137455461,0.1127584684,-0.0200510455\N,3.9682221164,-0.0112521566,-0.0019851183\C,4.6689369211,1.2311624734,0.1276132238\C,4.3244191733,2.2961534146,-0.7063444177\C,5.6475397762,1.3904983844,1.1108287676\C,4.9752436892,3.5172930846,-0.5641643591\C,6.2957868662,2.6157201466,1.2414203539\C,5.9648116632,3.6800387656,0.4047005423\C,4.3329709559,-3.659474734,-0.2738834128\C,5.9848196178,-1.3976196724,-0.3241156629\C,5.7032015058,-3.8035224818,-0.4081227885\C,6.5263413282,-2.6707448068,-0.4453529313\H,-2.4024352879,-2.737156246

7,-0.1855263246\H,0.4569861115,1.3068302197,0.0451562149\H,-5.8688593156,-0.6385397834,-1.5191947047\H,-3.810011226,-2.350091974,1.8288951856\H,-7.6043817551,-2.4083725279,-1.3575480167\H,-5.5291684958,-4.1195250677,1.9896258781\H,-7.4313058839,-4.1586268413,0.3950228266\H,0.0526146392,-2.9541765356,-0.2011045035\H,3.5481591126,2.1594712942,-1.4475505588\H,5.8835721897,0.5711877856,1.7781596002\H,4.7086653141,4.3427669442,-1.2137981547\H,7.050372949,2.7403203632,2.009281881\H,6.4692223074,4.6330973659,0.5123346385\H,6.1383201987,-4.7918899449,-0.4974094723\H,6.6272516008,-0.5294311878,-0.3660336489\H,3.6686182555,-4.5148135119,-0.2659555058\H,7.5964353648,-2.7810830462,-0.5745086138\H,-3.8685777317,2.8698419162,-0.1315884418\\Version=ES64L-G09RevD.01\State=1-A\HF=-1330.3533258\S2=1.029548\S2-1=0.\S2A=0.238037\RMSD=6.503e-09\RMSF=5.177e-06\Dipole=1.1216363,-0.7520401,0.0018747\Quadrupole=17.6638818,-3.6169005,-14.0469812,16.2112572,3.8486397,-2.9220864\PG=C01 [X(C26H18N6)]\\@

I[3,6]H,H,Ph -S, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C26H18N6\PKASZYNSKI\10-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benzo[e][1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer syn\\0,1\C,0.0480779379,1.0882715168,0.0588888213\C,0.4660230447,-0.2521378852,-0.0392534708\C,-1.2965129742,1.4204531512,0.0719324995\C,-0.4969657627,-1.254265149,-0.0999520575\C,-2.2683699426,0.4137218506,-0.0212073976\C,-1.8666040117,-0.9523886213,-0.0766766155\N,-2.7872927355,-1.9728750891,-0.0772250687\N,-3.640325536,0.655927306,-0.0333806807\N,-4.5541504683,-0.3582003479,0.0599516764\C,-4.0530059776,-1.5858440157,0.0298996151\C,-4.2193263616,1.963867217,-0.0821856012\C,-5.1970749886,2.3079676043,0.852968743\C,-3.8512446905,2.865387488,-1.0831393014\C,-5.7922898209,3.5637046282,0.794243589\C,-4.4498749989,4.1215649054,-1.1297029135\C,-5.4180731844,4.4757595076,-0.1918984057\C,1.9084133222,-0.6087062431,-0.0614974732\C,3.5658467146,-2.1935820235,-0.1443573064\C,4.5532858822,-1.1798686104,0.0041845816\N,2.2316615896,-1.8950635695,-0.2046011296\N,2.7498741474,0.4211600888,0.055668186\N,4.0766282617,0.1339008545,0.0242160184\C,4.9301815771,1.283225691,0.0802345938\C,4.7285229855,2.2327980188,1.0830246107\C,5.9219705781,1.4715556244,-0.883997185\C,5.5341843438,3.3661747097,1.1266828048\C,6.7258996269,2.6070269224,-0.8283490552\C,6.5367206599,3.5546316844,0.1760302632\C,3.9873974476,-3.5350359963,-0.2012376766\C,5.9034085249,-1.5214745399,0.1517606931\C,5.3274365255,-3.8635314514,-0.0853851306\C,6.2829648497,-2.8570114795,0.102699045\H,-1.5917018067,2.4563883635,0.1593930188\H,-0.201980441,-2.292767554,-0.1538024446\H,-5.4868066752,1.5861365053,1.6049834722\H,-3.1194820699,2.5794283049,-1.8282015703\H,-6.5492524695,3.8301494829,1.5227292126\H,-4.1671738845,4.8177358112,-1.9107660466\H,-5.8837856443,5.4533812789,-0.2341665833\H,0.7938440287,1.8682905644,0.1256250771\H,3.9434250489,2.076316254,1.8111667462\H,6.0502959773,0.7458869087,-1.6773759649\H,5.3801833033,4.1014633076,1.9078585967\H,7.4920013632,2.7554589085,-1.5803672654\H,7.1628019259,4.4383427182,0.2139561549\H,5.6362552301,-4.9013386678,-0.1280676051\H,6.6463021271,-0.7522949455,0.309018654\H,3.2234380831,-4.2927685073,-0.3243140083\H,7.3290951406,-3.1152880917,0.2159472456\H,-4.8085691533,-2.3637254286,0.0916926685\\Version=ES64L-G09RevD.01\State=1-A\HF=-1330.3536324\S2=1.000141\S2-1=0.\S2A=0.224184\RMSD=7.931e-09\RMSF=7.022e-06\Dipole=1.6680736,1.9920457,0.1272551\Quadrupole=12.31879,-1.3092161,-11.0095739,-10.9175646,-4.0688378,0.0375521\PG=C01 [X(C26H18N6)]\\@

I[3,6]CF_3,H,Ph -T, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C27H17F3N6(3)\PKASZYNSKI\
10-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,
NoAngle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-CF3-1-Ph-benzo[e]
[1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer anti\\
0,3\C,-0.411306476,-1.9636225982,-0.0990565836\C,0.4229513371,-0.83216
54801,-0.0368066389\C,-1.7906686629,-1.8432695866,-0.08239352\C,-0.159
4067768,0.4316293966,0.0153634218\C,-2.3777202954,-0.5738858384,0.0018
203345\C,-1.5508966206,0.5868590093,0.0186148284\N,-2.0963623183,1.848
9819674,0.0079726405\N,-3.7539929,-0.3575556183,0.0429666022\N,-4.2897
81744,0.8902284339,-0.0587329808\C,-3.4171673279,1.8812466649,-0.06958
41217\C,-4.7244512559,-1.4090794413,0.1363486342\C,-5.7716832517,-1.44
91573779,-0.7847654299\C,-4.6458454133,-2.3486652328,1.1654151478\C,-6
.7331291888,-2.4493432849,-0.6834802575\C,-5.6112597249,-3.347793495,1
.2542285536\C,-6.6531864916,-3.4033134954,0.3303481858\C,1.8985953477,
-1.0082569091,-0.0474195663\C,3.7347208437,-2.3795216146,-0.1711005915
\C,4.5905897747,-1.2426147134,-0.1646287481\N,2.3741684742,-2.25497119
67,-0.0833277692\N,2.6080605437,0.1207919053,-0.0069344741\N,3.9607312
445,-0.006702329,-0.0005333041\C,4.6685693072,1.2327088062,0.127458678
8\C,4.3378283637,2.295246034,-0.714655099\C,5.64234705,1.3885160329,1.
1155876772\C,4.9975464343,3.5120451525,-0.5747500423\C,6.2999700792,2.
609014504,1.2435491072\C,5.982478096,3.6714546161,0.3992768519\C,4.314
3160744,-3.6550612543,-0.3001620401\C,5.970750446,-1.3961065641,-0.346
9219553\C,5.6831285317,-3.8009198148,-0.4481336966\C,6.5082082697,-2.6
698005363,-0.4832372336\H,-2.4085543821,-2.7278125189,-0.1416898714\H,
0.4506698428,1.3234501932,0.0434356192\H,-5.8276137925,-0.6951827444,-
1.5588002842\H,-3.8505157199,-2.2876985162,1.897601409\H,-7.5454061364
,-2.4830592632,-1.3999527075\H,-5.5542138708,-4.074499398,2.0560348158
\H,-7.4041722277,-4.1809410552,0.4049504694\H,0.0480090862,-2.94030956
72,-0.1641639292\H,3.5656193977,2.1608637556,-1.4606663149\H,5.8684213
438,0.5703952437,1.7879798429\H,4.7415157259,4.3363324168,-1.230031756
9\H,7.0511595096,2.7315628065,2.0150516398\H,6.4938174484,4.6209928763
,0.505143666\H,6.1153616703,-4.7893769398,-0.5493350543\H,6.6149802041
,-0.5291935668,-0.386797942\H,3.6478779996,-4.5088025686,-0.2931729016
\H,7.5769397829,-2.7814763879,-0.6220124855\C,-4.0241418807,3.27564967
69,-0.1669052878\F,-5.359688991,3.2553540597,-0.2858964089\F,-3.723329
7059,4.0049952492,0.9271899187\F,-3.5313456235,3.9367740266,-1.2345301
481\\Version=ES64L-G09RevD.01\State=3-A\HF=-1667.488449\S2=2.02811\S2-
1=0.\S2A=2.000457\RMSD=6.900e-09\RMSF=3.217e-06\Dipole=1.7141867,-2.01
00368,0.0604649\Quadrupole=19.788302,-7.8608695,-11.9274324,24.8147757
,3.1649637,-2.4727874\PG=C01 [X(C27H17F3N6)]\\@

I[3,6]CF_3,H,Ph -T, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C27H17F3N6(3)\PKASZYNSKI\
11-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,
NoAngle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-CF3-1-Ph-benzo[e]
[1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer syn\\0
,3\C,0.0397936508,1.0852126727,0.0928010381\C,0.4619850671,-0.25461143
48,-0.0041028722\C,-1.3041553989,1.4169865591,0.0923107176\C,-0.498728
1329,-1.2582740211,-0.0759619602\C,-2.2720822844,0.4085365451,-0.01436
68972\C,-1.8662236645,-0.9550274522,-0.0694341504\N,-2.7902508667,-1.9
738404497,-0.0868041209\N,-3.6451012605,0.6515363291,-0.0429029936\N,-
4.5550491289,-0.3593330889,0.0306320724\C,-4.0499359683,-1.5793949034,
0.0033821078\C,-4.2257552639,1.9611421069,-0.0936481458\C,-5.215187723
5,2.2984194278,0.8307992067\C,-3.8420504633,2.8649223802,-1.0859109601
\C,-5.8073621823,3.5555450748,0.7707076614\C,-4.4381937317,4.122163035
6,-1.1331269098\C,-5.4176380275,4.4718720733,-0.2054526221\C,1.9072319

117,-0.6054833422,-0.0175607128\C,3.5635352464,-2.1923369049,-0.084753
806\C,4.5516201336,-1.1753655419,0.0383388473\N,2.228856501,-1.8942540
462,-0.137996628\N,2.7477418241,0.4268601336,0.0797821133\N,4.07694725
33,0.1368954798,0.0466849604\C,4.9317761143,1.2862594105,0.0804242744\
C,4.7550496068,2.2377312344,1.0858399003\C,5.9002990276,1.4713241683,-
0.9074216118\C,5.562645743,3.3704072629,1.1079086418\C,6.7064714587,2.
6061197141,-0.873567897\C,6.5424059948,3.555807931,0.1332032507\C,3.98
27230457,-3.534814364,-0.1269924809\C,5.9040589913,-1.515993569,0.1704
57826\C,5.3238171672,-3.8621717089,-0.0250812561\C,6.2814123561,-2.852
2225392,0.134324681\H,-1.6018814143,2.4521063418,0.1786571735\H,-0.202
1479116,-2.2962488424,-0.1277193018\H,-5.5158471334,1.5728045257,1.574
873771\H,-3.1015247474,2.5809085831,-1.8228590364\H,-6.5740210595,3.81
91093236,1.4897502806\H,-4.1452068089,4.8222780271,-1.9066008624\H,-5.
8815764371,5.4502138568,-0.2485310764\H,0.7842139998,1.865855792,0.168
4751698\H,3.9879105915,2.0835528488,1.8334974557\H,6.0092845874,0.7436
112175,-1.7019646818\H,5.4279470621,4.1074115076,1.8910533796\H,7.4545
560676,2.7522834039,-1.6439615994\H,7.1700434733,4.4389792805,0.154422
2643\H,5.6325845609,-4.9002595143,-0.0570108144\H,6.6497770404,-0.7451
497392,0.3050536946\H,3.2165996394,-4.2933211213,-0.229554643\H,7.3290
981465,-3.1092599732,0.2356415926\C,-5.0791439008,-2.7027734771,0.0435
606724\F,-4.7748543512,-3.6009017808,1.0005546897\F,-6.3224432057,-2.2
602010475,0.2837224221\F,-5.1032331351,-3.3652259756,-1.1325589047\\Ve
rsion=ES64L-G09RevD.01\State=3-A\HF=-1667.4877678\S2=2.028236\S2-1=0.\
S2A=2.00046\RMSD=9.751e-09\RMSF=2.582e-06\Dipole=2.6933513,2.9341096,0
.0946985\Quadrupole=9.3715771,-0.1789749,-9.1926023,-18.3428431,-4.007
6349,0.0849199\PG=C01 [X(C27H17F3N6)]\\@

I[3,6]CF$_3$,H,Ph -S, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C27H17F3N6\PKASZYNSKI\11-
Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoA
ngle) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-CF
3-1-Ph-benzo[e][1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, c
onformer anti\\0,1\C,-0.410352848,-1.9678931795,-0.1044321704\C,0.4233
926371,-0.8370037599,-0.0381599712\C,-1.7906173446,-1.8463552655,-0.08
79638735\C,-0.1578786413,0.4260741991,0.0174307214\C,-2.3769608422,-0.
5782224725,0.0001445475\C,-1.5509266246,0.5819244549,0.0198985297\N,-2
.0925354044,1.8443406023,0.0089853642\N,-3.7562403194,-0.3596737708,0.
0417605512\N,-4.2869690148,0.8887031875,-0.0652270759\C,-3.4144608932,
1.878519457,-0.0745766893\C,-4.7282058233,-1.4084690269,0.1372949903\C
,-5.7845494703,-1.4400243772,-0.774059728\C,-4.6430410554,-2.355420021
9,1.1594069184\C,-6.747930266,-2.4380123914,-0.6701016456\C,-5.6104291
09,-3.3523220293,1.250724613\C,-6.6613011546,-3.3990143471,0.336502290
2\C,1.9018354988,-1.0102593076,-0.0478311262\C,3.7385091904,-2.3792802
208,-0.1700656802\C,4.593325526,-1.2413467303,-0.1643258168\N,2.377835
7746,-2.2555234242,-0.0822548488\N,2.6089411758,0.119642452,-0.0081934
036\N,3.9627126809,-0.0066800316,-0.0004457461\C,4.6688164448,1.233390
5464,0.1287465974\C,4.3348781726,2.2971439292,-0.7106656688\C,5.644088
279,1.3888753837,1.1155253316\C,4.9931085783,3.5145897597,-0.569667339
3\C,6.3000648592,2.6101197398,1.24464194\C,5.9795541957,3.6736595671,0
.4029028709\C,4.3190779803,-3.6544125246,-0.2983698853\C,5.9738833749,
-1.3939976813,-0.3471548986\C,5.687884712,-3.7991608851,-0.446613187\C
,6.5120432921,-2.6671654714,-0.4827976362\H,-2.4085544656,-2.730710430
6,-0.1501164888\H,0.4521803746,1.3178493641,0.0481673036\H,-5.84569237
08,-0.6809718399,-1.542684298\H,-3.8411468057,-2.3015593176,1.88489812
65\H,-7.5669557754,-2.4646501292,-1.3791770804\H,-5.5478672631,-4.0843
397729,2.0472932059\H,-7.4137140863,-4.1750673442,0.4130507625\H,0.048
3022453,-2.9446753827,-0.1720896113\H,3.5614710247,2.1630243671,-1.455

454868\H,5.8724818142,0.5699590102,1.7861481523\H,4.7346951098,4.33972
31163,-1.222946436\H,7.0523532711,2.732344427,2.0151226456\H,6.4896527
517,4.6237626954,0.5096604606\H,6.1210323049,-4.7872565658,-0.54733363
78\H,6.6173731686,-0.5265939391,-0.3880213417\H,3.6533304246,-4.508677
1791,-0.2906908807\H,7.5807902276,-2.778149322,-0.6220484179\C,-4.0186
752679,3.2733296938,-0.177691539\F,-5.3539342073,3.2548789921,-0.29960
94538\F,-3.7189302018,4.0058199409,0.9146330838\F,-3.5222543841,3.9301
471767,-1.2464096625\\Version=ES64L-G09RevD.01\State=1-A\HF=-1667.4878
297\S2=1.029338\S2-1=0.\S2A=0.236708\RMSD=4.299e-09\RMSF=4.022e-06\Dip
ole=1.7434141,-1.9763727,0.0639182\Quadrupole=19.8420996,-7.8427231,-1
1.9993765,24.4775892,3.1353748,-2.4455835\PG=C01 [X(C27H17F3N6)]\\@

I[3,6]CF_3,H,Ph -S, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C27H17F3N6\PKASZYNSKI\14-
Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoA
ngle) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-CF
3-1-Ph-benzo[e][1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, c
onformer syn\\0,1\C,0.0448088074,1.0823700883,0.0906891329\C,0.4634874
025,-0.2578486899,-0.0057061954\C,-1.3000816201,1.4159144888,0.0907601
576\C,-0.4974590783,-1.2605384861,-0.0783160604\C,-2.2688708196,0.4101
658981,-0.0155757809\C,-1.8658844656,-0.9553624882,-0.0710991482\N,-2.
7885241167,-1.9716969521,-0.0876876964\N,-3.643374186,0.6539258545,-0.
0445240159\N,-4.5525430733,-0.3568989359,0.0302859069\C,-4.0501086489,
-1.5761288869,0.003472388\C,-4.2235379815,1.9634604539,-0.0943837713\C
,-5.215194698,2.2997604884,0.8281378208\C,-3.8371144183,2.8690791643,-
1.0840398785\C,-5.8071605331,3.5570274386,0.7684489332\C,-4.432929711,
4.1264508926,-1.1307612592\C,-5.4148258173,4.4749006556,-0.2051597068\
C,1.906809643,-0.614088795,-0.0185206311\C,3.5648952985,-2.1980587049,
-0.083295684\C,4.5511629334,-1.1795772047,0.037878701\N,2.2292100242,-
1.9028751316,-0.1362069885\N,2.7457907367,0.4188924402,0.0768478356\N,
4.0720839244,0.1332493684,0.0464526132\C,4.9253881452,1.2845506913,0.0
804060744\C,4.750234465,2.2325392154,1.0891541817\C,5.8899382696,1.473
4746293,-0.9103957002\C,5.555653119,3.3668024953,1.1112477891\C,6.6937
226465,2.6099526369,-0.8766019637\C,6.5312733546,3.5566358813,0.133284
2864\C,3.9885995223,-3.5389655178,-0.1241736575\C,5.9044882128,-1.5147
488042,0.1691538214\C,5.3311714483,-3.8618723759,-0.0228782884\C,6.286
5843159,-2.8499203424,0.1344017445\H,-1.5959351903,2.4516336833,0.1764
666216\H,-0.2016639465,-2.2986895257,-0.1307268946\H,-5.5178387952,1.5
732081365,1.5704945895\H,-3.0946112782,2.5863249343,-1.8194592213\H,-6
.5756171576,3.81950836,1.4859802911\H,-4.137744621,4.8277768512,-1.902
3141131\H,-5.8784470714,5.4534109437,-0.2478504451\H,0.7903340609,1.86
18872157,0.1651066944\H,3.9863473274,2.0746626859,1.839410147\H,5.9976
721742,0.7476664259,-1.7068347352\H,5.4224696995,4.1014361512,1.896846
0762\H,7.4387787363,2.7596680339,-1.6492182995\H,7.1572036182,4.441009
7852,0.1545062959\H,5.6424926275,-4.8992868821,-0.0538919023\H,6.64752
82945,-0.7409901445,0.3020919448\H,3.2251697007,-4.3003710104,-0.22526
81082\H,7.3350472602,-3.1038308479,0.2349292791\C,-5.0788762477,-2.699
2108879,0.0463214759\F,-4.7771337473,-3.5922631507,1.009037237\F,-6.32
29318448,-2.255705138,0.2803733534\F,-5.0991446411,-3.3680256756,-1.12
62823271\\Version=ES64L-G09RevD.01\State=1-A\HF=-1667.4881376\S2=0.999
349\S2-1=0.\S2A=0.223137\RMSD=9.899e-09\RMSF=5.307e-06\Dipole=2.722041
9,2.9571091,0.0937719\Quadrupole=9.5541676,-0.3344085,-9.2197591,-17.7
356338,-3.9866923,0.0899983\PG=C01 [X(C27H17F3N6)]\\@

I[3,6]Me_2N,H,Ph -T, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C28H23N7(3)\PKASZYNSKI\12

