Supplementary Geometric Structure and Property Information for

Theoretical Studies of a Novel Carbazole-Fluorene Macrocycle as a Host Material for Phosphorescent Organic Light-Emitting Diodes and the Effects of Substituent

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To characterize the excited states in our study, we employed Natural Transition Orbital (NTO) analysis, which provides a comprehensive description of electronic transitions through singular value decomposition of the particle-hole transition density matrix. The highest occupied (HONTO) and lowest unoccupied (LUNTO) NTO pairs were identified as the dominant contributors to each excited state, governing the nature of electronic transitions. The orbital overlap metric (I_{ST}) serves as a quantitative measure to classify excited states into three distinct categories: charge transfer (CT, 0-40%), hybrid local-charge transfer (HLCT, 40-75%), and localized excitation (LE, 75-100%).

We performed NTO analyses on the triplet excitation patterns of the unsubstituted host material a1 and the substituted host material c (which exhibits the most pronounced delocalization separation after substitution) using both the B3LYP and CAM-B3LYP functionals at the 6-31G(d) basis set level (Figure S1). For a1, the two dominant NTO pairs are 212-213 and 211-214. The corresponding calculated orbital overlap metric (I_{ST}) values under the B3LYP functional are 82.74% and 84.08%, while those under CAM-

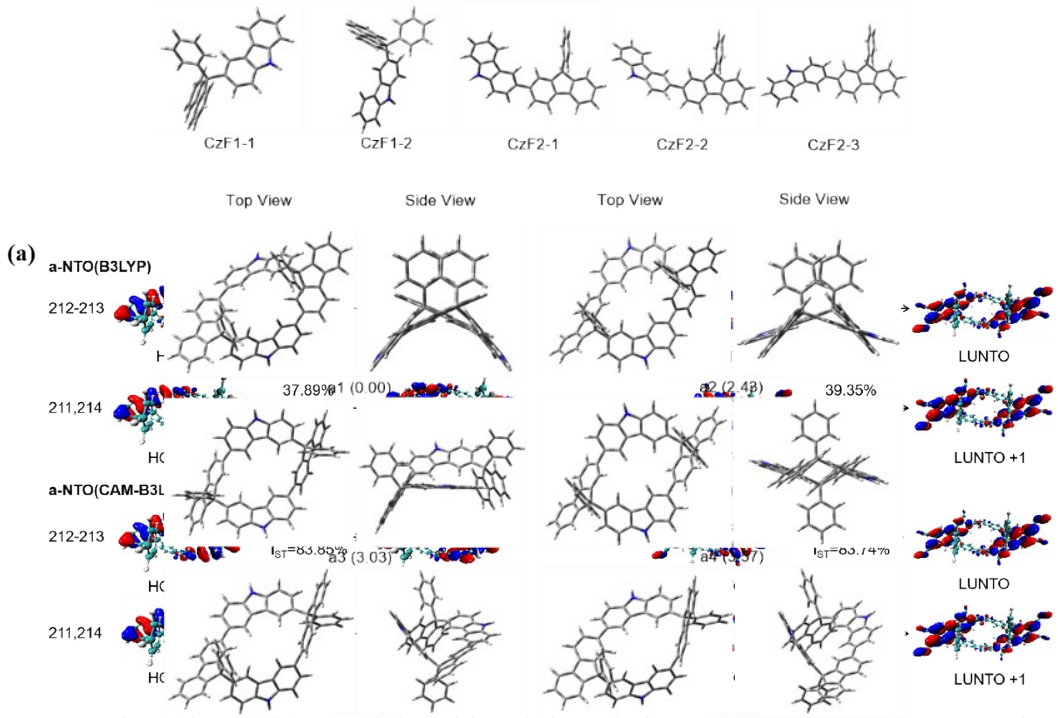

Figure S1. Natural Transition Orbital (NTO) analysis of triplet excitation modes for a1 and c at the B3LYP and CAM-B3LYP/6-31G(d)

[c]**Figure S2**. Optimized geometric conformations of CzF1, CzF2 and CzFMC(a1~a6). (The units for all relative energies are kcal/mol.)

B3LYP are 83.85% and 84.50%, respectively. The I_{ST} values obtained from both functionals show minimal discrepancies and are all greater than 75%, indicating that the excited states of a1 are predominantly characterized by localized π-π* transitions, thus confirming its distinct localized excitation (LE) nature. For the substituted host material c, the primary NTO pairs are 248-249 and 247-250. The I_{ST} values derived from B3LYP are 78.81% and 80.84%, whereas those from CAM-B3LYP are 83.74% and 84.24%. All calculated I_{ST} values remain above 75%, still classifying c within the LE category. However, the introduction of substituents induces slight delocalization, as evidenced by an approximate 5% decrease in I_{ST} values compared to a1. The spatial distributions of the HONTO and LUNTO reveal over 80% overlap on the conjugated backbone. This clearly demonstrates that the designed host materials in this work unequivocally belong to the localized excitation (LE) type. The B3LYP functional has been demonstrated to exhibit reasonable accuracy for obvious localized excitation (LE).”

We employed a strategy combining rigid potential energy surface (PES) scanning with full geometry optimization. Through molecular structure analysis, we selected two dihedral angles at the junctions between the benzene rings and the fluorene skeleton as scanning variables. A rigid PES scan was performed from 0° to +180° with a step size of 10°. Geometry optimizations were conducted at the DFT/B3LYP/6-31G(d) level, where frequency analyses were used to eliminate structures with imaginary frequencies. This process ultimately identified six stable conformations through energy ranking. Although the 10° scanning step size might have missed some minor conformations, the subsequent full optimization ensured coverage of the main energy regions. To enhance the reproducibility of this study, we have provided xyz structural data of optimized conformations.

Table S1. Dihedral angles of Fluorene-Carbazole (Φ_1) and Fluorene-Benzene (Φ_2) in CzF1 and CzFMCs, as well as Fluorene-Carbazole (Φ_3) in CzF2 and CzFMCs.

	Φ_1	Φ_2	Φ_3
CzF1-1	87.0	84.3	
CzF1-2	-18.8	163.5	
CzF2-1			142.6
CzF2-2			142.1
CzF2-3			38.1
a1	78.3, 78.3	87.2, 87.2	149.0, 149.0
a2	51.9, 51.9	106.7, 106.7	148.2, 148.2
a3	-5.5, -5.5	160.7, 160.7	109.6, 109.6
a4	60.1, 60.1	99.4, 99.4	124.8, 124.8
a5	75.0, 1.8	90.9, 155.7	149.9, 75.0
a6	80.9, -15.9	82.9, 165.5	157.3, 67.0

All values of dihedral angles are in degree.

Table S2. Comparison of E_T for the host material calculated using different functionals (B3LYP, ωB97XD, and CAM-B3LYP) at the same 6-31G(d) basis set level. Supplementary comparison of E_T for host a1calculated under the B3LYP functional level with the 6-31+G(d) basis set and the 6-31G(d) basis set.

	E_T B3LYP/ 6-31G(d)	E_T ωB97XD/ 6-31G(d)	E_T CAM-B3LYP/ 6-31G(d)	E_T B3LYP/ 6-31+G(d)
a1	2.61	2.91	2.82	2.57
b1	2.98	2.80	2.71	
b2	3.15	2.90	2.82	
b3	3.13	2.98	2.89	
b4	3.15	3.02	2.92	
b5	2.58	2.89	2.80	
c	2.89	2.85	2.87	
d	2.60	2.82	2.77	
e	2.44	2.69	2.64	
f	2.62	2.91	2.82	
Cz-4	2.67	2.98	2.90	

All values of E_T are in eV.

Table S2 presents the adiabatic triplet energy (E_T) of all host molecules calculated using three different functionals (B3LYP、ωB97XD and CAM-B3LYP) at the 6-31G(d) basis set level, with all computations employing the ΔSCF method. Additionally, we have supplemented the comparison of E_T calculated at the same B3LYP functional level using the 6-31+G(d) basis set (with diffuse functions) and the 6-31G(d) basis set (without diffuse functions) for material a1. The observed energy difference is 0.04 eV, which falls within the commonly accepted chemical accuracy range of 0.05–0.1 eV. This indicates that the 6-31G(d) basis set is relatively reliable for this calculation under the given conditions.

In Table S2, to further validate the reliability of the B3LYP functional, we employed the ΔSCF method to calculate the ET of Cz-4—a molecule previously reported by research group—and benchmarked the results against experimental data. The molecular framework of Cz-4 is also constructed from carbazole and fluorene moieties, exhibiting structural symmetrical analogous to the host molecules designed in this work. For Cz-4, the calculated ET values using CAM-B3LYP and ωB97XD are 2.90 eV and 2.98 eV, respectively, both deviating from the experimental value of 2.64 eV by over 0.25 eV. In contrast, the B3LYP calculation yields a value of 2.67 eV, with an error of only 0.03 eV. This discrepancy lies well within the chemical accuracy threshold (0.05–0.1 eV), robustly validating the reliability of the B3LYP functional for the systems investigated in this work.

Table S3. Spin-squared values ($\langle \hat{S}^2 \rangle$) and spin contamination in the ΔSCF method for E_T

	$\langle \hat{S}^2 \rangle$	$\Delta \langle \hat{S}^2 \rangle$	Spin contamination
a1	2.0308	0.0308	1.5%
b1	2.0105	0.0105	0.5%
b2	2.0137	0.0137	0.7%
b3	2.0125	0.0125	0.6%
b4	2.0124	0.0124	0.6%
b5	2.0349	0.0349	1.7%
c	2.0108	0.0108	0.5%
d	2.0266	0.0266	1.3%
e	2.0329	0.0329	1.6%
f	2.0293	0.0293	1.5%
Cz-4	2.0233	0.0233	1.2%

Figure S3 presents a comparative analysis of the normalized absorption spectra of a1 in vacuum versus chloroform ($CHCl_3$) solvent, where the Polarizable Continuum Model (PCM) was employed as the solvent framework. All calculations were uniformly performed at the B3LYP/6-31+G(d) level with a full width at half maximum (FWHM) set to 0.3 eV. The results indicate that the normalized absorption spectrum of a1 in $CHCl_3$ solvent exhibits a slight redshift of approximately 10 nm compared to that in vacuum. However, the overall shape and intensity of the absorption spectrum remain largely unchanged, demonstrating no significant distinction between the absorption spectrum under these two conditions. This demonstrates that solvent effects exert negligible influence on the absorption spectra of the molecular system under investigation.

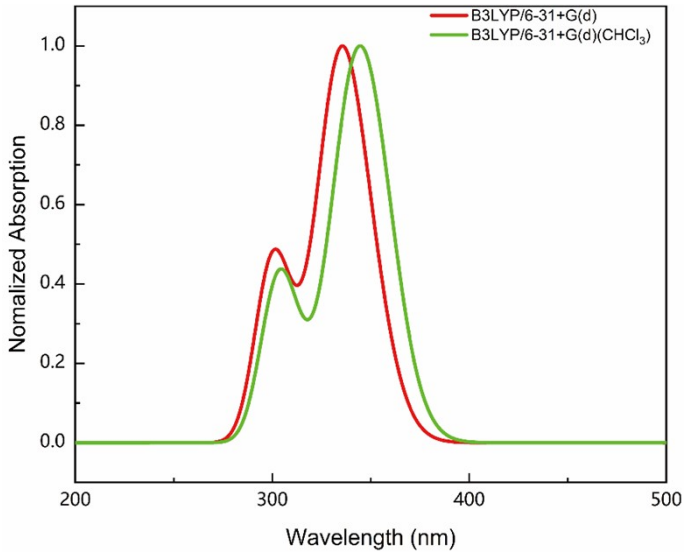

Figure S3. Comparison of the normalized simulated absorption spectra of host material a1 in vacuum and in chloroform ($CHCl_3$) solvent. (FWHM=0.3 eV)

Figure S4 presents a comparative analysis of simulated absorption spectra calculated using the long-range corrected (LC) functionals CAM-B3LYP and ωB97XD versus B3LYP. By adjusting the ratio of short-range to long-range exchange energy, LC functionals (CAM-B3LYP and ωB97XD) effectively mitigate artifacts inherent to low Hartree-Fock (HF) exchange functionals. Notably, the higher HF exchange content in CAM-B3LYP and ωB97XD induces a blueshift in the absorption bands compared to B3LYP. However, this comparison crucially demonstrates that the observed absorption bands are not ghost states, thereby confirming the genuine existence of the 301 nm absorption band calculated with B3LYP. This analysis robustly confirms that compound a1 reliably exhibits two absorption bands.

