Supplementary Information

Molecular design and properties of bridged energetic pyridines derivatives

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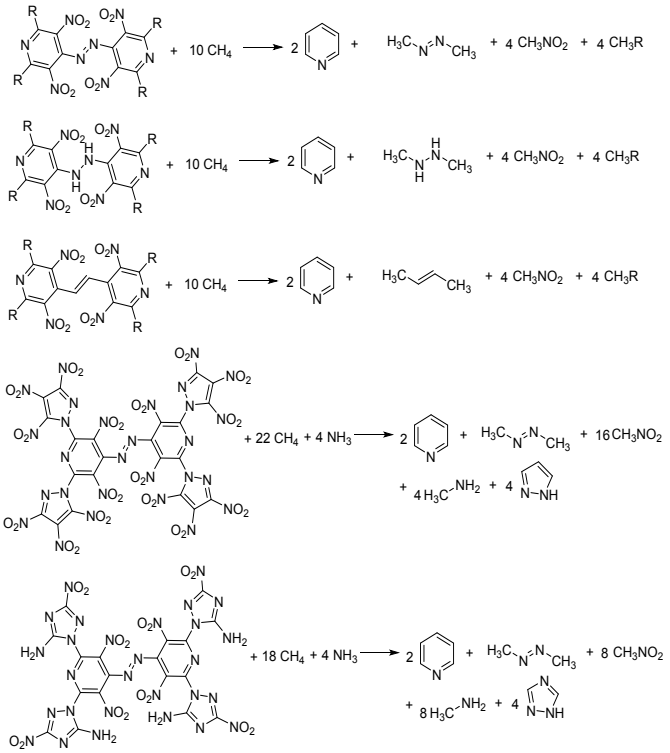
Index



Scheme s1 Representative isodesmic reactions for designed compounds

Computational methods

The method of dispersion correction as an add-on to density functional theory (DFT-D3) method has been demonstrated as an economical and liable tool in predicting physical and chemical properties of energetic materials[1-3]. The optimized molecular structures, accurate energies, frontier molecular orbitals, heats of formation, vibrational frequencies, energetic properties, bond dissociation energies and thermodynamic parameters of the designed compounds were carried out by using the hybrid DFT/B3LYP functional with 6-311G(d,p) basis set[4,5], in combination with the DFT-D3(BJ) dispersion correction[6,7]. All calculations were performed on the Gaussian 16 software[8] and the optimized structures were characterized to be the local energy minimum on the potential energy surface without imaginary frequencies. Isodesmic reactions and related equations (Scheme s1) were designed to predict accurate gas-phase HOFs (Δ*H*f,gas) of the designed compound.

$$\Delta \mathrm{H}_{298K} = \sum \Delta H_{f,p} - \sum \Delta H_{f,R} \quad (1)$$

$$\Delta H_{298K} = \Delta E_{298K} + \Delta(PV) = \Delta E_0 + \Delta ZPE + \Delta H_T + \Delta nRT \quad (2)$$

where ΔH_{298K}, HOFs that need to be calculated; $\Delta H_{f,p}$ and $\Delta H_{f,R}$, HOFs of products and reactants; ΔE_0, energy changes between products and reactants; ΔZPE, difference between the zero-point energy (ZPE) of products and reactants; ΔH_T, thermal correction from 0 to 298 K; n, number of the energetic groups; Δ(*PV*) equals to Δ*nRT*.

However, energetic materials were always in condensed phase while HOFs that obtained from the isodesmic reactions were in gas-phase. According to Hess's law of constant heat summation, the values of $\Delta H_{f,gas}$ and heat of sublimation (ΔH_{sub}) can be used to evaluate the accurate data of solid-phase HOFs ($\Delta H_{f,solid}$) based on the following equation:[9]

$$\Delta H_{\mathrm{f,solid}} = \Delta H_{f,gas} - \Delta H_{sub} \quad (3)$$

where, ΔH_{sub} is heat of sublimation. Politzer et al. proposed that ΔH_{sub} can also be correlated with molecular surface area A and electrostatic interaction index $v\sigma_{tot}^2$ by the empirical expression:[10]

$$\Delta H_{sub} = aA^2 + b(v\sigma_{tot}^2)^{0.5} + c \quad (4)$$

where *a*, *b* and *c* are coefficients and represented as 2.670×10^{-4} kcal mol^{-1} Å^{-4}, 1.650 kcal mol^{-1}, and 2.966 kcal mol^{-1};[11] *A* is the surface area of 0.001 e bohr^{-3} isosurface of electronic density of the molecule; *v* is the degree of balance between positive and negative potential on the isosurface; σ_{tot}^2 is the measure of variability of the electrostatic potential on molecular surface, which can be obtained via the Multiwfn program[12].

Densities (*ρ*) that used to calculate the detonation velocity and detonation pressure were obtained by an improved equation proposed by Politzer et al:[13]

$$\rho = \beta_1\left(\frac{M}{V}\right) + \beta_2(v\sigma_{tot}^2) + \beta_3 \quad (5)$$

where β_1, β_2, and β_3 are coefficients and represented as 0.9183, 0.0028, and 0.0443, respectively, *M* stands for the molecular mass (g mol^{-1}), *V* stands for the volume of a molecule (m^3 mol^{-1}), *v* stands for the degree of balance between positive and negative potential on the isosurface and σ_{tot}^2 stands for measure of variability of the electrostatic potential on the molecular surface.

Energetic properties (detonation velocity and detonation pressures) were estimated by the Kamlet-Jacobs equations:[14]

$$D = 1.01(N\overline{M}^{0.5}Q^{0.5})^{0.5}(1 + 1.3\rho) \quad (6)$$

$$P = 1.558\rho^2 N\overline{M}^{0.5}Q^{0.5} \quad (7)$$

where D is the detonation velocity (km s-1); P is the detonation pressure (GPa); *N*, $\overline{M}$ and *Q* are the moles of

detonation gases per-gram explosive (mol g^{-1}), the average molecular weight of these gases (g mol^{-1}) and heat of detonation (cal g^{-1}), respectively.

Bond dissociation energy (BDE), regarded as the strength of bonding, is an important indicator in predicting the way of bond cleavage and thermal decomposition mechanism of high energy density material. The homolytic BDEs were presented by the following equation:

$$BDE_0(A–B)=E_0(A\cdot)+E_0(B\cdot)–E_0(A–B) \quad (8)$$

The BDEs with zero-point energy (ZPE) corrections were finally calculated based on the folowing equation:

$$BDE(A–B)_{ZPE} = BDE_0(A–B) + \Delta E_{ZPE} \quad (9)$$

where ΔE_{ZPE} is the difference between ZPEs of products and reactants.

References

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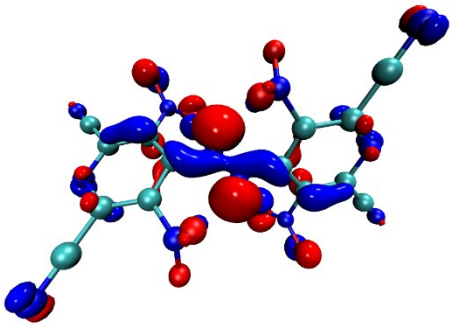
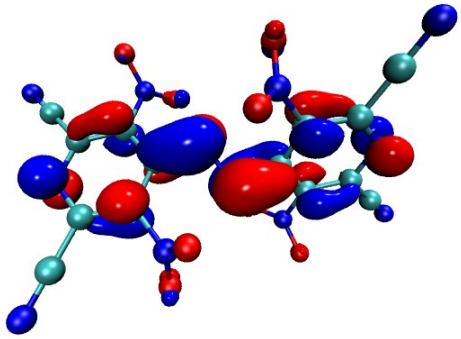
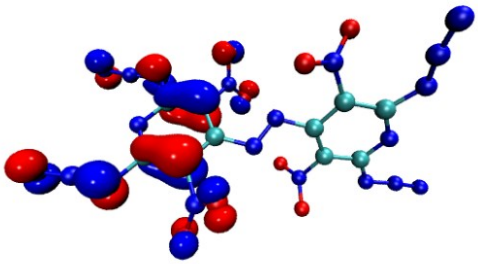
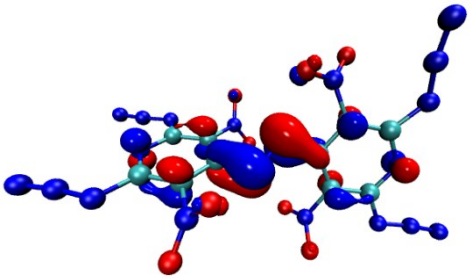
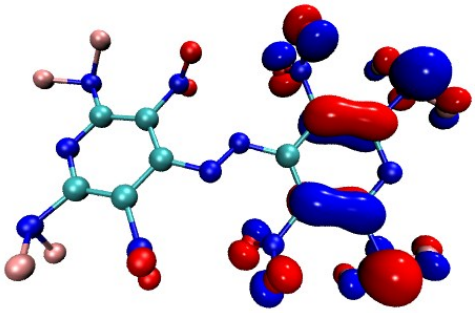
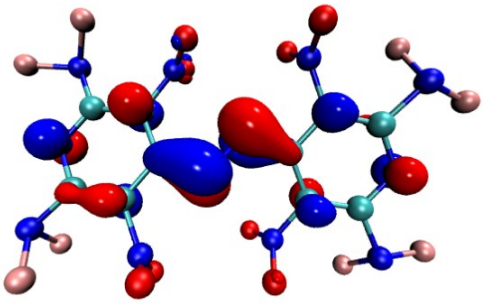
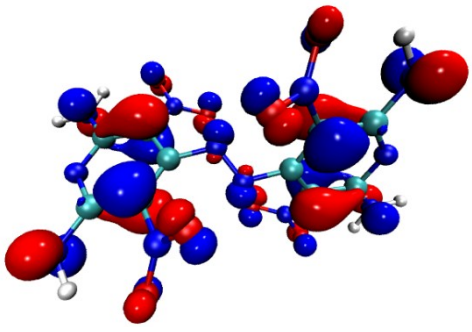
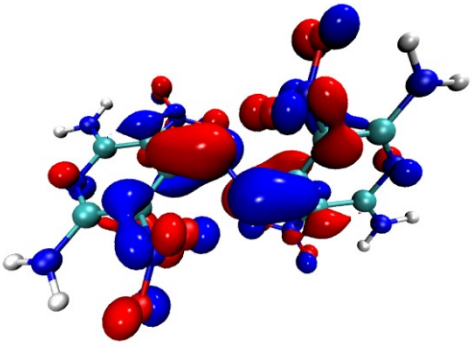
Table S1. The HOMO-LUMO pictures of B1, B2, B3, B4, B5, B8, B9 and B12.