-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,No
Angle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-NMe2-1-Ph-benzo[e][
1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer anti\\0
,3\C,-0.4343226784,-1.8830654719,-0.2474116963\C,0.4008308942,-0.74818
06843,-0.1987177953\C,-1.809965544,-1.7536485538,-0.2490644748\C,-0.17
85535794,0.5170528038,-0.1787065944\C,-2.3960079471,-0.4769056798,-0.1
949899875\C,-1.5731711521,0.6866008946,-0.1937745955\N,-2.1061959384,1
.94277809,-0.2181395749\N,-3.7624854597,-0.2492483102,-0.1751044546\N,
-4.3093988109,0.9921362144,-0.3059507912\C,-3.4362596474,2.0232785555,
-0.2998614515\C,-4.7340219189,-1.2989628043,-0.0889485575\C,-5.7568710
598,-1.3622390706,-1.0364507622\C,-4.6835727508,-2.2198163157,0.958904
5333\C,-6.7187008671,-2.3630348312,-0.9426857229\C,-5.6491892854,-3.21
95775292,1.0419031324\C,-6.6660252181,-3.2966278313,0.0919464456\C,1.8
74622795,-0.9256181375,-0.1856918527\C,3.7124485914,-2.3037072293,-0.2
395670769\C,4.5728114685,-1.1704062925,-0.2608580144\N,2.3524445227,-2
.1731965995,-0.1721182498\N,2.5906163067,0.2029263519,-0.1753551871\N,
3.9440088868,0.0706840875,-0.1449956491\C,4.6524243664,1.3112767682,-0
.0469482055\C,4.3246173362,2.3533008216,-0.9160042993\C,5.6242427374,1
.4931284475,0.9391054991\C,4.9846291569,3.5729251374,-0.8056550118\C,6
.2822641273,2.7161481508,1.0375752974\C,5.9676695316,3.7571818535,0.16
59857143\C,4.2902627393,-3.5849020089,-0.3185883172\C,5.9546212262,-1.
3347355154,-0.4230476176\C,5.6599871098,-3.7403805512,-0.4459069259\C,
6.4896443178,-2.6137425064,-0.5103244454\H,-2.4325746892,-2.6357979124
,-0.2996882631\H,0.4376448566,1.404895504,-0.1571460368\H,-5.790078233
1,-0.6253805233,-1.8279533764\H,-3.9058116104,-2.1439169099,1.70832464
8\H,-7.5096828582,-2.4144993393,-1.6819584592\H,-5.611390776,-3.930854
328,1.858779363\H,-7.4170216865,-4.0749050269,0.1611902183\H,0.0216115
658,-2.8624279283,-0.2876023272\H,3.5534991255,2.2001234113,-1.6594194
824\H,5.8482832515,0.6926017938,1.6329404866\H,4.7307200287,4.38017664
63,-1.4827874907\H,7.0316899139,2.8576702128,1.807643866\H,6.479596512
7,4.7087689464,0.2486262129\H,6.0896058385,-4.7332869062,-0.5082962389
\H,6.6023401725,-0.4716919326,-0.4855094912\H,3.6204585986,-4.43561705
2,-0.2900680406\H,7.559515486,-2.7332200856,-0.6335673609\N,-4.0089039
341,3.2693948205,-0.3579589113\C,-5.4431024443,3.4283041424,-0.5392825
587\H,-5.977830242,2.6368538364,-0.020489981\H,-5.7415594476,4.3944058
077,-0.1260538736\H,-5.7312620607,3.4030497679,-1.5996570702\C,-3.1931
366154,4.4465547016,-0.6134969006\H,-2.1580710535,4.2266162743,-0.3715
084106\H,-3.2538152284,4.7550201179,-1.6666164069\H,-3.5446296876,5.27
58507577,0.0069443047\\Version=ES64L-G09RevD.01\State=3-A\HF=-1464.371
7023\S2=2.028012\S2-1=0.\S2A=2.000448\RMSD=5.913e-09\RMSF=9.758e-07\Di
pole=0.3313355,0.1655577,-0.103781\Quadrupole=19.6951224,-1.0626146,-1
8.6325078,7.963302,4.7235502,-3.9825854\PG=C01 [X(C28H23N7)]\\@

I[3,6]Me$_2$N,H,Ph -T, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C28H23N7(3)\PKASZYNSKI\12
-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,No
Angle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-NMe2-1-Ph-benzo[e][
1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer syn\\0,
3\C,0.0155168775,1.0442378527,-0.0823027352\C,0.4321102651,-0.29869048
79,-0.1964221205\C,-1.326210974,1.3737488974,-0.0851563059\C,-0.530627
6471,-1.2982602834,-0.2892275416\C,-2.2981833214,0.3651965321,-0.20952
79717\C,-1.9035964695,-1.0002293238,-0.2840120773\N,-2.8206760821,-2.0
11849473,-0.3348330203\N,-3.6635402025,0.6025443938,-0.2407171492\N,-4
.5915421765,-0.3946315858,-0.2149778996\C,-4.1031046209,-1.6550874007,
-0.2466004835\C,-4.2342609494,1.9168188195,-0.2622076792\C,-5.18674680
78,2.2605702363,0.6982320445\C,-3.8751810685,2.8258662759,-1.258573757
7\C,-5.7661104987,3.5250227824,0.669300009\C,-4.4583074054,4.090334457

6,-1.2769680039\C,-5.4014563758,4.4443524274,-0.3139254387\C,1.8747711
164,-0.6527661744,-0.2052109498\C,3.5329411483,-2.2407018863,-0.284857
7776\C,4.5225264404,-1.229977466,-0.126171765\N,2.2007702314,-1.939519
0494,-0.3519745612\N,2.7202103749,0.3746979782,-0.0763530402\N,4.04997
6031,0.0821435931,-0.1024190882\C,4.9042533862,1.2295562228,-0.0401647
142\C,4.6954226455,2.181533181,0.9591630176\C,5.9042207331,1.416792222
8,-0.9962652726\C,5.5017293926,3.3141634752,1.0080663657\C,6.708790495
3,2.551591195,-0.9355791182\C,6.5128222266,3.5006676343,0.06601516\C,3
.9505514825,-3.5836620697,-0.3469731113\C,5.87148213,-1.5785387525,0.0
24707842\C,5.2883781934,-3.9180261576,-0.2279262339\C,6.2461524356,-2.
914780478,-0.0305367755\H,-1.6255362225,2.4076567424,0.0146877161\H,-0
.2325047125,-2.3348813687,-0.3579780927\H,-5.4644231073,1.5344347977,1
.4508845186\H,-3.1589848269,2.5393610398,-2.018370431\H,-6.5020643068,
3.7931413603,1.4184946481\H,-4.1825016428,4.7937455151,-2.0540102481\H
,-5.8549423376,5.4284849569,-0.3333290001\H,0.760605971,1.8223578296,0
.0081236768\H,3.9028382719,2.0275219957,1.6796493065\H,6.0383258355,0.
690753006,-1.7883969064\H,5.3408375649,4.0508700035,1.7866076642\H,7.4
80808549,2.698545822,-1.6819397349\H,7.1392476058,4.3840009833,0.10798
16804\H,5.5942951962,-4.956487272,-0.2753591788\H,6.6167606926,-0.8129
822959,0.1888965549\H,3.183636482,-4.3370821714,-0.477755309\H,7.29110
26861,-3.176993509,0.0855099866\N,-5.0490327981,-2.6489778921,-0.18069
72037\C,-6.4671301944,-2.3459792384,-0.305902493\H,-7.0379412248,-3.11
36623843,0.2216512843\H,-6.685048442,-1.3756352562,0.1305901763\H,-6.7
920603936,-2.3346079224,-1.3559311103\C,-4.6696117849,-4.0323234858,-0
.4256425511\H,-4.799201718,-4.3078055099,-1.4818830897\H,-3.6277994373
,-4.1773419396,-0.1567859006\H,-5.2998968613,-4.6880927951,0.180449440
2\\Version=ES64L-G09RevD.01\State=3-A\HF=-1464.3710246\S2=2.027914\S2-
1=0.\S2A=2.000444\RMSD=6.715e-09\RMSF=5.490e-06\Dipole=0.6619903,1.286
7238,0.0817538\Quadrupole=19.2978417,-0.9474252,-18.3504165,-0.1504102
,-3.1608662,0.8636599\PG=C01 [X(C28H23N7)]\\@

I[3,6]Me$_2$N,H,Ph -S, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C28H23N7\PKASZYNSKI\12-Ja
n-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAng
le) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-NMe2
-1-Ph-benzo[e][1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, co
nformer anti\\0,1\C,-0.4336619572,-1.887758361,-0.2566878976\C,0.40088
07767,-0.7536455539,-0.1982137732\C,-1.810076574,-1.7574179727,-0.2593
185844\C,-0.1776535075,0.510539628,-0.1700863013\C,-2.3958866997,-0.48
21085192,-0.1961420918\C,-1.573734472,0.6804240571,-0.1863432018\N,-2.
103130467,1.937409838,-0.2051139028\N,-3.7650679279,-0.2526581553,-0.1
758240746\N,-4.3069280542,0.9907758476,-0.3101120025\C,-3.4333399199,2
.0202340509,-0.2953356523\C,-4.7384098868,-1.2992347826,-0.0913205967\
C,-5.7739279956,-1.3468954781,-1.0264468794\C,-4.6792325532,-2.2343308
272,0.9439009996\C,-6.7384536223,-2.3450713293,-0.9334400029\C,-5.6476
583038,-3.2313203478,1.0259669811\C,-6.6767394024,-3.292464076,0.08806
3894\C,1.8778740536,-0.9287398419,-0.1832138184\C,3.7166192378,-2.3039
282777,-0.2307488951\C,4.5755046737,-1.1694002241,-0.2569848936\N,2.35
64328915,-2.174609989,-0.1633986668\N,2.5910413121,0.2006009544,-0.177
6856286\N,3.9449767736,0.0707116971,-0.1454375256\C,4.6510320437,1.312
8285367,-0.0508429281\C,4.3194743807,2.3525914425,-0.9212430537\C,5.62
40892607,1.4984613261,0.9333212326\C,4.9772745119,3.573680782,-0.81431
82162\C,6.2796517494,2.723043869,1.0284417744\C,5.9615303929,3.7617640
235,0.1553731595\C,4.2963063977,-3.5845099976,-0.3044989371\C,5.957704
2107,-1.3323468822,-0.4194650112\C,5.6661879399,-3.7383530759,-0.43187
90044\C,6.4943546121,-2.6107686261,-0.501663892\H,-2.4324316071,-2.639
2966314,-0.3176485482\H,0.4381674659,1.3984796274,-0.141595686\H,-5.81

42418617,-0.599797782,-1.8078866649\H,-3.8927538669,-2.1710322637,1.68
52744382\H,-7.5387645005,-2.3837889947,-1.6634309443\H,-5.6024922597,-
3.9530091121,1.8333127908\H,-7.4298404011,-4.0687554632,0.1566604943\H
,0.0217427372,-2.8670691546,-0.3033371973\H,3.5473531668,2.1964256462,
-1.6629681566\H,5.8508252581,0.6997929641,1.6284027648\H,4.720631609,4
.3791255952,-1.4925628162\H,7.0299633758,2.8675875212,1.7970764088\H,6
.4716296966,4.7145504212,0.235395932\H,6.0972618652,-4.7308700764,-0.4
902855432\H,6.6040392207,-0.4685868977,-0.4861345752\H,3.627855339,-4.
4361364403,-0.2720722615\H,7.5642840114,-2.7293652001,-0.6251733253\N,
-4.0030913925,3.2678927188,-0.3532321505\C,-5.4362645226,3.4288480555,
-0.5404771138\H,-5.9745042995,2.6408572713,-0.0199005608\H,-5.73406066
51,4.3973934545,-0.1326266289\H,-5.7210607885,3.3991906766,-1.60166201
14\C,-3.1842843225,4.4433382303,-0.6073051666\H,-2.1504727258,4.222112
6198,-0.3611342295\H,-3.240513154,4.7507938564,-1.6609950968\H,-3.5365
122129,5.2739266725,0.010944969\\Version=ES64L-G09RevD.01\State=1-A\HF
=-1464.3709154\S2=1.026317\S2-1=0.\S2A=0.212813\RMSD=6.351e-09\RMSF=3.
116e-06\Dipole=0.3999182,0.2065598,-0.112619\Quadrupole=19.6180656,-0.
9539399,-18.6641258,7.6832782,4.7544846,-4.0041705\PG=C01 [X(C28H23N7)
]\\@

I[3,6]Me$_2$N,H,Ph -S, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C28H23N7\PKASZYNSKI\13-Ja
n-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAng
le) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-NMe2
-1-Ph-benzo[e][1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, co
nformer syn\\0,1\C,0.0205245921,1.0405836263,-0.0857516293\C,0.4337790
042,-0.3028948066,-0.1992560398\C,-1.3216187818,1.3723527319,-0.087657
772\C,-0.5289728172,-1.3011930919,-0.291460308\C,-2.2951599671,0.36641
17613,-0.2107967458\C,-1.9029942957,-1.0008315144,-0.2844354398\N,-2.8
186185551,-2.0102743066,-0.3311079427\N,-3.6610776612,0.6042939744,-0.
2426088445\N,-4.5890192923,-0.3934781397,-0.2151964105\C,-4.1029143728
,-1.65253967,-0.2420827967\C,-4.2315990281,1.9181874105,-0.2669319303\
C,-5.189913656,2.2616712224,0.6879360619\C,-3.8666890531,2.8280321105,
-1.260628756\C,-5.7693189297,3.5260217226,0.656059577\C,-4.4499026608,
4.0923467703,-1.2819325955\C,-5.3989332848,4.445901052,-0.3244705991\C
,1.8750671517,-0.6629292094,-0.2086008806\C,3.535245467,-2.2470188462,
-0.2887960096\C,4.5226213071,-1.2348447445,-0.1290120624\N,2.201799260
8,-1.9489097418,-0.3558584369\N,2.7178370908,0.3655856898,-0.079016680
6\N,4.0449951442,0.0781536035,-0.1028657999\C,4.8970906939,1.227658955
6,-0.0376604259\C,4.6885835275,2.1743429058,0.9665426162\C,5.894025530
3,1.4208765749,-0.995578939\C,5.4921473231,3.3088564645,1.0180416528\C
,6.6956935742,2.5575715372,-0.9323717101\C,6.499956289,3.5018632178,0.
0738235218\C,3.9583202151,-3.5878813469,-0.3521254502\C,5.8723064169,-
1.577373592,0.021675752\C,5.2979357325,-3.9174263059,-0.2331663784\C,6
.2528798464,-2.9124207965,-0.0347747828\H,-1.6187849716,2.4069403771,0
.0114229274\H,-0.2317508317,-2.3380391426,-0.3603193863\H,-5.471903671
,1.5353660465,1.4387885527\H,-3.1459361019,2.5422290846,-2.0163365137\
H,-6.5097791086,3.7936429088,1.4009868537\H,-4.1695445605,4.7960992116
,-2.0570400937\H,-5.8524010072,5.4299908556,-0.3461510921\H,0.76703224
84,1.8173508742,0.0031443618\H,3.8986670856,2.0149958471,1.6888460296\
H,6.0279659836,0.6980768705,-1.7906766095\H,5.3317361413,4.0417477811,
1.8002532008\H,7.4653954599,2.7096658883,-1.6800706897\H,7.1242742154,
4.3865841889,0.1178270886\H,5.6067689179,-4.9550542347,-0.2818312513\H
,6.6143210355,-0.8087094396,0.1865038739\H,3.1947078706,-4.3445070414,
-0.4838218489\H,7.2986991686,-3.1710944326,0.08075961\N,-5.0476596088,
-2.6470804776,-0.1705303955\C,-6.465804334,-2.3401843398,-0.2846480257
\H,-7.0348812414,-3.123085725,0.2215644844\H,-6.6833508419,-1.38303022

49,0.1808597623\H,-6.7935632165,-2.2970993706,-1.3329468776\C,-4.67132
93534,-4.0296510106,-0.4256911875\H,-4.8143327588,-4.3011113974,-1.481
2506471\H,-3.6262911984,-4.1755655364,-0.1703381529\H,-5.2934712817,-4
.6880341796,0.1859074615\\Version=ES64L-G09RevD.01\State=1-A\HF=-1464.
3712461\S2=0.995505\S2-1=0.\S2A=0.198741\RMSD=8.347e-09\RMSF=5.330e-06
\Dipole=0.6121817,1.3226374,0.0835743\Quadrupole=19.3450718,-1.0730649
,-18.272007,0.6552245,-3.1594378,0.8577918\PG=C01 [X(C28H23N7)]\\@

I[3,6]Me$_2$N,CF$_3$,Ph -T, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C29H22F3N7(3)\PKASZYNSKI\
14-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,
NoAngle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-NMe2-1-Ph-benzo[e
][1,2,4]triazinyl-6-)-1-Ph-7-CF3_benzo[e][1,2,4] triazinyl, conformer
anti\\0,3\C,-0.6181726143,-1.8196773677,-0.0835866667\C,0.2554507716,-
0.714899305,-0.0185899364\C,-1.9882949558,-1.6433539209,-0.0678712282\
C,-0.2794049783,0.5693002484,0.0407693733\C,-2.5293274013,-0.348683586
5,0.0232282964\C,-1.6670082656,0.7861897509,0.0488790501\N,-2.15660142
4,2.0594919315,0.0693749759\N,-3.8856624807,-0.0754000616,0.0592654247
\N,-4.3919765592,1.1870022916,-0.0160858551\C,-3.4843935422,2.18845036
42,0.0148387043\C,-4.8932821192,-1.0946759071,0.1061306543\C,-5.902966
8316,-1.098160775,-0.856908904\C,-4.8897246971,-2.041593016,1.13121364
8\C,-6.901666205,-2.0650057814,-0.8007671782\C,-5.8918137314,-3.007564
0438,1.176301304\C,-6.8973375525,-3.0240300274,0.2115771201\C,1.719785
1452,-0.9410221184,-0.0308467032\C,3.5059589054,-2.3805305069,-0.12835
44079\C,4.4047836484,-1.2774325681,-0.1491418306\N,2.1569437205,-2.206
0159444,-0.0404108679\N,2.4760179796,0.1612549255,-0.0192742649\N,3.82
27804696,-0.0178229426,-0.0141175625\C,4.5807349177,1.1963043248,0.073
283189\C,4.3017312682,2.2366539726,-0.8134728466\C,5.5542280302,1.3469
924918,1.0620124741\C,5.0151538838,3.4270756403,-0.7175685465\C,6.2653
263399,2.5410714012,1.1460916779\C,6.0004425865,3.5810543901,0.2570575
989\C,4.0413968241,-3.6803700618,-0.2294198044\C,5.7763860401,-1.48223
87873,-0.3309656054\C,5.3994782945,-3.8817807798,-0.3762598282\C,6.264
8138648,-2.7791530908,-0.4388346728\H,-2.6414050012,-2.5020699085,-0.1
335923883\H,0.3669434787,1.4349540613,0.0770613752\H,-5.8984377145,-0.
3419710489,-1.6307570353\H,-4.1207853091,-2.0118489622,1.8930670111\H,
-7.6832636363,-2.07002233,-1.551654202\H,-5.8914038602,-3.7394943098,1
.9756041733\H,-7.6769029949,-3.7757790739,0.2520047924\H,-0.197051804,
-2.8129632477,-0.1512463934\H,3.5292921878,2.1052962616,-1.5597478174\
H,5.739729804,0.5469520055,1.7679053664\H,4.8019114853,4.234537923,-1.
4081448156\H,7.0179386017,2.6605379105,1.9164941676\H,6.5543774737,4.5
097464511,0.3275970563\H,5.7963425674,-4.8854916275,-0.4613538936\H,6.
4530963064,-0.6436490494,-0.3962065129\H,3.3473792603,-4.5107903527,-0
.2030942882\N,-4.0144025389,3.4534707942,0.0149139916\C,-5.4432011273,
3.6717144637,-0.1498484368\H,-6.0027883181,2.8624069481,0.311532614\H,
-5.7103998797,4.6147055178,0.3325469689\H,-5.7311268439,3.7330437203,-
1.2087282348\C,-3.1592814316,4.6136878986,-0.183809171\H,-2.1356511957
,4.3560696006,0.0691910794\H,-3.1901020834,4.9614649225,-1.2258299998\
H,-3.4998058329,5.4295075181,0.4598012358\C,7.7400098305,-3.0136660451
,-0.5819570894\F,8.3052104737,-3.4103442524,0.5867066644\F,8.406293840
9,-1.9065818433,-0.976106078\F,8.0130061894,-3.9856644059,-1.482523861
5\\Version=ES64L-G09RevD.01\State=3-A\HF=-1801.5109542\S2=2.028057\S2-
1=0.\S2A=2.000454\RMSD=3.805e-09\RMSF=5.110e-06\Dipole=-1.2520179,0.69
08881,0.013547\Quadrupole=3.0547902,6.898852,-9.9536422,17.5161618,6.6
119883,-4.4684685\PG=C01 [X(C29H22F3N7)]\\@