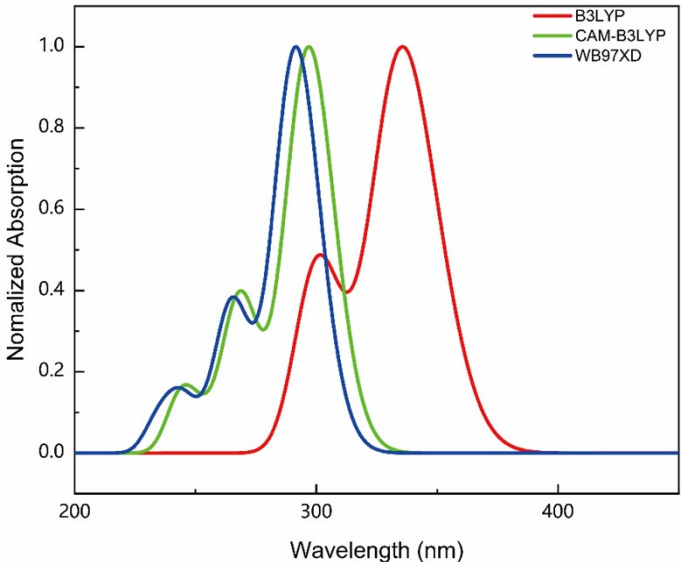

Figure S4. Comparison of normalized simulated absorption spectra of a1 under three different functionals (B3LYP, CAM-B3LYP, and ωB97XD) with the basis set uniformly set to 6-31+G(d). (FWHM=0.3 eV)

Table S4. Electronic transition, maximum absorption peak wavelength(nm), oscillator strength(f) and main transition behavior of the absorption spectra

	Electronic transition	λ (nm)	f	Main transition configuration
a1	S_0-S_2	347.03	0.3262	HOMO→LUMO (83%)
	S_0-S_6	332.08	0.6615	HOMO-1→LUMO+1 (90%)
	S_0-S_{12}	301.30	0.3269	HOMO-3→LUMO (38%)
b1	S_0-S_2	380.05	0.2948	HOMO→LUMO (88%)
	S_0-S_4	369.77	0.8230	HOMO-1→LUMO+1 (90%),
	S_0-S_9	333.41	0.1851	HOMO→LUMO+2 (36%)
b2	S_0-S_2	354.71	0.3141	HOMO→LUMO (92%)
	S_0-S_5	346.01	0.3205	HOMO→LUMO+2 (51%)
	S_0-S_8	336.12	0.2826	HOMO→LUMO+3 (89%)
b3	S_0-S_1	371.32	0.1120	HOMO→LUMO (84%)
	S_0-S_6	332.43	0.5178	HOMO→LUMO+2 (80%)
	S_0-S_{10}	320.18	0.7382	HOMO-1→LUMO+3 (48%)
b4	S_0-S_6	335.57	0.3956	HOMO→LUMO+2 (76%)
	S_0-S_{10}	320.52	0.3562	HOMO-1→LUMO+3 (59%)
	S_0-S_{11}	310.75	0.2159	HOMO-3→LUMO (72%)

Table S4 presents the calculated wavelengths, main transition configurations, and oscillator strengths for the most relevant singlet excited states of a1 and b1~b4.

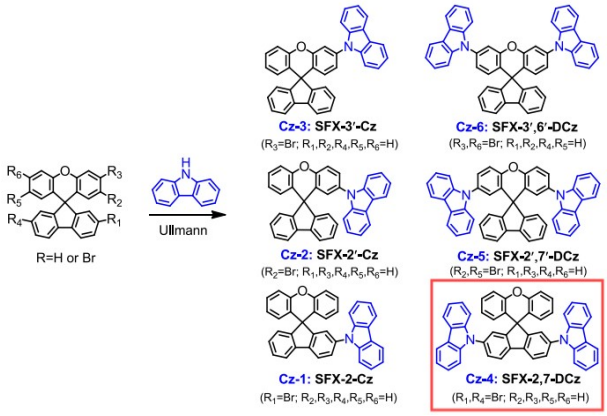

Figure S5. The chemical structure of molecule Cz-4, enclosed in a red square box.

Coordinates of DFT Optimized Geometries

Coordinates of geometry optimized structure of a1

C	3.33455200	0.66927200	4.75949200
C	3.64732900	1.80018100	4.00390300
C	4.03338500	1.67035000	2.66993600
C	4.11620500	0.40890000	2.05976500
C	3.80354300	-0.71860700	2.83075200
C	3.41520600	-0.58990200	4.16569000
C	5.42717900	-1.87145000	-0.21080800
C	4.27962500	-1.07925500	-0.03067600
C	4.63760100	0.27945500	0.60720700
C	6.17217500	0.15829400	0.67759300
C	6.59857800	-1.10894200	0.23117000
C	7.09861300	1.08029500	1.15237300
C	8.45626800	0.73989500	1.16582900
C	8.87893100	-0.51702700	0.72069600
C	7.95263400	-1.45084700	0.25254700

C	5.30693600	-3.15047300	-0.76002600
C	4.04953100	-3.61710000	-1.14187400
C	2.89492500	-2.81986300	-1.01012700
C	3.03840800	-1.53785100	-0.44174100
C	0.85827900	3.08866600	-1.44350200
C	0.94373200	3.97690400	-2.54590000
N	2.27772400	4.10537400	-2.90668100
C	3.05470300	3.27303100	-2.10979800
C	2.20919000	2.64345400	-1.16124300
C	4.42008600	2.99218300	-2.15085800
C	4.92572500	2.05479000	-1.24910800
C	4.11078500	1.41454900	-0.29335600
C	2.74910000	1.73775200	-0.24772200
C	-0.38897400	2.76066700	-0.91290500
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C	-0.85824000	-3.08850600	-1.44386000
C	-0.94366700	-3.97662500	-2.54635600
N	-2.27765200	-4.10506300	-2.90717800
C	-3.05464800	-3.27280000	-2.11022800
C	-2.20915800	-2.64332400	-1.16158600
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C	1.56206500	-3.27085300	-1.48823700
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C	0.20604500	-4.53488300	-3.10911200
C	-5.42717300	1.87147200	-0.21074500
C	-4.27962300	1.07926100	-0.03066500
C	-4.63761400	-0.27952000	0.60706200
C	-6.17219100	-0.15836800	0.67741900
C	-6.59858300	1.10891400	0.23111800
C	-7.09863900	-1.08042300	1.15207400
C	-8.45629500	-0.74002700	1.16552600
C	-8.87894900	0.51694100	0.72051500
C	-7.95264100	1.45081400	0.25249300
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H	-3.17323300	1.48021700	4.73979300
H	-3.58739600	-2.79007900	4.44992200
H	-4.25924000	-2.56164400	2.09184100
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Coordinates of geometry optimized structure of a2

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C	5.32127700	-1.54143300	-1.24602600
C	4.31036000	-1.06752900	-0.38772700
C	4.84084900	0.08749200	0.48842900
C	6.34840200	-0.01404600	0.18719300
C	6.58725800	-0.89912900	-0.88198200
C	7.41154500	0.61452900	0.82608800
C	8.71410800	0.39626300	0.35993600
C	8.94611300	-0.44912200	-0.72952100
C	7.88503600	-1.11035700	-1.35222500
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C	4.25665400	1.43599400	-0.03365000

C	2.87599400	1.57443300	-0.22196400
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H	9.96175900	-0.60891500	-1.08186200
H	8.07271800	-1.79332100	-2.17690700
H	5.80177900	-2.90124300	-2.85893500
H	3.52767800	-3.84684100	-2.96107300
H	2.31528300	-1.38411500	0.34984300
H	5.23772800	4.61125600	-0.92344800
H	6.15131900	2.46444500	-0.17948400
H	2.21138000	0.74124700	-0.02680600
H	-0.34327500	1.56080500	-0.70063900
H	-2.16149200	5.26739500	-1.92585400
H	0.03674100	6.37724800	-2.00296900
H	-5.23770000	-4.61116100	-0.92408200
H	-6.15131400	-2.46442600	-0.17992500
H	-2.21138200	-0.74124000	-0.02695600
H	0.34329400	-1.56072800	-0.70079800

H	-0.03668100	-6.37703800	-2.00363400
H	-7.23795000	-1.25753900	1.68487300
H	-9.55086500	-0.88224400	0.85429900
H	-9.96172900	0.60903500	-1.08208800
H	-8.07265500	1.79354900	-2.17696000
H	-5.80169200	2.90154200	-2.85880600
H	-3.52758800	3.84715100	-2.96077500
H	-2.31529700	1.38408300	0.34992500
H	-5.02656800	2.22436700	1.92248700
H	-4.70048700	2.59621500	4.33726100
H	-3.75393100	-1.56821900	4.84384800
H	-4.07265800	-1.93369200	2.42781000
H	2.78294000	5.87002000	-1.57911300
H	-4.05815800	0.70061300	5.82233800
H	4.05798900	-0.70124800	5.82238200
H	-2.78289500	-5.86984700	-1.57983400
H	2.16155000	-5.26719000	-1.92634400

Coordinates of geometry optimized structure of a3

C	-6.99803300	-1.66543300	-3.57087300
C	-7.64304000	-1.73580400	-2.33597500
C	-7.07520300	-1.14242900	-1.20741200
C	-5.85191700	-0.46279400	-1.28902600
C	-5.21093900	-0.40296400	-2.53577600
C	-5.77682200	-0.99710300	-3.66421400
C	-4.83234500	-1.35079100	1.87285500
C	-4.32221500	-0.99428000	0.61154000
C	-5.16896600	0.12691500	-0.02789900
C	-6.17757100	0.40062100	1.11044900
C	-5.96351800	-0.47642100	2.19124900
C	-7.20391200	1.33820000	1.17639900
C	-8.00734000	1.39902100	2.32057200
C	-7.78943000	0.52795300	3.39244000
C	-6.76468300	-0.41735300	3.33363800
C	-4.25796000	-2.39495500	2.59965200
C	-3.15043200	-3.05889100	2.07369400
C	-2.60471500	-2.68965600	0.83289000
C	-3.21686800	-1.66052000	0.09397300
C	-1.00207200	3.21902900	-0.18189300
C	-0.94619700	4.54394500	-0.68912300
N	-2.20451900	4.88365300	-1.16519600
C	-3.07085200	3.81559900	-0.98571600
C	-2.36812400	2.76412600	-0.34880100
C	-4.41041700	3.66565100	-1.35131000
C	-5.03346500	2.45892300	-1.05384800
C	-4.37491900	1.40587900	-0.37301200
C	-3.03473800	1.57538100	-0.02459500
C	0.16301000	2.62386400	0.30936400
C	1.36225500	3.34278300	0.32409700
C	1.37752200	4.67347900	-0.14853500
C	0.23705200	5.28487100	-0.66444000
C	1.00205600	-3.21899700	-0.18272200
C	0.94617400	-4.54381400	-0.69020900
N	2.20448300	-4.88341900	-1.16639000
C	3.07082400	-3.81540800	-0.98669100
C	2.36810100	-2.76405400	-0.34957600
C	4.41039200	-3.66539800	-1.35225000
C	5.03344600	-2.45872900	-1.05455900

C	4.37489600	-1.40580000	-0.37354800
C	3.03471700	-1.57536800	-0.02515700
C	-0.16301500	-2.62393800	0.30869100
C	-1.36225300	-3.34287200	0.32333100
C	-1.37752600	-4.67347400	-0.14956800
C	-0.23706900	-5.28475300	-0.66563600
C	4.83242200	1.35031600	1.87296300
C	4.32223000	0.99412300	0.61158400
C	5.16895000	-0.12690700	-0.02818500
C	6.17762900	-0.40088100	1.11003200
C	5.96362300	0.47587800	2.19107100
C	7.20399200	-1.33845800	1.17567600
C	8.00748500	-1.39956400	2.31978900
C	7.78961900	-0.52878000	3.39189700
C	6.76485400	0.41652500	3.33340000
C	4.25806600	2.39429100	2.60005400
C	3.15051000	3.05835800	2.07431800
C	2.60473800	2.68944000	0.83344500
C	3.21685900	1.66049200	0.09423800
C	5.85182800	0.46313000	-1.28919800
C	7.07527300	1.14246600	-1.20749900
C	7.64307500	1.73615800	-2.33591200
C	6.99786700	1.66642100	-3.57074000
C	5.77648900	0.99840900	-3.66416100
C	5.21064200	0.40394800	-2.53587300
H	-8.59498400	-2.25306000	-2.24594400
H	-7.59110700	-1.20973700	-0.25537700
H	-4.26522200	0.12171000	-2.62796700
H	-5.26029600	-0.93317900	-4.61866400
H	-7.38897800	2.02391300	0.35639500
H	-8.80750700	2.13240400	2.37454800
H	-8.42025500	0.58784200	4.27539100
H	-6.59275000	-1.09413700	4.16673500
H	-4.65620200	-2.68215900	3.56958700
H	-2.67900000	-3.85771200	2.63985400
H	-2.81431500	-1.39826000	-0.88040600
H	-4.95093700	4.45521300	-1.86662100
H	-6.05920400	2.31683000	-1.37826100
H	-2.50096200	0.78781300	0.49488000
H	0.14310700	1.60472500	0.68662900
H	2.31384300	5.22429500	-0.13032600
H	0.27583900	6.30244200	-1.04419100
H	4.95091200	-4.45486800	-1.86770200
H	6.05919100	-2.31659000	-1.37893100
H	2.50094300	-0.78789800	0.49446900
H	-0.14310500	-1.60487600	0.68616500
H	-2.31383900	-5.22430400	-0.13142600
H	-0.27586100	-6.30225000	-1.04558300
H	7.38901900	-2.02395400	0.35548300
H	8.80766700	-2.13294700	2.37352800
H	8.42049400	-0.58888800	4.27479700
H	6.59296000	1.09309300	4.16668100
H	4.65635600	2.68125300	3.57004200
H	2.67910300	3.85703400	2.64070200
H	2.81426300	1.39848200	-0.88019100
H	7.59133300	1.20928200	-0.25551300
H	8.59514800	2.25316500	-2.24581800
H	5.25980100	0.93498700	-4.61855700

H	4.26478500	-0.12046000	-2.62812600
H	-2.44149900	5.75654100	-1.60995200
H	2.44149300	-5.75627200	-1.61119700
H	7.44189800	2.12571200	-4.44999200
H	-7.44209200	-2.12447500	-4.45024000