Comp.	LUMO	HOMO
B1		
B2		
B3		
B4		

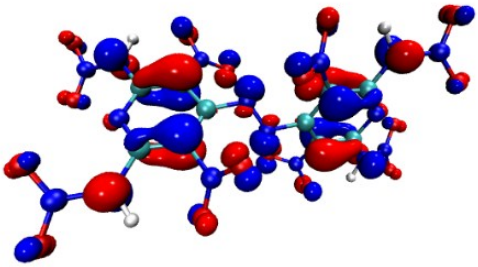
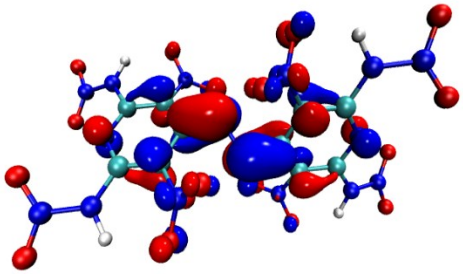
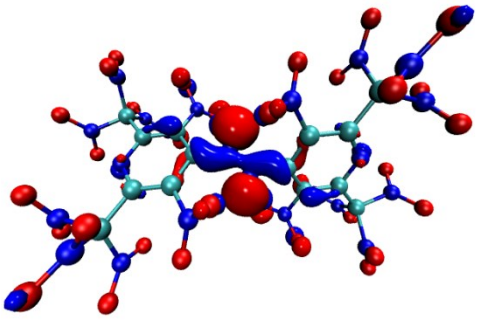
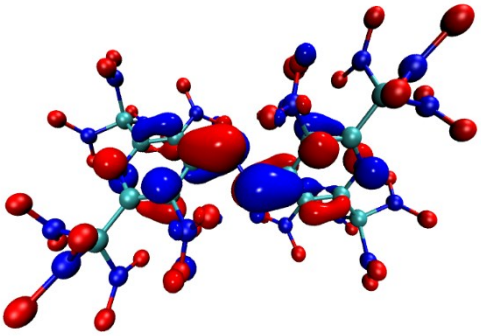
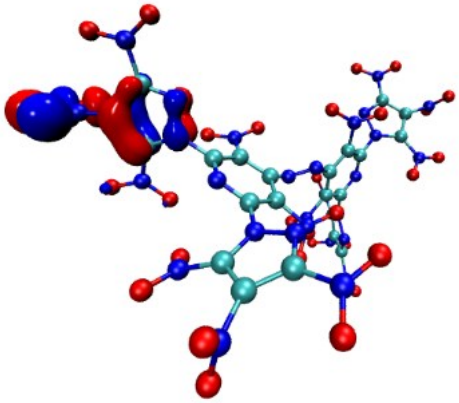
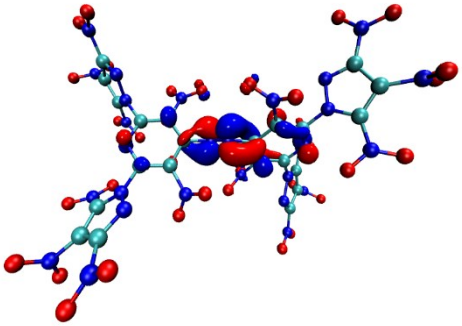
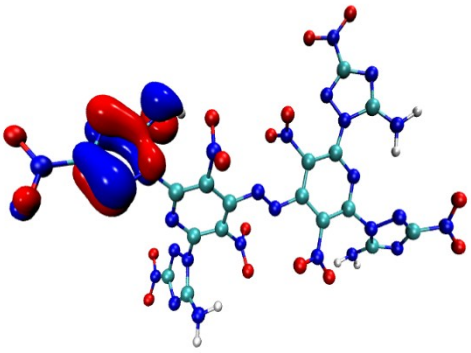
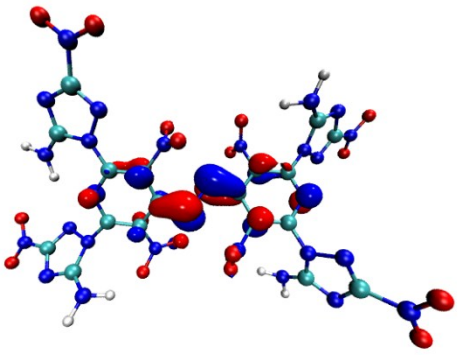
Comp.	LUMO	HOMO
B5		
B8		
B9		
B12		

Table S2. DFT/B3LYP/6-311G(d,p) optimized geometries of B9, B10, B11 and B12.

[B9]

0 1

N	0.43002200	0.33972700	0.66380600
N	-0.35562400	0.22052800	-0.28508000
C	1.79215400	0.19650200	0.30556400
C	-1.73479100	0.23819600	0.03941600
C	2.29259400	-0.77247000	-0.56863100
C	3.67334200	-0.86487400	-0.73705700
N	4.53534300	-0.06999000	-0.13754400
C	4.07209800	0.85617200	0.67898200
C	2.71918600	1.02264200	0.94611900
C	-2.35827000	-0.78940900	0.75269700
C	-3.74666900	-0.75676400	0.88155200
N	-4.50620000	0.18701400	0.36081000
C	-3.93430900	1.11354400	-0.38136000
C	-2.55899800	1.19603700	-0.56502400
C	-5.89967900	3.90075800	-0.99971600
N	-5.03234000	3.23074500	-0.26004800
N	-4.81484300	2.09586600	-0.93147800
C	-5.53574700	2.03712400	-2.09201200
C	-6.25881400	3.20262700	-2.16765500
C	-4.81044800	-2.86455200	3.40102600
N	-3.94462000	-2.01763200	2.88736000
N	-4.41345700	-1.73757700	1.65866800
C	-5.58293200	-2.40503100	1.39680200
C	-5.87118900	-3.14755700	2.51449600
C	5.98417300	3.58896800	1.59294000
N	4.97424100	3.04049100	0.94450000
N	5.02864400	1.73867400	1.25509200
C	6.06534100	1.45798800	2.10482000
C	6.71510300	2.64520700	2.34019200
C	4.62693000	-3.86704700	-2.16110700
N	3.93325900	-3.16414700	-1.28779500
N	4.21943400	-1.88334100	-1.56564400
C	5.09314900	-1.77110900	-2.61500600
C	5.38413000	-3.04944800	-3.02409900
N	1.39787800	-1.68846100	-1.31949300
O	1.55733200	-1.70323800	-2.52334800
O	0.60623100	-2.34232400	-0.67113200
N	-1.59420600	-1.94509900	1.29213400
O	-1.95124400	-3.03370000	0.88663100
O	-0.70412600	-1.70034300	2.07902000
N	2.24092300	2.05281200	1.89389600
O	1.28011800	2.70552100	1.53768200
O	2.85143000	2.14225400	2.94335800
N	-1.94493700	2.25072600	-1.39708700
O	-2.58880400	2.65201200	-2.34922200
O	-0.83266800	2.61895300	-1.06281200
N	-6.37795800	5.21947900	-0.58778000
O	-5.97906000	5.65693700	0.47054300
O	-7.14598200	5.75235500	-1.37494100
N	-5.41053300	0.95315900	-3.03573900
O	-4.54748400	0.11740700	-2.79562600
O	-6.16659400	0.97981000	-3.98666000
N	-7.18239500	3.60748600	-3.23643800
O	-8.34969300	3.33595100	-3.05209600
O	-6.67894600	4.16744000	-4.18654800
N	-4.59441300	-3.43735700	4.73199500
O	-3.75134200	-2.91878700	5.43182200
O	-5.29780300	-4.40035600	4.99334500
N	-6.27809200	-2.36738300	0.12220600
O	-5.61245300	-2.08405000	-0.86059000
O	-7.46081900	-2.64753800	0.16200600
N	-7.02647900	-4.03007700	2.71571400
O	-7.05049800	-5.04017200	2.04412100
O	-7.83803400	-3.64847700	3.53235100
N	6.23544800	5.02831900	1.51314100
O	5.54543600	5.67677700	0.75646500
O	7.13273400	5.42947400	2.23890300
N	6.29473900	0.15206100	2.68211900
O	5.39304900	-0.66672900	2.56601100

[B10]