I[3,6]Me$_2$N,CF$_3$,Ph -T, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C29H22F3N7(3)\PKASZYNSKI\
15-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,
NoAngle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-NMe2-1-Ph-benzo[e
][1,2,4]triazinyl-6-)-1-Ph-7-CF3_benzo[e][1,2,4] triazinyl, conformer
syn\\0,3\C,0.179871227,0.9871865789,-0.0685242472\C,-0.2943232831,-0.3
388964766,0.0181696062\C,1.5347473713,1.2557535763,-0.0769597448\C,0.6
232180263,-1.3835493781,0.0717173804\C,2.4616545773,0.2012274308,0.006
2812132\C,2.0077126437,-1.1472701018,0.0515317778\N,2.8790117581,-2.19
8841859,0.0602879741\N,3.8355027186,0.3765770195,0.0227121985\N,4.7182
682511,-0.6587009641,-0.0422207746\C,4.1750027557,-1.8976427336,-0.038
8145979\C,4.464033755,1.6642886118,0.0718455122\C,5.4043994126,1.99969
12453,-0.9029349052\C,4.172639663,2.5518307128,1.1086077213\C,6.041580
6689,3.2350340622,-0.8463123691\C,4.8134054751,3.7874027715,1.15468171
53\C,5.746182632,4.1332195332,0.1787220083\C,-1.7486384004,-0.62928446
16,0.036946067\C,-3.4685279523,-2.1482603591,0.1065347357\C,-4.4165667
743,-1.0952243031,-0.0331144517\N,-2.1294628896,-1.9048510429,0.169463
3015\N,-2.5533189265,0.432869651,-0.0706808138\N,-3.8922742952,0.19534
78118,-0.0412590719\C,-4.7030174819,1.3769286199,-0.0844453852\C,-4.46
8442415,2.3262693978,-1.0798433387\C,-5.6843075742,1.5916670088,0.8846
886803\C,-5.232771582,3.4882339936,-1.1112002933\C,-6.4469160209,2.755
79161,0.8408422936\C,-6.2254939996,3.7041201116,-0.1560413239\C,-3.943
4564223,-3.4743388332,0.1516887895\C,-5.7771386388,-1.3813762091,-0.18
51258611\C,-5.2909398631,-3.7522066218,0.033905924\C,-6.2052246166,-2.
703618167,-0.1463591862\H,1.8799199017,2.2772333598,-0.1543922794\H,0.
2795147926,-2.4071931972,0.1196301635\H,5.6289182685,1.289889935,-1.68
82751466\H,3.4647029959,2.2708486442,1.8783438085\H,6.7685658773,3.496
9148223,-1.6063604385\H,4.5906200491,4.4738779071,1.963249962\H,6.2446
883262,5.0946224308,0.2200167901\H,-0.5303281626,1.8000400886,-0.12942
0569\H,-3.6911610189,2.1475641746,-1.8111650596\H,-5.8368067313,0.8649
201364,1.6729148584\H,-5.0543971376,4.2243215886,-1.8863023787\H,-7.20
5990362,2.9248365419,1.595447863\H,-6.8197114051,4.609835419,-0.185089
1246\H,-5.6424202403,-4.7755962369,0.0614248853\H,-6.4915660121,-0.586
8724586,-0.3406907019\H,-3.2115913197,-4.2637092583,0.2662530611\N,5.0
73323526,-2.9294296961,-0.147560632\C,6.5069410686,-2.6948579651,-0.05
8922014\H,7.0252964741,-3.463924289,-0.6364110807\H,6.7542337468,-1.71
7461908,-0.4625496161\H,6.8650945151,-2.7428269642,0.9790202197\C,4.63
88536206,-4.30236123,0.0627350457\H,4.7998638395,-4.6221571958,1.10185
9925\H,3.5810557714,-4.3885821793,-0.1656258757\H,5.2115272188,-4.9635
434376,-0.5928294646\C,-7.6705739083,-3.0123928303,-0.2439386456\F,-8.
2362575954,-3.1705305304,0.9800821503\F,-8.366135397,-2.0334834825,-0.
8636254199\F,-7.9043349716,-4.1589245148,-0.9212106501\\Version=ES64L-
G09RevD.01\State=3-A\HF=-1801.5101926\S2=2.027984\S2-1=0.\S2A=2.000453
\RMSD=8.607e-09\RMSF=3.145e-06\Dipole=0.9482227,1.861725,-0.0015491\Qu
adrupole=1.1514852,8.3806609,-9.532146,-9.3787684,-4.6173055,-0.703965
6\PG=C01 [X(C29H22F3N7)]\\@

I[3,6]Me$_2$N,CF$_3$,Ph -S, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C29H22F3N7\PKASZYNSKI\15-
Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoA
ngle) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-NM
e2-1-Ph-benzo[e][1,2,4]triazinyl-6-)-1-Ph-7-CF3_benzo[e][1,2,4] triazi
nyl, conformer anti\\0,1\C,-0.6183625439,-1.8234739962,-0.0916952682\C
,0.255097519,-0.7197968889,-0.0172718863\C,-1.989000509,-1.6459959594,
-0.0771501269\C,-0.2788260986,0.5633373787,0.049461425\C,-2.5294538035
,-0.3525999093,0.0223493453\C,-1.6675850232,0.7808451153,0.0563197249\
N,-2.1538279974,2.0549508342,0.0824734017\N,-3.8881211602,-0.077635777
4,0.0582772404\N,-4.3899568497,1.1865970794,-0.019022935\C,-3.48158415

08,2.1862854386,0.0204803434\C,-4.8971662098,-1.0942511917,0.1023118\C
,-5.9161263022,-1.0844456154,-0.8512982372\C,-4.8873665697,-2.05344667
81,1.1163068865\C,-6.9169292992,-2.0491457474,-0.7970054528\C,-5.89159
69594,-3.0171785601,1.1593836591\C,-6.9061339987,-3.019991506,0.203958
6661\C,1.7224369245,-0.9450238927,-0.0269564644\C,3.5093948762,-2.3822
480699,-0.1169515825\C,4.4069649603,-1.2780854443,-0.1456111011\N,2.16
04439867,-2.20873267,-0.0275736675\N,2.4761942805,0.1577789131,-0.0222
547186\N,3.8229519758,-0.0187384874,-0.0154520089\C,4.5787595276,1.196
9762134,0.0676644423\C,4.2942721024,2.2356225201,-0.8194058192\C,5.555
4345614,1.3508606943,1.052812755\C,5.0056228401,3.4275653872,-0.727551
0196\C,6.264165031,2.54658147,1.1328968376\C,5.9939962433,3.5848423161
,0.2434232036\C,4.0470258421,-3.6816542661,-0.2114502214\C,5.778482309
5,-1.4813445855,-0.3297647863\C,5.4051812667,-3.8813763959,-0.36025370
66\C,6.2689027118,-2.7779538679,-0.4314144264\H,-2.6421762105,-2.50407
57543,-0.150406511\H,0.3673243669,1.4288824298,0.0924464786\H,-5.91674
46104,-0.3193884387,-1.6163402142\H,-4.1120584588,-2.0345404875,1.8719
780417\H,-7.7053871998,-2.0432584763,-1.5407090846\H,-5.8858819011,-3.
7581095925,1.9503532013\H,-7.6873806483,-3.7700685895,0.2428858588\H,-
0.1979102367,-2.816634603,-0.1653623096\H,3.5195000672,2.1016563077,-1
.5627618321\H,5.7450183497,0.5522330229,1.7591830944\H,4.7883360061,4.
2336671088,-1.4184439269\H,7.0191372277,2.6686504332,1.9005644636\H,6.
5462323554,4.5147712441,0.3108264333\H,5.8034211395,-4.884974531,-0.44
03943272\H,6.4534828408,-0.6419106118,-0.4015395801\H,3.3546929435,-4.
5132402379,-0.178800003\N,-4.0093138439,3.4524455627,0.02171773\C,-5.4
371153177,3.6727403873,-0.148651197\H,-5.9998743369,2.8663615918,0.314
1414083\H,-5.7038744498,4.6180937109,0.3292594503\H,-5.7218139233,3.73
03753322,-1.208622289\C,-3.1516338804,4.6114070289,-0.1734651802\H,-2.
129139158,4.3517603183,0.0820294209\H,-3.1790699947,4.9605449378,-1.21
51487738\H,-3.4922693961,5.4270807164,0.4702628337\C,7.7439354684,-3.0
110909288,-0.5772185367\F,8.3127631313,-3.4023452976,0.5915572036\F,8.
4077358932,-1.9046355911,-0.9774534228\F,8.0160755534,-3.9863301636,-1
.4745516721\\Version=ES64L-G09RevD.01\State=1-A\HF=-1801.5101608\S2=1.
024434\S2-1=0.\S2A=0.209165\RMSD=9.766e-09\RMSF=4.183e-06\Dipole=-1.19
65568,0.7311135,0.0049412\Quadrupole=2.7764736,7.1281687,-9.9046423,17
.3516136,6.6579739,-4.4857314\PG=C01 [X(C29H22F3N7)]\\@

I[3,6]Me$_2$N,CF$_3$,Ph -S, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C29H22F3N7\PKASZYNSKI\16-
Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoA
ngle) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-NM
e2-1-Ph-benzo[e][1,2,4]triazinyl-6-)-1-Ph-7-CF3_benzo[e][1,2,4] triazi
nyl, conformer syn\\0,1\C,0.1745566025,0.9808507573,-0.0662184977\C,-0
.2957429504,-0.3464795745,0.0198388184\C,1.5294025538,1.2527993195,-0.
0756932127\C,0.6223736847,-1.3894767874,0.0730037571\C,2.458705652,0.2
01050523,0.0061438054\C,2.0076587956,-1.1501043076,0.0509841951\N,2.87
86835392,-2.1979887098,0.056914927\N,3.8319941237,0.3775926958,0.02312
3926\N,4.7160778638,-0.6566403167,-0.0398885446\C,4.1765086443,-1.8949
48375,-0.0407214901\C,4.4590778718,1.6661251159,0.0729081681\C,5.39930
7824,2.0028265325,-0.9014709298\C,4.1660601953,2.5528527764,1.10986945
08\C,6.0350745691,3.2388837995,-0.8441271235\C,4.8055696941,3.78899877
25,1.1567506988\C,5.7383293307,4.1362113675,0.181225999\C,-1.748071674
6,-0.643085877,0.0390823403\C,-3.4699595291,-2.1578238886,0.1054153853
\C,-4.4157996698,-1.1027337895,-0.0327307228\N,-2.1300232177,-1.918311
2188,0.1688700878\N,-2.5494344082,0.4206811135,-0.0663638237\N,-3.8852
654113,0.1891907032,-0.0395512248\C,-4.6930764802,1.3732076218,-0.0830
406882\C,-4.456961166,2.320724929,-1.0796953157\C,-5.6728790238,1.5911
372894,0.8868154572\C,-5.2178645592,3.4849743458,-1.1111402619\C,-6.43

18787829,2.7575850149,0.8429567492\C,-6.2087034289,3.7045162369,-0.154
9185011\C,-3.9511821612,-3.4814519768,0.1480756482\C,-5.7761736376,-1.
3815618549,-0.1858550826\C,-5.3004795092,-3.7534717656,0.0294181932\C,
-6.2113542716,-2.7028224157,-0.1494567373\H,1.8719816228,2.2751906546,
-0.1522675432\H,0.2797648345,-2.4134300818,0.1215431535\H,5.6249159763
,1.2936787851,-1.6870959581\H,3.4578783547,2.2708894426,1.8790092435\H
,6.7620164904,3.5019155153,-1.6038032519\H,4.581754964,4.4749137207,1.
965496631\H,6.2357309181,5.0981539102,0.2231040096\H,-0.537825034,1.79
17317042,-0.1255199425\H,-3.6814365282,2.1389193881,-1.8121736119\H,-5
.8270847426,0.8650127319,1.6752570301\H,-5.0383954589,4.219792097,-1.8
871857258\H,-7.1897746714,2.9293859539,1.5981146171\H,-6.8003658469,4.
6118983376,-0.1840423886\H,-5.6553091769,-4.7757838868,0.0555335077\H,
-6.486790425,-0.5833299554,-0.3405061588\H,-3.2233002369,-4.2746920698
,0.2613543711\N,5.0745575956,-2.926301665,-0.1517747156\C,6.5077581972
,-2.6865579059,-0.0686147712\H,7.0268448513,-3.4706329035,-0.624418295
1\H,6.7540019445,-1.7203974938,-0.4996287616\H,6.8661799952,-2.7039776
272,0.9701297595\C,4.6434489821,-4.2992617433,0.0672430853\H,4.8107058
519,-4.6140687049,1.1068540899\H,3.5846674151,-4.3884902366,-0.1552564
335\H,5.2134118086,-4.9623550625,-0.5886125974\C,-7.6777503537,-3.0027
210563,-0.2451439611\F,-8.2524669661,-3.1210420803,0.9797702621\F,-8.3
624605848,-2.0354272338,-0.8956752103\F,-7.9189353099,-4.1658846807,-0
.8908157142\\Version=ES64L-G09RevD.01\State=1-A\HF=-1801.5107022\S2=0.
981945\S2-1=0.\S2A=0.1898\RMSD=9.135e-09\RMSF=3.824e-06\Dipole=1.13127
34,1.9207695,-0.0015241\Quadrupole=1.1231369,8.3839102,-9.5070471,-10.
0513113,-4.6265708,-0.6853731\PG=C01 [X(C29H22F3N7)]\\@

I[3,6]H,H,2-Pyr -T, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C24H16N8(3)\PKASZYNSKI\17
-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,No
Angle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benzo[e][1,2
,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer anti\\0,3\
C,1.2038345278,1.2767320932,-0.074311114\C,0.1974510091,0.294268039,-0
.0440234467\C,2.5462204791,0.9403246905,-0.0865526443\C,0.5760227603,-
1.0422543005,-0.0420426011\C,2.9345554914,-0.4089638777,-0.0692017307\
C,1.9264334355,-1.419813935,-0.0682650506\N,2.2323749939,-2.759366945,
-0.1132803201\N,4.2613946131,-0.864023656,-0.0936910968\N,4.5541815209
,-2.1962312453,-0.2062596128\C,3.5255341447,-3.0306166004,-0.204185867
\C,5.429980874,-0.043634864,-0.0408428571\C,6.6177106961,-0.5105052527
,-0.6242489078\C,7.7444611967,0.2901315689,-0.5256415039\C,6.434449884
4,1.8817131867,0.6730668869\C,7.6627593344,1.5142601181,0.138560617\C,
-1.2317499688,0.701907815,-0.0233037942\C,-2.8317874616,2.3408617579,0
.0042115249\C,-3.8671306801,1.3617096209,-0.0293100455\N,-1.5067954399
,2.0049623572,0.0301870116\N,-2.1123718544,-0.2968218037,-0.0523508234
\N,-3.4336043233,0.0232401095,-0.0122213899\C,-4.2820558333,-1.1264884
105,0.0042292752\C,-3.8292044241,-2.3175376663,-0.5824107206\C,-4.6566
30618,-3.4271645219,-0.5141598377\C,-6.2464504427,-2.0925850529,0.6604
573695\C,-5.8932790976,-3.3240284501,0.1232982113\C,-3.1850069137,3.70
46157596,-0.010834673\C,-5.2057535171,1.769904274,-0.1182050263\C,-4.5
082362521,4.0946298831,-0.080957502\C,-5.5150330072,3.1227578802,-0.14
3262223\H,3.2938708123,1.7143834126,-0.0800753691\H,-0.1613456583,-1.8
321975661,-0.0269955172\H,6.6366564719,-1.4670222899,-1.1224298715\H,8
.6782978006,-0.0374699671,-0.9675606496\H,6.3171181558,2.8242496197,1.
1991146659\H,8.5227631201,2.1643434471,0.2373451563\H,0.9102438477,2.3
174705377,-0.0836219639\H,-2.8646382325,-2.3533473452,-1.064379925\H,-
4.3401190947,-4.363476932,-0.9587700469\H,-7.1988545958,-1.9592846299,
1.1645049546\H,-6.5641718785,-4.1702768112,0.1990069301\H,-4.766196903

3,5.1470784182,-0.0933267259\H,-5.9912559347,1.034025831,-0.1363718617
\H,-2.3770046624,4.4247950242,0.0235635415\H,-6.5544543052,3.422337738
9,-0.2076705422\H,3.8150493029,-4.0748057464,-0.2798507486\N,-5.459960
5132,-1.0122300013,0.6095807984\N,5.3376041395,1.1212166877,0.59255506
69\\Version=ES64L-G09RevD.01\State=3-A\HF=-1362.4443209\S2=2.02996\S2-
1=0.\S2A=2.000536\RMSD=8.582e-09\RMSF=5.200e-06\Dipole=-0.0109823,0.07
86922,-0.6749128\Quadrupole=28.6470937,-5.7280515,-22.9190422,13.38065
69,-1.9151679,2.4975652\PG=C01 [X(C24H16N8)]\\@

I[3,6]H,H,2-Pyr -T, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C24H16N8(3)\PKASZYNSKI\17
-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,No
Angle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benzo[e][1,2
,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer syn\\0,3\C
,0.8174069221,0.5192453542,-0.0304534542\C,0.145856557,-0.717992217,-0
.0238761059\C,2.1984863337,0.593409395,-0.0618906011\C,0.9009888106,-1
.8820193824,-0.0666171089\C,2.9672178625,-0.5817429352,-0.0919377686\C
,2.3028083889,-1.8437163053,-0.1172085507\N,2.9897484688,-3.0308357267
,-0.2158607598\N,4.3691089704,-0.6224428179,-0.1424720728\N,5.03919045
54,-1.8029859587,-0.317021862\C,4.3023836947,-2.9038109639,-0.33666420
66\C,5.2432891126,0.5034531867,-0.0566137472\C,6.50511889,0.4355812022
,-0.6669258766\C,7.3472037267,1.5280492819,-0.5337680516\C,5.648016117
9,2.6052098279,0.7463280672\C,6.9202687841,2.6418411989,0.1899071596\C
,-1.3386532293,-0.7933463834,0.0205623223\C,-3.260306006,-2.0327960875
,0.1543129541\C,-4.0544338025,-0.8534045396,0.0517541907\N,-1.89442713
83,-1.996264786,0.1618365401\N,-1.9764425402,0.3715477955,-0.081380501
9\N,-3.3368011783,0.353293104,-0.0217409669\C,-3.9140492656,1.65726013
7,-0.0976884114\C,-3.2347511989,2.6654423066,-0.797368166\C,-3.8011401
934,3.9301665012,-0.8215239248\C,-5.6016548794,3.0806946584,0.49228424
56\C,-5.0094107521,4.1542247762,-0.1610985701\C,-3.9054566788,-3.28334
63963,0.2295123668\C,-5.4511357444,-0.9604604445,-0.0142488059\C,-5.28
24891824,-3.3748805086,0.1794063604\C,-6.0508165582,-2.2104451824,0.04
87170405\H,2.6859096724,1.5524992176,-0.0310807675\H,0.4195832304,-2.8
496992048,-0.0759756493\H,6.7961144687,-0.4491181489,-1.2111312644\H,8
.3279929611,1.5114423578,-0.9946575226\H,5.2677204967,3.4460240776,1.3
185002602\H,7.5521949485,3.5115349798,0.3175137695\H,0.2386136973,1.43
2226567,0.0025225103\H,-2.3028193362,2.4464311989,-1.2953195996\H,-3.3
06836832,4.7327364445,-1.356511489\H,-6.5435223311,3.2022247509,1.0185
980379\H,-5.4800784839,5.1290924191,-0.1557785731\H,-5.7667650418,-4.3
426346641,0.2357810884\H,-6.0557707083,-0.0723611474,-0.08382608\H,-3.
2753279838,-4.1598124372,0.3155239863\H,-7.1313531383,-2.2770932486,0.
0003689996\H,4.8849080519,-3.812174424,-0.4607196811\N,-5.0683977456,1
.8550066571,0.5314294537\N,4.8226923266,1.5593715143,0.6328997867\\Ver
sion=ES64L-G09RevD.01\State=3-A\HF=-1362.4434409\S2=2.030052\S2-1=0.\S
2A=2.000539\RMSD=8.969e-09\RMSF=5.159e-06\Dipole=-0.1975762,2.4661864,
-0.7334503\Quadrupole=21.785319,-1.6655061,-20.1198128,5.4852533,-1.91
08974,-1.2663472\PG=C01 [X(C24H16N8)]\\@

I[3,6]H,H,2-Pyr -S, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C24H16N8\PKASZYNSKI\18-Ja
n-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAng
le) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-H-1-
Pyr-benzo[e][1,2,4]triazinyl-6-)-1-Pyr-benzo[e][1,2,4]triazinyl, confo
rmer anti\\0,1\C,1.202613353,1.2818788104,-0.0779934233\C,0.1969748119
,0.2994300634,-0.048747786\C,2.5458348209,0.9446768055,-0.091170845\C,
0.5750631322,-1.0363516926,-0.0488574822\C,2.93439926,-0.4035015179,-0
.0762355329\C,1.9269683624,-1.4142128371,-0.0767537958\N,2.2290052408,