Coordinates of geometry optimized structure of a4

C	5.50390900	0.09804800	4.46740000
C	5.52439700	1.25120600	3.68025700
C	5.35103700	1.16457800	2.29990300
C	5.14757700	-0.07461800	1.67281600
C	5.13528500	-1.22511800	2.47280200
C	5.31185800	-1.13975000	3.85618500
C	5.20868300	1.72089700	-1.40215800
C	4.35484000	1.08435300	-0.48097900
C	5.03641700	-0.15881300	0.13163300
C	6.44344200	-0.03386900	-0.48412000
C	6.49852900	1.02450700	-1.41033200
C	7.58549900	-0.77773600	-0.20500200
C	8.77186000	-0.49269400	-0.89118600
C	8.81531900	0.53569400	-1.83824500
C	7.68108800	1.30747000	-2.09755700
C	4.80232900	2.88799800	-2.05279500
C	3.55695700	3.43843200	-1.75252200
C	2.70573200	2.83680400	-0.80909400
C	3.11817500	1.64435700	-0.18471500
C	0.93941900	-3.30170500	-0.11813000
C	0.91019600	-4.63834600	-0.59690500
N	2.16663100	-4.95921800	-1.08799600
C	3.01496800	-3.87279700	-0.93646600
C	2.29745600	-2.82311900	-0.30630100
C	4.35066000	-3.71204500	-1.29518200
C	4.97298000	-2.50297000	-0.98408600
C	4.30775500	-1.45873600	-0.30858100
C	2.95703000	-1.63589600	0.01750300
C	-0.23601400	-2.72099500	0.36609400
C	-1.42088300	-3.46646400	0.40375000
C	-1.40077400	-4.81342700	-0.02610900
C	-0.25123000	-5.41016100	-0.53455700
C	-0.93942300	3.30166400	0.11819400
C	-0.91019700	4.63830100	0.59698200
N	-2.16660300	4.95913300	1.08816800
C	-3.01496700	3.87274700	0.93654800
C	-2.29746100	2.82308000	0.30636000
C	-4.35066500	3.71199900	1.29524500
C	-4.97299000	2.50293500	0.98411800
C	-4.30776300	1.45870300	0.30860900
C	-2.95703800	1.63586600	-0.01746800
C	0.23600500	2.72095600	-0.36604100
C	1.42086900	3.46643100	-0.40372100
C	1.40075800	4.81339700	0.02612800
C	0.25122400	5.41012300	0.53460700
C	-5.20871300	-1.72093200	1.40213300
C	-4.35485700	-1.08438900	0.48096500
C	-5.03642100	0.15878800	-0.13164100
C	-6.44346400	0.03382900	0.48407100
C	-6.49856300	-1.02454900	1.41028100
C	-7.58552700	0.77767300	0.20491400

C	-8.77190200	0.49261800	0.89106800
C	-8.81537100	-0.53576400	1.83813200
C	-7.68113700	-1.30752500	2.09747600
C	-4.80236800	-2.88803300	2.05277500
C	-3.55699000	-3.43846600	1.75252200
C	-2.70575100	-2.83683600	0.80910700
C	-3.11818500	-1.64439000	0.18472300
C	-5.14753800	0.07466300	-1.67282900
C	-5.13480100	1.22519400	-2.47275900
C	-5.31134000	1.13995500	-3.85615400
C	-5.50380400	-0.09774600	-4.46743500
C	-5.52473800	-1.25093400	-3.68034800
C	-5.35140800	-1.16443400	-2.29998100
H	5.67414800	2.22426600	4.14125700
H	5.37207200	2.07061500	1.70233500
H	4.97777400	-2.19649600	2.01627000
H	5.29290600	-2.04746900	4.45415300
H	7.56254100	-1.56444500	0.54436300
H	9.66748300	-1.07078400	-0.67989400
H	9.74292300	0.74675700	-2.36379100
H	7.72532000	2.12456200	-2.81320100
H	5.45565100	3.38013200	-2.76901000
H	3.23633700	4.35075500	-2.24845900
H	2.48178000	1.22116400	0.58552400
H	4.90296000	-4.50052300	-1.79953000
H	6.00992600	-2.37783800	-1.26930600
H	2.41613800	-0.86209100	0.54990500
H	-0.23837900	-1.69161600	0.71515600
H	-2.32548200	-5.38306200	-0.00013100
H	-0.26848500	-6.43689300	-0.89037200
H	-4.90296200	4.50046800	1.79960800
H	-6.00994000	2.37780600	1.26932700
H	-2.41614300	0.86206600	-0.54987400
H	0.23836800	1.69157700	-0.71510300
H	2.32546200	5.38303900	0.00013000
H	0.26848400	6.43685200	0.89043100
H	-7.56256200	1.56437500	-0.54445800
H	-9.66752800	1.07069200	0.67974700
H	-9.74298600	-0.74683800	2.36365400
H	-7.72537700	-2.12461600	2.81312000
H	-5.45570200	-3.38017000	2.76897700
H	-3.23637800	-4.35079000	2.24846000
H	-2.48177800	-1.22119600	-0.58550600
H	-4.97695900	2.19649400	-2.01617100
H	-5.29203500	2.04769500	-4.45407900
H	-5.67481700	-2.22391800	-4.14140100
H	-5.37279900	-2.07049100	-1.70246000
H	2.41716600	-5.83774400	-1.51378000
H	-2.41726900	5.83782400	1.51353400
H	-5.63457400	-0.16505300	-5.54425700
H	5.63470700	0.16545300	5.54421100

Coordinates of geometry optimized structure of a5

C	7.56108100	-1.33348600	-3.23661100
C	7.95011000	-1.61694800	-1.92648400
C	7.19076000	-1.15784600	-0.85027300
C	6.02799900	-0.40137700	-1.05821900
C	5.64444900	-0.12827400	-2.37915400

C	6.40253400	-0.58908000	-3.45723300
C	4.41191900	-1.51051900	1.85889500
C	4.21611400	-1.13091900	0.51870700
C	5.14246100	0.03564400	0.13169400
C	5.94399500	0.20386300	1.44713600
C	5.47551500	-0.68560800	2.43345300
C	7.00178300	1.05946000	1.74571500
C	7.56549900	1.04009400	3.02634200
C	7.08000700	0.17051100	4.00741500
C	6.03247800	-0.70252400	3.71402200
C	3.65119100	-2.53398000	2.42414300
C	2.66980700	-3.15204200	1.65021400
C	2.46311900	-2.78297000	0.31109800
C	3.27114500	-1.78427800	-0.26123800
C	0.99117900	3.18176100	-0.52523700
C	1.06900100	4.58552500	-0.74187000
N	2.39721100	4.95914800	-0.80755700
C	3.19660800	3.84295300	-0.64698000
C	2.37178000	2.70965300	-0.42861000
C	4.58639800	3.74099700	-0.70541600
C	5.15057300	2.49250600	-0.49542000
C	4.37671700	1.34847400	-0.18774100
C	2.98234700	1.46811100	-0.17066000
C	-0.27432000	2.57183000	-0.51387100
C	-1.43761700	3.34288000	-0.68659500
C	-1.30351500	4.74791000	-0.82173000
C	-0.07048200	5.37913800	-0.86202900
C	-1.09277400	-3.14051300	-0.82268900
C	-0.97533700	-4.03016800	-1.91966700
N	-2.23047400	-4.16622700	-2.50419700
C	-3.13142600	-3.32038900	-1.86532900
C	-2.46182000	-2.68327200	-0.79135000
C	-4.46444300	-3.02208800	-2.14384400
C	-5.09695200	-2.05148400	-1.36410600
C	-4.44453600	-1.38950400	-0.30225800
C	-3.12432400	-1.74007400	-0.00949000
C	0.03350300	-2.80025300	-0.07904800
C	1.28546900	-3.30063000	-0.44385000
C	1.38395400	-4.18245200	-1.54059200
C	0.26293300	-4.56906900	-2.27781000
C	-5.45187800	1.79089300	-0.88930100
C	-4.47373800	1.09417600	-0.15619500
C	-5.07922100	-0.19428800	0.45148500
C	-6.56327700	-0.00978300	0.09288400
C	-6.74606400	1.12626000	-0.71728200
C	-7.65001200	-0.79640400	0.45668100
C	-8.92525600	-0.45146600	-0.00660100
C	-9.10593700	0.67061500	-0.82240300
C	-8.01823000	1.46943700	-1.18123800
C	-5.10095400	2.93459300	-1.60655600
C	-3.78835000	3.39183500	-1.55374000
C	-2.80380500	2.75285800	-0.76845000
C	-3.17030000	1.57789200	-0.08035800
C	-4.92311100	-0.30413400	1.97924000
C	-4.96178200	-1.55185500	2.61949600
C	-4.90557800	-1.64729200	4.01093600
C	-4.80922900	-0.49574400	4.79238900
C	-4.77404500	0.75162900	4.16768300

C	-4.83286300	0.84551700	2.77702300
H	8.84987500	-2.19717300	-1.73773800
H	7.50679500	-1.38932900	0.16188900
H	4.75046400	0.45751500	-2.56764600
H	6.08476600	-0.36016500	-4.47138700
H	7.40741800	1.73543000	1.00085200
H	8.39158500	1.70760800	3.25660100
H	7.52563500	0.16859000	4.99861800
H	5.66102300	-1.38970400	4.46994700
H	3.80373800	-2.83665400	3.45705200
H	2.04270100	-3.92522800	2.08564900
H	3.11075800	-1.50010200	-1.29776700
H	5.20914800	4.60592300	-0.91802400
H	6.22632500	2.39419900	-0.58381300
H	2.36423900	0.60433600	0.04742600
H	-0.35175700	1.49183500	-0.41999500
H	-2.19822000	5.35772400	-0.88614100
H	0.00137700	6.45684400	-0.98266900
H	-4.99817400	-3.50362300	-2.95890500
H	-6.12267300	-1.79321000	-1.60070800
H	-2.60132600	-1.25940500	0.81160300
H	-0.04496700	-2.10648500	0.75373300
H	2.36051600	-4.56882100	-1.81935100
H	0.36333200	-5.24895400	-3.11970800
H	-7.51599800	-1.66386300	1.09722900
H	-9.78194800	-1.05822800	0.27430800
H	-10.10205000	0.92760300	-1.17309700
H	-8.16442700	2.34824000	-1.80430400
H	-5.83648300	3.46421900	-2.20697100
H	-3.51467900	4.25978400	-2.14468500
H	-2.43325100	1.07242000	0.53628400
H	-5.02315500	-2.45790900	2.02464300
H	-4.93310500	-2.62663000	4.48207500
H	-4.69867500	1.65825600	4.76265700
H	-4.80615500	1.82319900	2.30661400
H	2.72985700	5.89144400	-0.99767900
H	-2.41244000	-4.65046400	-3.36956800
H	-4.75960200	-0.56941700	5.87554500
H	8.15485900	-1.68804900	-4.07501800

Coordinates of geometry optimized structure of a6

C	8.06049600	-1.30346800	-2.50316800
C	8.30224700	-1.38122600	-1.13230100
C	7.35336300	-0.91641600	-0.21896300
C	6.14382800	-0.36051100	-0.65592900
C	5.91137500	-0.29157700	-2.03907500
C	6.85708600	-0.75664100	-2.95208900
C	4.17016000	-1.59060500	1.88116900
C	4.11473100	-1.13481000	0.55160200
C	5.04070400	0.07468400	0.34198200
C	5.57864000	0.27023200	1.77341400
C	5.07261700	-0.71880700	2.63945400
C	6.43909300	1.24831500	2.26058500
C	6.79976000	1.23042800	3.61281000
C	6.30082100	0.24419700	4.47001300
C	5.43166900	-0.73650000	3.98902600
C	3.40042500	-2.68458500	2.28059900
C	2.53613200	-3.27685600	1.35938600

C	2.45054300	-2.80961700	0.03653200
C	3.28420900	-1.75379300	-0.37129900
C	0.95113400	3.18699700	-0.65437600
C	1.03894100	4.46011700	-1.28148200
N	2.36822100	4.77621100	-1.48128800
C	3.16010900	3.73069100	-1.04300800
C	2.32712900	2.70870400	-0.51516800
C	4.54702000	3.60065600	-1.09620400
C	5.10234500	2.41180200	-0.64486700
C	4.31381500	1.35323700	-0.13803600
C	2.92539300	1.52090300	-0.05930300
C	-0.31839400	2.68096400	-0.33120300
C	-1.48326100	3.40004200	-0.65984100
C	-1.33368400	4.64064600	-1.33107200
C	-0.09662300	5.18779300	-1.63086900
C	-1.01471700	-3.00726600	-1.34172300
C	-0.82347900	-3.61467100	-2.60608800
N	-2.03821600	-3.58286500	-3.28901200
C	-2.97432900	-2.87821000	-2.53368100
C	-2.37458000	-2.53460500	-1.29905700
C	-4.27807800	-2.46662200	-2.82026600
C	-4.94295500	-1.67770100	-1.87663100
C	-4.35270600	-1.31408900	-0.64770500
C	-3.06705200	-1.77618500	-0.36178000
C	0.05438700	-2.84735100	-0.46742000
C	1.33733000	-3.23499300	-0.85922900
C	1.51291500	-3.84565700	-2.12019800
C	0.44357100	-4.06102500	-2.99405400
C	-5.52644200	2.01970800	-0.04551200
C	-4.45574300	1.11164700	0.03995100
C	-4.98556500	-0.31169100	0.32768100
C	-6.50172200	-0.08919500	0.18122500
C	-6.78924500	1.28163600	0.03223500
C	-7.53510900	-1.01736900	0.24642400
C	-8.85914000	-0.57235500	0.15364700
C	-9.14394000	0.78969200	0.01221200
C	-8.11055400	1.72662000	-0.04853300
C	-5.26533300	3.38007000	-0.20764400
C	-3.94805300	3.80897900	-0.33935400
C	-2.86104400	2.90671300	-0.36432000
C	-3.14573000	1.54124300	-0.14508000
C	-4.74197800	-0.72869700	1.80411600
C	-4.92241900	-2.06702600	2.18993300
C	-4.78214100	-2.45796300	3.52033400
C	-4.45676900	-1.51768800	4.50008500
C	-4.27507800	-0.18621400	4.13070000
C	-4.41711600	0.20442400	2.79672400
H	9.23401500	-1.80408300	-0.76514600
H	7.55998400	-0.98857000	0.84340600
H	4.98688600	0.14297100	-2.40632100
H	6.65192900	-0.68776300	-4.01750000
H	6.82771900	2.02359200	1.60688100
H	7.47160900	1.99217400	3.99930700
H	6.58806700	0.24386900	5.51817900
H	5.03864900	-1.49799900	4.65789900
H	3.44422700	-3.05391000	3.30214500
H	1.89466500	-4.09714500	1.67013500
H	3.21072800	-1.38363000	-1.38975300