0 1

N	-0.51253200	-0.52728100	-0.13064100
N	0.22624500	0.40145900	-0.49376300
C	-1.89277900	-0.21854600	-0.13163000
C	1.61274800	0.15149600	-0.36552500
C	-2.75533700	-1.26970500	-0.44687400
C	-4.12876800	-1.02750900	-0.44623100
N	-4.62949600	0.12829100	-0.02345200
C	-3.82507300	1.12149200	0.34380100
C	-2.43123800	1.01488200	0.24425300
C	2.18430500	-0.57720700	0.67099800
C	3.59197500	-0.64078200	0.73641000
N	4.34936400	-0.01280500	-0.14664300
C	3.83048800	0.67257000	-1.15440600
C	2.45235000	0.77451900	-1.31133100
C	-5.69761600	-3.60409100	-2.09610200
N	-4.63303700	-2.90833900	-1.83556500
N	-5.04969200	-1.96997700	-0.90691100
C	-6.39150900	-2.08792700	-0.60371100
C	-6.83816700	-3.16090600	-1.37991500
N	-7.08474700	-1.30121600	0.23514700
C	-4.57427700	4.09766800	1.89597800
N	-3.74118100	3.13736900	1.63609300
N	-4.45506600	2.26555200	0.82872700
C	-5.75350100	2.69671900	0.60577500
C	-5.84177200	3.91544600	1.29073000
N	-6.68019800	2.06834500	-0.11602100
C	6.83444600	0.98491300	-2.68304100
N	5.81346200	0.25934300	-2.34388300
N	4.80550600	1.17889100	-2.05013100
C	5.26249900	2.48372100	-2.14944700
C	6.58254000	2.37558800	-2.60626400
N	4.57666000	3.57017400	-1.78268900
C	4.56930800	-2.30103700	3.57716300
N	3.66284600	-1.65918300	2.90562700
N	4.28439700	-1.34207900	1.70771300
C	5.60485200	-1.79035600	1.65210500
C	5.79400000	-2.44076700	2.88031100
N	6.44324200	-1.64723400	0.63354400
N	-2.16930600	-2.60208100	-0.71903500
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O	-2.51268600	-3.48520200	0.04122500
N	1.31832300	-1.31413000	1.62990200
O	1.30234600	-2.51701500	1.48311500
O	0.70581800	-0.64728200	2.43580000
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O	-3.74403300	5.00850000	3.82584200
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O	-8.00219100	4.32730300	0.75379300
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O	8.53667800	-0.49248300	-2.31786600
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O	8.95453200	2.92398600	2.60774900	N	7.02325100	-2.98393700	3.33283700
O	7.68058200	2.94091700	4.38187500	O	7.09545600	-3.34916900	4.49546200
N	4.53673800	-5.32814600	-2.18899900	O	7.94400900	-3.04020100	2.50629500
O	3.93485600	-5.86873500	-1.28661800	H	-6.59372200	-0.73734300	0.90985000
O	5.08675100	-5.85395300	-3.14455500	H	-8.02368800	-1.63212600	0.43158800
N	5.49387400	-0.50649800	-3.19719700	H	-6.52235600	1.14168600	-0.47641600
O	6.47677600	-0.54169500	-3.91195700	H	-7.56499500	2.55174600	-0.21077300
O	4.79828600	0.46405200	-2.93606600	H	3.56919100	3.53521000	-1.85876600
N	6.27401700	-3.44631100	-4.12320100	H	5.04748800	4.44088600	-2.00366600
O	7.35595000	-3.87921200	-3.78882100	H	6.22457300	-1.05826300	-0.15796000
O	5.83489200	-3.29489600	-5.24361100	H	7.35479400	-2.07351500	0.74886200

[B11]

0 1

N	0.38150100	-0.48977900	-0.17965000
N	-0.38152200	0.48979900	-0.17967900
C	1.75440500	-0.15677700	-0.11820700
C	-1.75442400	0.15679600	-0.11822900
C	2.27720100	0.89401200	0.64247600
C	3.66113500	1.03428500	0.71207400
N	4.50202700	0.23968800	0.07680100
C	4.02671500	-0.73393900	-0.67346300
C	2.65813700	-0.98637500	-0.78897900
C	-2.27720400	-0.89400100	0.64245100
C	-3.66113600	-1.03427800	0.71206900
N	-4.50204000	-0.23968400	0.07680900
C	-4.02674200	0.73394500	-0.67346300
C	-2.65816500	0.98639300	-0.78898600
C	4.66503800	3.03755200	3.32911000
N	3.85626800	2.14813900	2.78613600
N	4.23737100	2.04554500	1.51442400
C	5.32111100	2.86677800	1.23281900
C	5.63908700	3.54991300	2.41132400
N	6.59188000	4.46010000	2.62130500
C	6.68131700	-2.84357600	-1.31160200
N	5.90704500	-2.13523700	-0.51026200
N	5.02087700	-1.53770200	-1.29888200
C	5.22654700	-1.86079700	-2.63408200
C	6.32373700	-2.72569200	-2.69195400
N	6.89690400	-3.27961300	-3.76180300
C	-6.68136300	2.84357400	-1.31153900
N	-5.90708100	2.13522300	-0.51022100
N	-5.02092200	1.53770100	-1.29886200
C	-5.22663700	1.86078500	-2.63405900
C	-6.32381900	2.72569100	-2.69190100
N	-6.89699200	3.27964300	-3.76173000
C	-4.66500500	-3.03757900	3.32909700
N	-3.85626900	-2.14812300	2.78613800
N	-4.23735600	-2.04554900	1.51442100
C	-5.32104600	-2.86683800	1.23279500
C	-5.63900900	-3.54999000	2.41129400
N	-6.59176500	-4.46022100	2.62125900
N	1.40378500	1.85144100	1.36563800
O	1.50873100	3.01342000	1.02207400
O	0.68887200	1.39798500	2.23376800
N	-1.40377100	-1.85143400	1.36558600
O	-0.68880000	-1.39797700	2.23366600
O	-1.50882100	-3.01342900	1.02210800
N	2.13694100	-2.09828100	-1.60767900
O	2.77597800	-3.13962900	-1.57504000
O	1.11983600	-1.89060600	-2.23865800
N	-2.13697300	2.09832300	-1.60765900
O	-2.77603300	3.13965700	-1.57501900
O	-1.11984300	1.89068300	-2.23860800
N	4.52489500	3.41667300	4.71603700
O	3.66620600	2.88357100	5.38528000
O	5.32030300	4.27860400	5.10527900
N	5.81157600	3.14270600	-0.06385800
O	5.21180400	2.69717400	-1.03439100
O	6.82291200	3.85382100	-0.11196700
N	7.76953900	-3.63081400	-0.78472200
O	7.96094200	-3.64330100	0.41312000
O	8.43231400	-4.24156600	-1.63086400

[B12]

0 1

N	-0.42755300	-0.64772900	-0.07971300
N	0.31661700	0.28977600	-0.41903900
C	-1.80953200	-0.36407300	-0.11371300
C	1.69395100	0.03015300	-0.27205000
C	-2.67401900	-1.41825000	-0.48985500
C	-4.05133300	-1.23171500	-0.35080000
N	-4.53446900	-0.07165900	0.06905900
C	-3.75452400	0.95478700	0.36224400
C	-2.34873400	0.84543900	0.30390300
C	2.30185800	-1.13059800	0.21592000
C	3.69377800	-1.20886200	0.24734700
N	4.46890100	-0.18674300	-0.08419400
C	3.92230900	0.94516300	-0.49928200
C	2.54136000	1.06980300	-0.65073400
C	-7.08025900	-2.52092900	-1.02502200
N	-6.18002600	-1.61683500	-1.28814200
N	-5.06044500	-2.16143000	-0.67970200
C	-5.43911700	-3.34717500	-0.04137800
N	-6.71001300	-3.59244100	-0.29390100
N	-4.64402000	-4.05345900	0.78832100
C	-4.77905400	3.97474700	1.53144600
N	-3.79762500	3.12386900	1.40592700
N	-4.42526300	2.10108400	0.73074900
C	-5.77647300	2.44355400	0.51491900
N	-5.98530400	3.64230800	1.02611000
N	-6.66525500	1.68990600	-0.13332100
C	6.55679200	2.81637300	-1.53592000
N	5.79164800	1.77991800	-1.74731100
N	4.79108400	2.00564400	-0.82564900
C	5.07567500	3.16380900	-0.10920900
N	6.18861700	3.69116800	-0.57145500
N	4.34524200	3.59742900	0.94703000
C	5.81440900	-3.47810700	1.62669400
N	5.20309400	-2.33004100	1.74263000
N	4.33374600	-2.39174300	0.67570800
C	4.53133500	-3.58169800	-0.01342000
N	5.45980900	-4.28396100	0.59859100
N	3.90522200	-3.89403100	-1.17646000
N	-2.08814900	-2.55944100	-1.18808500
O	-2.64758500	-3.64660500	-1.08726900
O	-1.09079500	-2.34592400	-1.85576100
N	1.51102200	-2.25217000	0.77098800
O	1.30938000	-3.20031600	0.02681800
O	1.15680400	-2.14192700	1.92210400
N	-1.45025800	1.98849100	0.61910300
O	-0.81274000	1.91078000	1.64951600
O	-1.42360800	2.86809400	-0.21250600
N	1.94573600	2.27370500	-1.27245800
O	1.59871400	2.16481100	-2.42587200
O	1.86340000	3.26617700	-0.56555300
N	-8.45589300	-2.34044400	-1.51425400
O	-9.14105500	-3.34008200	-1.59693500
O	-8.78585700	-1.19614000	-1.78674600
N	-4.55512100	5.25848700	2.22264300
O	-5.49337500	6.03228900	2.23927100
O	-3.45201500	5.42643000	2.71115600
N	7.77439500	3.01534400	-2.33928500
O	8.50505100	3.92603400	-1.99534400
O	7.94516900	2.24994400	-3.27197600