-2.7530124172,-0.1258223419\N,4.263845474,-0.861146289,-0.1017000551\N
,4.5512862202,-2.1934034688,-0.2199949914\C,3.5229555677,-3.0263254994
,-0.2199031517\C,5.4336075917,-0.0447963899,-0.0434215822\C,6.62764820
21,-0.5204758007,-0.60793432\C,7.7550987618,0.2781588069,-0.5043061176
\C,6.4357988329,1.8858097019,0.6615527062\C,7.6693835049,1.5096631646,
0.1459344505\C,-1.2349764412,0.7039341703,-0.0259732968\C,-2.835747880
7,2.3410005996,0.0050103907\C,-3.8703210144,1.3607717779,-0.028897717\
N,-1.5105268528,2.005810713,0.0296826572\N,-2.1136547212,-0.2958111653
,-0.0555333771\N,-3.4361388737,0.0234133886,-0.0128821805\C,-4.2832548
523,-1.126997523,0.0055693429\C,-3.8291863363,-2.3186951278,-0.5789241
921\C,-4.6555294229,-3.4290121568,-0.5088080901\C,-6.2466977402,-2.094
0514301,0.6634996789\C,-5.8922929,-3.3260839313,0.1284535602\C,-3.1895
9095,3.7045996515,-0.0084138822\C,-5.2094590443,1.768648356,-0.1170057
051\C,-4.5129482064,4.0938716002,-0.0775897056\C,-5.5191651148,3.12117
36193,-0.1405855616\H,3.2935702219,1.7185663992,-0.083367363\H,-0.1619
519131,-1.8266492125,-0.0347614353\H,6.6503453401,-1.4819307816,-1.096
1945728\H,8.6930861375,-0.0567244229,-0.9318057383\H,6.3146569015,2.83
43338047,1.1759305661\H,8.5299714031,2.1584698269,0.2478540561\H,0.909
472635,2.3227188217,-0.0851593688\H,-2.8645835114,-2.3543494954,-1.060
7795186\H,-4.3380302039,-4.3657642236,-0.9517856904\H,-7.1991918407,-1
.9608610415,1.1674170963\H,-6.5622892352,-4.1729025803,0.2056646126\H,
-4.7717079667,5.1461187939,-0.0888301751\H,-5.9946114768,1.0324445995,
-0.1357400538\H,-2.3819000437,4.4250988792,0.0262851179\H,-6.558761181
2,3.4202932756,-0.2044723857\H,3.8103746336,-4.070640279,-0.3002439476
\N,-5.4613511974,-1.0130084494,0.6107704544\N,5.3377855116,1.127594103
4,0.5760366923\\Version=ES64L-G09RevD.01\State=1-A\HF=-1362.4438771\S2
=1.032217\S2-1=0.\S2A=0.265006\RMSD=7.132e-09\RMSF=5.961e-06\Dipole=-0
.0689727,0.0495004,-0.6559861\Quadrupole=28.3175933,-5.4368074,-22.880
7859,12.938528,-1.760259,2.4608703\PG=C01 [X(C24H16N8)]\\@

I[3,6]H,H,2-Pyr -S, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C24H16N8\PKASZYNSKI\19-Ja
n-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAng
le) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-H-1-
Pyr-benzo[e][1,2,4]triazinyl-6-)-1-Pyr-benzo[e][1,2,4]triazinyl, confo
rmer syn\\0,1\C,0.8120392122,0.5184319828,-0.0456424244\C,0.1435547899
,-0.7195706655,-0.0201411399\C,2.1942699861,0.5942735753,-0.0737808063
\C,0.8999474549,-1.8827192729,-0.0395785186\C,2.9653300104,-0.57836363
29,-0.0807788449\C,2.3032270841,-1.8429642503,-0.085658948\N,2.9892424
196,-3.0293541475,-0.1591404144\N,4.3693782031,-0.6193414813,-0.125540
4377\N,5.0387510107,-1.803796503,-0.2725109456\C,4.3044986692,-2.90426
78562,-0.274694304\C,5.243872985,0.507127006,-0.0616141427\C,6.5154605
498,0.4191546572,-0.6497420701\C,7.3563955274,1.5148042839,-0.53913143
56\C,5.6390475342,2.6344157622,0.6780402827\C,6.9197429293,2.652260403
1,0.1408184569\C,-1.3405445207,-0.7999642638,0.0197304076\C,-3.2633971
754,-2.0386902295,0.1317672741\C,-4.0555404534,-0.8576412747,0.0390240
977\N,-1.8969330234,-2.0039031742,0.1453257016\N,-1.9766603208,0.36657
93912,-0.0702096765\N,-3.3347186186,0.3496082799,-0.017888921\C,-3.910
8547918,1.6554430375,-0.0809923315\C,-3.2327875774,2.6680237803,-0.774
8850275\C,-3.7973844155,3.9338115099,-0.7860743599\C,-5.5940379261,3.0
755111022,0.5277121359\C,-5.0026687537,4.1536781658,-0.1189104596\C,-3
.9117910401,-3.2881548779,0.1894238067\C,-5.4517736579,-0.9598940093,-
0.0352411924\C,-5.2891564595,-3.375846963,0.1317011072\C,-6.0550452233
,-2.2090992228,0.0106088436\H,2.6798577634,1.5545379765,-0.0580460018\
H,0.4198521207,-2.8510177374,-0.0330201164\H,6.814343729,-0.4825716197
,-1.1605194908\H,8.3441986633,1.4823624569,-0.9839583189\H,5.250613859
7,3.4937525686,1.2162673092\H,7.5504994359,3.5253699383,0.249416902\H,

0.2318011035,1.4308055294,-0.0300847792\H,-2.3031608265,2.451903241,-1
.2785460829\H,-3.3041465271,4.7402810984,-1.3161206326\H,-6.5336027903
,3.1939022219,1.0587844155\H,-5.4719294659,5.1291170521,-0.1034712687\
H,-5.7753414707,-4.343377279,0.1747232853\H,-6.0539262298,-0.069504867
7,-0.097947912\H,-3.2844874525,-4.167331271,0.2681196936\H,-7.13543197
11,-2.2729794321,-0.0435790555\H,4.8873105051,-3.8149172734,-0.3778867
532\N,-5.0623144254,1.8487909912,0.5542705746\N,4.8143825709,1.5859502
937,0.5860015186\\Version=ES64L-G09RevD.01\State=1-A\HF=-1362.4437285\
S2=1.010773\S2-1=0.\S2A=0.255261\RMSD=7.281e-09\RMSF=6.737e-06\Dipole=
-0.1980337,2.4708399,-0.7479297\Quadrupole=21.6966014,-1.4608664,-20.2
35735,4.6683124,-1.9706513,-1.1983063\PG=C01 [X(C24H16N8)]\\@

I[3,6]H,H,4-Me2NPh -T, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C30H28N8(3)\PKASZYNSKI\17
-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,No
Angle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benzo[e][1,2
,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer anti\\0,3\
C,1.1763423735,1.3010104865,-0.1910578057\C,0.1598102791,0.3295777378,
-0.1461146907\C,2.5137699953,0.9425635182,-0.1905506542\C,0.5187897994
,-1.0172239944,-0.1262886128\C,2.8761839154,-0.4123249256,-0.139530406
4\C,1.8617313283,-1.4140966956,-0.1382491742\N,2.1786309673,-2.7541641
166,-0.175770775\N,4.1924960825,-0.8580252428,-0.1146590021\N,4.508837
0294,-2.1849951041,-0.2349313839\C,3.4753997729,-3.0187701413,-0.25788
98122\C,5.321901376,0.0147241213,-0.019779116\C,6.351276197,-0.0784151
897,-0.9565663087\C,5.4409044672,0.929526715,1.0267307845\C,7.46843895
05,0.7360232953,-0.8646764479\C,6.5530436559,1.7527022977,1.1248287413
\C,7.6064489104,1.6774658362,0.1834192755\C,-1.2634367227,0.754774473,
-0.1386111173\C,-2.8414894444,2.42082909,-0.2098869323\C,-3.8780684489
,1.4451667111,-0.2191058739\N,-1.5211124611,2.065763109,-0.1441565602\
N,-2.1560642104,-0.2376889057,-0.1130128809\N,-3.4691673311,0.11716533
66,-0.0952545469\C,-4.3800235958,-0.9836744716,-0.0098344464\C,-4.2713
078499,-2.0453028203,-0.9081308735\C,-5.3473595577,-1.0426582737,0.993
354109\C,-5.1180769806,-3.1381750881,-0.8189311085\C,-6.2036562838,-2.
1300379499,1.0881387842\C,-6.1106910967,-3.2173526012,0.187353174\C,-3
.1997448048,3.7786347549,-0.2990983394\C,-5.2149229318,1.835440763,-0.
3721135567\C,-4.5263812031,4.1584168672,-0.4210216237\C,-5.531685735,3
.1850212664,-0.4686285446\H,3.2769253235,1.7064833445,-0.2359632215\H,
-0.2362889996,-1.7905999429,-0.1110060458\H,6.2723277744,-0.8016030229
,-1.7583042332\H,4.6643121998,0.9950501723,1.779304221\H,8.2389659635,
0.638397135,-1.616083535\H,6.605250761,2.4484250954,1.9500417204\H,0.8
924524521,2.3437305234,-0.2291156561\H,-3.5103471558,-2.0125406103,-1.
6776508608\H,-5.4265198288,-0.239829675,1.7166530558\H,-5.0035582973,-
3.9360366704,-1.5387522556\H,-6.9377522199,-2.1373415433,1.8812279143\
H,-4.7852726893,5.2084551814,-0.4911566134\H,-5.994992542,1.0886942884
,-0.419907236\H,-2.3985149954,4.507394957,-0.2815660037\H,-6.567973064
2,3.4793959608,-0.5859083143\H,3.7656222261,-4.0624203964,-0.343715297
9\N,8.723869154,2.4780193197,0.2885777066\N,-6.9422792467,-4.310715240
4,0.291636826\C,-6.9019270662,-5.3551247876,-0.7199502268\H,-7.6047511
21,-6.1404507044,-0.4481088941\H,-7.1737089683,-4.9830576317,-1.717004
1198\H,-5.9075918559,-5.8083941749,-0.7859061801\C,-8.0235644702,-4.31
36212033,1.2640322082\H,-8.7557200646,-3.5157207322,1.0792900131\H,-8.
5433034331,-5.2686865502,1.2147385149\H,-7.6432660116,-4.1956693344,2.
2839908523\C,9.7152965414,2.4844028942,-0.7759350542\H,9.2996073738,2.
8233347503,-1.7346763486\H,10.5265772552,3.1559923026,-0.5010341712\H,
10.1455705602,1.4890450439,-0.9249415775\C,8.7760816529,3.5223143406,1
.2997118917\H,9.7427528559,4.0199796493,1.2467092691\H,7.9920000969,4.

279816523,1.1630957852\H,8.6735934674,3.1054852997,2.3066294024\\Versi
on=ES64L-G09RevD.01\State=3-A\HF=-1598.3614653\S2=2.02724\S2-1=0.\S2A=
2.000431\RMSD=6.088e-09\RMSF=1.893e-06\Dipole=-0.631541,0.6392554,0.12
46918\Quadrupole=48.5423343,-14.9765823,-33.5657521,43.9739111,-3.7787
248,4.1569793\PG=C01 [X(C30H28N8)]\\@

I I[3,6]H,H,4-Me2NPh -T, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C30H28N8(3)\PKASZYNSKI\17
-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,No
Angle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benzo[e][1,2
,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, conformer syn\\0,3\C
,0.8616978853,0.351004468,-0.0459857302\C,0.1745326305,-0.8758346379,0
.0243767486\C,2.244450405,0.4015604022,-0.0117116702\C,0.9129868309,-2
.0538685465,0.1038369704\C,2.9880581328,-0.7841073994,0.1013888628\C,2
.3135968793,-2.0383444458,0.1293360578\N,3.0101284106,-3.2272301493,0.
1520009861\N,4.3769476319,-0.8204211939,0.1639892445\N,5.0712339262,-1
.9996973802,0.1026259504\C,4.3288062572,-3.1010325413,0.0991507133\C,5
.1989648645,0.3473374563,0.2377895231\C,6.2505995151,0.5118365926,-0.6
639419644\C,5.0159887149,1.2991117563,1.2414470752\C,7.0867927642,1.61
37314544,-0.5845098253\C,5.8445825631,2.4086163985,1.3254193183\C,6.89
97513738,2.6083582799,0.4046686459\C,-1.3109384772,-0.927238149,-0.000
0954842\C,-3.2551254961,-2.1478484445,0.0153914743\C,-4.0128854655,-0.
9528308347,-0.1398733483\N,-1.8902610836,-2.1247325028,0.1100298817\N,
-1.9248293066,0.2534711669,-0.1183081423\N,-3.2869844059,0.2369766777,
-0.1306364741\C,-3.8985126511,1.5295436656,-0.1956011747\C,-3.54290395
18,2.4190029513,-1.2092277758\C,-4.8205373799,1.9357262682,0.768865711
1\C,-4.1041675826,3.6847917293,-1.269424742\C,-5.3921007374,3.19859358
05,0.7147606162\C,-5.044532264,4.1171627461,-0.3037808765\C,-3.9398380
909,-3.3769420105,0.0446472218\C,-5.4019535892,-1.0142152603,-0.314967
4515\C,-5.3161710097,-3.4273781954,-0.101617944\C,-6.0440699965,-2.246
0489836,-0.2919718423\H,2.7503903574,1.354431218,-0.077128436\H,0.4108
351816,-3.0105710152,0.1362373663\H,6.4192766752,-0.2420937961,-1.4221
481794\H,4.2334722719,1.1651717165,1.9786394727\H,7.8917250828,1.69828
10186,-1.3005363423\H,5.6755186606,3.113585232,2.126837096\H,0.2926706
501,1.2668859316,-0.1288788798\H,-2.8191309834,2.1119549436,-1.9538375
76\H,-5.0895676345,1.2640749025,1.5754542553\H,-3.8102634829,4.3405660
944,-2.0763783853\H,-6.1027149901,3.4743468633,1.4805671292\H,-5.82894
46079,-4.3818398644,-0.0798620993\H,-5.9687051254,-0.1072087975,-0.471
8915716\H,-3.3471532958,-4.2744932024,0.1724666455\H,-7.1185368689,-2.
286357058,-0.4271738256\H,4.9149491305,-4.0152341542,0.0602155803\N,-5
.5904236688,5.3826610127,-0.3476923776\N,7.7102013273,3.7240091304,0.4
669334483\C,-5.3304873377,6.246348886,-1.4892475136\H,-5.7153898685,5.
82853106,-2.4297651007\H,-5.8111344054,7.2086764372,-1.322493033\H,-4.
2585767203,6.429264001,-1.6121078184\C,-6.6592688268,5.7433899183,0.57
08181273\H,-6.9346594677,6.783255033,0.4043343248\H,-7.5572318616,5.12
47015688,0.4357435212\H,-6.3359568123,5.6500668273,1.6122155903\C,7.61
14377061,4.6264990467,1.6038198312\H,8.2929027363,5.4620543344,1.45295
62406\H,6.6014848587,5.0370876971,1.6946110815\H,7.8690822335,4.139722
0893,2.5549331487\C,8.8965588587,3.8020992321,-0.371892376\H,9.3807000
416,4.7639798254,-0.2120034428\H,9.6246200737,3.0091895907,-0.15038918
11\H,8.6352844146,3.7372849784,-1.4322163562\\Version=ES64L-G09RevD.01
\State=3-A\HF=-1598.3607813\S2=2.027362\S2-1=0.\S2A=2.000433\RMSD=4.66
9e-09\RMSF=4.395e-06\Dipole=-0.8743767,4.5141832,-0.10696\Quadrupole=3
4.2128195,-10.4947338,-23.7180856,7.6687456,-0.2760324,1.1870938\PG=C0
1 [X(C30H28N8)]\\@

I[3,6]H,H,4-Me2NPh -S, *anti*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C30H28N8\PKASZYNSKI\18-Ja
n-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAng
le) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-H-1-
PhNme2-benzo[e][1,2,4]triazinyl-6-)-1-PhNme2-benzo[e][1,2,4]triazinyl,
conformer anti\\0,1\C,1.1741708362,1.3068619754,-0.1951598801\C,0.158
2260693,0.3356951268,-0.1494132367\C,2.5122145669,0.9471025847,-0.1954
516481\C,0.516307012,-1.0103634886,-0.1297502528\C,2.8740109822,-0.406
7712961,-0.1443507182\C,1.8604625622,-1.4080057905,-0.1429184703\N,2.1
739477058,-2.7478735423,-0.1830843508\N,4.1927024412,-0.8549368015,-0.
1200098494\N,4.5046491754,-2.1816536376,-0.2472703868\C,3.4712122539,-
3.0141552445,-0.2703630483\C,5.3229470224,0.0153569387,-0.0230897166\C
,6.3569606512,-0.0829502707,-0.9544699137\C,5.4390804524,0.9341623022,
1.0204924541\C,7.4755317518,0.7292933713,-0.8599093378\C,6.5523895091,
1.7554681278,1.1208581648\C,7.6103942915,1.6744334879,0.1851626463\C,-
1.2682300428,0.7591417744,-0.1400375759\C,-2.8471761422,2.4231261369,-
0.2067444379\C,-3.8828944281,1.4463402132,-0.2188492926\N,-1.526546843
5,2.0688018148,-0.1411133199\N,-2.1586396163,-0.2344542732,-0.11722128
19\N,-3.4727928165,0.1190703247,-0.0970131537\C,-4.3818313387,-0.98286
60823,-0.0105355944\C,-4.2687991022,-2.0472110539,-0.9052073757\C,-5.3
516308735,-1.0405838838,0.9904687374\C,-5.1140249048,-3.1411200975,-0.
814967612\C,-6.2061277666,-2.1292067903,1.0864075963\C,-6.1091708717,-
3.2189589857,0.1889648238\C,-3.206716198,3.7807245313,-0.2929697682\C,
-5.2202062136,1.8357583343,-0.3727051938\C,-4.5335996184,4.1593834166,
-0.415288433\C,-5.5380259701,3.1850584221,-0.4664231623\H,3.2754843375
,1.7109423674,-0.2411917147\H,-0.2387246546,-1.7838142807,-0.113981551
3\H,6.2804229343,-0.8087556819,-1.7540542485\H,4.6592317493,1.00412146
95,1.7692529917\H,8.2494949425,0.6272093944,-1.6071924879\H,6.60190080
28,2.4542503168,1.9436582486\H,0.8908747174,2.3497326362,-0.2327008896
\H,-3.5058619869,-2.0154542421,-1.672773304\H,-5.4339030033,-0.2359232
59,1.7113475467\H,-4.9963401397,-3.9409118352,-1.5321297272\H,-6.94202
45132,-2.1355629995,1.8778283902\H,-4.793511141,5.2093133143,-0.483199
399\H,-5.999454627,1.088357244,-0.4233977523\H,-2.4062616349,4.5102590
501,-0.273026494\H,-6.574412412,3.4787967448,-0.584393086\H,3.75954775
13,-4.0578165947,-0.3611865221\N,8.7291420208,2.4731006528,0.292927079
6\N,-6.9393173321,-4.3132255366,0.294232368\C,-6.8946675662,-5.3606219
505,-0.7141144166\H,-7.5970812882,-6.1461577275,-0.4418436602\H,-7.164
3099198,-4.9918718126,-1.7129633947\H,-5.8995052599,-5.8126344946,-0.7
760194505\C,-8.0228607144,-4.3151823984,1.264155254\H,-8.7556055128,-3
.5187123597,1.0756997229\H,-8.5412315418,-5.2710416233,1.2160033828\H,
-7.6450800082,-4.1941997863,2.2846950457\C,9.7251414639,2.4742134912,-
0.7672695408\H,9.3144031775,2.8109552158,-1.7289457574\H,10.5365997522
,3.1450134533,-0.4909291231\H,10.1540701404,1.4775421258,-0.9112949056
\C,8.7780571977,3.5215635494,1.2998434853\H,9.7460592633,4.0169992942,
1.2500072347\H,7.9962984559,4.2801565365,1.1559102481\H,8.6693200828,3
.1091975015,2.3079368254\\Version=ES64L-G09RevD.01\State=1-A\HF=-1598.
3607868\S2=1.027361\S2-1=0.\S2A=0.2206\RMSD=7.162e-09\RMSF=5.065e-06\D
ipole=-0.6810968,0.604258,0.1291332\Quadrupole=48.4205272,-14.8149849,
-33.6055423,43.7829854,-3.7675184,4.1546959\PG=C01 [X(C30H28N8)]\\@

I[3,6]H,H,4-Me2NPh -S, *syn*

1\1\GINC-GAUSIANDELL\FOpt\UB3LYP\6-311G(d,p)\C30H28N8\PKASZYNSKI\18-Ja
n-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAng
le) fcheck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-H-1-
Ph-benzo[e][1,2,4]triazinyl-6-)-1-Ph-benzo[e][1,2, 4]triazi nyl, confo
rmer syn\\0,1\C,0.8544817564,0.3477223559,-0.0421144089\C,0.1710760876
,-0.8805758536,0.0269685761\C,2.2383564014,0.4004341333,-0.0086671243\
C,0.910184393,-2.0575533496,0.1059890963\C,2.9837885967,-0.7828259228,