H	5.17427000	4.39192400	-1.49822000
H	6.17723200	2.28126500	-0.71647800
H	2.30517200	0.72101100	0.33182900
H	-0.39645000	1.72974800	0.18739000
H	-2.21625600	5.18018500	-1.65364900
H	-0.02012000	6.14282000	-2.14389000
H	-4.76170900	-2.72047600	-3.75980800
H	-5.94250900	-1.32340200	-2.10745900
H	-2.59315000	-1.52071700	0.58069100
H	-0.08804100	-2.34858700	0.48724300
H	2.51118200	-4.14961800	-2.42356300
H	0.60943300	-4.52947100	-3.96058900
H	-7.32470100	-2.07608400	0.36856000
H	-9.67197900	-1.29244200	0.19533300
H	-10.17696100	1.12104400	-0.05315400
H	-8.33418900	2.78423000	-0.16343600
H	-6.07488400	4.10530800	-0.23343800
H	-3.76406100	4.87388500	-0.42815100
H	-2.34048700	0.81427800	-0.16527000
H	-5.15842600	-2.81447600	1.43849400
H	-4.92385200	-3.50150600	3.79011500
H	-4.01798500	0.55840300	4.87977700
H	-4.27029100	1.24574400	2.53211400
H	2.70466000	5.60411400	-1.94759900
H	-2.15578800	-3.83096100	-4.25922600
H	-4.34304800	-1.82185100	5.53721400
H	8.80035900	-1.66222600	-3.21382800

Löwdin population analysis

Population of atoms for a1

Atom	Alpha pop.	Beta pop.	Spin pop.	Atomic charge
1(C)	3.08060	3.07822	0.00237	-0.15882
2(C)	3.08002	3.07813	0.00189	-0.15815
3(C)	3.08423	3.08321	0.00102	-0.16744
4(C)	3.00272	2.99535	0.00737	0.00194
5(C)	3.08537	3.08016	0.00521	-0.16553
6(C)	3.07892	3.07836	0.00056	-0.15728
7(C)	3.17175	2.84324	0.32851	-0.01499
8(C)	3.04272	2.94878	0.09394	0.00850
9(C)	2.98746	2.99453	-0.00707	0.01800
10(C)	3.07336	2.91824	0.15511	0.00840
11(C)	3.03956	2.97806	0.06150	-0.01763
12(C)	3.05542	3.11117	-0.05575	-0.16659
13(C)	3.21070	2.95831	0.25239	-0.16901
14(C)	3.04704	3.10271	-0.05567	-0.14976
15(C)	3.17055	3.00043	0.17012	-0.17098
16(C)	3.14092	3.03151	0.10941	-0.17244
17(C)	3.10934	3.03840	0.07094	-0.14774
18(C)	3.18634	2.83096	0.35538	-0.01730
19(C)	3.12081	3.05546	0.06535	-0.17627
20(C)	3.01651	3.01647	0.00004	-0.03298
21(C)	2.97568	2.97584	-0.00017	0.04848
22(N)	3.61036	3.60957	0.00079	-0.21993
23(C)	2.97765	2.97556	0.00209	0.04679
24(C)	3.01718	3.01655	0.00063	-0.03373

25(C)	3.09607	3.09665	-0.00058	-0.19272
26(C)	3.08211	3.07772	0.00439	-0.15984
27(C)	3.01019	3.00458	0.00562	-0.01477
28(C)	3.08046	3.07946	0.00101	-0.15992
29(C)	3.07756	3.07717	0.00039	-0.15473
30(C)	3.01019	3.00988	0.00031	-0.02007
31(C)	3.07879	3.07892	-0.00013	-0.15770
32(C)	3.09477	3.09438	0.00038	-0.18915
33(C)	3.00161	3.02474	-0.02313	-0.02635
34(C)	3.03531	2.92093	0.11438	0.04376
35(N)	3.63041	3.57574	0.05467	-0.20615
36(C)	2.97337	2.98214	-0.00877	0.04449
37(C)	3.02603	3.00612	0.01991	-0.03215
38(C)	3.10191	3.08599	0.01591	-0.18790
39(C)	3.07448	3.08442	-0.00993	-0.15890
40(C)	3.01426	2.99696	0.01730	-0.01122
41(C)	3.07517	3.08157	-0.00640	-0.15674
42(C)	3.16367	2.99872	0.16495	-0.16239
43(C)	3.02620	2.98204	0.04416	-0.00825
44(C)	3.11696	3.03605	0.08091	-0.15301
45(C)	3.08298	3.10081	-0.01782	-0.18379
46(C)	3.00836	3.00761	0.00076	-0.01597
47(C)	2.99978	2.99879	0.00099	0.00143
48(C)	2.99128	2.99167	-0.00039	0.01704
49(C)	3.00061	3.00026	0.00035	-0.00086
50(C)	3.00469	3.00479	-0.00010	-0.00948
51(C)	3.07907	3.07919	-0.00012	-0.15826
52(C)	3.08068	3.08039	0.00029	-0.16107
53(C)	3.07670	3.07681	-0.00011	-0.15351
54(C)	3.08126	3.08102	0.00024	-0.16228
55(C)	3.08098	3.08113	-0.00015	-0.16211
56(C)	3.08133	3.08066	0.00067	-0.16199
57(C)	2.99873	2.99879	-0.00007	0.00248
58(C)	3.08307	3.08301	0.00006	-0.16608
59(C)	2.99898	2.99856	0.00043	0.00246
60(C)	3.08222	3.08221	0.00001	-0.16443
61(C)	3.07759	3.07752	0.00007	-0.15511
62(C)	3.07864	3.07860	0.00004	-0.15723
63(C)	3.07804	3.07801	0.00003	-0.15604
64(C)	3.08443	3.08420	0.00022	-0.16863
65(H)	0.42235	0.42234	0.00001	0.15531
66(H)	0.41907	0.41905	0.00002	0.16189
67(H)	0.41730	0.41744	-0.00015	0.16526
68(H)	0.42163	0.42159	0.00004	0.15678
69(H)	0.42102	0.41950	0.00152	0.15948
70(H)	0.41743	0.42525	-0.00782	0.15733
71(H)	0.42330	0.42174	0.00157	0.15496
72(H)	0.41945	0.42490	-0.00544	0.15565
73(H)	0.41911	0.42274	-0.00363	0.15815
74(H)	0.42037	0.42272	-0.00235	0.15692
75(H)	0.42090	0.42080	0.00010	0.15830
76(H)	0.41748	0.41752	-0.00004	0.16500
77(H)	0.41919	0.41920	-0.00001	0.16161
78(H)	0.42126	0.42127	-0.00001	0.15748
79(H)	0.41973	0.42023	-0.00051	0.16004
80(H)	0.41665	0.41637	0.00028	0.16697
81(H)	0.41650	0.41630	0.00021	0.16720
82(H)	0.41565	0.42064	-0.00499	0.16371

83(H)	0.41748	0.42015	-0.00266	0.16237
84(H)	0.42057	0.41998	0.00059	0.15945
85(H)	0.41976	0.41976	-0.00000	0.16048
86(H)	0.42055	0.42056	-0.00001	0.15889
87(H)	0.42207	0.42207	0.00000	0.15586
88(H)	0.42151	0.42151	-0.00001	0.15698
89(H)	0.42108	0.42106	0.00002	0.15786
90(H)	0.42159	0.42161	-0.00002	0.15681
91(H)	0.41805	0.41801	0.00004	0.16394
92(H)	0.41673	0.41673	0.00000	0.16655
93(H)	0.42081	0.42081	0.00000	0.15838
94(H)	0.42178	0.42177	0.00000	0.15645
95(H)	0.41917	0.41914	0.00003	0.16168
96(H)	0.35218	0.35367	-0.00149	0.29416
97(H)	0.42229	0.42228	0.00000	0.15543
98(H)	0.42296	0.42301	-0.00005	0.15403
99(H)	0.41736	0.41954	-0.00217	0.16310
100(H)	0.35406	0.35408	-0.00002	0.29186
101(H)	0.41726	0.41703	0.00023	0.16572
102(H)	0.42021	0.42020	0.00000	0.15959

Total net charge: 0.00000006 Total spin electrons: 2.00000001

Population of atoms for b1

Atom	Alpha pop.	Beta pop.	Spin pop.	Atomic charge
1(C)	3.07761	3.07736	0.00025	-0.15497
2(C)	3.07740	3.07621	0.00119	-0.15361
3(C)	3.08422	3.08430	-0.00008	-0.16852
4(C)	3.00254	2.99844	0.00411	-0.00098
5(C)	3.08388	3.08216	0.00172	-0.16603
6(C)	3.07743	3.07691	0.00052	-0.15434
7(C)	3.06031	2.94752	0.11278	-0.00783
8(C)	3.01727	2.97788	0.03940	0.00485
9(C)	2.98903	2.99252	-0.00349	0.01845
10(C)	3.02558	2.97080	0.05478	0.00362
11(C)	3.03585	2.98011	0.05573	-0.01596
12(C)	3.07239	3.07550	-0.00310	-0.14789
13(C)	3.07660	2.95973	0.11687	-0.03632
14(C)	3.06117	3.07265	-0.01148	-0.13382
15(C)	3.11283	3.04979	0.06304	-0.16262
16(C)	3.10344	3.06502	0.03842	-0.16846
17(C)	3.09066	3.05750	0.03317	-0.14816
18(C)	3.06510	2.94616	0.11894	-0.01126
19(C)	3.09103	3.07745	0.01358	-0.16848
20(C)	3.01394	3.01115	0.00279	-0.02510
21(C)	2.99595	2.95582	0.04013	0.04823
22(N)	3.62777	3.56738	0.06039	-0.19514
23(C)	2.97520	2.98071	-0.00551	0.04410
24(C)	3.02417	3.00755	0.01662	-0.03172
25(C)	3.10090	3.07957	0.02133	-0.18047
26(C)	3.07659	3.08178	-0.00519	-0.15837
27(C)	3.01656	2.98933	0.02723	-0.00588
28(C)	3.07938	3.07328	0.00610	-0.15265
29(C)	3.11571	3.04021	0.07550	-0.15592
30(C)	3.02512	2.97750	0.04763	-0.00262
31(C)	3.08326	3.07029	0.01296	-0.15355
32(C)	3.09713	3.08188	0.01525	-0.17901
33(C)	3.01395	3.01115	0.00279	-0.02510
34(C)	2.99595	2.95582	0.04013	0.04823

35(N)	3.62777	3.56737	0.06039	-0.19514
36(C)	2.97520	2.98071	-0.00551	0.04410
37(C)	3.02417	3.00755	0.01662	-0.03172
38(C)	3.10090	3.07957	0.02133	-0.18047
39(C)	3.07659	3.08178	-0.00519	-0.15837
40(C)	3.01656	2.98933	0.02723	-0.00588
41(C)	3.07938	3.07328	0.00610	-0.15265
42(C)	3.11571	3.04021	0.07550	-0.15592
43(C)	3.02512	2.97750	0.04763	-0.00262
44(C)	3.08326	3.07029	0.01296	-0.15355
45(C)	3.09713	3.08188	0.01525	-0.17901
46(C)	3.06031	2.94752	0.11278	-0.00783
47(C)	3.01727	2.97788	0.03940	0.00485
48(C)	2.98903	2.99252	-0.00349	0.01845
49(C)	3.02558	2.97080	0.05478	0.00362
50(C)	3.03585	2.98011	0.05573	-0.01596
51(C)	3.07239	3.07550	-0.00310	-0.14789
52(C)	3.07660	2.95973	0.11687	-0.03632
53(C)	3.06117	3.07265	-0.01148	-0.13382
54(C)	3.11283	3.04979	0.06304	-0.16261
55(C)	3.10344	3.06502	0.03842	-0.16846
56(C)	3.09066	3.05750	0.03317	-0.14816
57(C)	3.06510	2.94616	0.11893	-0.01126
58(C)	3.09103	3.07745	0.01358	-0.16848
59(C)	3.00254	2.99844	0.00411	-0.00098
60(C)	3.08388	3.08216	0.00172	-0.16603
61(C)	3.07743	3.07691	0.00052	-0.15434
62(C)	3.07761	3.07736	0.00025	-0.15497
63(C)	3.07740	3.07621	0.00119	-0.15361
64(C)	3.08422	3.08430	-0.00008	-0.16852
65(H)	0.42059	0.42059	-0.00000	0.15882
66(H)	0.41889	0.41881	0.00008	0.16230
67(H)	0.41724	0.41726	-0.00002	0.16551
68(H)	0.42025	0.42023	0.00002	0.15952
69(H)	0.41439	0.41440	-0.00001	0.17121
70(H)	0.41523	0.41497	0.00025	0.16980
71(H)	0.41834	0.42039	-0.00205	0.16127
72(H)	0.41872	0.42008	-0.00136	0.16120
73(H)	0.41978	0.42080	-0.00102	0.15942
74(H)	0.41762	0.41820	-0.00058	0.16418
75(H)	0.41578	0.41593	-0.00015	0.16829
76(H)	0.41631	0.41857	-0.00226	0.16512
77(H)	0.41831	0.41878	-0.00047	0.16292
78(H)	0.41762	0.41820	-0.00058	0.16418
79(H)	0.41522	0.41483	0.00039	0.16995
80(H)	0.41578	0.41593	-0.00015	0.16829
81(H)	0.41631	0.41857	-0.00226	0.16512
82(H)	0.41741	0.41793	-0.00052	0.16467
83(H)	0.41831	0.41878	-0.00047	0.16292
84(H)	0.41439	0.41440	-0.00001	0.17121
85(H)	0.41523	0.41497	0.00025	0.16980
86(H)	0.41834	0.42039	-0.00205	0.16127
87(H)	0.41872	0.42008	-0.00136	0.16120
88(H)	0.41978	0.42080	-0.00102	0.15942
89(H)	0.41821	0.41868	-0.00047	0.16311
90(H)	0.41724	0.41726	-0.00002	0.16551
91(H)	0.42025	0.42023	0.00002	0.15952
92(H)	0.42059	0.42059	-0.00000	0.15882