N	4.50869200	-1.31501800	-3.71046200	N	6.84584700	-3.87235200	2.60026500
O	3.60152600	-0.51903400	-3.46270000	O	7.45407100	-4.89818300	2.35608900
O	4.84771800	-1.67817200	-4.84030400	O	7.00143700	-3.13764100	3.55963100
N	-7.76958200	3.63080200	-0.78463300	H	-3.67468000	-4.13729400	0.51169600
O	-7.96095300	3.64329500	0.41321500	H	-5.07527700	-4.90062400	1.13010600
O	-8.43241100	4.24151200	-1.63076500	H	-6.45544900	0.74703500	-0.43160900
N	-4.50885700	1.31495600	-3.71046400	H	-7.58507000	2.07658600	-0.27262600
O	-3.60145500	0.51923800	-3.46271300	H	3.33864700	3.52047700	0.87451100
O	-4.84763700	1.67843800	-4.84027400	H	4.67143300	4.47788600	1.31931200
N	-4.52486800	-3.41669600	4.71602600	H	2.92253900	-3.66272500	-1.24546000
O	-3.66620900	-2.88356000	5.38528400	H	4.14023700	-4.81634800	-1.51453900
O	-5.32022300	-4.27868500	5.10524600				
N	-5.81148300	-3.14277400	-0.06389000				
O	-5.21173100	-2.69718300	-1.03440900				
O	-6.82277600	-3.85394900	-0.11202100				
H	7.18480300	4.72116000	1.84816400				
H	6.63230200	4.91139300	3.52194900				
H	6.51771600	-3.07435900	-4.67342200				
H	7.70081000	-3.87137400	-3.62049300				
H	-6.51789700	3.07430000	-4.67336900				
H	-7.70096300	3.87131200	-3.62040900				
H	-7.18464800	-4.72132300	1.84810200				
H	-6.63217000	-4.91152800	3.52189600				

Table S3. The specific data of bond order for all designed compounds

A1					A2				
The bond order >=		0.050000			The bond order >=		0.050000		
#	1:	1(N)	2(N):	1.435992	#	1:	1(N)	2(N):	1.433785
#	2:	1(N)	3(C):	0.931659	#	2:	1(N)	3(C):	0.931831
#	3:	2(N)	4(C):	0.931634	#	3:	2(N)	4(C):	0.931843
#	4:	3(C)	5(C):	1.369661	#	4:	3(C)	5(C):	1.393289
#	5:	3(C)	9(C):	1.410072	#	5:	3(C)	9(C):	1.369963
#	6:	4(C)	10(C):	1.369668	#	6:	4(C)	10(C):	1.393264
#	7:	4(C)	14(C):	1.410092	#	7:	4(C)	14(C):	1.369957
#	8:	5(C)	6(C):	1.376092	#	8:	5(C)	6(C):	1.370248
#	9:	5(C)	19(N):	0.676061	#	9:	5(C)	21(N):	0.669566
#	10:	6(C)	7(N):	1.181516	#	10:	6(C)	7(N):	1.202321
#	11:	6(C)	15(C):	1.256907	#	11:	6(C)	15(N):	0.922941
#	12:	7(N)	8(C):	1.235409	#	12:	7(N)	8(C):	1.200353
#	13:	8(C)	9(C):	1.469657	#	13:	8(C)	9(C):	1.477924
#	14:	8(C)	31(H):	0.854104	#	14:	8(C)	33(H):	0.853763
#	15:	9(C)	22(N):	0.694726	#	15:	9(C)	24(N):	0.707046
#	16:	10(C)	11(C):	1.376109	#	16:	10(C)	11(C):	1.370237
#	17:	10(C)	28(N):	0.676059	#	17:	10(C)	30(N):	0.669568
#	18:	11(C)	12(N):	1.181508	#	18:	11(C)	12(N):	1.202307
#	19:	11(C)	17(C):	1.256899	#	19:	11(C)	18(N):	0.922964
#	20:	12(N)	13(C):	1.235422	#	20:	12(N)	13(C):	1.200366
#	21:	13(C)	14(C):	1.469646	#	21:	13(C)	14(C):	1.477918
#	22:	13(C)	32(H):	0.854100	#	22:	13(C)	34(H):	0.853765
#	23:	14(C)	25(N):	0.694721	#	23:	14(C)	27(N):	0.707061
#	24:	15(C)	16(N):	2.536295	#	24:	15(N)	16(N):	1.129553
#	25:	17(C)	18(N):	2.536289	#	25:	16(N)	17(N):	2.255729
#	26:	19(N)	20(O):	0.999048	#	26:	18(N)	19(N):	1.129545
#	27:	19(N)	21(O):	0.986694	#	27:	19(N)	20(N):	2.255736
#	28:	22(N)	23(O):	0.969806	#	28:	21(N)	22(O):	1.001757
#	29:	22(N)	24(O):	0.969011	#	29:	21(N)	23(O):	0.981808
#	30:	25(N)	26(O):	0.969829	#	30:	24(N)	25(O):	0.948798
#	31:	25(N)	27(O):	0.969106	#	31:	24(N)	26(O):	0.958205
#	32:	28(N)	29(O):	0.986750	#	32:	27(N)	28(O):	0.948809
#	33:	28(N)	30(O):	0.999088	#	33:	27(N)	29(O):	0.958190
					#	34:	30(N)	31(O):	0.981792
					#	35:	30(N)	32(O):	1.001755
#	17:	10(C)	28(N):	0.676059					
					#	9:	5(C)	21(N):	0.669566

A3					A4				
The bond order >=		0.050000			The bond order >=		0.050000		
#	1:	1(N)	2(N):	1.451800	#	1:	1(N)	2(N):	1.450038

#	2:	1(N)	3(C):	0.909725	#	2:	1(N)	3(C):	0.916689
#	3:	2(N)	4(C):	0.922133	#	3:	2(N)	4(C):	0.916693
#	4:	3(C)	5(C):	1.372403	#	4:	3(C)	5(C):	1.365069
#	5:	3(C)	9(C):	1.366314	#	5:	3(C)	9(C):	1.377648
#	6:	4(C)	10(C):	1.373823	#	6:	4(C)	10(C):	1.365269
#	7:	4(C)	14(C):	1.391631	#	7:	4(C)	14(C):	1.377579
#	8:	5(C)	6(C):	1.364136	#	8:	5(C)	6(C):	1.285230
#	9:	5(C)	21(N):	0.657592	#	9:	5(C)	17(N):	0.687387
#	10:	6(C)	7(N):	1.278487	#	10:	6(C)	7(N):	1.139389
#	11:	6(C)	15(N):	0.870213	#	11:	6(C)	15(N):	1.163596
#	12:	7(N)	8(C):	1.193591	#	12:	7(N)	8(C):	1.258812
#	13:	8(C)	9(C):	1.486765	#	13:	8(C)	9(C):	1.443163
#	14:	8(C)	33(H):	0.853479	#	14:	8(C)	29(H):	0.850743
#	15:	9(C)	24(N):	0.687955	#	15:	9(C)	20(N):	0.714729
#	16:	10(C)	11(C):	1.361827	#	16:	10(C)	11(C):	1.285399
#	17:	10(C)	30(N):	0.666991	#	17:	10(C)	26(N):	0.687218
#	18:	11(C)	12(N):	1.284135	#	18:	11(C)	12(N):	1.139581
#	19:	11(C)	18(N):	0.868045	#	19:	11(C)	16(N):	1.163155
#	20:	12(N)	13(C):	1.191912	#	20:	12(N)	13(C):	1.258599
#	21:	13(C)	14(C):	1.492669	#	21:	13(C)	14(C):	1.443354
#	22:	13(C)	34(H):	0.852723	#	22:	13(C)	30(H):	0.850711
#	23:	14(C)	27(N):	0.697173	#	23:	14(C)	23(N):	0.714667
#	24:	15(N)	16(F):	0.172805	#	24:	15(N)	31(H):	0.680217
#	25:	15(N)	17(F):	0.137554	#	25:	15(N)	32(H):	0.677012
#	26:	18(N)	19(F):	0.174206	#	26:	16(N)	33(H):	0.680195
#	27:	18(N)	20(F):	0.137272	#	27:	16(N)	34(H):	0.677128
#	28:	21(N)	22(O):	0.983067	#	28:	17(N)	18(O):	0.903864
#	29:	21(N)	23(O):	0.993098	#	29:	17(N)	19(O):	1.003637
#	30:	24(N)	25(O):	0.968509	#	30:	20(N)	21(O):	0.936992
#	31:	24(N)	26(O):	0.959524	#	31:	20(N)	22(O):	0.951051
#	32:	27(N)	28(O):	0.957974	#	32:	23(N)	24(O):	0.936966
#	33:	27(N)	29(O):	0.969758	#	33:	23(N)	25(O):	0.951254
#	34:	30(N)	31(O):	0.985177	#	34:	26(N)	27(O):	1.003769
#	35:	30(N)	32(O):	1.003272	#	35:	26(N)	28(O):	0.903867
#	27:	18(N)	20(F):	0.137272	#	25:	15(N)	32(H):	0.677012

A5					A6				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	1.431017	#	1:	1(N)	2(N):	1.443614
#	2:	1(N)	3(C):	0.918927	#	2:	1(N)	3(C):	0.920124
#	3:	2(N)	4(C):	0.918961	#	3:	2(N)	4(C):	0.920109
#	4:	3(C)	5(C):	1.357790	#	4:	3(C)	5(C):	1.381285
#	5:	3(C)	9(C):	1.400666	#	5:	3(C)	9(C):	1.362902
#	6:	4(C)	10(C):	1.357758	#	6:	4(C)	10(C):	1.381157