0.102742407\C,2.3120943985,-2.0398178695,0.1303207039\N,3.0085630968,-3.2254644358,0.1510886329\N,4.3738317123,-0.8182690254,0.1651656784\N,5.0683100614,-1.9968146458,0.1022004314\C,4.3290926231,-3.0981939484,0.0975884071\C,5.1947308973,0.3501952442,0.2379320626\C,6.245782924,0.5156431506,-0.6643110121\C,5.0109807223,1.302345007,1.241143034\C,7.0809742699,1.618396875,-0.5854801007\C,5.8384336464,2.4127094668,1.3244313836\C,6.893185477,2.6131925764,0.40333694\C,-1.3135918529,-0.9380864858,0.0024872756\C,-3.2587550431,-2.155319407,0.0142055202\C,-4.0144689614,-0.9591312541,-0.1384654918\N,-1.8934331013,-2.1354914713,0.1091274805\N,-1.9255296544,0.2431254486,-0.1125364335\N,-3.2837536334,0.2309181324,-0.127414847\C,-3.892862492,1.525021181,-0.1930968016\C,-3.5343481868,2.413262421,-1.2066893009\C,-4.8149756172,1.9330399176,0.7704616379\C,-4.0926771897,3.6802771034,-1.2675782706\C,-5.3832956065,3.1972834262,0.7157869052\C,-5.0326865027,4.114988434,-0.3026035048\C,-3.9477479852,-3.3818533595,0.0402771265\C,-5.4028493919,-1.0147256517,-0.3143221795\C,-5.3246592172,-3.4274295498,-0.1065784538\C,-6.0498385211,-2.2446185766,-0.2944419401\H,2.7423310384,1.3544407326,-0.0727339372\H,0.4088756831,-3.0146640122,0.13858618\H,6.415014692,-0.2382271441,-1.4224728134\H,4.2286144676,1.1680791444,1.978426495\H,7.8856234804,1.7034892571,-1.3017664643\H,5.6687337853,3.1179138015,2.1255140518\H,0.2836340384,1.2624914927,-0.1228754657\H,-2.8109936895,2.1043064803,-1.9509363081\H,-5.0864304875,1.2620114617,1.5767261336\H,-3.7968755342,4.3350767507,-2.0746091352\H,-6.0940196029,3.4747304756,1.4808600988\H,-5.8397264038,-4.3807922588,-0.0870332363\H,-5.9661940863,-0.1052870556,-0.4695697356\H,-3.3584834313,-4.2819511094,0.1660244093\H,-7.1243319075,-2.2814005078,-0.4298975866\H,4.9153855167,-4.01205575,0.0569203698\N,-5.5755728117,5.3815848546,-0.3471358896\N,7.7023673382,3.7298195955,0.4649128898\C,-5.3121809868,6.2448745473,-1.4882658268\H,-5.696939596,5.8280267306,-2.4292301116\H,-5.7908058113,7.2082766035,-1.3219659673\H,-4.2397004387,6.425303789,-1.6097348331\C,-6.6441053222,5.7452482471,0.5706873652\H,-6.916545634,6.785826942,0.4039186803\H,-7.5435631001,5.1289604092,0.4349194761\H,-6.3217078593,5.6510872556,1.6122727692\C,7.6033406873,4.6322686548,1.6018142749\H,8.2841707162,5.4682981432,1.4507236597\H,6.5931419736,5.0421740613,1.6929602864\H,7.8616459339,4.1456722922,2.5528311779\C,8.8882092202,3.8090811403,-0.3745392144\H,9.371060822,4.7717371648,-0.215446478\H,9.6174763316,3.0173080075,-0.1529574599\H,8.6264284706,3.7432813564,-1.4346703638\\Version=ES64L-G09RevD.01\State=1-A\HF=-1598.3612001\S2=0.993946\S2-1=0.\S2A=0.206646\RMSD=8.313e-09\RMSF=4.065e-06\Dipole=-0.8416555,4.5497667,-0.1083241\Quadrupole=34.0582833,-10.4154488,-23.6428345,6.9879687,-0.2884925,1.1712735\PG=C01 [X(C30H28N8)]\\@

I[3,7]H,H,Ph -T, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C26H18N6(3)\PIOTR\10-Jan-2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benzo[e][1,2,4]triazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer anti\\0,3\C,-1.6608206894,0.0216492238,-0.026875033\C,-2.9916743303,1.8885721357,-0.1724527051\C,-4.1554064498,1.0758207003,-0.0659313014\C,-0.3100352416,-0.5908734465,0.040516259\C,-0.1468829215,-1.9871832002,0.1405567404\C,0.8171386643,0.2324228486,-0.0040526627\C,1.1149253864,-2.5427082767,0.168825743\C,2.0963992165,-0.3213940292,0.0617579288\C,2.2683452824,-1.7357281869,0.1123822859\N,3.5055802689,-2.3169069807,0.0732183321\N,3.2723022951,0.4393011967,0.0504756106\N,4.50039751,-0.1421376907,-0.0909831952\C,4.5196555571,-1.4649981195,-0.0690827321\C,3.3011803871,1.8670638544,0.123641798\C,4.078684635,2.5784014606,-0.7928516767\C,2.6045290085,2.5411232454,1.1293550234\C,4.1422496623,3.9652274582,-0.71039626

72\C,2.6717735345,3.9296780631,1.1996548132\C,3.4362834,4.646139114,0.
2806838696\N,-3.9341263636,-0.3006699471,-0.0236576856\N,-2.6841428625
,-0.8331040721,0.0575020952\N,-1.7356294777,1.346662145,-0.176287613\C
,-5.4236328779,1.6653270093,0.0197786591\C,-3.1526180288,3.2847167396,
-0.2491260282\C,-4.4113070496,3.8580166398,-0.1939378571\C,-5.54443343
6,3.0472642026,-0.0480052097\C,-4.9885653145,-1.2704703758,-0.00074803
49\C,-5.0145838631,-2.2237602163,1.0180590033\C,-5.9508753364,-1.28821
8913,-1.0116369885\C,-6.0177815006,-3.1876091259,1.0304081943\C,-6.953
2440925,-2.2544114015,-0.9875847996\C,-6.9912398193,-3.2036481911,0.03
22170332\H,-1.0254479641,-2.6165810201,0.1762823142\H,0.6717297561,1.2
980828281,-0.0932830104\H,1.2611830394,-3.6147245157,0.2164073587\H,4.
6301421441,2.0373282059,-1.5500509172\H,2.029837268,1.9844649421,1.858
4379601\H,4.7432540179,4.5149183087,-1.4255213567\H,2.1333210927,4.449
1063165,1.9837478683\H,3.4872619453,5.726982009,0.3406593645\H,-4.5201
030489,4.9345456788,-0.251898127\H,-2.2561591905,3.8856241001,-0.34031
11739\H,-6.3034920973,1.0496645853,0.1433084276\H,-4.2488241854,-2.204
3070667,1.7825025253\H,-5.904095783,-0.5651776374,-1.8164062353\H,-6.0
395811432,-3.9259298452,1.8234997715\H,-7.6966631494,-2.271348002,-1.7
75993531\H,-7.7710434765,-3.956042581,0.0451888616\H,-6.5282714481,3.4
965133156,0.0174796603\H,5.5145921297,-1.8882816161,-0.1703876396\\Ver
sion=ES64L-G09RevD.01\State=3-A\HF=-1330.3544679\S2=2.032336\S2-1=0.\S
2A=2.000596\RMSD=5.768e-09\RMSF=8.257e-06\Dipole=-2.3604791,0.9758774,
0.0689085\Quadrupole=5.0344836,2.8864202,-7.9209038,13.9626166,-1.0274
444,-1.6167709\PG=C01 [X(C26H18N6)]\\@

I[3,7]H,H,Ph -T, *syn*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C26H18N6(3)\PIOTR\10-Jan-20
24\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle)
fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benzo[e][1,2,4]tria
zinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer syn\\0,3\C,1.65615
19242,-1.4854044193,-0.0747685705\C,3.7146563134,-2.5037519056,-0.0457
158019\C,4.3478958568,-1.2375217944,0.0986336124\C,0.1763036424,-1.583
0966818,-0.1196568742\C,-0.4361750628,-2.8475516837,-0.2157903621\C,-0
.6186908868,-0.4346027578,-0.0637467579\C,-1.8109224556,-2.960054561,-
0.2289127573\C,-2.0091098017,-0.5391126576,-0.1126889168\C,-2.63554541
68,-1.8206876158,-0.1601929252\N,-3.9938115421,-1.9640202041,-0.109895
3103\N,-2.8716995032,0.56336044,-0.0894085197\N,-4.2215677884,0.415699
5425,0.0596432952\C,-4.6729939774,-0.8276882992,0.0380366352\C,-2.4338
900204,1.9230746268,-0.1592650303\C,-2.9332472709,2.8446853846,0.76365
97597\C,-1.5604684462,2.3381771511,-1.1672308475\C,-2.542445114,4.1771
188907,0.6853024731\C,-1.1717739232,3.6731510231,-1.2328495226\C,-1.65
73950534,4.5953903512,-0.307789999\N,3.5026982674,-0.1266626691,0.0589
391125\N,2.1485378344,-0.2473843301,0.032649614\N,2.3558421293,-2.6196
101178,-0.1576491228\C,5.73217612,-1.1581961659,0.2979671254\C,4.51775
76411,-3.6595247549,-0.0439285444\C,5.8891905072,-3.5708836671,0.12225
42827\C,6.4931490132,-2.3203485476,0.3045230523\C,3.9720017653,1.22605
56371,0.1080413513\C,3.4511769208,2.0928771167,1.0698822307\C,4.905633
9163,1.6820971261,-0.8243139109\C,3.8807503169,3.4156603155,1.10595134
15\C,5.3326838486,3.0065391101,-0.7762682051\C,4.8248445444,3.87499495
3,0.1882832757\H,0.1946919219,-3.7242249247,-0.2656013903\H,-0.1385046
667,0.5282840035,0.0167910813\H,-2.3004838272,-3.9249093405,-0.2768226
426\H,-3.6284100884,2.5091298419,1.5215144319\H,-1.201799818,1.6285555
197,-1.9017072578\H,-2.9295206558,4.88948508,1.4046844318\H,-0.4960688
443,3.9920728116,-2.0177542068\H,-1.3542481291,5.6342719301,-0.3648282
857\H,6.4944375952,-4.4696401474,0.1237789827\H,4.0189467708,-4.613351
6997,-0.1640360485\H,6.2066928968,-0.1994148621,0.4523048033\H,2.71440
76276,1.7252360758,1.7719662269\H,5.2799427751,1.0118488414,-1.5879496

615\H,3.478367095,4.0873381381,1.8552514489\H,6.0540792615,3.361103686
5,-1.5031820006\H,5.1579936927,4.9057058787,0.2206251894\H,7.563562175
6,-2.2515630049,0.4576190459\H,-5.7510185915,-0.9024508238,0.145275598
5\\Version=ES64L-G09RevD.01\State=3-A\HF=-1330.3546883\S2=2.032652\S2-
1=0.\S2A=2.000607\RMSD=6.233e-09\RMSF=5.856e-06\Dipole=2.3764892,1.769
5337,0.1098247\Quadrupole=-1.0572453,6.0403894,-4.983144,-4.4035415,-4
.4876705,1.2861475\PG=C01 [X(C26H18N6)]\\@

I[3,7]H,H,Ph -S, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C26H18N6\PIOTR\10-Jan-2024\
0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fch
eck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-tBu-1-Ph-be
nzo[e][1,2,4]triazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer a
nti\\0,1\C,-1.6597672716,0.0319339345,-0.0310486955\C,-2.9922524611,1.
896347504,-0.1724325361\C,-4.1545309677,1.0821917521,-0.0656024531\C,-
0.3115881146,-0.5881282368,0.0374569956\C,-0.1528593638,-1.984096591,0
.1339649329\C,0.8157515639,0.2336221628,-0.0033659143\C,1.1091832464,-
2.5423753552,0.1637756499\C,2.0951047421,-0.3234748497,0.063225852\C,2
.2629849459,-1.7385088891,0.1123326583\N,3.5022997619,-2.3208608917,0.
0778578439\N,3.2697007462,0.4346077401,0.0542108697\N,4.499256629,-0.1
463201041,-0.0787340561\C,4.5162000845,-1.470835761,-0.0570967891\C,3.
2990792073,1.8632419568,0.1248027987\C,4.0727809523,2.5720423658,-0.79
65274672\C,2.6070121718,2.5386636755,1.1323942829\C,4.1366704521,3.959
0479172,-0.7172089691\C,2.6747238566,3.9273732359,1.1997409189\C,3.435
1863745,4.6417364509,0.2758383432\N,-3.9286608644,-0.2965365853,-0.025
4407764\N,-2.6810348743,-0.8236244112,0.0499715261\N,-1.7347052136,1.3
568020046,-0.1776238327\C,-5.4243752363,1.6657400096,0.0234206335\C,-3
.1588490956,3.2916197807,-0.2475070881\C,-4.4200866546,3.8604848649,-0
.1895545013\C,-5.5509801307,3.0477075151,-0.0425127204\C,-4.9818020989
,-1.268657929,-0.0023053029\C,-5.0059758537,-2.2211144179,1.01711488\C
,-5.9434716483,-1.2882806494,-1.0136175565\C,-6.0070753616,-3.18718019
27,1.0293914283\C,-6.9433913128,-2.2569731309,-0.9897809526\C,-6.97970
20338,-3.2058255882,0.0304806801\H,-1.0326089719,-2.6118029023,0.16626
8174\H,0.6716296261,1.2995778441,-0.0914459105\H,1.2528441962,-3.61481
45971,0.209754643\H,4.6208701596,2.0292542893,-1.5549609453\H,2.035291
1581,1.9832399828,1.8647678703\H,4.7344436475,4.5073890144,-1.43603522
11\H,2.1397518141,4.4484864862,1.9850614615\H,3.4865038157,5.722690780
5,0.3334532583\H,-4.5315963183,4.9368919544,-0.2464199992\H,-2.2651601
876,3.8965183579,-0.3395275573\H,-6.3015302354,1.0462775159,0.14765461
61\H,-4.2408992974,-2.1993413411,1.7822237151\H,-5.8980655388,-0.56503
93195,-1.8182532309\H,-6.02782287,-3.9250613354,1.8228912339\H,-7.6864
14344,-2.2759501471,-1.778490981\H,-7.7578488532,-3.9599254807,0.04334
39289\H,-6.5360183895,3.4938274912,0.0249277327\H,5.5118894716,-1.8941
860111,-0.151747751\\Version=ES64L-G09RevD.01\State=1-A\HF=-1330.35444
45\S2=0.992568\S2-1=0.\S2A=0.191907\RMSD=9.777e-09\RMSF=9.559e-06\Dipo
le=-2.3470247,0.9455662,0.0726091\Quadrupole=5.238664,2.7247542,-7.963
4183,14.6672879,-1.061518,-1.5865629\PG=C01 [X(C26H18N6)]\\@

I[3,7]H,H,Ph -S, *syn*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C26H18N6\PIOTR\10-Jan-2024\
0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fch
eck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benz
o[e][1,2,4]triazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer syn
\\0,1\C,1.6575185205,-1.4875736701,-0.0742395622\C,3.7157574848,-2.503
3315778,-0.0520356146\C,4.3479112313,-1.2368882061,0.0971236239\C,0.17
35108826,-1.5863707887,-0.1169545982\C,-0.4393200375,-2.8496693161,-0.
2094641842\C,-0.6188711713,-0.4377595915,-0.0627941398\C,-1.81547954,-

2.9600360711,-0.2206628352\C,-2.0110061791,-0.5410369429,-0.1105223413
\C,-2.6373689324,-1.8205164208,-0.1548743464\N,-3.9999204802,-1.961421
472,-0.1030861763\N,-2.8700976371,0.5638198381,-0.0868093679\N,-4.2199
54911,0.4197838891,0.0656430507\C,-4.6738932779,-0.8253330505,0.045359
5001\C,-2.4293676055,1.9221977877,-0.1618739104\C,-2.9266293279,2.8480
90126,0.7579952519\C,-1.5558265155,2.332072828,-1.171956967\C,-2.53302
04029,4.1793428337,0.674849121\C,-1.1644612636,3.6660378478,-1.2423670
163\C,-1.6476172787,4.5923925468,-0.3201749786\N,3.5011594201,-0.12736
83408,0.0620085133\N,2.1472180253,-0.2502760228,0.0371748241\N,2.35685
52794,-2.6196926942,-0.1632724145\C,5.7323663518,-1.1561758626,0.29631
61373\C,4.5206858783,-3.657688006,-0.0559820109\C,5.892124419,-3.56751
33608,0.1097499796\C,6.4948807811,-2.3170655494,0.2973838244\C,3.96833
4091,1.2259857898,0.1136648852\C,3.4448989783,2.0904047738,1.076266334
\C,4.9021785175,1.6848321758,-0.8171212875\C,3.8723998587,3.4137603053
,1.1148383286\C,5.3268291384,3.0099271008,-0.7666763114\C,4.8166181573
,3.8760225811,0.1987575078\H,0.1902005305,-3.7273549137,-0.2579702987\
H,-0.1379121074,0.5248675905,0.0165596343\H,-2.3059609051,-3.924624922
8,-0.2652767473\H,-3.622152743,2.5164790918,1.5172179979\H,-1.19966737
01,1.6193849296,-1.9046695834\H,-2.9182515793,4.8949961023,1.391949096
\H,-0.4887686104,3.9809345288,-2.0288993248\H,-1.3424676371,5.63046903
21,-0.381015604\H,6.4985965372,-4.4654616033,0.1068966786\H,4.02347248
51,-4.6118480214,-0.1799293749\H,6.2053404873,-0.1973043889,0.45479918
3\H,2.7080278561,1.7204468636,1.7770039758\H,5.2782886704,1.0163919087
,-1.5814304905\H,3.4682449213,4.0836252276,1.8647943067\H,6.0482633955
,3.3668373611,-1.492388779\H,5.148030938,4.907226588,0.2330021619\H,7.
5652616122,-2.2477328325,0.4503142854\H,-5.7521774461,-0.8960301813,0.
1544049938\\Version=ES64L-G09RevD.01\State=1-A\HF=-1330.3536144\S2=1.0
25333\S2-1=0.\S2A=0.208133\RMSD=9.797e-09\RMSF=1.435e-05\Dipole=2.4139
126,1.8082518,0.1103612\Quadrupole=-1.1879511,6.0549917,-4.8670406,-4.
4853437,-4.4726779,1.2766807\PG=C01 [X(C26H18N6)]\\@

I[3,7]CF_3,H,Ph -T, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C27H17F3N6(3)\PIOTR\11-Jan-
2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle
) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-CF3-1-Ph-benzo[e][1,2,4]
triazinyl-7-)-1-Ph-benzo[e][1,2,4]triazinyl, conformer anti\\0,3\C,-1.
660948325,0.0212066977,0.0047550578\C,-2.9904228001,1.8907221542,-0.09
06496229\C,-4.1535918439,1.0739847651,-0.0131795456\C,-0.3094599177,-0
.5916106419,0.0677829434\C,-0.1458616399,-1.9872508386,0.1763915615\C,
0.816682171,0.2327496131,0.0145847985\C,1.1155380014,-2.5435008878,0.2
092898355\C,2.0943016501,-0.3207849432,0.0797672111\C,2.2659012518,-1.
7344639618,0.1456169155\N,3.5037814314,-2.3114248055,0.113208603\N,3.2
717468574,0.4420768114,0.0561278968\N,4.4930606466,-0.139568586,-0.075
1557617\C,4.5091538979,-1.4549884817,-0.0385212298\C,3.3024094801,1.87
3305244,0.100778601\C,4.0782990056,2.5624837634,-0.8330280052\C,2.6097
774325,2.5653808218,1.0961846619\C,4.1447512564,3.9504677279,-0.777310
9644\C,2.6799457186,3.9549291366,1.1386852079\C,3.442926202,4.65093571
63,0.2029899341\N,-3.9321903466,-0.3038807047,-0.0187143181\N,-2.68252
11452,-0.8366788317,0.0553078351\N,-1.733777271,1.349599394,-0.1076486
471\C,-5.4217242465,1.6597493898,0.092591809\C,-3.1514128019,3.2883717
086,-0.1213411252\C,-4.4103526946,3.8589374126,-0.0475650106\C,-5.5429
988596,3.04314499,0.0713241774\C,-4.9860791548,-1.2743499747,-0.046377
3391\C,-5.0157368987,-2.2768025602,0.9240822596\C,-5.9438209901,-1.242
4497794,-1.0614597527\C,-6.0179687978,-3.2410068023,0.8834637464\C,-6.
9455422078,-2.2090115863,-1.0897971018\C,-6.9870538298,-3.207842639,-0
.1186229386\H,-1.0242338929,-2.616486563,0.2169653639\H,0.6700614929,1

.2977276877,-0.0794586114\H,1.2622207473,-3.6147964382,0.2662542194\H,
4.627164176,2.0060786428,-1.5810496908\H,2.0379995028,2.0238856909,1.8
387312049\H,4.7450339435,4.4851087605,-1.5040708365\H,2.1460568684,4.4
91035181,1.9144549533\H,3.4964905459,5.7325593223,0.2420316657\H,-4.51
96982299,4.9366843459,-0.0697504529\H,-2.2551162328,3.8922883115,-0.19
15971102\H,-6.3011636374,1.039916752,0.1954839644\H,-4.2539510669,-2.2
942155462,1.6924564201\H,-5.8940505704,-0.4803592498,-1.8291394303\H,-
6.0425118251,-4.0179262417,1.6386341036\H,-7.6853248054,-2.1875862687,
-1.8814273474\H,-7.7661160311,-3.9605445641,-0.1464409176\H,-6.5269687
775,3.4894558672,0.1522491168\C,5.8873998303,-2.0915017081,-0.15712194
03\F,6.8521678848,-1.1980043082,-0.4195815201\F,6.2188849851,-2.725094
8218,0.9880348827\F,5.9070411009,-3.0126931741,-1.1411909302\\Version=
ES64L-G09RevD.01\State=3-A\HF=-1667.4890833\S2=2.032437\S2-1=0.\S2A=2.
0006\RMSD=6.155e-09\RMSF=2.712e-06\Dipole=-3.6654894,1.6389522,0.10446
53\Quadrupole=-1.193174,6.3909012,-5.1977272,19.6043208,-0.5126154,-1.
6771973\PG=C01 [X(C27H17F3N6)]\\@