93(H)	0.41889	0.41881	0.00008	0.16230
94(H)	0.35021	0.35184	-0.00163	0.29794
95(H)	0.42136	0.42136	-0.00000	0.15727
96(H)	0.42136	0.42136	-0.00000	0.15727
97(H)	0.41821	0.41868	-0.00047	0.16311
98(H)	0.35021	0.35184	-0.00163	0.29794
99(H)	0.41522	0.41483	0.00039	0.16995
100(H)	0.41741	0.41793	-0.00052	0.16467
101(C)	3.00539	3.01665	-0.01126	-0.02204
102(N)	3.60476	3.53526	0.06951	-0.14002
103(C)	3.00539	3.01665	-0.01126	-0.02204
104(N)	3.60476	3.53526	0.06951	-0.14002

Total net charge: 0.00000004 Total spin electrons: 1.99999998

Population of atoms for b2

Atom	Alpha pop.	Beta pop.	Spin pop.	Atomic charge
1(C)	3.07835	3.07731	0.00103	-0.15566
2(C)	3.07800	3.07712	0.00088	-0.15511
3(C)	3.08488	3.08452	0.00036	-0.16941
4(C)	3.00364	2.99736	0.00628	-0.00101
5(C)	3.08387	3.08142	0.00245	-0.16530
6(C)	3.07698	3.07701	-0.00003	-0.15399
7(C)	3.07483	2.93860	0.13623	-0.01343
8(C)	3.01508	2.98264	0.03244	0.00228
9(C)	2.98932	2.99327	-0.00395	0.01741
10(C)	3.03691	2.95443	0.08249	0.00866
11(C)	3.02377	2.99523	0.02854	-0.01900
12(C)	3.06377	3.09246	-0.02869	-0.15624
13(C)	3.14364	3.01299	0.13065	-0.15662
14(C)	3.00153	3.01769	-0.01617	-0.01922
15(C)	3.09884	3.04347	0.05537	-0.14231
16(C)	3.09506	3.07192	0.02314	-0.16699
17(C)	3.10017	3.04949	0.05068	-0.14966
18(C)	3.06731	2.94712	0.12019	-0.01443
19(C)	3.09503	3.07336	0.02167	-0.16839
20(C)	3.01295	3.01201	0.00094	-0.02496
21(C)	3.00100	2.95331	0.04769	0.04569
22(N)	3.62902	3.56466	0.06436	-0.19367
23(C)	2.97678	2.98079	-0.00402	0.04243
24(C)	3.02600	3.00566	0.02034	-0.03167
25(C)	3.10141	3.07956	0.02185	-0.18097
26(C)	3.07864	3.08203	-0.00339	-0.16068
27(C)	3.01893	2.98754	0.03138	-0.00647
28(C)	3.07875	3.07400	0.00475	-0.15275
29(C)	3.12766	3.03268	0.09498	-0.16034
30(C)	3.03160	2.97103	0.06057	-0.00264
31(C)	3.08137	3.07122	0.01015	-0.15259
32(C)	3.10071	3.07924	0.02147	-0.17995
33(C)	3.01295	3.01201	0.00094	-0.02496
34(C)	3.00100	2.95331	0.04769	0.04569
35(N)	3.62902	3.56466	0.06436	-0.19367
36(C)	2.97678	2.98079	-0.00402	0.04243
37(C)	3.02600	3.00566	0.02034	-0.03167
38(C)	3.10141	3.07956	0.02185	-0.18097
39(C)	3.07864	3.08203	-0.00339	-0.16068
40(C)	3.01893	2.98754	0.03138	-0.00647
41(C)	3.07875	3.07400	0.00475	-0.15275
42(C)	3.12766	3.03268	0.09498	-0.16034

43(C)	3.03160	2.97104	0.06057	-0.00264
44(C)	3.08137	3.07122	0.01015	-0.15259
45(C)	3.10071	3.07924	0.02147	-0.17995
46(C)	3.07483	2.93860	0.13623	-0.01343
47(C)	3.01508	2.98264	0.03244	0.00228
48(C)	2.98932	2.99327	-0.00395	0.01741
49(C)	3.03691	2.95443	0.08249	0.00866
50(C)	3.02377	2.99523	0.02854	-0.01900
51(C)	3.06377	3.09246	-0.02869	-0.15624
52(C)	3.14364	3.01299	0.13065	-0.15662
53(C)	3.00153	3.01769	-0.01617	-0.01922
54(C)	3.09884	3.04347	0.05537	-0.14231
55(C)	3.09506	3.07192	0.02314	-0.16699
56(C)	3.10017	3.04949	0.05068	-0.14966
57(C)	3.06731	2.94712	0.12019	-0.01443
58(C)	3.09503	3.07336	0.02168	-0.16839
59(C)	3.00364	2.99736	0.00628	-0.00101
60(C)	3.08387	3.08142	0.00245	-0.16530
61(C)	3.07698	3.07701	-0.00003	-0.15399
62(C)	3.07835	3.07731	0.00103	-0.15566
63(C)	3.07800	3.07712	0.00088	-0.15511
64(C)	3.08488	3.08452	0.00036	-0.16941
65(H)	0.42111	0.42108	0.00003	0.15781
66(H)	0.41940	0.41930	0.00010	0.16129
67(H)	0.41675	0.41678	-0.00003	0.16648
68(H)	0.42030	0.42025	0.00005	0.15945
69(H)	0.41774	0.41694	0.00080	0.16533
70(H)	0.41198	0.41604	-0.00407	0.17198
71(H)	0.41378	0.41559	-0.00181	0.17062
72(H)	0.41905	0.41995	-0.00090	0.16100
73(H)	0.41983	0.42139	-0.00156	0.15878
74(H)	0.41807	0.41865	-0.00058	0.16327
75(H)	0.41574	0.41584	-0.00010	0.16842
76(H)	0.41647	0.41931	-0.00285	0.16422
77(H)	0.41851	0.41917	-0.00067	0.16232
78(H)	0.41807	0.41865	-0.00058	0.16327
79(H)	0.41602	0.41572	0.00030	0.16827
80(H)	0.41574	0.41584	-0.00010	0.16842
81(H)	0.41647	0.41931	-0.00285	0.16422
82(H)	0.41761	0.41808	-0.00047	0.16431
83(H)	0.41851	0.41917	-0.00067	0.16232
84(H)	0.41774	0.41694	0.00080	0.16533
85(H)	0.41198	0.41604	-0.00407	0.17198
86(H)	0.41378	0.41559	-0.00181	0.17062
87(H)	0.41905	0.41995	-0.00090	0.16100
88(H)	0.41983	0.42139	-0.00156	0.15878
89(H)	0.41843	0.41908	-0.00066	0.16249
90(H)	0.41675	0.41678	-0.00003	0.16648
91(H)	0.42030	0.42025	0.00005	0.15945
92(H)	0.42111	0.42108	0.00003	0.15781
93(H)	0.41940	0.41930	0.00010	0.16129
94(H)	0.35044	0.35215	-0.00172	0.29741
95(H)	0.42153	0.42156	-0.00003	0.15691
96(H)	0.42153	0.42156	-0.00003	0.15691
97(H)	0.41843	0.41908	-0.00066	0.16249
98(H)	0.35044	0.35215	-0.00172	0.29741
99(H)	0.41602	0.41572	0.00030	0.16827
100(H)	0.41761	0.41808	-0.00047	0.16431

101(C)	3.00913	3.00537	0.00376	-0.01449
102(N)	3.56233	3.56656	-0.00424	-0.12889
103(C)	3.00913	3.00537	0.00376	-0.01449
104(N)	3.56233	3.56656	-0.00424	-0.12889

Total net charge: 0.00000004 Total spin electrons: 2.00000002

Population of atoms for b3

Atom	Alpha pop.	Beta pop.	Spin pop.	Atomic charge
1(C)	3.07779	3.07785	-0.00006	-0.15564
2(C)	3.07732	3.07722	0.00010	-0.15453
3(C)	3.08409	3.08369	0.00041	-0.16778
4(C)	2.99997	2.99913	0.00084	0.00090
5(C)	3.08266	3.08255	0.00011	-0.16520
6(C)	3.07724	3.07707	0.00017	-0.15430
7(C)	3.03688	2.96330	0.07358	-0.00018
8(C)	2.99689	2.99484	0.00204	0.00827
9(C)	2.99056	2.99209	-0.00153	0.01735
10(C)	3.01216	2.98101	0.03115	0.00684
11(C)	3.00596	3.00418	0.00178	-0.01014
12(C)	3.07267	3.08498	-0.01230	-0.15765
13(C)	3.10027	3.05282	0.04745	-0.15309
14(C)	3.06912	3.08031	-0.01119	-0.14942
15(C)	3.09576	3.06269	0.03307	-0.15845
16(C)	3.08416	3.07934	0.00483	-0.16350
17(C)	3.09181	3.05276	0.03905	-0.14457
18(C)	3.01693	2.97750	0.03942	0.00557
19(C)	3.09695	3.06907	0.02787	-0.16602
20(C)	3.02513	3.00760	0.01754	-0.03273
21(C)	2.98377	2.95379	0.02999	0.06244
22(N)	3.62777	3.54620	0.08156	-0.17397
23(C)	2.98018	2.97665	0.00353	0.04317
24(C)	3.03497	2.99695	0.03802	-0.03193
25(C)	3.10349	3.07402	0.02947	-0.17751
26(C)	3.09952	3.07429	0.02523	-0.17380
27(C)	3.01475	2.98660	0.02814	-0.00135
28(C)	3.09690	3.06661	0.03029	-0.16351
29(C)	3.19956	2.98739	0.21217	-0.18694
30(C)	3.02606	2.96935	0.05671	0.00459
31(C)	3.09188	3.05828	0.03361	-0.15016
32(C)	3.07749	2.98492	0.09256	-0.06241
33(C)	3.02513	3.00759	0.01754	-0.03273
34(C)	2.98377	2.95379	0.02999	0.06244
35(N)	3.62777	3.54620	0.08156	-0.17397
36(C)	2.98018	2.97665	0.00353	0.04317
37(C)	3.03497	2.99695	0.03802	-0.03193
38(C)	3.10349	3.07402	0.02947	-0.17751
39(C)	3.09952	3.07429	0.02523	-0.17380
40(C)	3.01475	2.98660	0.02814	-0.00135
41(C)	3.09690	3.06661	0.03029	-0.16351
42(C)	3.19956	2.98739	0.21217	-0.18694
43(C)	3.02606	2.96935	0.05671	0.00459
44(C)	3.09189	3.05828	0.03361	-0.15016
45(C)	3.07749	2.98492	0.09256	-0.06241
46(C)	3.03688	2.96330	0.07358	-0.00018
47(C)	2.99689	2.99484	0.00204	0.00827
48(C)	2.99056	2.99209	-0.00153	0.01735
49(C)	3.01216	2.98101	0.03115	0.00684
50(C)	3.00596	3.00418	0.00178	-0.01014

51(C)	3.07267	3.08498	-0.01231	-0.15765
52(C)	3.10027	3.05282	0.04745	-0.15309
53(C)	3.06912	3.08031	-0.01119	-0.14942
54(C)	3.09576	3.06269	0.03307	-0.15845
55(C)	3.08416	3.07934	0.00483	-0.16350
56(C)	3.09181	3.05276	0.03905	-0.14457
57(C)	3.01693	2.97750	0.03943	0.00557
58(C)	3.09695	3.06907	0.02788	-0.16602
59(C)	2.99997	2.99913	0.00084	0.00090
60(C)	3.08266	3.08254	0.00011	-0.16520
61(C)	3.07724	3.07707	0.00017	-0.15430
62(C)	3.07779	3.07785	-0.00006	-0.15564
63(C)	3.07731	3.07722	0.00010	-0.15453
64(C)	3.08410	3.08369	0.00041	-0.16778
65(H)	0.42091	0.42091	-0.00000	0.15818
66(H)	0.41861	0.41856	0.00005	0.16283
67(H)	0.41734	0.41734	-0.00000	0.16531
68(H)	0.42028	0.42028	-0.00001	0.15944
69(H)	0.41857	0.41819	0.00037	0.16324
70(H)	0.41802	0.41945	-0.00143	0.16253
71(H)	0.42046	0.42015	0.00032	0.15939
72(H)	0.41946	0.42050	-0.00104	0.16003
73(H)	0.41860	0.41886	-0.00026	0.16255
74(H)	0.41798	0.41884	-0.00086	0.16317
75(H)	0.41722	0.41810	-0.00088	0.16468
76(H)	0.41598	0.41692	-0.00094	0.16711
77(H)	0.41584	0.42217	-0.00634	0.16199
78(H)	0.41722	0.41810	-0.00088	0.16468
79(H)	0.41632	0.41717	-0.00085	0.16650
80(H)	0.41598	0.41692	-0.00094	0.16711
81(H)	0.41584	0.42217	-0.00634	0.16199
82(H)	0.41337	0.41456	-0.00119	0.17207
83(H)	0.41857	0.41819	0.00037	0.16324
84(H)	0.41802	0.41945	-0.00143	0.16253
85(H)	0.42046	0.42015	0.00032	0.15939
86(H)	0.41946	0.42050	-0.00104	0.16003
87(H)	0.41860	0.41886	-0.00026	0.16255
88(H)	0.41799	0.41884	-0.00086	0.16317
89(H)	0.41719	0.41645	0.00073	0.16636
90(H)	0.41734	0.41734	-0.00000	0.16531
91(H)	0.42028	0.42028	-0.00001	0.15944
92(H)	0.42091	0.42091	-0.00000	0.15818
93(H)	0.41861	0.41856	0.00005	0.16283
94(H)	0.34555	0.34777	-0.00222	0.30667
95(H)	0.42158	0.42158	0.00000	0.15684
96(H)	0.42158	0.42158	0.00000	0.15684
97(H)	0.41719	0.41645	0.00073	0.16636
98(H)	0.34555	0.34777	-0.00222	0.30667
99(H)	0.41632	0.41717	-0.00085	0.16650
100(H)	0.41337	0.41456	-0.00119	0.17207
101(C)	3.01320	3.01645	-0.00325	-0.02966
102(N)	3.60289	3.54069	0.06220	-0.14358
103(C)	3.01320	3.01645	-0.00325	-0.02965
104(N)	3.60289	3.54069	0.06220	-0.14358
Total net charge:	0.00000007		Total spin electrons:	2.00000000