#	7:	4(C)	14(C):	1.400585	#	7:	4(C)	14(C):	1.362947
#	8:	5(C)	6(C):	1.315583	#	8:	5(C)	6(C):	1.257529
#	9:	5(C)	23(N):	0.681059	#	9:	5(C)	19(N):	0.684104
#	10:	6(C)	7(N):	1.220290	#	10:	6(C)	7(N):	1.145817
#	11:	6(C)	15(N):	0.955249	#	11:	6(C)	15(N):	1.116853
#	12:	7(N)	8(C):	1.235218	#	12:	7(N)	8(C):	1.236206
#	13:	8(C)	9(C):	1.463826	#	13:	8(C)	9(C):	1.459897
#	14:	8(C)	35(H):	0.854038	#	14:	8(C)	31(H):	0.853906
#	15:	9(C)	26(N):	0.698143	#	15:	9(C)	22(N):	0.716741
#	16:	10(C)	11(C):	1.315385	#	16:	10(C)	11(C):	1.257441
#	17:	10(C)	32(N):	0.681083	#	17:	10(C)	28(N):	0.684150
#	18:	11(C)	12(N):	1.220228	#	18:	11(C)	12(N):	1.145748
#	19:	11(C)	19(N):	0.955435	#	19:	11(C)	17(N):	1.116957
#	20:	12(N)	13(C):	1.235258	#	20:	12(N)	13(C):	1.236315
#	21:	13(C)	14(C):	1.463836	#	21:	13(C)	14(C):	1.459844
#	22:	13(C)	36(H):	0.854033	#	22:	13(C)	32(H):	0.853887
#	23:	14(C)	29(N):	0.698146	#	23:	14(C)	25(N):	0.716741
#	24:	15(N)	16(N):	0.569774	#	24:	15(N)	16(N):	0.610011
#	25:	15(N)	37(H):	0.656090	#	25:	15(N)	33(H):	0.676855
#	26:	16(N)	17(O):	0.989141	#	26:	16(N)	34(H):	0.692132
#	27:	16(N)	18(O):	1.033978	#	27:	16(N)	35(H):	0.696103
#	28:	19(N)	20(N):	0.569548	#	28:	17(N)	18(N):	0.610026
#	29:	19(N)	38(H):	0.655995	#	29:	17(N)	36(H):	0.676784
#	30:	20(N)	21(O):	0.989141	#	30:	18(N)	37(H):	0.692069
#	31:	20(N)	22(O):	1.033968	#	31:	18(N)	38(H):	0.696077
#	32:	23(N)	24(O):	0.920368	#	32:	19(N)	20(O):	0.906535
#	33:	23(N)	25(O):	1.014927	#	33:	19(N)	21(O):	1.006827
#	34:	26(N)	27(O):	0.961579	#	34:	22(N)	23(O):	0.937508
#	35:	26(N)	28(O):	0.963760	#	35:	22(N)	24(O):	0.951166
#	36:	29(N)	30(O):	0.961536	#	36:	25(N)	26(O):	0.937505
#	37:	29(N)	31(O):	0.963630	#	37:	25(N)	27(O):	0.951188
#	38:	32(N)	33(O):	1.014848	#	38:	28(N)	29(O):	1.006809
#	39:	32(N)	34(O):	0.920302	#	39:	28(N)	30(O):	0.906531
#	28:	19(N)	20(N):	0.569548	#	24:	15(N)	16(N):	0.610011

A7

The bond order >= 0.050000

#	1:	1(N)	2(N):	1.445170
#	2:	1(N)	3(C):	0.932417
#	3:	2(N)	4(C):	0.932332
#	4:	3(C)	5(C):	1.350126
#	5:	3(C)	9(C):	1.412862
#	6:	4(C)	10(C):	1.350070
#	7:	4(C)	14(C):	1.412922

A8

The bond order >= 0.050000

#	1:	1(N)	2(N):	1.455527
#	2:	1(N)	3(C):	0.916896
#	3:	2(N)	4(C):	0.916891
#	4:	3(C)	5(C):	1.356549
#	5:	3(C)	9(C):	1.406590
#	6:	4(C)	10(C):	1.356528
#	7:	4(C)	14(C):	1.406568

#	8:	5(C)	6(C):	1.392307	#	8:	5(C)	6(C):	1.356465
#	9:	5(C)	29(N):	0.678386	#	9:	5(C)	35(N):	0.677518
#	10:	6(C)	7(N):	1.208959	#	10:	6(C)	7(N):	1.208259
#	11:	6(C)	15(C):	1.043793	#	11:	6(C)	15(C):	1.004239
#	12:	7(N)	8(C):	1.227169	#	12:	7(N)	8(C):	1.219923
#	13:	8(C)	9(C):	1.472152	#	13:	8(C)	9(C):	1.493808
#	14:	8(C)	41(H):	0.853754	#	14:	8(C)	47(H):	0.855092
#	15:	9(C)	32(N):	0.686197	#	15:	9(C)	38(N):	0.689686
#	16:	10(C)	11(C):	1.392335	#	16:	10(C)	11(C):	1.356427
#	17:	10(C)	38(N):	0.678385	#	17:	10(C)	44(N):	0.677527
#	18:	11(C)	12(N):	1.208927	#	18:	11(C)	12(N):	1.208278
#	19:	11(C)	22(C):	1.043794	#	19:	11(C)	25(C):	1.004231
#	20:	12(N)	13(C):	1.227182	#	20:	12(N)	13(C):	1.219916
#	21:	13(C)	14(C):	1.472100	#	21:	13(C)	14(C):	1.493808
#	22:	13(C)	42(H):	0.853750	#	22:	13(C)	48(H):	0.855106
#	23:	14(C)	35(N):	0.686184	#	23:	14(C)	41(N):	0.689697
#	24:	15(C)	16(N):	0.539343	#	24:	15(C)	16(N):	0.525784
#	25:	15(C)	19(N):	0.544332	#	25:	15(C)	19(N):	0.460026
#	26:	15(C)	43(H):	0.833264	#	26:	15(C)	22(N):	0.457366
#	27:	16(N)	17(O):	0.999667	#	27:	16(N)	17(O):	0.978970
#	28:	16(N)	18(O):	1.011059	#	28:	16(N)	18(O):	1.043573
#	29:	19(N)	20(O):	0.984811	#	29:	19(N)	20(O):	1.001090
#	30:	19(N)	21(O):	1.035391	#	30:	19(N)	21(O):	1.059882
#	31:	22(C)	23(N):	0.539326	#	31:	22(N)	23(O):	1.047508
#	32:	22(C)	26(N):	0.544358	#	32:	22(N)	24(O):	1.027488
#	33:	22(C)	44(H):	0.833258	#	33:	25(C)	26(N):	0.525769
#	34:	23(N)	24(O):	0.999666	#	34:	25(C)	29(N):	0.460108
#	35:	23(N)	25(O):	1.011045	#	35:	25(C)	32(N):	0.457311
#	36:	26(N)	27(O):	0.984812	#	36:	26(N)	27(O):	0.978933
#	37:	26(N)	28(O):	1.035389	#	37:	26(N)	28(O):	1.043552
#	38:	29(N)	30(O):	0.951933	#	38:	29(N)	30(O):	1.001108
#	39:	29(N)	31(O):	0.998961	#	39:	29(N)	31(O):	1.059894
#	40:	32(N)	33(O):	0.970471	#	40:	32(N)	33(O):	1.047496
#	41:	32(N)	34(O):	0.969807	#	41:	32(N)	34(O):	1.027508
#	42:	35(N)	36(O):	0.970359	#	42:	35(N)	36(O):	0.946419
#	43:	35(N)	37(O):	0.969946	#	43:	35(N)	37(O):	1.027890
#	44:	38(N)	39(O):	0.999147	#	44:	38(N)	39(O):	0.976203
#	45:	38(N)	40(O):	0.951974	#	45:	38(N)	40(O):	0.975395
					#	46:	41(N)	42(O):	0.976210
					#	47:	41(N)	43(O):	0.975368
#	31:	22(C)	23(N):	0.539326	#	48:	44(N)	45(O):	1.027850
					#	49:	44(N)	46(O):	0.946418
					#	35:	25(C)	32(N):	0.457311
A9					A10				