I[3,7]CF_3,H,Ph -T, *syn*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C27H17F3N6(3)\PIOTR\11-Jan-
2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle
) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-CF3-1-Ph-benzo[e][1,2,4]
triazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer syn\\0,3\C,1.6
544872834,-1.4781664835,-0.0700604933\C,3.7210011392,-2.4764154663,-0.
0095273734\C,4.3393558234,-1.2022060163,0.1279145404\C,0.1754852455,-1
.5902386,-0.1258530455\C,-0.4236004234,-2.8613366207,-0.2197523031\C,-
0.6300836774,-0.4484229122,-0.080769511\C,-1.7968632161,-2.9896511752,
-0.2396464897\C,-2.0172894108,-0.5689033264,-0.1346945407\C,-2.6299237
682,-1.8573400483,-0.1794681138\N,-3.9859074462,-2.009852866,-0.131961
7312\N,-2.892103917,0.5272058122,-0.1206956833\N,-4.2340073534,0.36593
81902,0.0220387974\C,-4.6668763784,-0.8765593508,0.0079261788\C,-2.467
799986,1.8938936894,-0.1856767511\C,-2.9737146816,2.8036911064,0.74448
10101\C,-1.6035112893,2.3194762494,-1.1962464681\C,-2.5975097505,4.140
4443089,0.6694846049\C,-1.2301850662,3.6590524534,-1.2581523064\C,-1.7
221665865,4.5713995644,-0.3266365836\N,3.4840413084,-0.0998832999,0.06
76447417\N,2.1320890628,-0.2346714232,0.0291273107\N,2.3641097659,-2.6
069006008,-0.1348001759\C,5.7202435161,-1.1060160948,0.3406333719\C,4.
5351862254,-3.6236808027,0.0136002499\C,5.9037776824,-3.5189872089,0.1
941534738\C,6.4927193527,-2.2603097949,0.3686483654\C,3.940596639,1.25
80436277,0.1004116513\C,3.4126598329,2.1306773471,1.0528184963\C,4.868
1426325,1.7118977034,-0.8389211156\C,3.8279196214,3.4583770732,1.07161
38255\C,5.280557305,3.0414672786,-0.8083542211\C,4.7648458127,3.916461
2692,0.1461054089\H,0.216950075,-3.7313094255,-0.2614734977\H,-0.16003
05759,0.5199274959,-0.0045107316\H,-2.2761779242,-3.9594594947,-0.2847
245663\H,-3.661822027,2.4585735459,1.5046277003\H,-1.2414702365,1.6161
527829,-1.935159493\H,-2.9889114706,4.8458869276,1.3930760186\H,-0.562
5711651,3.9892404441,-2.0451573352\H,-1.4310347238,5.6137868834,-0.381
2537991\H,6.5181004712,-4.4113188761,0.212621351\H,4.0473653334,-4.583
7067742,-0.1013741834\H,6.1831885112,-0.1405878553,0.4885495344\H,2.68
17985981,1.7639106564,1.7615843106\H,5.2493668735,1.036204914,-1.59443
2412\H,3.4201088571,4.134720388,1.813711199\H,5.996740432,3.3945719133
,-1.5410913304\H,5.0867240248,4.9510544214,0.1646899351\H,7.5606396063
,-2.178785092,0.5323717606\C,-6.1731092127,-1.0437143687,0.154932267\F
,-6.4643965851,-1.8289055733,1.2128113785\F,-6.8120690597,0.1220960791
,0.3287257869\F,-6.6966300997,-1.6372865748,-0.9375110135\\Version=ES6
4L-G09RevD.01\State=3-A\HF=-1667.4892457\S2=2.032692\S2-1=0.\S2A=2.000
607\RMSD=5.874e-09\RMSF=2.400e-06\Dipole=3.8225311,2.0283545,0.0200622
\Quadrupole=-10.0347625,12.0574069,-2.0226444,-5.0854767,-3.3531714,1.

2652698\PG=C01 [X(C27H17F3N6)]\\@

I[3,7]CF_3,H,Ph -S, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C27H17F3N6\PIOTR\12-Jan-202
4\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) f
check guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-CF3-1-Ph-
benzo[e][1,2,4]triazinyl-7-)-1-Ph-benzo[e][1,2,4]triazinyl, conformer
anti\\0,1\C,-1.6598978853,0.0321659101,-0.0098434778\C,-2.9912829415,1
.8988683897,-0.1021016778\C,-4.1528488851,1.0808388111,-0.0196362043\C
,-0.3109954614,-0.5887009689,0.0513582145\C,-0.1518912739,-1.984471234
6,0.1486400378\C,0.815351994,0.2344309199,0.0075143096\C,1.1098285357,
-2.5435232533,0.1812941655\C,2.0931473249,-0.3226187329,0.0720202041\C
,2.2605490398,-1.737259695,0.1288208395\N,3.5007854691,-2.3151248783,0
.0997444186\N,3.269165897,0.4378402692,0.056448282\N,4.4926021185,-0.1
426556291,-0.0682276969\C,4.5060076614,-1.459842142,-0.0385300708\C,3.
3004612971,1.8694751376,0.1061198544\C,4.0742442049,2.5609175548,-0.82
75303756\C,2.6109704443,2.5580214408,1.1058481186\C,4.1411237282,3.948
7105158,-0.7676539467\C,2.6817831922,3.9474167978,1.1527607364\C,3.442
2994716,4.6460382925,0.2170378141\N,-3.9266373659,-0.2989543391,-0.023
4611438\N,-2.6794901683,-0.8257808677,0.042502701\N,-1.7332759443,1.36
03259568,-0.1219111252\C,-5.4226093291,1.6607084359,0.0900109657\C,-3.
1582389687,3.2955665012,-0.134766802\C,-4.4195687373,3.8615277007,-0.0
573259132\C,-5.5497959466,3.0438476409,0.067076553\C,-4.9793912063,-1.
2720425802,-0.0431312911\C,-5.004050753,-2.2686520801,0.9331816566\C,-
5.9394799953,-1.2470003441,-1.0559748342\C,-6.0042743881,-3.2352549888
,0.9003820357\C,-6.9387707628,-2.2162565096,-1.0766697756\C,-6.9755422
042,-3.2097378975,-0.0997824271\H,-1.0313449971,-2.612447306,0.1812220
548\H,0.6701589701,1.3002116566,-0.0797309468\H,1.2538362727,-3.615570
5565,0.2305515657\H,4.620964679,2.0065722963,-1.5786605735\H,2.0409560
703,2.0140787844,1.8479818451\H,4.7394975602,4.4856109233,-1.494300867
2\H,2.1502749103,4.4812428339,1.9317059696\H,3.4963351506,5.7275128445
,0.2594471652\H,-4.5318529525,4.9390354376,-0.0810667882\H,-2.26494903
71,3.9034081,-0.2092396288\H,-6.2990138218,1.0372142969,0.1970078859\H
,-4.2405973055,-2.2798361804,1.7000637476\H,-5.8933590772,-0.488485317
9,-1.8273791983\H,-6.0254862468,-4.007892374,1.6599918792\H,-7.6805954
509,-2.2008950703,-1.8664911948\H,-7.7529950543,-3.9642861817,-0.12159
96\H,-6.5347994777,3.4871723814,0.150596369\C,5.8859130451,-2.09588721
09,-0.1465762128\F,6.8510758682,-1.2029739775,-0.4098666054\F,6.212333
9181,-2.7214638422,1.0045124657\F,5.911566055,-3.0231846712,-1.1243546
773\\Version=ES64L-G09RevD.01\State=1-A\HF=-1667.4889943\S2=0.991819\S
2-1=0.\S2A=0.189243\RMSD=4.887e-09\RMSF=2.973e-06\Dipole=-3.7014358,1.
6076943,0.108157\Quadrupole=-0.8884877,6.147606,-5.2591183,20.3585492,
-0.6019195,-1.6234591\PG=C01 [X(C27H17F3N6)]\\@

I[3,7]CF_3,H,Ph -S, *syn*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C27H17F3N6\PIOTR\12-Jan-202
4\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) f
check guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-CF3-1-Ph-
benzo[e][1,2,4]triazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer
syn\\0,1\C,1.6565856525,-1.4804728698,-0.0710707583\C,3.7229956575,-2
.4758212143,-0.0202105436\C,4.3399898586,-1.2016084164,0.1251291347\C,
0.173296567,-1.5937619134,-0.1244376231\C,-0.4260336533,-2.8638482037,
-0.2137888717\C,-0.6298104111,-0.4520112902,-0.0813831853\C,-1.8006829
124,-2.9904383064,-0.2305655318\C,-2.0188579336,-0.5716042308,-0.13322
3948\C,-2.6312098076,-1.8580761142,-0.1731925375\N,-3.9913277726,-2.00
82075061,-0.122391827\N,-2.890334442,0.526534592,-0.1195063325\N,-4.23
22395514,0.368939435,0.0291647398\C,-4.6671567249,-0.8753162962,0.0183

762312\C,-2.4635716169,1.8918363229,-0.19370453\C,-2.9672612059,2.8084
504014,0.7310732151\C,-1.5998372492,2.309558272,-1.2081175116\C,-2.588
6486208,4.1439263678,0.6472801592\C,-1.2242745024,3.648069456,-1.27884
41085\C,-1.713568838,4.5670593232,-0.3524965343\N,3.4828656224,-0.1006
610875,0.0721856224\N,2.1311707508,-0.2378536513,0.0351325458\N,2.3660
711542,-2.6068307794,-0.1449794461\C,5.7210661453,-1.104316764,0.33796
60811\C,4.5393232305,-3.6215826712,-0.00570091\C,5.9078915587,-3.51554
7175,0.1745436625\C,6.4953704719,-2.2572464548,0.3575417809\C,3.936807
3434,1.2579328552,0.1111161477\C,3.4054342877,2.1256414717,1.066154637
7\C,4.8649627827,1.7173059116,-0.8249741511\C,3.8181842966,3.453984510
2,1.0910332335\C,5.2744779357,3.047590198,-0.7884563377\C,4.7555960159
,3.9176595413,0.1687877892\H,0.2133628722,-3.7347341228,-0.2542889702\
H,-0.1591249252,0.5162327324,-0.0072040586\H,-2.2807519262,-3.96009727
07,-0.2712683781\H,-3.6552953647,2.4692152725,1.4938848248\H,-1.240534
0677,1.6011819066,-1.9435186899\H,-2.9780129832,4.854630754,1.36680414
69\H,-0.5571918836,3.9721923383,-2.0688065037\H,-1.4207398309,5.608581
1817,-0.4140288872\H,6.5236477601,-4.4070303108,0.1863317353\H,4.05332
15741,-4.5817610608,-0.1268310183\H,6.1822411488,-0.1390908025,0.49257
4347\H,2.6741516321,1.7545099405,1.7721778674\H,5.2487033949,1.0454964
757,-1.5826396911\H,3.4079416922,4.1264856017,1.8352673965\H,5.9909960
451,3.4051141369,-1.5187078762\H,5.0753838457,4.9527997036,0.192060664
6\H,7.5632374508,-2.1753643672,0.5212885791\C,-6.1740412089,-1.0375822
681,0.170329926\F,-6.4644058407,-1.8246793647,1.2268479344\F,-6.808341
9813,0.1299724253,0.3498279094\F,-6.7033864924,-1.6258206152,-0.922143
5505\\Version=ES64L-G09RevD.01\State=1-A\HF=-1667.488117\S2=1.024924\S
2-1=0.\S2A=0.205352\RMSD=5.444e-09\RMSF=3.418e-06\Dipole=3.8438701,2.0
661458,0.0153554\Quadrupole=-10.0847669,12.0446838,-1.9599169,-5.00545
73,-3.2682994,1.2518007\PG=C01 [X(C27H17F3N6)]\\@

I[3,7]Me$_2$N,H,Ph -T, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C28H23N7(3)\PIOTR\13-Jan-20
24\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle)
fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-NMe2-1-Ph-benzo[e][1,2,4]t
riazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer anti\\0,3\C,-1.
663034531,-0.0086958302,-0.1723644063\C,-2.9949360592,1.8630340835,-0.
2461170189\C,-4.1587474685,1.050826405,-0.1349051044\C,-0.3143862201,-
0.6232359996,-0.1375360001\C,-0.1478816257,-2.0227177988,-0.0542198092
\C,0.813743363,0.1948437175,-0.1926721121\C,1.111369262,-2.580339056,-
0.0477817324\C,2.094616452,-0.362683471,-0.1509957096\C,2.2717845338,-
1.7764887837,-0.1133535261\N,3.497724064,-2.3551584156,-0.1568771532\N
,3.2707025234,0.3876208877,-0.1779795795\N,4.4976841559,-0.180460717,-
0.3447306982\C,4.5401978215,-1.5261468901,-0.3021732719\C,3.3003333157
,1.8165606797,-0.1207390821\C,4.0530614427,2.5208669422,-1.0631759505\
C,2.6277644518,2.4995681115,0.8951683319\C,4.1163183184,3.9086221819,-
0.9958447195\C,2.6948285314,3.888947048,0.9510011957\C,3.435142448,4.5
979510096,0.0068049611\N,-3.9393154113,-0.3264384603,-0.1381215141\N,-
2.6887189489,-0.8630122955,-0.0904672612\N,-1.7413703158,1.3202353431,
-0.2919789144\C,-5.4225677193,1.641415743,0.0000534585\C,-3.1545599497
,3.26155835,-0.2816035407\C,-4.4094790948,3.8363074799,-0.1798857146\C
,-5.5413930969,3.0247634892,-0.0269933658\C,-4.9936479345,-1.295437813
8,-0.1309445038\C,-4.9899739808,-2.3002717227,0.8380162357\C,-5.986535
1517,-1.2636561513,-1.1120451739\C,-5.9927292058,-3.2646443526,0.83099
07647\C,-6.9884199136,-2.2304973462,-1.106986699\C,-6.9964021795,-3.23
07773174,-0.1364828646\H,-1.0254436081,-2.6533925039,-0.0113870292\H,0
.6709248234,1.261761978,-0.2706821258\H,1.2519546317,-3.6537075337,-0.
0079543054\H,4.583261473,1.9728582517,-1.8303870291\H,2.0712129704,1.9

485272024,1.6422345393\H,4.6970110282,4.452655134,-1.7319187198\H,2.17
51237778,4.4151158243,1.7432760116\H,3.4858884774,5.6794439014,0.05541
28481\H,-4.5161921166,4.9143635337,-0.2062619288\H,-2.2583423409,3.862
0601343,-0.3779257958\H,-6.3007828255,1.0249143991,0.1303616902\H,-4.2
006890685,-2.3192323417,1.5779714053\H,-5.9636123617,-0.5013462149,-1.
8807156957\H,-5.9903479241,-4.04268964,1.5855173166\H,-7.7549190297,-2
.2083094295,-1.8728719665\H,-7.7757736056,-3.9837495837,-0.1382781295\
H,-6.5218523074,3.4743565732,0.0763853706\N,5.7933524231,-2.0761851697
,-0.392986321\C,6.9593981626,-1.2425516018,-0.640694365\H,6.8518056345
,-0.2861370392,-0.1353396656\H,7.8427428591,-1.7562886875,-0.255242456
7\H,7.1110389944,-1.0522008977,-1.71234373\C,5.9619940653,-3.503735266
8,-0.6201840822\H,5.0625937681,-4.0274152227,-0.3120884122\H,6.1536066
764,-3.7209030834,-1.6802373445\H,6.8128354859,-3.8662316258,-0.036788
0604\\Version=ES64L-G09RevD.01\State=3-A\HF=-1464.3725843\S2=2.027929\
S2-1=0.\S2A=2.000447\RMSD=5.047e-09\RMSF=2.527e-06\Dipole=-0.9957303,0
.501265,-0.0484289\Quadrupole=18.9476968,-2.1351625,-16.8125343,4.5995
628,-3.2857001,-0.7391353\PG=C01 [X(C28H23N7)]\\@

I[3,7]Me$_2$N,H,Ph -T, *syn*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C28H23N7(3)\PIOTR\13-Jan-20
24\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle)
fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-NMe2-1-Ph-benzo[e][1,2,4]t
riazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer syn\\0,3\C,1.59
47955136,-1.4705939021,-0.2456646583\C,3.6550900517,-2.4869135216,-0.1
901752737\C,4.2856387641,-1.2225352747,-0.0199413402\C,0.1177965768,-1
.5677344858,-0.3132397241\C,-0.4973664398,-2.8320325478,-0.4253022968\
C,-0.6799192726,-0.4230257066,-0.2624394282\C,-1.8701228813,-2.9462088
003,-0.4579537985\C,-2.0714828314,-0.529807333,-0.3287433532\C,-2.7027
629274,-1.8076464452,-0.391412024\N,-4.0515010428,-1.9506001869,-0.369
4009573\N,-2.9361353382,0.5640001679,-0.3134467877\N,-4.2879147613,0.4
328960855,-0.2099071269\C,-4.7654190272,-0.8264733521,-0.2228577882\C,
-2.4930385811,1.9238742044,-0.3606706901\C,-2.975928287,2.829334714,0.
5864462031\C,-1.6284835436,2.3542542484,-1.3692983837\C,-2.5796205076,
4.1613672594,0.530335391\C,-1.2348946876,3.688901925,-1.4142883618\C,-
1.7059603574,4.595264143,-0.4661950634\N,3.4408684398,-0.1123252887,-0
.0676960572\N,2.0867148055,-0.2327180071,-0.1160391644\N,2.2996761765,
-2.6022225353,-0.3310406954\C,5.6653896476,-1.1453834813,0.2111265496\
C,4.4594836821,-3.6422221971,-0.1836290726\C,5.8269011539,-3.555606165
6,0.013759266\C,6.4267304684,-2.3071623273,0.2227393306\C,3.9080591821
,1.2399422061,-0.0085592777\C,3.3615619464,2.1083587931,0.9377342094\C
,4.8639315491,1.6972076832,-0.9178920143\C,3.7866871229,3.432227259,0.
981680376\C,5.2858163606,3.0229780171,-0.8624445801\C,4.7520067131,3.8
92619944,0.0869203556\H,0.1328716217,-3.7095593838,-0.4721774856\H,-0.
2045283887,0.5415558444,-0.1708044418\H,-2.3539641551,-3.9133383333,-0
.5201872939\H,-3.6584371703,2.4807357358,1.3500552671\H,-1.2796419476,
1.6550880154,-2.1184671134\H,-2.9524480908,4.8610411171,1.2695697705\H
,-0.5664424858,4.0202373421,-2.2003393521\H,-1.3985888745,5.6337481689
,-0.5067973421\H,6.431997489,-4.4545720693,0.0189461072\H,3.9634285034
,-4.5946312637,-0.3246764222\H,6.1361067291,-0.1881851373,0.3860750774
\H,2.6072644188,1.7404175269,1.6206564396\H,5.259452426,1.0269312659,-
1.6707870087\H,3.3635170561,4.104182519,1.7192537824\H,6.023762456,3.3
776745735,-1.5725957648\H,5.0812440602,4.9244227381,0.1248483435\H,7.4
934874912,-2.2398162989,0.4004324601\N,-6.1246140559,-0.9418858356,-0.
072915284\C,-6.977982822,0.2370696175,-0.1016274124\H,-7.9123278547,0.
002346481,0.4121119313\H,-6.492035367,1.0675356107,0.4033842403\H,-7.2
148021082,0.5496088859,-1.1281777458\C,-6.7818627058,-2.2176592268,-0.
3173196661\H,-6.0867841714,-3.0279064609,-0.1201733089\H,-7.6461268545

,-2.3070628243,0.3454909132\H,-7.1319586169,-2.3016510599,-1.355793044
1\\Version=ES64L-G09RevD.01\State=3-A\HF=-1464.3725554\S2=2.028199\S2-
1=0.\S2A=2.000453\RMSD=5.008e-09\RMSF=1.915e-06\Dipole=0.9253791,1.772
5707,0.1277543\Quadrupole=15.6877513,-1.8803477,-13.8074035,2.0227545,
-3.7748903,1.5072788\PG=C01 [X(C28H23N7)]\\@