Population of atoms for b4

Atom	Alpha pop.	Beta pop.	Spin pop.	Atomic charge

1(C)	3.07789	3.07834	-0.00046	-0.15623
2(C)	3.07881	3.07682	0.00199	-0.15562
3(C)	3.08346	3.08338	0.00008	-0.16683
4(C)	3.00089	2.99794	0.00295	0.00116
5(C)	3.08373	3.08327	0.00046	-0.16701
6(C)	3.07818	3.07656	0.00162	-0.15474
7(C)	3.03787	2.96263	0.07525	-0.00050
8(C)	3.00706	2.99001	0.01705	0.00294
9(C)	2.99059	2.99220	-0.00161	0.01721
10(C)	3.01445	2.97969	0.03477	0.00586
11(C)	3.00461	3.00333	0.00128	-0.00794
12(C)	3.07157	3.08562	-0.01405	-0.15718
13(C)	3.09529	3.05550	0.03979	-0.15079
14(C)	3.07064	3.07917	-0.00853	-0.14981
15(C)	3.08937	3.06527	0.02410	-0.15464
16(C)	3.07074	3.08509	-0.01435	-0.15583
17(C)	3.09804	3.04152	0.05652	-0.13956
18(C)	3.01381	2.98172	0.03209	0.00447
19(C)	3.08385	3.07575	0.00810	-0.15959
20(C)	3.06385	2.97580	0.08805	-0.03965
21(C)	2.99033	2.95993	0.03039	0.04974
22(N)	3.63980	3.54469	0.09511	-0.18448
23(C)	2.97117	2.98158	-0.01042	0.04725
24(C)	3.01749	3.01276	0.00473	-0.03025
25(C)	3.12373	3.06339	0.06034	-0.18712
26(C)	3.09678	3.07132	0.02546	-0.16810
27(C)	3.01537	2.98639	0.02898	-0.00176
28(C)	3.13249	3.04161	0.09088	-0.17410
29(C)	3.08494	3.06581	0.01913	-0.15076
30(C)	3.02917	2.95751	0.07166	0.01331
31(C)	3.08127	2.97598	0.10530	-0.05725
32(C)	3.12522	3.04614	0.07907	-0.17136
33(C)	3.06385	2.97580	0.08804	-0.03965
34(C)	2.99033	2.95993	0.03040	0.04974
35(N)	3.63980	3.54469	0.09511	-0.18448
36(C)	2.97117	2.98158	-0.01042	0.04725
37(C)	3.01748	3.01276	0.00472	-0.03025
38(C)	3.12373	3.06339	0.06033	-0.18712
39(C)	3.09678	3.07132	0.02546	-0.16810
40(C)	3.01537	2.98639	0.02898	-0.00176
41(C)	3.13248	3.04162	0.09087	-0.17410
42(C)	3.08494	3.06581	0.01913	-0.15076
43(C)	3.02917	2.95751	0.07166	0.01331
44(C)	3.08127	2.97598	0.10530	-0.05725
45(C)	3.12521	3.04614	0.07907	-0.17136
46(C)	3.03787	2.96263	0.07524	-0.00050
47(C)	3.00705	2.99001	0.01705	0.00294
48(C)	2.99059	2.99220	-0.00161	0.01721
49(C)	3.01445	2.97969	0.03476	0.00586
50(C)	3.00461	3.00333	0.00128	-0.00794
51(C)	3.07157	3.08562	-0.01405	-0.15718
52(C)	3.09529	3.05550	0.03979	-0.15080
53(C)	3.07064	3.07917	-0.00853	-0.14981
54(C)	3.08937	3.06527	0.02410	-0.15464
55(C)	3.07074	3.08509	-0.01435	-0.15583
56(C)	3.09803	3.04152	0.05651	-0.13956
57(C)	3.01381	2.98173	0.03208	0.00447
58(C)	3.08385	3.07575	0.00810	-0.15960

59(C)	3.00089	2.99794	0.00295	0.00117
60(C)	3.08374	3.08328	0.00046	-0.16702
61(C)	3.07818	3.07656	0.00161	-0.15474
62(C)	3.07789	3.07834	-0.00045	-0.15623
63(C)	3.07880	3.07682	0.00199	-0.15562
64(C)	3.08345	3.08337	0.00008	-0.16682
65(H)	0.42112	0.42114	-0.00003	0.15774
66(H)	0.41921	0.41909	0.00012	0.16170
67(H)	0.41719	0.41721	-0.00002	0.16561
68(H)	0.42047	0.42051	-0.00003	0.15902
69(H)	0.41887	0.41837	0.00051	0.16276
70(H)	0.41823	0.41943	-0.00119	0.16234
71(H)	0.42047	0.42023	0.00024	0.15929
72(H)	0.41872	0.41948	-0.00076	0.16180
73(H)	0.41793	0.41756	0.00036	0.16451
74(H)	0.41072	0.41239	-0.00166	0.17689
75(H)	0.41777	0.41959	-0.00182	0.16264
76(H)	0.41534	0.41806	-0.00272	0.16660
77(H)	0.41631	0.41700	-0.00069	0.16669
78(H)	0.41261	0.41510	-0.00249	0.17229
79(H)	0.41777	0.41959	-0.00182	0.16264
80(H)	0.41664	0.41749	-0.00085	0.16587
81(H)	0.41534	0.41806	-0.00272	0.16660
82(H)	0.41631	0.41700	-0.00069	0.16669
83(H)	0.41261	0.41510	-0.00248	0.17229
84(H)	0.41888	0.41837	0.00051	0.16275
85(H)	0.41823	0.41943	-0.00119	0.16234
86(H)	0.42047	0.42023	0.00024	0.15929
87(H)	0.41872	0.41948	-0.00076	0.16180
88(H)	0.41793	0.41756	0.00036	0.16451
89(H)	0.41072	0.41239	-0.00166	0.17689
90(H)	0.41709	0.41622	0.00087	0.16669
91(H)	0.41719	0.41720	-0.00002	0.16561
92(H)	0.42047	0.42051	-0.00003	0.15902
93(H)	0.42112	0.42114	-0.00003	0.15774
94(H)	0.41921	0.41909	0.00012	0.16169
95(H)	0.34902	0.35159	-0.00257	0.29939
96(H)	0.42169	0.42168	0.00001	0.15663
97(H)	0.42169	0.42168	0.00001	0.15663
98(H)	0.41709	0.41622	0.00087	0.16669
99(H)	0.34902	0.35159	-0.00257	0.29939
100(H)	0.41664	0.41749	-0.00085	0.16587
101(C)	3.01463	3.01523	-0.00060	-0.02986
102(N)	3.61354	3.54588	0.06765	-0.15942
103(C)	3.01463	3.01523	-0.00060	-0.02986
104(N)	3.61354	3.54588	0.06766	-0.15942

Total net charge: 0.00000005 Total spin electrons: 2.00000001

Population of atoms for b5

Atom	Alpha pop.	Beta pop.	Spin pop.	Atomic charge
1(C)	3.07808	3.07831	-0.00023	-0.15639
2(C)	3.07829	3.07707	0.00122	-0.15536
3(C)	3.08424	3.08423	0.00001	-0.16847
4(C)	3.00559	2.99541	0.01018	-0.00100
5(C)	3.08353	3.08241	0.00112	-0.16594
6(C)	3.07753	3.07683	0.00070	-0.15436
7(C)	3.06963	2.94733	0.12230	-0.01696
8(C)	3.05044	2.95671	0.09373	-0.00715

9(C)	2.98930	2.99361	-0.00431	0.01709
10(C)	3.02709	2.97067	0.05642	0.00225
11(C)	3.01005	2.99947	0.01057	-0.00952
12(C)	3.06733	3.09136	-0.02403	-0.15870
13(C)	3.11704	3.04007	0.07697	-0.15711
14(C)	3.06736	3.08229	-0.01492	-0.14965
15(C)	3.10197	3.05702	0.04495	-0.15900
16(C)	3.05374	3.07955	-0.02581	-0.13330
17(C)	3.06857	2.96665	0.10192	-0.03522
18(C)	3.07683	2.93484	0.14200	-0.01167
19(C)	3.07027	3.08658	-0.01631	-0.15685
20(C)	3.01606	3.01054	0.00552	-0.02660
21(C)	3.00478	2.95058	0.05420	0.04463
22(N)	3.62899	3.56107	0.06791	-0.19006
23(C)	2.97801	2.98081	-0.00280	0.04119
24(C)	3.02144	3.00778	0.01366	-0.02922
25(C)	3.10393	3.07644	0.02749	-0.18037
26(C)	3.07427	3.08385	-0.00958	-0.15811
27(C)	3.02285	2.98485	0.03801	-0.00770
28(C)	3.08322	3.07225	0.01097	-0.15547
29(C)	3.11166	3.04127	0.07039	-0.15293
30(C)	3.03120	2.97054	0.06066	-0.00175
31(C)	3.08478	3.06234	0.02244	-0.14712
32(C)	3.09525	3.07931	0.01593	-0.17456
33(C)	3.01606	3.01054	0.00551	-0.02660
34(C)	3.00478	2.95058	0.05420	0.04464
35(N)	3.62899	3.56108	0.06791	-0.19006
36(C)	2.97801	2.98080	-0.00280	0.04119
37(C)	3.02144	3.00778	0.01366	-0.02922
38(C)	3.10393	3.07644	0.02749	-0.18037
39(C)	3.07427	3.08384	-0.00958	-0.15811
40(C)	3.02285	2.98485	0.03800	-0.00770
41(C)	3.08322	3.07225	0.01097	-0.15547
42(C)	3.11167	3.04127	0.07040	-0.15293
43(C)	3.03120	2.97054	0.06066	-0.00174
44(C)	3.08478	3.06234	0.02243	-0.14712
45(C)	3.09525	3.07931	0.01593	-0.17456
46(C)	3.06963	2.94733	0.12229	-0.01696
47(C)	3.05042	2.95672	0.09370	-0.00715
48(C)	2.98930	2.99361	-0.00431	0.01709
49(C)	3.02708	2.97067	0.05642	0.00225
50(C)	3.01005	2.99948	0.01057	-0.00952
51(C)	3.06734	3.09136	-0.02403	-0.15870
52(C)	3.11703	3.04007	0.07696	-0.15711
53(C)	3.06736	3.08229	-0.01492	-0.14965
54(C)	3.10197	3.05702	0.04495	-0.15900
55(C)	3.05375	3.07955	-0.02581	-0.13330
56(C)	3.06856	2.96665	0.10191	-0.03522
57(C)	3.07682	2.93485	0.14197	-0.01167
58(C)	3.07027	3.08657	-0.01630	-0.15685
59(C)	3.00559	2.99541	0.01018	-0.00100
60(C)	3.08353	3.08241	0.00112	-0.16594
61(C)	3.07753	3.07683	0.00070	-0.15436
62(C)	3.07808	3.07831	-0.00023	-0.15639
63(C)	3.07829	3.07707	0.00122	-0.15536
64(C)	3.08424	3.08423	0.00001	-0.16847
65(H)	0.42122	0.42112	0.00010	0.15766
66(H)	0.41966	0.41950	0.00016	0.16084

67(H)	0.41693	0.41692	0.00002	0.16615
68(H)	0.42040	0.42033	0.00006	0.15927
69(H)	0.41933	0.41867	0.00067	0.16200
70(H)	0.41834	0.42071	-0.00237	0.16095
71(H)	0.42108	0.42066	0.00042	0.15826
72(H)	0.41888	0.42035	-0.00146	0.16077
73(H)	0.41424	0.41361	0.00064	0.17215
74(H)	0.41818	0.41892	-0.00074	0.16290
75(H)	0.41536	0.41556	-0.00020	0.16908
76(H)	0.41637	0.41851	-0.00214	0.16513
77(H)	0.41756	0.41799	-0.00043	0.16445
78(H)	0.41818	0.41892	-0.00074	0.16290
79(H)	0.41631	0.41586	0.00045	0.16783
80(H)	0.41536	0.41556	-0.00020	0.16908
81(H)	0.41637	0.41851	-0.00214	0.16513
82(H)	0.41081	0.41168	-0.00087	0.17751
83(H)	0.41756	0.41799	-0.00043	0.16445
84(H)	0.41933	0.41867	0.00067	0.16200
85(H)	0.41834	0.42071	-0.00237	0.16095
86(H)	0.42108	0.42066	0.00042	0.15826
87(H)	0.41888	0.42035	-0.00146	0.16077
88(H)	0.41424	0.41361	0.00064	0.17215
89(H)	0.41692	0.41671	0.00021	0.16637
90(H)	0.41693	0.41692	0.00002	0.16615
91(H)	0.42040	0.42033	0.00006	0.15927
92(H)	0.42122	0.42112	0.00010	0.15766
93(H)	0.41966	0.41950	0.00016	0.16085
94(H)	0.35021	0.35206	-0.00185	0.29772
95(H)	0.42171	0.42169	0.00002	0.15660
96(H)	0.42171	0.42169	0.00002	0.15660
97(H)	0.41692	0.41671	0.00021	0.16637
98(H)	0.35021	0.35206	-0.00185	0.29772
99(H)	0.41631	0.41586	0.00045	0.16783
100(H)	0.41080	0.41168	-0.00087	0.17752
101(C)	3.00944	3.01489	-0.00545	-0.02433
102(N)	3.60375	3.54221	0.06153	-0.14596
103(C)	3.00944	3.01489	-0.00545	-0.02433
104(N)	3.60374	3.54222	0.06152	-0.14596