The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	1.441145	#	1:	1(N)	2(N):	1.448633
#	2:	1(N)	3(C):	0.933444	#	2:	1(N)	3(C):	0.917237
#	3:	2(N)	4(C):	0.933474	#	3:	2(N)	4(C):	0.915558
#	4:	3(C)	5(C):	1.357322	#	4:	3(C)	5(C):	1.374541
#	5:	3(C)	9(C):	1.406011	#	5:	3(C)	9(C):	1.382316
#	6:	4(C)	10(C):	1.357334	#	6:	4(C)	10(C):	1.374756
#	7:	4(C)	14(C):	1.405994	#	7:	4(C)	14(C):	1.382095
#	8:	5(C)	6(C):	1.424333	#	8:	5(C)	6(C):	1.342194
#	9:	5(C)	25(N):	0.674178	#	9:	5(C)	27(N):	0.658330
#	10:	6(C)	7(N):	1.287324	#	10:	6(C)	7(N):	1.205285
#	11:	6(C)	17(N):	0.770972	#	11:	6(C)	17(N):	0.903439
#	12:	7(N)	8(C):	1.197860	#	12:	7(N)	8(C):	1.183823
#	13:	8(C)	9(C):	1.477578	#	13:	8(C)	9(C):	1.503623
#	14:	8(C)	55(H):	0.853964	#	14:	8(C)	51(H):	0.854448
#	15:	9(C)	28(N):	0.690918	#	15:	9(C)	30(N):	0.701427
#	16:	10(C)	11(C):	1.424320	#	16:	10(C)	11(C):	1.339318
#	17:	10(C)	34(N):	0.674182	#	17:	10(C)	36(N):	0.656969
#	18:	11(C)	12(N):	1.287343	#	18:	11(C)	12(N):	1.204053
#	19:	11(C)	22(N):	0.770979	#	19:	11(C)	23(N):	0.904502
#	20:	12(N)	13(C):	1.197848	#	20:	12(N)	13(C):	1.183567
#	21:	13(C)	14(C):	1.477594	#	21:	13(C)	14(C):	1.504462
#	22:	13(C)	56(H):	0.853975	#	22:	13(C)	52(H):	0.854815
#	23:	14(C)	31(N):	0.690916	#	23:	14(C)	33(N):	0.702773
#	24:	15(C)	16(N):	1.305302	#	24:	15(C)	16(N):	1.421387
#	25:	15(C)	19(C):	1.275639	#	25:	15(C)	19(C):	1.228763
#	26:	15(C)	37(N):	0.761978	#	26:	15(C)	39(N):	0.745632
#	27:	16(N)	17(N):	0.799940	#	27:	16(N)	17(N):	0.623670
#	28:	17(N)	18(C):	0.937279	#	28:	17(N)	18(C):	0.878308
#	29:	18(C)	19(C):	1.438278	#	29:	18(C)	19(C):	1.355949
#	30:	18(C)	40(N):	0.805649	#	30:	18(C)	20(N):	1.208018
#	31:	19(C)	43(N):	0.734640	#	31:	19(C)	42(N):	0.860199
#	32:	20(C)	21(N):	1.305299	#	32:	20(N)	53(H):	0.667357
#	33:	20(C)	24(C):	1.275637	#	33:	20(N)	54(H):	0.659989
#	34:	20(C)	46(N):	0.761981	#	34:	21(C)	22(N):	1.423730
#	35:	21(N)	22(N):	0.799939	#	35:	21(C)	25(C):	1.229870
#	36:	22(N)	23(C):	0.937306	#	36:	21(C)	45(N):	0.743918
#	37:	23(C)	24(C):	1.438276	#	37:	22(N)	23(N):	0.613887
#	38:	23(C)	49(N):	0.805663	#	38:	23(N)	24(C):	0.877353
#	39:	24(C)	52(N):	0.734641	#	39:	24(C)	25(C):	1.354760
#	40:	25(N)	26(O):	0.980627	#	40:	24(C)	26(N):	1.211329
#	41:	25(N)	27(O):	1.006775	#	41:	25(C)	48(N):	0.867711
#	42:	28(N)	29(O):	0.971521	#	42:	26(N)	55(H):	0.665695
#	43:	28(N)	30(O):	0.975022	#	43:	26(N)	56(H):	0.659358
#	44:	31(N)	32(O):	0.971517	#	44:	27(N)	28(O):	1.000088

#	45:	31(N)	33(O):	0.974985	#	45:	27(N)	29(O):	1.011718
#	46:	34(N)	35(O):	1.006755	#	46:	30(N)	31(O):	0.956094
#	47:	34(N)	36(O):	0.980631	#	47:	30(N)	32(O):	0.964356
#	48:	37(N)	38(O):	1.001490	#	48:	33(N)	34(O):	0.955322
#	49:	37(N)	39(O):	0.953085	#	49:	33(N)	35(O):	0.964983
#	50:	40(N)	41(O):	0.949179	#	50:	36(N)	37(O):	1.011066
#	51:	40(N)	42(O):	0.979100	#	51:	36(N)	38(O):	1.001687
#	52:	43(N)	44(O):	1.005368	#	52:	39(N)	40(O):	0.991163
#	53:	43(N)	45(O):	1.012600	#	53:	39(N)	41(O):	0.989692
#	54:	46(N)	47(O):	1.001493	#	54:	42(N)	43(O):	0.855229
#	55:	46(N)	48(O):	0.953085	#	55:	42(N)	44(O):	0.967409
#	56:	49(N)	50(O):	0.949172	#	56:	45(N)	46(O):	0.997394
#	57:	49(N)	51(O):	0.979097	#	57:	45(N)	47(O):	0.992451
#	58:	52(N)	53(O):	1.005372	#	58:	48(N)	49(O):	0.961300
#	59:	52(N)	54(O):	1.012601	#	59:	48(N)	50(O):	0.854289
#	9:	5(C)	25(N):	0.674178	#	37:	22(N)	23(N):	0.613887

A11

The bond order >= 0.050000

#	1:	1(N)	2(N):	1.434955
#	2:	1(N)	3(C):	0.934342
#	3:	2(N)	4(C):	0.934325
#	4:	3(C)	5(C):	1.360966
#	5:	3(C)	9(C):	1.400285
#	6:	4(C)	10(C):	1.360962
#	7:	4(C)	14(C):	1.400296
#	8:	5(C)	6(C):	1.409234
#	9:	5(C)	27(N):	0.670905
#	10:	6(C)	7(N):	1.273005
#	11:	6(C)	17(N):	0.811083
#	12:	7(N)	8(C):	1.206180
#	13:	8(C)	9(C):	1.476147
#	14:	8(C)	51(H):	0.854098
#	15:	9(C)	30(N):	0.698070
#	16:	10(C)	11(C):	1.409240
#	17:	10(C)	36(N):	0.670904
#	18:	11(C)	12(N):	1.272996
#	19:	11(C)	23(N):	0.811081
#	20:	12(N)	13(C):	1.206185
#	21:	13(C)	14(C):	1.476141
#	22:	13(C)	52(H):	0.854098
#	23:	14(C)	33(N):	0.698063
#	24:	15(C)	16(N):	1.289229
#	25:	15(C)	19(C):	1.216253

A12

The bond order >= 0.050000

#	1:	1(N)	2(N):	1.433901
#	2:	1(N)	3(C):	0.925211
#	3:	2(N)	4(C):	0.925213
#	4:	3(C)	5(C):	1.358574
#	5:	3(C)	9(C):	1.407724
#	6:	4(C)	10(C):	1.358568
#	7:	4(C)	14(C):	1.407712
#	8:	5(C)	6(C):	1.399530
#	9:	5(C)	27(N):	0.666404
#	10:	6(C)	7(N):	1.256292
#	11:	6(C)	17(N):	0.845521
#	12:	7(N)	8(C):	1.219015
#	13:	8(C)	9(C):	1.466036
#	14:	8(C)	45(H):	0.853776
#	15:	9(C)	30(N):	0.697431
#	16:	10(C)	11(C):	1.399539
#	17:	10(C)	36(N):	0.666393
#	18:	11(C)	12(N):	1.256292
#	19:	11(C)	23(N):	0.845524
#	20:	12(N)	13(C):	1.219007
#	21:	13(C)	14(C):	1.466042
#	22:	13(C)	46(H):	0.853776
#	23:	14(C)	33(N):	0.697433
#	24:	15(C)	16(N):	1.406403

#	26:	15(C)	39(N):	0.804728	#	25:	15(C)	19(N):	1.078961
#	27:	16(N)	17(N):	0.850319	#	26:	15(C)	39(N):	0.737892
#	28:	17(N)	18(C):	0.849501	#	27:	16(N)	17(N):	0.655335
#	29:	18(C)	19(C):	1.357090	#	28:	17(N)	18(C):	0.852181
#	30:	18(C)	42(N):	0.898312	#	29:	18(C)	19(N):	1.287325
#	31:	19(C)	20(N):	1.159469	#	30:	18(C)	20(N):	1.098892
#	32:	20(N)	53(H):	0.675862	#	31:	20(N)	47(H):	0.669389
#	33:	20(N)	54(H):	0.673853	#	32:	20(N)	48(H):	0.677619
#	34:	21(C)	22(N):	1.289227	#	33:	21(C)	22(N):	1.406405
#	35:	21(C)	25(C):	1.216253	#	34:	21(C)	25(N):	1.078964
#	36:	21(C)	45(N):	0.804728	#	35:	21(C)	42(N):	0.737897
#	37:	22(N)	23(N):	0.850321	#	36:	22(N)	23(N):	0.655337
#	38:	23(N)	24(C):	0.849506	#	37:	23(N)	24(C):	0.852193
#	39:	24(C)	25(C):	1.357089	#	38:	24(C)	25(N):	1.287325
#	40:	24(C)	48(N):	0.898313	#	39:	24(C)	26(N):	1.098888
#	41:	25(C)	26(N):	1.159464	#	40:	26(N)	49(H):	0.669377
#	42:	26(N)	55(H):	0.675865	#	41:	26(N)	50(H):	0.677617
#	43:	26(N)	56(H):	0.673855	#	42:	27(N)	28(O):	1.038469
#	44:	27(N)	28(O):	0.976710	#	43:	27(N)	29(O):	0.919390
#	45:	27(N)	29(O):	1.006438	#	44:	30(N)	31(O):	0.970817
#	46:	30(N)	31(O):	0.960397	#	45:	30(N)	32(O):	0.967212
#	47:	30(N)	32(O):	0.973416	#	46:	33(N)	34(O):	0.970808
#	48:	33(N)	34(O):	0.960394	#	47:	33(N)	35(O):	0.967204
#	49:	33(N)	35(O):	0.973439	#	48:	36(N)	37(O):	0.919371
#	50:	36(N)	37(O):	1.006428	#	49:	36(N)	38(O):	1.038436
#	51:	36(N)	38(O):	0.976720	#	50:	39(N)	40(O):	0.972784
#	52:	39(N)	40(O):	1.001962	#	51:	39(N)	41(O):	0.969235
#	53:	39(N)	41(O):	0.878949	#	52:	42(N)	43(O):	0.972786
#	54:	42(N)	43(O):	0.926672	#	53:	42(N)	44(O):	0.969220
#	55:	42(N)	44(O):	0.870806					
#	56:	45(N)	46(O):	1.001964					
#	57:	45(N)	47(O):	0.878950	#	27:	16(N)	17(N):	0.655335
#	58:	48(N)	49(O):	0.926671					
#	59:	48(N)	50(O):	0.870800					
#	17:	10(C)	36(N):	0.670904					

B1					B2				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	1.434088	#	1:	1(N)	2(N):	1.441534
#	2:	1(N)	3(C):	0.928649	#	2:	1(N)	3(C):	0.921804
#	3:	2(N)	4(C):	0.928614	#	3:	2(N)	4(C):	0.928238
#	4:	3(C)	5(C):	1.377553	#	4:	3(C)	5(C):	1.372777
#	5:	3(C)	9(C):	1.420188	#	5:	3(C)	9(C):	1.401054
#	6:	4(C)	10(C):	1.377486	#	6:	4(C)	10(C):	1.402102