I[3,7]Me$_2$N,H,Ph -S, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C28H23N7\PIOTR\14-Jan-2024\
0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fch
eck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-NMe2-1-Ph-b
enzo[e][1,2,4]triazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer
anti\\0,1\C,-1.6608951205,0.0003675457,-0.1735130757\C,-2.9941941136,1
.8703843219,-0.2299356566\C,-4.1566181847,1.0562214404,-0.1237724652\C
,-0.3150659499,-0.6205425779,-0.1424677911\C,-0.1522096799,-2.01991306
58,-0.0668623267\C,0.8133553985,0.1965338569,-0.1937252818\C,1.1073530
874,-2.5801262941,-0.0615131282\C,2.0939859971,-0.3643649542,-0.155376
0796\C,2.2681954232,-1.7790957029,-0.1215712858\N,3.4958013874,-2.3579
915241,-0.1628806977\N,3.2688567305,0.3837049159,-0.1820339375\N,4.497
3876444,-0.1822915676,-0.3361941978\C,4.5386514611,-1.5299427307,-0.29
68402947\C,3.2968623858,1.8142582083,-0.1329893068\C,4.0306970165,2.51
37292309,-1.093114287\C,2.640819272,2.5003613655,0.8909200516\C,4.0918
774111,3.9020595269,-1.034925208\C,2.7057391874,3.8902568064,0.9378807
576\C,3.4274384685,4.5951070436,-0.0236514706\N,-3.9334956878,-0.32303
65703,-0.1388827743\N,-2.6848710265,-0.8555399858,-0.0996299517\N,-1.7
39268484,1.3298115476,-0.281594065\C,-5.4215569162,1.6406204695,0.0187
746811\C,-3.1585540309,3.2682903687,-0.2533444096\C,-4.4155531799,3.83
85981627,-0.1442635773\C,-5.5453809449,3.0242488754,0.0038716712\C,-4.
9869958169,-1.2936463186,-0.137962802\C,-4.9830698434,-2.3034259708,0.
8256353921\C,-5.9787521462,-1.2571274225,-1.1199102916\C,-5.9845655909
,-3.2690927267,0.8120555849\C,-6.9791854619,-2.2254493404,-1.121537561
9\C,-6.9869235971,-3.2311276246,-0.1565834722\H,-1.0308518114,-2.64914
02511,-0.0281889175\H,0.6716548662,1.2639648392,-0.266884795\H,1.24546
3241,-3.6539715865,-0.0258710181\H,4.5481312753,1.9623759682,-1.866751
5435\H,2.0980991033,1.951536824,1.6497887126\H,4.6576757413,4.44343342
81,-1.7843904238\H,2.1988596811,4.4200275379,1.7359981687\H,3.47652583
45,5.6769715739,0.0179345745\H,-4.5244606606,4.9167099145,-0.161448446
5\H,-2.2646908874,3.8728800668,-0.3461141591\H,-6.2974089464,1.0198622
831,0.1451667982\H,-4.1949260372,-2.3251539574,1.5667800034\H,-5.95609
87767,-0.4900248725,-1.8837951529\H,-5.9822260641,-4.0512141218,1.5623
365111\H,-7.7449138871,-2.1999674289,-1.8880758003\H,-7.7653358918,-3.
9850587349,-0.1635005651\H,-6.5268231067,3.4702594515,0.1126479955\N,5
.7926087273,-2.0783330773,-0.3789679931\C,6.9611922384,-1.2455403665,-
0.6181271271\H,6.845795569,-0.2848189904,-0.1230266058\H,7.8398769096,
-1.7547446325,-0.2162429718\H,7.1269356773,-1.0652408657,-1.6893668394
\C,5.9644143279,-3.5070951998,-0.595383798\H,5.0625273411,-4.029425808
1,-0.2923104013\H,6.1657538026,-3.7305784021,-1.6522427416\H,6.8103185
775,-3.8651127608,-0.0020946665\\Version=ES64L-G09RevD.01\State=1-A\HF
=-1464.3728141\S2=0.993044\S2-1=0.\S2A=0.186496\RMSD=8.020e-09\RMSF=4.
893e-06\Dipole=-0.9182452,0.4790998,-0.0436372\Quadrupole=19.1204134,-
2.29212,-16.8282934,5.2351056,-3.2103377,-0.7712505\PG=C01 [X(C28H23N7
)]\\@

I[3,7]Me$_2$N,H,Ph -S, *syn*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C28H23N7\PIOTR\15-Jan-2024\
0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fch
eck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-NMe2-1-Ph-b
enzo[e][1,2,4]triazinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer

syn\\0,1\C,1.5958974252,-1.4719038096,-0.2462941702\C,3.656640416,-2.4
852232877,-0.1980518703\C,4.2857161568,-1.2207232801,-0.0219522834\C,0
.116106767,-1.5716505016,-0.3123775275\C,-0.4991871024,-2.8350982565,-
0.4195492256\C,-0.6803352497,-0.4268639968,-0.2650524162\C,-1.87334371
65,-2.9478830292,-0.4511931344\C,-2.0728260987,-0.5336726193,-0.330625
0897\C,-2.7042011208,-1.8096376831,-0.3895225715\N,-4.0566253996,-1.95
00806735,-0.3690715572\N,-2.9351121773,0.5626658789,-0.3161485492\N,-4
.2858356491,0.4351487546,-0.2104912498\C,-4.7664589854,-0.826325895,-0
.2242388534\C,-2.4881516655,1.9214331931,-0.3654609271\C,-2.963732951,
2.8281192674,0.5841046911\C,-1.6272294743,2.3489191327,-1.3783314515\C
,-2.5634609848,4.158873577,0.526161907\C,-1.2296264906,3.6823468955,-1
.4251206927\C,-1.6932731119,4.5900001843,-0.4746489354\N,3.4395502356,
-0.1119705348,-0.0644515032\N,2.0851225918,-0.2344497243,-0.1110667742
\N,2.3012326684,-2.601195241,-0.338774373\C,5.6656794022,-1.1427710923
,0.2092780745\C,4.4626895204,-3.63931755,-0.1977627283\C,5.8300356369,
-3.5516381838,-0.000504838\C,6.4284149698,-2.3034002795,0.2147321123\C
,3.9044272984,1.2408072598,-0.0011098542\C,3.3548986672,2.1058415019,0
.9465852844\C,4.8609020542,1.7020326182,-0.9078576746\C,3.7778951043,3
.430214315,0.9947286542\C,5.2803896244,3.0283637298,-0.8483052047\C,4.
7437804374,3.8945760894,0.1026157767\H,0.1298928504,-3.7136039643,-0.4
636865261\H,-0.204745699,0.537912831,-0.1759807979\H,-2.3574643388,-3.
9151445523,-0.5097514392\H,-3.6434706488,2.4814403284,1.3510794292\H,-
1.284609726,1.6486052328,-2.1293194225\H,-2.930360284,4.8597006884,1.2
672552975\H,-0.5639566193,4.0117175947,-2.2143393949\H,-1.3828398624,5
.6275152644,-0.516668992\H,6.4364103028,-4.4497610193,-0.000142824\H,3
.9680205921,-4.5917518862,-0.3433655814\H,6.1350106055,-0.1858180898,0
.3891813393\H,2.6001183199,1.7348094976,1.6272645074\H,5.2585871495,1.
0345019169,-1.6620285445\H,3.3525608793,4.0995002787,1.7334773836\H,6.
0187152452,3.3861903224,-1.5564820829\H,5.0712559223,4.9268118813,0.14
37784313\H,7.4951219916,-2.2356768171,0.3925382279\N,-6.1261030623,-0.
9362372737,-0.0762350313\C,-6.9822615537,0.2403365057,-0.1163840288\H,
-7.8967274,0.0261191201,0.4409168105\H,-6.4782251619,1.0890025818,0.33
69626644\H,-7.2587964783,0.5113870519,-1.1448427503\C,-6.7845545797,-2
.214926539,-0.2998782256\H,-6.0902182431,-3.0228876237,-0.0909438655\H
,-7.6488191454,-2.2925508883,0.3645457208\H,-7.1353356041,-2.314386562
1,-1.3367039399\\Version=ES64L-G09RevD.01\State=1-A\HF=-1464.3717536\S
2=1.02479\S2-1=0.\S2A=0.200309\RMSD=9.582e-09\RMSF=4.915e-06\Dipole=0.
9491776,1.8192746,0.1343321\Quadrupole=15.723039,-1.9625729,-13.760466
,1.8418387,-3.7807869,1.4548569\PG=C01 [X(C28H23N7)]\\@

I[3,7]Me_2N,CF_3,Ph -T, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C29H22F3N7(3)\PIOTR\15-Jan-
2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle
) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-NMe2-1-Ph-benzo[e][1,2,4
]triazinyl-7-)-1-Ph-7-CF3-benzo[e][1,2, 4]triazinyl, conformer anti\\0
,3\C,-1.4449713902,-0.0082473573,-0.0137126542\C,-2.7010352055,1.91162
48058,-0.1287511895\C,-3.8974786408,1.1452019191,-0.0401881939\C,-0.12
35572002,-0.671172469,0.0481868339\C,-0.0112994648,-2.0757948488,0.140
3792331\C,1.0356187701,0.104590149,0.0074811117\C,1.2256161781,-2.6798
228051,0.1708508163\C,2.2929585198,-0.500568493,0.0724639844\C,2.41659
41005,-1.9199851092,0.12153307\N,3.6200993674,-2.5431517175,0.10448298
75\N,3.4960809887,0.2050688982,0.0589522456\N,4.7043006529,-0.40758278
16,-0.0742953976\C,4.696405344,-1.7546469145,-0.0214224126\C,3.5741597
952,1.6336156238,0.0984622791\C,4.3414718467,2.3012303128,-0.858045326
\C,2.9301812351,2.3488737133,1.1101944234\C,4.4476545148,3.6872797882,
-0.8091313302\C,3.0403571748,3.7361558238,1.1479761114\C,3.7952074135,

4.4096185116,0.1894502452\N,-3.7320622228,-0.2374003942,-0.0196325758\
N,-2.5056354037,-0.8208648073,0.0521856377\N,-1.4721194932,1.324581074
5,-0.1390517025\C,-5.1413477852,1.7791716052,0.0525575245\C,-2.8091724
575,3.3163350789,-0.1812874825\C,-4.0400583587,3.9382008669,-0.1207920
251\C,-5.2053696376,3.1666172561,0.0073329048\C,-4.8270814766,-1.16308
48982,-0.0051190257\C,-4.8922322838,-2.1213405586,1.0068528989\C,-5.78
98726334,-1.1296582066,-1.0147439067\C,-5.937502507,-3.0392436491,1.01
40703984\C,-6.8345543874,-2.0501239257,-0.9952948419\C,-6.9128006833,-
3.0034668538,0.0181526947\H,-0.9123129578,-2.6732017585,0.1714091342\H
,0.9353671211,1.1756717205,-0.0793952406\H,1.3251267931,-3.7573107896,
0.2194757912\H,4.8489770106,1.7272834944,-1.6218154288\H,2.3621657087,
1.8240886671,1.8676936605\H,5.0393855684,4.2040155234,-1.5559315037\H,
2.5430629061,4.2881797654,1.9369890935\H,3.8798081649,5.4894982318,0.2
23838595\H,-4.1086727985,5.0181698828,-0.1547515199\H,-1.8916050231,3.
8857721405,-0.2571390667\H,-6.0461048659,1.2013280841,0.166382203\H,-4
.1252972311,-2.1410898462,1.7700793325\H,-5.7123001151,-0.4041760345,-
1.8150389304\H,-5.9913252212,-3.7814916279,1.8018566912\H,-7.579834327
1,-2.0275270904,-1.7816097685\H,-7.7261678623,-3.7194256441,0.02811643
67\N,5.9284789502,-2.350985747,-0.0795970387\C,7.1332561851,-1.5674209
783,-0.3060400627\H,7.0394863879,-0.5904728071,0.1608420997\H,7.981553
5663,-2.0969046767,0.1332984497\H,7.3339020779,-1.4225766896,-1.376550
5031\C,6.050691226,-3.7890128104,-0.2678996525\H,5.1244858776,-4.27277
75933,0.025837134\H,6.2643956341,-4.0377006512,-1.3165116662\H,6.87129
03847,-4.1669821318,0.3481244312\C,-6.5369353638,3.857004452,0.0530476
025\F,-7.5246593341,3.0525706078,0.502307256\F,-6.9212451754,4.2954015
462,-1.1726076502\F,-6.5148333771,4.9472991329,0.8541185143\\Version=E
S64L-G09RevD.01\State=3-A\HF=-1801.5118744\S2=2.027375\S2-1=0.\S2A=2.0
00436\RMSD=9.230e-09\RMSF=4.550e-06\Dipole=0.4121895,-0.3779793,-0.083
3407\Quadrupole=8.2639208,-0.2614983,-8.0024225,18.6188127,-2.6424533,
-0.9948487\PG=C01 [X(C29H22F3N7)]\\@

I[3,7]Me$_2$N,CF$_3$,Ph -T, *syn*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C29H22F3N7(3)\PIOTR\18-Jan-
2024\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle
) fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-NMe2-1-Ph-benzo[e][1,2,4
]triazinyl-7-)-1-Ph-7-CF3_benzo[e][1,2,4] triazinyl, conformer syn\\0,
3\C,-1.4644042198,-1.4825339388,0.0495158403\C,-3.5472734976,-2.448881
9272,0.0042481734\C,-4.151353597,-1.1651985048,-0.1163980379\C,0.00753
2746,-1.6185680149,0.0897094902\C,0.5903657761,-2.8999653844,0.1822137
206\C,0.8346100011,-0.4941958048,0.0342013533\C,1.959506528,-3.0504100
069,0.1970338053\C,2.2231367093,-0.6383204832,0.0790483827\C,2.8211545
396,-1.9331805808,0.1286536302\N,4.1640186145,-2.1111121522,0.09315170
24\N,3.116254423,0.4315967877,0.0537095862\N,4.4627632448,0.2660864023
,-0.0578686535\C,4.9079911843,-1.0057827138,-0.0509630942\C,2.70715969
12,1.8031138104,0.1003657053\C,3.1877059188,2.688738947,-0.8659710573\
C,1.8771465389,2.2606708102,1.1254954684\C,2.8225574859,4.0298950453,-
0.8124597113\C,1.5138296176,3.6040562439,1.1674307181\C,1.9820558965,4
.4912742025,0.2001431773\N,-3.2808125553,-0.0776111841,-0.0574899315\N
,-1.9309647381,-0.2303903603,-0.0343530501\N,-2.1977021484,-2.60010893
82,0.1136928064\C,-5.5300189872,-1.0454276077,-0.3148714757\C,-4.38132
03329,-3.5842802873,-0.0201012374\C,-5.7472259933,-3.4617323566,-0.184
543672\C,-6.3185686121,-2.1909847064,-0.3433723556\C,-3.7216840433,1.2
86733625,-0.0756924426\C,-3.1918923771,2.1597710731,-1.0262829511\C,-4
.6369416155,1.741921107,0.8746985228\C,-3.5942997253,3.4915218809,-1.0
319667058\C,-5.0363006078,3.0756784105,0.8570548415\C,-4.5192703932,3.
9517898275,-0.0954848894\H,-0.0612927512,-3.7615367883,0.229907976\H,0
.3842702791,0.4832428474,-0.0449633946\H,2.4183448349,-4.030288517,0.2

474653848\H,3.8436619881,2.3183494571,-1.6425872327\H,1.531442224,1.57
60843902,1.8895035552\H,3.19363473,4.7148625157,-1.5661250382\H,0.8716
062358,3.9569222542,1.9658229213\H,1.6988616222,5.5366654772,0.2384638
504\H,-6.3758274558,-4.342418273,-0.2102816408\H,-3.9094522844,-4.5535
511922,0.0792386752\H,-5.9826871692,-0.0750469888,-0.4550328502\H,-2.4
700891166,1.7903873802,-1.742829694\H,-5.0190925458,1.0644486791,1.628
1548555\H,-3.1860436269,4.1693262148,-1.7724069522\H,-5.7439283304,3.4
303535454,1.5971447635\H,-4.8315649333,4.9894202416,-0.1047325509\N,6.
2616957941,-1.1559392567,-0.2055292542\C,7.147662432,-0.0008477315,-0.
2018956036\H,8.057457039,-0.2585097619,-0.748061113\H,6.6678650962,0.8
453770175,-0.6858970201\H,7.427738276,0.2979331447,0.817603684\C,6.891
6947426,-2.4476220392,0.0270440636\H,6.161446104,-3.2383105168,-0.1134
339571\H,7.714832891,-2.5794387508,-0.6799754045\H,7.2967406761,-2.519
278768,1.0459540725\C,-7.8060798138,-2.0605283156,-0.4897597349\F,-8.4
32432926,-2.0205789126,0.7145317472\F,-8.3452283835,-3.1007267143,-1.1
638541982\F,-8.1638449601,-0.9324829995,-1.143165989\\Version=ES64L-G0
9RevD.01\State=3-A\HF=-1801.5119007\S2=2.027766\S2-1=0.\S2A=2.000446\R
MSD=5.031e-09\RMSF=4.652e-06\Dipole=0.8166648,1.9719816,0.0365593\Quad
rupole=-5.4246896,10.5615306,-5.1368411,-5.1638255,-6.5720924,-1.57592
5\PG=C01 [X(C29H22F3N7)]\\@

I[3,7]Me$_2$N,CF$_3$,Ph -S, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C29H22F3N7\PIOTR\19-Jan-202
4\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) f
check guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-NMe2-1-Ph
-benzo[e][1,2,4]triazinyl-7-)-1-Ph-7-CF3-benzo[e][1,2, 4]triazinyl, co
nformer anti\\0,1\C,-1.441610519,0.0047698235,-0.0176283989\C,-2.69967
7139,1.9225368629,-0.1198197845\C,-3.894922362,1.15387219,-0.034429484
2\C,-0.1241536549,-0.664538107,0.0413270748\C,-0.0167060955,-2.0694813
479,0.1254576395\C,1.0357130987,0.1094750869,0.0051091043\C,1.21939492
26,-2.6773973768,0.1547606907\C,2.2922288351,-0.5000944005,0.066954126
2\C,2.411582757,-1.9212201645,0.1111566048\N,3.6151098218,-2.545389159
4,0.0958868477\N,3.4945475104,0.201245784,0.0554519804\N,4.7033490258,
-0.4103525679,-0.0650134999\C,4.6931765543,-1.7588687031,-0.0176991289
\C,3.5733557871,1.631373073,0.0901094496\C,4.3239713274,2.2953690863,-
0.88137839\C,2.9461492161,2.347920124,1.1106910587\C,4.430579683,3.681
6428242,-0.8380400694\C,3.0566871902,3.7353862128,1.1430801581\C,3.795
102657,4.4060270651,0.1699461526\N,-3.7247410823,-0.2318359925,-0.0222
117736\N,-2.4999799996,-0.8098544641,0.0421748641\N,-1.4692571946,1.33
8240627,-0.1340444531\C,-5.1397833559,1.781006139,0.0644781872\C,-2.81
40572875,3.3266849913,-0.1639315009\C,-4.0479585475,3.9440432148,-0.09
82282282\C,-5.2105353426,3.169811091,0.0274771805\C,-4.8183012735,-1.1
598609978,-0.0119428026\C,-4.8819651924,-2.1223529827,0.995947756\C,-5
.7807159391,-1.1235363119,-1.0217802916\C,-5.9251847758,-3.0426901894,
0.9984575258\C,-6.8231703022,-2.0465557319,-1.0071111513\C,-6.89981283
5,-3.0046496111,0.0020336399\H,-0.9194357411,-2.6642479751,0.151830495
7\H,0.9371073866,1.1811283479,-0.076551984\H,1.3155832151,-3.755378134
5,0.1986354749\H,4.8181705525,1.7194232724,-1.652445341\H,2.3902183298
,1.8244786849,1.8780870333\H,5.0091853823,4.1967486358,-1.5961052792\H
,2.5724170866,4.2896283039,1.9385571266\H,3.8799549499,5.4860137334,0.
1999938372\H,-4.1193573046,5.0239947996,-0.1257490097\H,-1.8991819209,
3.9008018894,-0.2372072962\H,-6.0418829139,1.1985285958,0.1772660199\H
,-4.1157778732,-2.143475576,1.7599416047\H,-5.7046402227,-0.3936688248
,-1.8181988963\H,-5.9779640235,-3.788412871,1.7830178307\H,-7.56820009
61,-2.0219884951,-1.7935976348\H,-7.711653978,-3.7223800678,0.00834489
63\N,5.9247269379,-2.355402746,-0.0684656773\C,7.1331403958,-1.5732801
766,-0.2810197562\H,7.0336983648,-0.594607579,0.1808635543\H,7.9750271

223,-2.1016610061,0.1718068652\H,7.3482170955,-1.4330497024,-1.3492428
501\C,6.0482708719,-3.7940603409,-0.2512022153\H,5.1165504725,-4.27586
9006,0.027899011\H,6.2791920992,-4.044689901,-1.2955596976\H,6.8580120
093,-4.1718920296,0.3791715132\C,-6.5471522664,3.8485418486,0.07036355
52\F,-7.5112722166,3.0619265308,0.5979987239\F,-6.975988963,4.20452812
49,-1.1679907337\F,-6.5166856604,4.9868315871,0.800943475\\Version=ES6
4L-G09RevD.01\State=1-A\HF=-1801.5124141\S2=0.979305\S2-1=0.\S2A=0.176
561\RMSD=9.485e-09\RMSF=3.722e-06\Dipole=0.6040721,-0.4403133,-0.07457
24\Quadrupole=8.4331243,-0.3327499,-8.1003743,19.0818943,-2.5195252,-1
.0087739\PG=C01 [X(C29H22F3N7)]\\@