Total net charge: 0.00000002 Total spin electrons: 2.00000000

Population of atoms for c

Atom	Alpha pop.	Beta pop.	Spin pop.	Atomic charge
1(C)	3.07566	3.07519	0.00047	-0.15085
2(C)	3.07564	3.07464	0.00100	-0.15028
3(C)	3.08456	3.08422	0.00034	-0.16878
4(C)	3.00719	2.99823	0.00896	-0.00543
5(C)	3.08464	3.08284	0.00180	-0.16748
6(C)	3.07579	3.07540	0.00039	-0.15119
7(C)	3.05122	2.95895	0.09227	-0.01017
8(C)	3.02785	2.96678	0.06107	0.00536
9(C)	2.98867	2.99304	-0.00437	0.01829
10(C)	3.03225	2.96191	0.07034	0.00584
11(C)	3.03020	2.98485	0.04535	-0.01505
12(C)	3.05859	3.07670	-0.01811	-0.13529
13(C)	3.06652	2.95399	0.11252	-0.02051
14(C)	3.00701	2.99846	0.00855	-0.00548
15(C)	3.07695	3.05333	0.02362	-0.13028
16(C)	3.06537	3.06642	-0.00105	-0.13179

17(C)	3.03362	2.98552	0.04810	-0.01915
18(C)	3.05761	2.94625	0.11137	-0.00386
19(C)	3.07693	3.08126	-0.00433	-0.15819
20(C)	3.01848	3.00582	0.01266	-0.02430
21(C)	2.99170	2.95644	0.03525	0.05186
22(N)	3.63127	3.54887	0.08239	-0.18014
23(C)	2.97391	2.98124	-0.00734	0.04485
24(C)	3.02185	3.00640	0.01545	-0.02825
25(C)	3.10271	3.06849	0.03422	-0.17120
26(C)	3.07209	3.08318	-0.01109	-0.15528
27(C)	3.02295	2.98090	0.04205	-0.00384
28(C)	3.08171	3.07050	0.01121	-0.15221
29(C)	3.10201	3.04625	0.05576	-0.14826
30(C)	3.02917	2.96832	0.06086	0.00251
31(C)	3.07521	3.06831	0.00690	-0.14353
32(C)	3.09708	3.07032	0.02676	-0.16739
33(C)	3.01848	3.00581	0.01267	-0.02430
34(C)	2.99170	2.95644	0.03526	0.05186
35(N)	3.63127	3.54887	0.08241	-0.18014
36(C)	2.97391	2.98124	-0.00734	0.04485
37(C)	3.02185	3.00640	0.01545	-0.02825
38(C)	3.10271	3.06848	0.03423	-0.17120
39(C)	3.07209	3.08319	-0.01109	-0.15528
40(C)	3.02295	2.98089	0.04206	-0.00384
41(C)	3.08171	3.07050	0.01121	-0.15221
42(C)	3.10201	3.04625	0.05576	-0.14826
43(C)	3.02918	2.96831	0.06086	0.00251
44(C)	3.07521	3.06831	0.00690	-0.14353
45(C)	3.09708	3.07031	0.02676	-0.16739
46(C)	3.05122	2.95894	0.09228	-0.01016
47(C)	3.02787	2.96677	0.06109	0.00536
48(C)	2.98867	2.99304	-0.00438	0.01829
49(C)	3.03226	2.96190	0.07035	0.00584
50(C)	3.03021	2.98485	0.04536	-0.01505
51(C)	3.05859	3.07670	-0.01811	-0.13529
52(C)	3.06653	2.95399	0.11254	-0.02051
53(C)	3.00702	2.99846	0.00855	-0.00548
54(C)	3.07695	3.05333	0.02362	-0.13028
55(C)	3.06537	3.06642	-0.00105	-0.13179
56(C)	3.03363	2.98552	0.04811	-0.01915
57(C)	3.05763	2.94624	0.11139	-0.00386
58(C)	3.07693	3.08126	-0.00434	-0.15819
59(C)	3.00719	2.99823	0.00896	-0.00543
60(C)	3.08464	3.08284	0.00180	-0.16749
61(C)	3.07579	3.07540	0.00039	-0.15119
62(C)	3.07566	3.07519	0.00047	-0.15085
63(C)	3.07564	3.07464	0.00100	-0.15028
64(C)	3.08455	3.08422	0.00034	-0.16877
65(H)	0.41889	0.41882	0.00007	0.16228
66(H)	0.41882	0.41868	0.00013	0.16250
67(H)	0.41757	0.41754	0.00002	0.16489
68(H)	0.41865	0.41859	0.00006	0.16276
69(H)	0.41109	0.41063	0.00046	0.17828
70(H)	0.41033	0.41118	-0.00084	0.17849
71(H)	0.41045	0.41057	-0.00013	0.17898
72(H)	0.41480	0.41572	-0.00092	0.16948
73(H)	0.41448	0.41472	-0.00023	0.17080
74(H)	0.41545	0.41713	-0.00168	0.16741

75(H)	0.41451	0.41529	-0.00078	0.17020
76(H)	0.41480	0.41572	-0.00092	0.16948
77(H)	0.41479	0.41422	0.00058	0.17099
78(H)	0.41448	0.41472	-0.00023	0.17080
79(H)	0.41545	0.41713	-0.00168	0.16741
80(H)	0.40948	0.40983	-0.00034	0.18069
81(H)	0.41451	0.41529	-0.00078	0.17020
82(H)	0.41109	0.41064	0.00046	0.17827
83(H)	0.41033	0.41118	-0.00084	0.17849
84(H)	0.41045	0.41057	-0.00013	0.17898
85(H)	0.41579	0.41584	-0.00005	0.16837
86(H)	0.41757	0.41754	0.00002	0.16489
87(H)	0.41865	0.41859	0.00006	0.16276
88(H)	0.41889	0.41882	0.00007	0.16228
89(H)	0.41882	0.41869	0.00013	0.16249
90(H)	0.34746	0.34970	-0.00224	0.30284
91(H)	0.41951	0.41952	-0.00001	0.16097
92(H)	0.41951	0.41952	-0.00001	0.16097
93(H)	0.41579	0.41584	-0.00005	0.16838
94(H)	0.34746	0.34970	-0.00224	0.30284
95(H)	0.41479	0.41422	0.00058	0.17099
96(H)	0.40949	0.40983	-0.00034	0.18068
97(C)	3.00644	3.01147	-0.00503	-0.01791
98(N)	3.57330	3.54660	0.02670	-0.11989
99(C)	3.00797	3.00701	0.00096	-0.01498
100(N)	3.55368	3.54586	0.00782	-0.09954
101(C)	3.00366	3.01634	-0.01268	-0.02001
102(N)	3.58641	3.52173	0.06468	-0.10815
103(C)	3.00644	3.01148	-0.00503	-0.01792
104(N)	3.57330	3.54659	0.02671	-0.11989
105(C)	3.00797	3.00701	0.00096	-0.01498
106(N)	3.55368	3.54586	0.00782	-0.09954
107(C)	3.00366	3.01635	-0.01269	-0.02001
108(N)	3.58642	3.52173	0.06469	-0.10815

Total net charge: 0.00000010 Total spin electrons: 2.00000002

Population of atoms for d

Atom	Alpha pop.	Beta pop.	Spin pop.	Atomic charge
1(C)	3.07465	3.07435	0.00030	-0.14900
2(C)	3.07501	3.07432	0.00069	-0.14933
3(C)	3.08428	3.08293	0.00135	-0.16721
4(C)	3.00343	3.00099	0.00243	-0.00442
5(C)	3.08354	3.08381	-0.00027	-0.16735
6(C)	3.07604	3.07477	0.00127	-0.15081
7(C)	3.00627	3.00468	0.00159	-0.01096
8(C)	3.00067	2.99383	0.00684	0.00551
9(C)	2.99028	2.99153	-0.00126	0.01819
10(C)	2.99380	2.99175	0.00204	0.01445
11(C)	2.99599	2.99611	-0.00012	0.00790
12(C)	3.06467	3.06445	0.00022	-0.12912
13(C)	3.00274	3.00203	0.00071	-0.00477
14(C)	2.99815	2.99838	-0.00023	0.00348
15(C)	3.06585	3.06527	0.00058	-0.13112
16(C)	3.07338	3.07338	-0.00000	-0.14676
17(C)	3.07172	3.06949	0.00223	-0.14121
18(C)	2.99934	2.99976	-0.00042	0.00090
19(C)	3.08219	3.07932	0.00288	-0.16151
20(C)	3.08804	2.97948	0.10857	-0.06752

21(C)	2.96169	2.95828	0.00341	0.08003
22(N)	3.66563	3.44593	0.21970	-0.11157
23(C)	2.98940	2.97403	0.01537	0.03658
24(C)	3.03435	2.97734	0.05702	-0.01169
25(C)	3.11588	3.03868	0.07720	-0.15455
26(C)	3.11908	3.06665	0.05242	-0.18573
27(C)	3.02828	2.94786	0.08042	0.02387
28(C)	3.12812	3.05221	0.07590	-0.18033
29(C)	3.23917	2.94016	0.29901	-0.17934
30(C)	3.02156	2.91354	0.10802	0.06489
31(C)	3.13883	2.94882	0.19001	-0.08765
32(C)	3.18154	2.85489	0.32666	-0.03643
33(C)	3.00924	3.00924	-0.00000	-0.01848
34(C)	2.96642	2.96645	-0.00003	0.06713
35(N)	3.59819	3.59821	-0.00003	-0.19640
36(C)	2.97135	2.97146	-0.00011	0.05719
37(C)	3.01645	3.01640	0.00005	-0.03286
38(C)	3.08804	3.08792	0.00012	-0.17596
39(C)	3.07405	3.07411	-0.00006	-0.14816
40(C)	3.00707	3.00718	-0.00011	-0.01426
41(C)	3.07834	3.07856	-0.00022	-0.15690
42(C)	3.06874	3.06880	-0.00006	-0.13753
43(C)	2.99911	2.99901	0.00011	0.00188
44(C)	3.00347	3.00349	-0.00003	-0.00696
45(C)	3.01507	3.01505	0.00001	-0.03012
46(C)	3.02340	2.97532	0.04809	0.00128
47(C)	2.99290	3.00361	-0.01071	0.00349
48(C)	2.99068	2.99073	-0.00005	0.01858
49(C)	2.99870	2.98348	0.01522	0.01782
50(C)	2.99319	3.00054	-0.00735	0.00627
51(C)	3.06078	3.06818	-0.00740	-0.12896
52(C)	3.00857	2.99192	0.01665	-0.00049
53(C)	2.99507	3.00117	-0.00610	0.00376
54(C)	3.07106	3.05578	0.01528	-0.12683
55(C)	3.06585	3.08049	-0.01464	-0.14633
56(C)	3.08147	3.04273	0.03873	-0.12420
57(C)	2.99700	2.99142	0.00558	0.01159
58(C)	3.09254	3.05736	0.03519	-0.14990
59(C)	3.00248	3.00300	-0.00052	-0.00548
60(C)	3.08387	3.08374	0.00013	-0.16760
61(C)	3.07518	3.07515	0.00004	-0.15033
62(C)	3.07465	3.07429	0.00036	-0.14894
63(C)	3.07470	3.07487	-0.00017	-0.14957
64(C)	3.08424	3.08382	0.00042	-0.16806
65(H)	0.41807	0.41806	0.00001	0.16387
66(H)	0.41836	0.41825	0.00011	0.16340
67(H)	0.41689	0.41686	0.00003	0.16625
68(H)	0.41824	0.41827	-0.00003	0.16349
69(H)	0.40922	0.40913	0.00010	0.18165
70(H)	0.40887	0.40888	-0.00001	0.18225
71(H)	0.41458	0.41449	0.00009	0.17094
72(H)	0.41108	0.41113	-0.00005	0.17779
73(H)	0.41169	0.41400	-0.00230	0.17431
74(H)	0.41390	0.41624	-0.00234	0.16986
75(H)	0.41257	0.42139	-0.00883	0.16604
76(H)	0.41350	0.41350	-0.00000	0.17300
77(H)	0.41553	0.41552	0.00001	0.16895
78(H)	0.41514	0.41514	0.00000	0.16972

79(H)	0.41372	0.41372	0.00000	0.17257
80(H)	0.40875	0.40853	0.00021	0.18272
81(H)	0.40783	0.40830	-0.00046	0.18387
82(H)	0.41370	0.41316	0.00053	0.17314
83(H)	0.40625	0.40738	-0.00114	0.18637
84(H)	0.41474	0.41467	0.00007	0.17060
85(H)	0.41708	0.41711	-0.00003	0.16582
86(H)	0.41799	0.41799	-0.00001	0.16402
87(H)	0.41815	0.41815	0.00000	0.16370
88(H)	0.41835	0.41837	-0.00001	0.16328
89(H)	0.34494	0.34494	0.00000	0.31013
90(H)	0.41878	0.41879	-0.00001	0.16244
91(H)	0.41889	0.41890	-0.00000	0.16221
92(H)	0.41636	0.41585	0.00051	0.16779
93(H)	0.33783	0.34377	-0.00594	0.31840
94(H)	0.41489	0.41670	-0.00182	0.16841
95(C)	3.00665	3.00664	0.00001	-0.01329
96(N)	3.54726	3.54724	0.00002	-0.09451
97(C)	3.01092	3.02419	-0.01327	-0.03511
98(N)	3.62440	3.51863	0.10578	-0.14303
99(C)	3.00726	3.00726	-0.00000	-0.01452
100(N)	3.54658	3.54657	0.00001	-0.09315
101(C)	3.00685	3.00681	0.00004	-0.01365
102(N)	3.54289	3.54298	-0.00009	-0.08586
103(C)	3.00653	3.00662	-0.00009	-0.01316
104(N)	3.54473	3.54439	0.00034	-0.08912
105(C)	2.99962	3.03264	-0.03302	-0.03227
106(N)	3.65575	3.46102	0.19473	-0.11678
107(C)	3.00756	3.00645	0.00111	-0.01401
108(N)	3.54025	3.54273	-0.00248	-0.08298
109(C)	3.00469	3.00797	-0.00328	-0.01266
110(N)	3.54679	3.53818	0.00861	-0.08497