#	7:	4(C)	14(C):	1.420267	#	7:	4(C)	14(C):	1.354201
#	8:	5(C)	6(C):	1.376462	#	8:	5(C)	6(C):	1.385534
#	9:	5(C)	15(N):	0.686632	#	9:	5(C)	15(N):	0.677386
#	10:	6(C)	7(N):	1.194480	#	10:	6(C)	7(N):	1.175107
#	11:	6(C)	29(C):	1.257036	#	11:	6(C)	30(N):	0.911940
#	12:	7(N)	8(C):	1.187270	#	12:	7(N)	8(C):	1.172232
#	13:	8(C)	9(C):	1.392581	#	13:	8(C)	9(C):	1.395901
#	14:	8(C)	27(C):	1.258694	#	14:	8(C)	27(N):	0.919381
#	15:	9(C)	21(N):	0.695103	#	15:	9(C)	21(N):	0.691385
#	16:	10(C)	11(C):	1.376491	#	16:	10(C)	11(C):	1.365456
#	17:	10(C)	18(N):	0.686644	#	17:	10(C)	18(N):	0.682614
#	18:	11(C)	12(N):	1.194442	#	18:	11(C)	12(N):	1.224275
#	19:	11(C)	31(C):	1.257021	#	19:	11(C)	33(N):	0.921132
#	20:	12(N)	13(C):	1.187325	#	20:	12(N)	13(C):	1.186377
#	21:	13(C)	14(C):	1.392572	#	21:	13(C)	14(C):	1.334723
#	22:	13(C)	33(C):	1.258681	#	22:	13(C)	36(N):	0.901361
#	23:	14(C)	24(N):	0.695082	#	23:	14(C)	24(N):	0.698008
#	24:	15(N)	16(O):	1.006830	#	24:	15(N)	16(O):	0.997255
#	25:	15(N)	17(O):	0.985859	#	25:	15(N)	17(O):	0.976812
#	26:	18(N)	19(O):	0.985971	#	26:	18(N)	19(O):	0.969647
#	27:	18(N)	20(O):	1.006834	#	27:	18(N)	20(O):	0.996348
#	28:	21(N)	22(O):	0.997048	#	28:	21(N)	22(O):	0.983245
#	29:	21(N)	23(O):	0.978481	#	29:	21(N)	23(O):	0.962478
#	30:	24(N)	25(O):	0.997102	#	30:	24(N)	25(O):	0.938026
#	31:	24(N)	26(O):	0.978656	#	31:	24(N)	26(O):	0.970137
#	32:	27(C)	28(N):	2.540722	#	32:	27(N)	28(N):	1.133482
#	33:	29(C)	30(N):	2.541503	#	33:	28(N)	29(N):	2.239904
#	34:	31(C)	32(N):	2.541502	#	34:	30(N)	31(N):	1.136246
#	35:	33(C)	34(N):	2.540736	#	35:	31(N)	32(N):	2.242783
					#	36:	33(N)	34(N):	1.129308
#	9:	5(C)	15(N):	0.686632	#	37:	34(N)	35(N):	2.259919
					#	38:	36(N)	37(N):	1.141414
					#	39:	37(N)	38(N):	2.210928
					#	9:	5(C)	15(N):	0.677386

B3					B4				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	1.416006	#	1:	1(N)	2(N):	1.458449
#	2:	1(N)	3(C):	0.923866	#	2:	1(N)	3(C):	0.904837
#	3:	2(N)	4(C):	0.927636	#	3:	2(N)	4(C):	0.904844
#	4:	3(C)	5(C):	1.355211	#	4:	3(C)	5(C):	1.364389
#	5:	3(C)	9(C):	1.394948	#	5:	3(C)	9(C):	1.363629
#	6:	4(C)	10(C):	1.349279	#	6:	4(C)	10(C):	1.364322
#	7:	4(C)	14(C):	1.402786	#	7:	4(C)	14(C):	1.363671

#	8:	5(C)	6(C):	1.383867	#	8:	5(C)	6(C):	1.249355
#	9:	5(C)	15(N):	0.671474	#	9:	5(C)	19(N):	0.712956
#	10:	6(C)	7(N):	1.254640	#	10:	6(C)	7(N):	1.182499
#	11:	6(C)	30(N):	0.865695	#	11:	6(C)	16(N):	1.157970
#	12:	7(N)	8(C):	1.253654	#	12:	7(N)	8(C):	1.173521
#	13:	8(C)	9(C):	1.410890	#	13:	8(C)	9(C):	1.268284
#	14:	8(C)	27(N):	0.852713	#	14:	8(C)	15(N):	1.170871
#	15:	9(C)	21(N):	0.674370	#	15:	9(C)	25(N):	0.745335
#	16:	10(C)	11(C):	1.393739	#	16:	10(C)	11(C):	1.249304
#	17:	10(C)	18(N):	0.672123	#	17:	10(C)	22(N):	0.713036
#	18:	11(C)	12(N):	1.242083	#	18:	11(C)	12(N):	1.182430
#	19:	11(C)	33(N):	0.869008	#	19:	11(C)	17(N):	1.158084
#	20:	12(N)	13(C):	1.247063	#	20:	12(N)	13(C):	1.173600
#	21:	13(C)	14(C):	1.397679	#	21:	13(C)	14(C):	1.268242
#	22:	13(C)	36(N):	0.878122	#	22:	13(C)	18(N):	1.170868
#	23:	14(C)	24(N):	0.667913	#	23:	14(C)	28(N):	0.745345
#	24:	15(N)	16(O):	0.999646	#	24:	15(N)	31(H):	0.667510
#	25:	15(N)	17(O):	1.018346	#	25:	15(N)	32(H):	0.684037
#	26:	18(N)	19(O):	0.993804	#	26:	16(N)	33(H):	0.684213
#	27:	18(N)	20(O):	1.010665	#	27:	16(N)	34(H):	0.672743
#	28:	21(N)	22(O):	1.008319	#	28:	17(N)	35(H):	0.684215
#	29:	21(N)	23(O):	1.011332	#	29:	17(N)	36(H):	0.672717
#	30:	24(N)	25(O):	1.018628	#	30:	18(N)	37(H):	0.667499
#	31:	24(N)	26(O):	0.996366	#	31:	18(N)	38(H):	0.684026
#	32:	27(N)	28(F):	0.148025	#	32:	19(N)	20(O):	0.875930
#	33:	27(N)	29(F):	0.145485	#	33:	19(N)	21(O):	0.996046
#	34:	30(N)	31(F):	0.177278	#	34:	22(N)	23(O):	0.995947
#	35:	30(N)	32(F):	0.138904	#	35:	22(N)	24(O):	0.875878
#	36:	33(N)	34(F):	0.175500	#	36:	25(N)	26(O):	0.854534
#	37:	33(N)	35(F):	0.138560	#	37:	25(N)	27(O):	0.950194
#	38:	36(N)	37(F):	0.141016	#	38:	28(N)	29(O):	0.854546
#	39:	36(N)	38(F):	0.174635	#	39:	28(N)	30(O):	0.950200

#	37:	33(N)	35(F):	0.138560	#	30:	18(N)	37(H):	0.667499

B5					B6				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	1.453213	#	1:	1(N)	2(N):	1.449391
#	2:	1(N)	3(C):	0.911214	#	2:	1(N)	3(C):	0.930275
#	3:	2(N)	4(C):	0.911222	#	3:	2(N)	4(C):	0.884835
#	4:	3(C)	5(C):	1.372423	#	4:	3(C)	5(C):	1.361627
#	5:	3(C)	9(C):	1.377907	#	5:	3(C)	9(C):	1.344637
#	6:	4(C)	10(C):	1.372446	#	6:	4(C)	10(C):	1.311649
#	7:	4(C)	14(C):	1.377928	#	7:	4(C)	14(C):	1.440838