I[3,7]Me$_2$N,CF$_3$,Ph -S, *syn*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C29H22F3N7\PIOTR\21-Jan-202
4\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) f
check guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-NMe2-1-Ph
-benzo[e][1,2,4]triazinyl-7-)-1-Ph-7-CF3_benzo[e][1,2,4] triazinyl, co
nformer syn\\0,1\C,-1.4657523122,-1.4846268117,0.0516752037\C,-3.54856
12146,-2.4488715905,0.0105495343\C,-4.1516223689,-1.1651116083,-0.1157
578844\C,0.0087847898,-1.6219312568,0.0914443755\C,0.5920878297,-2.902
2048803,0.1838213936\C,0.8347671968,-0.497605776,0.0360097863\C,1.9623
09684,-3.0511886531,0.1985748924\C,2.2240075622,-0.6412864808,0.081500
8499\C,2.8223301816,-1.9341474749,0.1312594375\N,4.1683214705,-2.11024
75864,0.0971449251\N,3.1152869093,0.4312844938,0.0548480636\N,4.460672
227,0.2681271806,-0.0607653085\C,4.9084912133,-1.0055491352,-0.0503810
927\C,2.7035215545,1.8019352938,0.1028245648\C,3.1831425236,2.68958547
85,-0.8622020278\C,1.872114164,2.2568293207,1.1280809429\C,2.815443647
6,4.0299481307,-0.8073757956\C,1.5062897883,3.5995079786,1.171239702\C
,1.9734423005,4.4886591135,0.2052361621\N,-3.2796899648,-0.0783982023,
-0.0597453184\N,-1.9302930773,-0.2329878534,-0.0367878528\N,-2.1992603
287,-2.6005214205,0.1214452117\C,-5.5299087987,-1.0442805894,-0.316560
2323\C,-4.38414006,-3.5832161384,-0.009580014\C,-5.7497221318,-3.45949
55999,-0.1759396318\C,-6.3198129502,-2.1888958862,-0.3410484351\C,-3.7
188134181,1.2864358101,-0.0801920679\C,-3.1852784535,2.1580289195,-1.0
300525847\C,-4.636012061,1.7434268389,0.8675074116\C,-3.5860722454,3.4
902312809,-1.0378241748\C,-5.033421825,3.0777030697,0.8478837886\C,-4.
5128115842,3.9523971596,-0.1040232778\H,-0.0585335578,-3.7645847711,0.
2314121635\H,0.3842108939,0.4797019582,-0.0441671468\H,2.4215682636,-4
.030923808,0.2486862765\H,3.8401727541,2.3212085964,-1.6388555033\H,1.
5276997473,1.5709166042,1.8914710963\H,3.1856752183,4.716429577,-1.560
0754374\H,0.8630391483,3.9503015902,1.9697112774\H,1.6883317545,5.5334
874557,0.2445817891\H,-6.3792968241,-4.3395967711,-0.1984923363\H,-3.9
137351735,-4.5527093531,0.0943339329\H,-5.9810886796,-0.0739104773,-0.
4615457644\H,-2.4621526987,1.7871263149,-1.7444519065\H,-5.0209765446,
1.0670499444,1.6204866508\H,-3.1751323674,4.1669282552,-1.7777817229\H
,-5.7424155249,3.4338828329,1.5859303105\H,-4.8237384029,4.9904181025,
-0.1148560887\N,6.2624371917,-1.1515820172,-0.205040027\C,7.1506640863
,0.0017705349,-0.1954939122\H,8.0440325659,-0.2405811135,-0.7752206454
\H,6.65797773,0.8615652485,-0.640216376\H,7.4615934378,0.2694481283,0.
8237271237\C,6.8928093998,-2.4455445633,0.0124803768\H,6.1648731483,-3
.2353843152,-0.1440710709\H,7.7208821826,-2.5647611366,-0.6909831217\H
,7.2913188193,-2.5318143524,1.0328163235\C,-7.8069056893,-2.0576809192
,-0.4896651979\F,-8.4350031281,-2.0135256919,0.7135955752\F,-8.3461271
427,-3.0994820055,-1.1612988667\F,-8.1628747165,-0.9312561126,-1.14697
67387\\Version=ES64L-G09RevD.01\State=1-A\HF=-1801.5111086\S2=1.023009
\S2-1=0.\S2A=0.196734\RMSD=6.190e-09\RMSF=6.950e-06\Dipole=0.8051151,2
.0152188,0.0301625\Quadrupole=-5.4341254,10.5331479,-5.0990225,-5.0265
647,-6.6397692,-1.5372332\PG=C01 [X(C29H22F3N7)]\\@

I[3,7]H,H,2-Pyr -T, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C24H16N8(3)\PIOTR\16-Jan-20
24\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle)
fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-H-1-Pyridine-benzo[e][1,2,
4]triazinyl-7-)-1-Pyridine-benzo[e][1,2, 4]triazinyl, conformer anti\\
0,3\C,-0.8286358334,-0.1090722907,-0.1200254729\C,-1.7148251012,1.9986
133265,-0.2776839836\C,-3.0330390846,1.481534618,-0.1122566155\C,0.348
5703328,-1.0146291408,-0.0990422909\C,0.1873206894,-2.4148083174,-0.07
41577712\C,1.6304006581,-0.4635640141,-0.1052503213\C,1.2899884648,-3.
2384683431,-0.0812194899\C,2.7558972264,-1.290847867,-0.0820376161\C,2
.5965789392,-2.7090970223,-0.1030586956\N,3.6574378375,-3.5673617533,-
0.1756528624\N,4.0866909926,-0.8274630145,-0.0838466009\N,5.1350480148
,-1.6884037254,-0.2471287964\C,4.8448075875,-2.9764070924,-0.279262177
9\C,4.4932448795,0.5328829326,0.052896383\C,5.6990327209,0.9495797212,
-0.5306217117\C,6.0823273881,2.2687871311,-0.3474957482\C,4.0931238791
,2.6063299069,0.9252876395\C,5.2694319626,3.124068725,0.3969566487\N,-
3.1231888101,0.0834811397,0.0019695293\N,-2.0116283006,-0.7020882204,0
.0403449378\N,-0.6112532316,1.1938157831,-0.3037498323\C,-4.1195404564
,2.3645093858,-0.0303555496\C,-1.5408259328,3.3918391932,-0.3990354285
\C,-2.6206067268,4.2502489716,-0.3335124368\C,-3.9077236566,3.73166202
17,-0.1398694237\C,-4.3340102232,-0.6610852509,0.141008739\C,-4.318016
6375,-1.8625114857,0.8648829786\C,-5.4999151467,-2.5813667229,0.951037
7807\C,-6.5530669522,-0.8870871411,-0.3563653547\C,-6.647823383,-2.093
315095,0.3262411951\H,-0.8106316652,-2.8310028051,-0.0690692221\H,1.73
16207074,0.6071066586,-0.1018797838\H,1.1950898914,-4.3171312615,-0.09
11262173\H,6.2984018477,0.2511622569,-1.0937399607\H,7.0057778169,2.62
77217965,-0.7869656296\H,3.4255370569,3.2296780051,1.5122969455\H,5.53
75069499,4.1600283139,0.5612388517\H,-2.4732822421,5.3198705695,-0.425
8067196\H,-0.5288613396,3.7532243704,-0.5331483261\H,-5.1177499091,1.9
788657335,0.0875495563\H,-3.4072676501,-2.2015796142,1.3338516031\H,-5
.5261871809,-3.5118204745,1.5061865099\H,-7.4180569913,-0.4634204843,-
0.8575579442\H,-7.5877803379,-2.6286034753,0.3697560901\H,-4.757844466
,4.4008870657,-0.0783798289\H,5.7137230481,-3.6173043909,-0.3951217079
\N,-5.4212183427,-0.1817393641,-0.4551688396\N,3.7091917102,1.33614774
07,0.7646109714\\Version=ES64L-G09RevD.01\State=3-A\HF=-1362.4444304\S
2=2.035353\S2-1=0.\S2A=2.000732\RMSD=4.944e-09\RMSF=3.509e-06\Dipole=-
1.1994957,1.0127766,0.2636564\Quadrupole=18.8917006,-1.3653862,-17.526
3145,18.9637181,-7.257821,-1.682891\PG=C01 [X(C24H16N8)]\\@

I[3,7]H,H,2-Pyr -T, *syn*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C24H16N8(3)\PIOTR\16-Jan-20
24\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle)
fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-H-1-Pyridine-benzo[e][1,2,
4]triazinyl-7-)-1-Pyridine-benzo[e][1,2, 4]triazinyl, conformer syn\\0
,3\C,-1.0118552752,-1.4677862637,0.0080621574\C,-3.2137644757,-2.09095
59284,0.1390929995\C,-3.6294025673,-0.731723835,0.0309922897\C,0.42759
27921,-1.8304088205,-0.0196212784\C,0.7987610313,-3.1892092939,-0.0059
947677\C,1.4120670105,-0.8404230918,-0.053005183\C,2.1279331812,-3.543
2335846,-0.0557838801\C,2.7645742733,-1.1883007427,-0.0792979856\C,3.1
423577445,-2.566412442,-0.1125112188\N,4.4420058702,-2.9706656014,-0.2
219686789\N,3.8294138886,-0.2644507429,-0.1165105597\N,5.1175326876,-0
.679323489,-0.3083299814\C,5.3241178731,-1.9826130719,-0.3447823146\C,
3.7135188333,1.1513902485,0.0106682872\C,4.6957805796,1.9739578088,-0.
5635924036\C,4.574776969,3.3431262605,-0.3891841293\C,2.5799650639,2.9
482326889,0.8565533434\C,3.4982734191,3.8525931594,0.3380467647\N,-2.5

895531418,0.212458353,-0.0578371431\N,-1.2842002579,-0.1676423335,-0.1
045126903\N,-1.8968926338,-2.4558029652,0.1463243793\C,-4.997144634,-0
.4274860109,-0.0239409394\C,-4.1953836636,-3.0983427745,0.2231827363\C
,-5.5398312984,-2.7850022688,0.181771276\C,-5.9354708162,-1.44772432,0
.0507195138\C,-2.7580392766,1.6268405216,-0.1653108882\C,-1.7979946082
,2.3778173548,-0.8604221688\C,-1.9697909986,3.7517880242,-0.9189636861
\C,-3.967349814,3.494611567,0.3581042414\C,-3.0737834057,4.3338346602,
-0.295232355\H,0.0214561652,-3.9395401621,0.0351947439\H,1.1178058145,
0.1927808939,-0.0195633016\H,2.4413826995,-4.5796092142,-0.0691276353\
H,5.5153654633,1.5370341123,-1.1121264855\H,5.3138370696,4.0080389768,
-0.8209770061\H,1.7237194517,3.2910051548,1.4294602171\H,3.3745018125,
4.9162400034,0.4975469064\H,-6.2847134221,-3.5693950733,0.2461182725\H
,-3.8479264782,-4.1201794327,0.3115851644\H,-5.3164580362,0.598088198,
-0.0944551172\H,-0.9586827972,1.8864619931,-1.3274936867\H,-1.25053279
78,4.3624368546,-1.4523375288\H,-4.8436030741,3.8971832806,0.857110868
1\H,-3.2395166629,5.403415937,-0.3180556644\H,-6.9886268373,-1.1955563
7,0.0107446197\H,6.3656307926,-2.2564355488,-0.4840874792\N,-3.8166616
577,2.1677668438,0.4294036728\N,2.6815781442,1.6240804863,0.7026987033
\\Version=ES64L-G09RevD.01\State=3-A\HF=-1362.4445932\S2=2.03603\S2-1=
0.\S2A=2.000759\RMSD=8.407e-09\RMSF=1.173e-05\Dipole=-0.8488013,2.6690
67,-0.6856223\Quadrupole=3.1890714,9.5733368,-12.7624082,9.1103056,-2.
4585244,-2.1629129\PG=C01 [X(C24H16N8)]\\@

I[3,7]H,H,2-Pyr -S, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C24H16N8\PIOTR\17-Jan-2024\
0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fch
eck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-H-1-Pyridin
e-benzo[e][1,2,4]triazinyl-7-)-1-Pyridine-benzo[e][1,2, 4]triazinyl, c
onformer anti\\0,1\C,-0.825175995,-0.1020113019,-0.1232716912\C,-1.711
9407777,2.0045536174,-0.2741686838\C,-3.029283978,1.4861371244,-0.1092
258163\C,0.3493470954,-1.0141132208,-0.09763405\C,0.1850050497,-2.4126
517867,-0.0688675469\C,1.6305270232,-0.4644568763,-0.1036835113\C,1.28
77277136,-3.238652948,-0.0725114352\C,2.7557441448,-1.294615305,-0.076
6763518\C,2.5934880174,-2.7120363676,-0.0937769336\N,3.6572645079,-3.5
718191881,-0.1609521538\N,4.0844134829,-0.8322631424,-0.079324881\N,5.
1343612991,-1.6922030967,-0.237292865\C,4.8424966868,-2.9821040185,-0.
2644791905\C,4.4896354799,0.5299512431,0.0517893201\C,5.68729142,0.947
9546575,-0.5462218187\C,6.0699467292,2.268323133,-0.3688864397\C,4.095
1063255,2.6023288728,0.9276976114\C,5.2639012636,3.1220964348,0.384452
2719\N,-3.1167785917,0.0857743078,-0.0015353268\N,-2.006929811,-0.6963
653987,0.0316050381\N,-0.607244892,1.2003966984,-0.3034447532\C,-4.118
0985505,2.364888697,-0.0204231983\C,-1.5422950565,3.3983947756,-0.3903
176793\C,-2.6246787312,4.2538793169,-0.3192517692\C,-3.9105367637,3.73
32163489,-0.124787265\C,-4.3278319335,-0.6607163799,0.1341408013\C,-4.
3132999347,-1.8584527656,0.8633770884\C,-5.4943294106,-2.5794262115,0.
9454262578\C,-6.5426909314,-0.8925487372,-0.3760341935\C,-6.6390504683
,-2.0960868578,0.3113230409\H,-0.813437564,-2.827389145,-0.0634001072\
H,1.7324779279,0.6062733282,-0.1050684239\H,1.1905353467,-4.3171521006
,-0.0789016565\H,6.281329076,0.2498578509,-1.1154703328\H,6.9873021073
,2.6290411277,-0.8194594336\H,3.4335008935,3.2246405312,1.5224627811\H
,5.5315933358,4.1587835834,0.544743761\H,-2.4793310069,5.3241652524,-0
.4078137711\H,-0.5317747983,3.7637443478,-0.5246530012\H,-5.1150227207
,1.9759405782,0.0985382275\H,-3.4046562349,-2.1935603962,1.3394617898\
H,-5.5223855498,-3.5074875465,1.5044284573\H,-7.4054235408,-0.47286861
18,-0.8843505177\H,-7.5782479508,-2.6329741325,0.3514112912\H,-4.76177
96451,4.4004807791,-0.0588678076\H,5.712357517,-3.6227749187,-0.375542
7382\N,-5.4116468096,-0.1853631758,-0.4707397944\N,3.7122902037,1.3311

380236,0.7727014007\\Version=ES64L-G09RevD.01\State=1-A\HF=-1362.44405
82\S2=1.00428\S2-1=0.\S2A=0.210615\RMSD=9.072e-09\RMSF=3.659e-06\Dipol
e=-1.2123485,0.9985051,0.2670575\Quadrupole=19.413008,-1.8201208,-17.5
928873,19.628793,-7.4438748,-1.6509069\PG=C01 [X(C24H16N8)]\\@

I[3,7]H,H,2-Pyr -S, *syn*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C24H16N8\PIOTR\17-Jan-2024\
0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fch
eck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-H-1-Pyridin
e-benzo[e][1,2,4]triazinyl-7-)-1-Pyridine-benzo[e][1,2, 4]triazinyl, c
onformer syn\\0,1\C,-1.0123778876,-1.4682042725,0.0070993007\C,-3.2127
369574,-2.0877504116,0.1538440084\C,-3.6275082056,-0.7291407,0.0331089
\C,0.4307169672,-1.8332870538,-0.0258011684\C,0.8015927294,-3.19093958
79,-0.0226868235\C,1.4131877082,-0.8433555714,-0.0529385038\C,2.132258
6427,-3.5439674257,-0.076787105\C,2.767317253,-1.1914537233,-0.0826802
985\C,3.1445617139,-2.5670933376,-0.1263637779\N,4.4489169522,-2.96919
91675,-0.241135586\N,3.8292359482,-0.2652460286,-0.1156327527\N,5.1173
487874,-0.6746618852,-0.3158046267\C,5.3258198027,-1.9803032333,-0.360
9976238\C,3.70919843,1.1493091753,0.0241271672\C,4.6800445739,1.979682
7028,-0.5575027773\C,4.5563527828,3.3470984007,-0.370747317\C,2.580935
7281,2.9343566955,0.9004630138\C,3.4883106283,3.846324073,0.3756732988
\N,-2.5871649462,0.2124656459,-0.0665632531\N,-1.2825176052,-0.1700144
163,-0.1171779591\N,-1.8958619055,-2.4531626155,0.1608776335\C,-4.9952
622624,-0.4236117601,-0.0226955055\C,-4.1953733439,-3.0927769061,0.250
9908736\C,-5.5394953991,-2.7779937151,0.2092724785\C,-5.9343491896,-1.
4417030215,0.0646276041\C,-2.7543593548,1.6264564009,-0.1813739715\C,-
1.7968525573,2.372189699,-0.8854304511\C,-1.9673086837,3.7460656258,-0
.9506673056\C,-3.9587715159,3.4982886111,0.3380273846\C,-3.0674083723,
4.3327755592,-0.3244766784\H,0.0249666504,-3.9422166379,0.0141988114\H
,1.1186029942,0.1896543539,-0.0132916943\H,2.445625581,-4.5802502671,-
0.0989242827\H,5.4933614104,1.5497826414,-1.1208388035\H,5.2865755279,
4.0183687845,-0.8076807729\H,1.731943318,3.269419755,1.4884912804\H,3.
3627069681,4.9081769091,0.5453802051\H,-6.2851221003,-3.5608174031,0.2
835837021\H,-3.8491842932,-4.11412665,0.3492749879\H,-5.3134967834,0.6
01532404,-0.1038196596\H,-0.9606064052,1.8770283742,-1.3539927273\H,-1
.2500326843,4.3529744825,-1.4909069997\H,-4.831879284,3.904711406,0.83
94053514\H,-3.2319099087,5.4024302995,-0.352250983\H,-6.9873500333,-1.
189059591,0.0239646317\H,6.3679658182,-2.2493964858,-0.5057784445\N,-3
.8093864871,2.1717277549,0.4158077791\N,2.6855392499,1.6118721135,0.73
50844402\\Version=ES64L-G09RevD.01\State=1-A\HF=-1362.4434538\S2=1.027
49\S2-1=0.\S2A=0.223173\RMSD=9.068e-09\RMSF=7.556e-06\Dipole=-0.876928
5,2.7266679,-0.6914541\Quadrupole=3.0102529,9.5634381,-12.5736909,9.28
25913,-2.4223897,-2.1783337\PG=C01 [X(C24H16N8)]\\@

I[3,7]H,H,4-Me2NPh -T, *anti*

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-311G(d,p)\C30H28N8(3)\PIOTR\17-Jan-20
24\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle)
fcheck freq #P SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benzo[e][1,2,4]tria
zinyl-7-)-1-Ph-benzo[e][1,2, 4]triazinyl, conformer anti\\0,3\C,-0.841
059632,-0.0906546249,0.0598892078\C,-1.6939000318,2.0395354006,-0.0309
068592\C,-3.0137442578,1.5220899491,0.1004209772\C,0.3272978169,-1.006
8159157,0.0918136845\C,0.1576014523,-2.3991517357,0.224643269\C,1.6162
553392,-0.4793090965,-0.0174479474\C,1.2512153442,-3.2401710662,0.2253
886237\C,2.7286691299,-1.3222083495,0.0155291567\C,2.5604378341,-2.735
4154244,0.1044045268\N,3.6214100905,-3.5971621912,0.0418669857\N,4.048
6375845,-0.8621211984,-0.0622761208\N,5.0977110996,-1.7250641567,-0.21

90273982\C,4.8018600619,-3.013133542,-0.1573457824\C,4.4126929906,0.51
89542181,-0.0549567745\C,5.2773702381,1.0110253039,-1.0338428325\C,3.9
661601703,1.3834959526,0.9456315557\C,5.6777247481,2.3371208864,-1.025
6894282\C,4.358207624,2.7138420794,0.959202508\C,5.2342662065,3.231831
8506,-0.0230250589\N,-3.1273131318,0.1331319532,0.1168982198\N,-2.0358
194956,-0.680768837,0.155764656\N,-0.6015991789,1.2167501243,-0.074426
7116\C,-4.1044253607,2.3929067607,0.2284206692\C,-1.5241532298,3.43540
49799,-0.0888492061\C,-2.6105857255,4.288888478,0.008439143\C,-3.89861
12546,3.7659394362,0.1787308088\C,-4.3820868523,-0.5541723816,0.147737
0332\C,-4.6369424788,-1.4936914112,1.1467587759\C,-5.3441771298,-0.338
9096477,-0.8391215429\C,-5.8307753736,-2.1967757686,1.1702044164\C,-6.
5452297169,-1.032614137,-0.8210354575\C,-6.8230644023,-1.9920024741,0.
1814359609\H,-0.8433756021,-2.7995595315,0.3090932761\H,1.7278113988,0
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I[3,7]H,H,4-Me2NPh -T, *syn*

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24\0\\#P UB3LYP/6-311G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle)
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I[3,7]H,H,4-Me2NPh -S, *anti*

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eck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-H-1-Ph-benz
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I[3,7]H,H,4-Me2NPh -S, *syn*

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eck guess(mix,always) #P freq SCRF=(solvent=Benzene)\\3-(3-H-1-PhNMe2-
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