Total net charge: -0.00000011 Total spin electrons: 1.99999999

Population of atoms for e

Atom	Alpha pop.	Beta pop.	Spin pop.	Atomic charge
1(C)	3.07776	3.07775	0.00001	-0.15552
2(C)	3.07717	3.07716	0.00000	-0.15433
3(C)	3.08314	3.08308	0.00006	-0.16622
4(C)	2.99947	2.99935	0.00012	0.00118
5(C)	3.08331	3.08331	-0.00000	-0.16661
6(C)	3.07708	3.07707	0.00002	-0.15415
7(C)	3.00702	3.00679	0.00023	-0.01381
8(C)	3.00015	2.99984	0.00031	0.00001
9(C)	2.99087	2.99099	-0.00012	0.01814
10(C)	2.99830	2.99817	0.00012	0.00353
11(C)	3.00195	3.00198	-0.00003	-0.00393
12(C)	3.07206	3.07210	-0.00004	-0.14416
13(C)	2.99699	2.99691	0.00007	0.00610
14(C)	2.99433	2.99436	-0.00003	0.01131
15(C)	3.07372	3.07366	0.00006	-0.14737
16(C)	3.08010	3.08016	-0.00006	-0.16027
17(C)	3.07409	3.07386	0.00023	-0.14796
18(C)	2.99877	2.99882	-0.00006	0.00241
19(C)	3.08241	3.08242	-0.00001	-0.16483
20(C)	3.00963	3.01886	-0.00922	-0.02849
21(C)	2.98735	2.95441	0.03294	0.05824
22(N)	3.61008	3.59239	0.01769	-0.20247

23(C)	2.97253	2.97677	-0.00424	0.05069
24(C)	3.01932	3.01345	0.00586	-0.03277
25(C)	3.09561	3.08984	0.00577	-0.18545
26(C)	3.07458	3.07909	-0.00451	-0.15367
27(C)	3.00953	3.00407	0.00546	-0.01360
28(C)	3.07833	3.08112	-0.00279	-0.15945
29(C)	3.09708	3.04904	0.04804	-0.14611
30(C)	3.00035	3.00705	-0.00670	-0.00741
31(C)	3.01818	2.97707	0.04110	0.00475
32(C)	3.00407	3.01504	-0.01097	-0.01910
33(C)	3.01496	3.01478	0.00018	-0.02973
34(C)	2.97099	2.97110	-0.00012	0.05791
35(N)	3.60335	3.60244	0.00091	-0.20579
36(C)	2.97530	2.97369	0.00162	0.05101
37(C)	3.01704	3.01660	0.00044	-0.03364
38(C)	3.09326	3.09367	-0.00042	-0.18693
39(C)	3.07882	3.07508	0.00373	-0.15390
40(C)	3.01255	3.00350	0.00905	-0.01605
41(C)	3.08113	3.07969	0.00144	-0.16082
42(C)	3.07411	3.07398	0.00013	-0.14809
43(C)	3.00472	3.00453	0.00020	-0.00925
44(C)	2.99740	2.99747	-0.00007	0.00514
45(C)	3.01049	3.01020	0.00029	-0.02069
46(C)	3.03842	2.96845	0.06997	-0.00687
47(C)	3.06256	2.92969	0.13287	0.00775
48(C)	2.98603	2.99557	-0.00954	0.01840
49(C)	3.11894	2.87456	0.24438	0.00650
50(C)	3.14611	2.87346	0.27265	-0.01958
51(C)	3.04612	3.10541	-0.05929	-0.15153
52(C)	3.19447	2.80888	0.38559	-0.00336
53(C)	3.08677	2.90549	0.18128	0.00774
54(C)	3.05165	3.09133	-0.03968	-0.14298
55(C)	3.14199	3.02154	0.12045	-0.16353
56(C)	3.05986	3.08171	-0.02185	-0.14157
57(C)	3.10343	2.89535	0.20808	0.00121
58(C)	3.06061	3.10747	-0.04686	-0.16808
59(C)	3.00670	2.99394	0.01276	-0.00064
60(C)	3.08959	3.07939	0.01020	-0.16898
61(C)	3.07648	3.07878	-0.00229	-0.15526
62(C)	3.08234	3.07443	0.00792	-0.15677
63(C)	3.07767	3.07772	-0.00005	-0.15539
64(C)	3.08433	3.08013	0.00419	-0.16446
65(H)	0.42095	0.42095	0.00000	0.15810
66(H)	0.41906	0.41905	0.00001	0.16189
67(H)	0.41657	0.41657	0.00000	0.16685
68(H)	0.42026	0.42026	0.00000	0.15948
69(H)	0.41451	0.41451	-0.00000	0.17098
70(H)	0.41547	0.41547	-0.00000	0.16905
71(H)	0.41967	0.41966	0.00000	0.16067
72(H)	0.41503	0.41503	-0.00001	0.16994
73(H)	0.41811	0.41829	-0.00018	0.16361
74(H)	0.41599	0.41590	0.00009	0.16811
75(H)	0.41503	0.41653	-0.00150	0.16844
76(H)	0.41870	0.41857	0.00013	0.16273
77(H)	0.41691	0.41641	0.00050	0.16668
78(H)	0.41650	0.41649	0.00001	0.16702
79(H)	0.41645	0.41645	-0.00000	0.16710
80(H)	0.41591	0.41470	0.00122	0.16939

81(H)	0.41599	0.41546	0.00054	0.16855
82(H)	0.41715	0.42104	-0.00389	0.16182
83(H)	0.41486	0.41432	0.00054	0.17082
84(H)	0.41728	0.41609	0.00119	0.16664
85(H)	0.41747	0.41750	-0.00003	0.16503
86(H)	0.42093	0.42075	0.00018	0.15833
87(H)	0.42138	0.42126	0.00012	0.15736
88(H)	0.41903	0.41901	0.00002	0.16196
89(H)	0.35009	0.35012	-0.00003	0.29979
90(H)	0.42189	0.42210	-0.00022	0.15601
91(H)	0.42155	0.42155	0.00000	0.15689
92(H)	0.41700	0.41700	0.00000	0.16600
93(H)	0.34947	0.34996	-0.00050	0.30057
94(H)	0.41649	0.41635	0.00013	0.16716
95(C)	3.01278	3.01283	-0.00006	-0.02561
96(C)	3.12195	3.12179	0.00016	-0.24374
97(H)	0.39519	0.39520	-0.00001	0.20961
98(C)	3.01230	3.01228	0.00002	-0.02458
99(C)	3.11757	3.11759	-0.00002	-0.23516
100(H)	0.39561	0.39560	0.00000	0.20879
101(C)	3.01371	3.01370	0.00001	-0.02741
102(C)	3.11633	3.11634	-0.00002	-0.23267
103(H)	0.39666	0.39666	0.00000	0.20668
104(C)	3.01354	3.01356	-0.00002	-0.02709
105(C)	3.11779	3.11773	0.00006	-0.23552
106(H)	0.39575	0.39575	-0.00000	0.20850
107(C)	2.98462	3.04059	-0.05597	-0.02522
108(C)	3.28293	2.95187	0.33107	-0.23480
109(H)	0.38998	0.40088	-0.01089	0.20914
110(C)	2.99651	3.02820	-0.03168	-0.02471
111(C)	3.19447	3.04033	0.15414	-0.23480
112(H)	0.39416	0.39928	-0.00512	0.20656
113(C)	3.00920	3.01631	-0.00712	-0.02551
114(C)	3.12765	3.10501	0.02264	-0.23266
115(H)	0.39486	0.39561	-0.00074	0.20953
116(C)	3.01435	3.01154	0.00281	-0.02588
117(C)	3.11797	3.12321	-0.00524	-0.24118
118(H)	0.39496	0.39479	0.00017	0.21025

Total net charge: -0.00000001 Total spin electrons: 1.99999999

Population of atoms for f

Atom	Alpha pop.	Beta pop.	Spin pop.	Atomic charge
1(C)	3.07808	3.07758	0.00050	-0.15566
2(C)	3.07811	3.07688	0.00123	-0.15499
3(C)	3.08457	3.08451	0.00006	-0.16908
4(C)	3.00238	2.99832	0.00407	-0.00070
5(C)	3.08387	3.08172	0.00215	-0.16559
6(C)	3.07746	3.07701	0.00046	-0.15447
7(C)	3.07789	2.93700	0.14089	-0.01489
8(C)	3.01515	2.98032	0.03483	0.00453
9(C)	2.98846	2.99215	-0.00369	0.01939
10(C)	3.03255	2.96292	0.06963	0.00452
11(C)	3.01981	2.99229	0.02752	-0.01210
12(C)	3.07975	3.10423	-0.02448	-0.18397
13(C)	2.99702	2.89048	0.10655	0.11250
14(C)	2.92761	2.94442	-0.01681	0.12797
15(C)	3.13427	3.06088	0.07338	-0.19515
16(C)	3.10025	3.06972	0.03053	-0.16996

17(C)	3.09578	3.05018	0.04560	-0.14596
18(C)	3.07249	2.93937	0.13311	-0.01186
19(C)	3.09858	3.07354	0.02505	-0.17212
20(C)	3.01096	3.01687	-0.00591	-0.02783
21(C)	3.01347	2.96684	0.04663	0.01968
22(N)	3.62250	3.56988	0.05262	-0.19238
23(C)	2.97721	2.97818	-0.00096	0.04461
24(C)	3.02603	3.00479	0.02124	-0.03081
25(C)	3.09836	3.08219	0.01617	-0.18055
26(C)	3.08045	3.08059	-0.00014	-0.16104
27(C)	3.01673	2.99096	0.02577	-0.00769
28(C)	3.07880	3.07645	0.00235	-0.15524
29(C)	3.13704	3.02974	0.10730	-0.16677
30(C)	3.04167	2.99050	0.05117	-0.03217
31(C)	2.94457	2.93606	0.00852	0.11937
32(C)	2.95980	2.94450	0.01530	0.09570
33(C)	3.01096	3.01687	-0.00591	-0.02783
34(C)	3.01347	2.96685	0.04663	0.01968
35(N)	3.62250	3.56988	0.05262	-0.19238
36(C)	2.97721	2.97818	-0.00096	0.04461
37(C)	3.02603	3.00479	0.02124	-0.03082
38(C)	3.09836	3.08219	0.01617	-0.18055
39(C)	3.08045	3.08059	-0.00014	-0.16104
40(C)	3.01673	2.99096	0.02577	-0.00770
41(C)	3.07880	3.07645	0.00235	-0.15525
42(C)	3.13704	3.02974	0.10731	-0.16678
43(C)	3.04167	2.99050	0.05117	-0.03217
44(C)	2.94457	2.93606	0.00852	0.11937
45(C)	2.95980	2.94450	0.01530	0.09570
46(C)	3.07789	2.93700	0.14089	-0.01489
47(C)	3.01515	2.98032	0.03483	0.00453
48(C)	2.98846	2.99215	-0.00369	0.01939
49(C)	3.03255	2.96293	0.06963	0.00452
50(C)	3.01981	2.99229	0.02752	-0.01210
51(C)	3.07974	3.10423	-0.02448	-0.18397
52(C)	2.99702	2.89048	0.10655	0.11250
53(C)	2.92761	2.94442	-0.01680	0.12797
54(C)	3.13427	3.06089	0.07338	-0.19515
55(C)	3.10025	3.06972	0.03053	-0.16996
56(C)	3.09578	3.05018	0.04561	-0.14596
57(C)	3.07248	2.93937	0.13311	-0.01186
58(C)	3.09858	3.07353	0.02505	-0.17211
59(C)	3.00238	2.99832	0.00407	-0.00070
60(C)	3.08386	3.08171	0.00215	-0.16557
61(C)	3.07746	3.07701	0.00046	-0.15447
62(C)	3.07808	3.07758	0.00050	-0.15566
63(C)	3.07811	3.07688	0.00123	-0.15499
64(C)	3.08458	3.08452	0.00007	-0.16910
65(H)	0.42097	0.42097	-0.00000	0.15806
66(H)	0.41940	0.41932	0.00008	0.16128
67(H)	0.41662	0.41664	-0.00002	0.16674
68(H)	0.42033	0.42031	0.00002	0.15936
69(H)	0.41212	0.41147	0.00065	0.17642
70(H)	0.41148	0.41390	-0.00242	0.17462
71(H)	0.41927	0.42040	-0.00113	0.16033
72(H)	0.41638	0.41776	-0.00138	0.16586
73(H)	0.41771	0.41815	-0.00044	0.16414
74(H)	0.41569	0.41575	-0.00006	0.16856

75(H)	0.41429	0.41747	-0.00318	0.16823
76(H)	0.41771	0.41815	-0.00044	0.16414
77(H)	0.41646	0.41630	0.00016	0.16724
78(H)	0.41569	0.41575	-0.00006	0.16856
79(H)	0.41430	0.41748	-0.00318	0.16823
80(H)	0.41211	0.41147	0.00065	0.17642
81(H)	0.41148	0.41390	-0.00242	0.17462
82(H)	0.41927	0.42040	-0.00113	0.16033
83(H)	0.41638	0.41776	-0.00138	0.16586
84(H)	0.41808	0.41877	-0.00068	0.16315
85(H)	0.41662	0.41664	-0.00003	0.16674
86(H)	0.42033	0.42031	0.00002	0.15937
87(H)	0.42097	0.42097	-0.00000	0.15806
88(H)	0.41939	0.41931	0.00008	0.16129
89(H)	0.34791	0.34932	-0.00141	0.30277
90(H)	0.42153	0.42154	-0.00001	0.15693
91(H)	0.42153	0.42154	-0.00001	0.15693
92(H)	0.41808	0.41877	-0.00068	0.16315
93(H)	0.34791	0.34932	-0.00141	0.30277
94(H)	0.41646	0.41630	0.00016	0.16724
95(F)	4.57025	4.55328	0.01696	-0.12353
96(F)	4.56238	4.56360	-0.00121	-0.12598
97(F)	4.56107	4.56040	0.00066	-0.12147
98(F)	4.56639	4.56361	0.00278	-0.13000
99(F)	4.57025	4.55328	0.01696	-0.12353
100(F)	4.56238	4.56360	-0.00121	-0.12598
101(F)	4.56107	4.56040	0.00066	-0.12147
102(F)	4.56639	4.56361	0.00278	-0.12999

Total net charge: 0.00000007 Total spin electrons: 2.00000000