#	8:	5(C)	6(C):	1.287784	#	8:	5(C)	6(C):	1.227359
#	9:	5(C)	15(N):	0.688881	#	9:	5(C)	15(N):	0.719833
#	10:	6(C)	7(N):	1.232452	#	10:	6(C)	7(N):	1.161915
#	11:	6(C)	31(N):	0.972160	#	11:	6(C)	29(N):	1.133331
#	12:	7(N)	8(C):	1.222413	#	12:	7(N)	8(C):	1.156651
#	13:	8(C)	9(C):	1.301920	#	13:	8(C)	9(C):	1.243060
#	14:	8(C)	27(N):	0.993184	#	14:	8(C)	27(N):	1.135626
#	15:	9(C)	21(N):	0.714419	#	15:	9(C)	21(N):	0.765333
#	16:	10(C)	11(C):	1.287763	#	16:	10(C)	11(C):	1.266531
#	17:	10(C)	18(N):	0.688868	#	17:	10(C)	18(N):	0.735104
#	18:	11(C)	12(N):	1.232445	#	18:	11(C)	12(N):	1.128516
#	19:	11(C)	35(N):	0.972158	#	19:	11(C)	31(N):	1.101832
#	20:	12(N)	13(C):	1.222418	#	20:	12(N)	13(C):	1.185519
#	21:	13(C)	14(C):	1.301946	#	21:	13(C)	14(C):	1.309160
#	22:	13(C)	39(N):	0.993170	#	22:	13(C)	33(N):	1.074593
#	23:	14(C)	24(N):	0.714410	#	23:	14(C)	24(N):	0.659961
#	24:	15(N)	16(O):	0.914820	#	24:	15(N)	16(O):	0.873875
#	25:	15(N)	17(O):	1.011794	#	25:	15(N)	17(O):	0.985396
#	26:	18(N)	19(O):	1.011803	#	26:	18(N)	19(O):	0.980804
#	27:	18(N)	20(O):	0.914829	#	27:	18(N)	20(O):	0.867632
#	28:	21(N)	22(O):	0.896810	#	28:	21(N)	22(O):	0.854546
#	29:	21(N)	23(O):	0.982720	#	29:	21(N)	23(O):	0.933903
#	30:	24(N)	25(O):	0.896805	#	30:	24(N)	25(O):	1.003151
#	31:	24(N)	26(O):	0.982734	#	31:	24(N)	26(O):	0.962450
#	32:	27(N)	28(N):	0.545837	#	32:	27(N)	28(N):	0.619149
#	33:	27(N)	43(H):	0.647109	#	33:	27(N)	35(H):	0.661898
#	34:	28(N)	29(O):	0.992197	#	34:	28(N)	36(H):	0.693199
#	35:	28(N)	30(O):	1.048751	#	35:	28(N)	37(H):	0.693808
#	36:	31(N)	32(N):	0.558281	#	36:	29(N)	30(N):	0.621848
#	37:	31(N)	44(H):	0.650215	#	37:	29(N)	38(H):	0.663573
#	38:	32(N)	33(O):	0.988754	#	38:	30(N)	39(H):	0.691928
#	39:	32(N)	34(O):	1.048239	#	39:	30(N)	40(H):	0.692470
#	40:	35(N)	36(N):	0.558307	#	40:	31(N)	32(N):	0.621656
#	41:	35(N)	45(H):	0.650224	#	41:	31(N)	41(H):	0.671765
#	42:	36(N)	37(O):	0.988748	#	42:	32(N)	42(H):	0.692061
#	43:	36(N)	38(O):	1.048228	#	43:	32(N)	43(H):	0.694268
#	44:	39(N)	40(N):	0.545869	#	44:	33(N)	34(N):	0.657362
#	45:	39(N)	46(H):	0.647106	#	45:	33(N)	44(H):	0.669941
#	46:	40(N)	41(O):	0.992186	#	46:	34(N)	45(H):	0.694408
#	47:	40(N)	42(O):	1.048750	#	47:	34(N)	46(H):	0.694773

#	32:	27(N)	28(N):	0.545837	#	32:	27(N)	28(N):	0.619149

B7	B8
The bond order >= 0.050000	The bond order >= 0.050000

#	1:	1(N)	2(N):	1.439134	#	1:	1(N)	2(N):	1.454131
#	2:	1(N)	3(C):	0.926231	#	2:	1(N)	3(C):	0.912691
#	3:	2(N)	4(C):	0.925490	#	3:	2(N)	4(C):	0.912693
#	4:	3(C)	5(C):	1.366436	#	4:	3(C)	5(C):	1.363563
#	5:	3(C)	9(C):	1.407804	#	5:	3(C)	9(C):	1.404293
#	6:	4(C)	10(C):	1.358347	#	6:	4(C)	10(C):	1.363573
#	7:	4(C)	14(C):	1.412038	#	7:	4(C)	14(C):	1.404305
#	8:	5(C)	6(C):	1.396610	#	8:	5(C)	6(C):	1.377265
#	9:	5(C)	15(N):	0.685382	#	9:	5(C)	15(N):	0.677810
#	10:	6(C)	7(N):	1.215819	#	10:	6(C)	7(N):	1.201490
#	11:	6(C)	34(C):	1.043763	#	11:	6(C)	37(C):	1.007115
#	12:	7(N)	8(C):	1.208468	#	12:	7(N)	8(C):	1.204289
#	13:	8(C)	9(C):	1.408980	#	13:	8(C)	9(C):	1.399269
#	14:	8(C)	27(C):	1.044678	#	14:	8(C)	27(C):	1.012998
#	15:	9(C)	21(N):	0.690997	#	15:	9(C)	21(N):	0.691529
#	16:	10(C)	11(C):	1.411994	#	16:	10(C)	11(C):	1.377258
#	17:	10(C)	18(N):	0.682632	#	17:	10(C)	18(N):	0.677802
#	18:	11(C)	12(N):	1.199065	#	18:	11(C)	12(N):	1.201501
#	19:	11(C)	41(C):	1.045804	#	19:	11(C)	47(C):	1.007110
#	20:	12(N)	13(C):	1.214107	#	20:	12(N)	13(C):	1.204289
#	21:	13(C)	14(C):	1.393711	#	21:	13(C)	14(C):	1.399273
#	22:	13(C)	48(C):	1.028379	#	22:	13(C)	57(C):	1.013003
#	23:	14(C)	24(N):	0.688861	#	23:	14(C)	24(N):	0.691556
#	24:	15(N)	16(O):	0.958139	#	24:	15(N)	16(O):	0.956421
#	25:	15(N)	17(O):	1.003376	#	25:	15(N)	17(O):	1.034093
#	26:	18(N)	19(O):	1.000914	#	26:	18(N)	19(O):	1.034060
#	27:	18(N)	20(O):	0.963310	#	27:	18(N)	20(O):	0.956422
#	28:	21(N)	22(O):	0.944245	#	28:	21(N)	22(O):	0.954012
#	29:	21(N)	23(O):	0.989519	#	29:	21(N)	23(O):	1.011803
#	30:	24(N)	25(O):	0.943000	#	30:	24(N)	25(O):	0.954016
#	31:	24(N)	26(O):	1.011115	#	31:	24(N)	26(O):	1.011767
#	32:	27(C)	28(N):	0.541590	#	32:	27(C)	28(N):	0.457241
#	33:	27(C)	31(N):	0.543987	#	33:	27(C)	31(N):	0.522536
#	34:	27(C)	55(H):	0.832409	#	34:	27(C)	34(N):	0.463598
#	35:	28(N)	29(O):	0.987437	#	35:	28(N)	29(O):	1.047357
#	36:	28(N)	30(O):	1.025437	#	36:	28(N)	30(O):	1.020500
#	37:	31(N)	32(O):	0.994125	#	37:	31(N)	32(O):	0.978608
#	38:	31(N)	33(O):	1.029766	#	38:	31(N)	33(O):	1.049346
#	39:	34(C)	35(N):	0.534155	#	39:	34(N)	35(O):	1.071828
#	40:	34(C)	38(N):	0.540465	#	40:	34(N)	36(O):	1.004603
#	41:	34(C)	56(H):	0.830808	#	41:	37(C)	38(N):	0.529236
#	42:	35(N)	36(O):	0.999706	#	42:	37(C)	41(N):	0.458740
#	43:	35(N)	37(O):	1.018683	#	43:	37(C)	44(N):	0.453161
#	44:	38(N)	39(O):	0.994918	#	44:	38(N)	39(O):	0.974044
#	45:	38(N)	40(O):	1.037786	#	45:	38(N)	40(O):	1.047543

#	46:	41(C)	42(N):	0.535470	#	46:	41(N)	42(O):	1.000328
#	47:	41(C)	45(N):	0.536991	#	47:	41(N)	43(O):	1.074560
#	48:	41(C)	57(H):	0.834003	#	48:	44(N)	45(O):	1.048630
#	49:	42(N)	43(O):	0.999635	#	49:	44(N)	46(O):	1.020287
#	50:	42(N)	44(O):	1.022820	#	50:	47(C)	48(N):	0.529203
#	51:	45(N)	46(O):	0.988872	#	51:	47(C)	51(N):	0.458740
#	52:	45(N)	47(O):	1.033770	#	52:	47(C)	54(N):	0.453172
#	53:	48(C)	49(N):	0.554592	#	53:	48(N)	49(O):	0.974049
#	54:	48(C)	52(N):	0.526082	#	54:	48(N)	50(O):	1.047553
#	55:	48(C)	58(H):	0.830761	#	55:	51(N)	52(O):	1.000354
#	56:	49(N)	50(O):	1.001370	#	56:	51(N)	53(O):	1.074594
#	57:	49(N)	51(O):	1.024049	#	57:	54(N)	55(O):	1.048619
#	58:	52(N)	53(O):	0.979629	#	58:	54(N)	56(O):	1.020291
#	59:	52(N)	54(O):	1.031181	#	59:	57(C)	58(N):	0.457237
					#	60:	57(C)	61(N):	0.522540
					#	61:	57(C)	64(N):	0.463595
#	54:	48(C)	52(N):	0.526082	#	62:	58(N)	59(O):	1.047354
					#	63:	58(N)	60(O):	1.020496
					#	64:	61(N)	62(O):	0.978600
					#	65:	61(N)	63(O):	1.049290
					#	66:	64(N)	65(O):	1.071839
					#	67:	64(N)	66(O):	1.004598
					#	43:	37(C)	44(N):	0.453161

B9					B10				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	1.464493	#	1:	1(N)	2(N):	1.444620
#	2:	1(N)	3(C):	0.928313	#	2:	1(N)	3(C):	0.923031
#	3:	2(N)	4(C):	0.911467	#	3:	2(N)	4(C):	0.916586
#	4:	3(C)	5(C):	1.365664	#	4:	3(C)	5(C):	1.397268
#	5:	3(C)	9(C):	1.397977	#	5:	3(C)	9(C):	1.362232
#	6:	4(C)	10(C):	1.366164	#	6:	4(C)	10(C):	1.397347
#	7:	4(C)	14(C):	1.372840	#	7:	4(C)	14(C):	1.337699
#	8:	5(C)	6(C):	1.413401	#	8:	5(C)	6(C):	1.405187
#	9:	5(C)	35(N):	0.670127	#	9:	5(C)	39(N):	0.679252
#	10:	6(C)	7(N):	1.266353	#	10:	6(C)	7(N):	1.179462
#	11:	6(C)	32(N):	0.804657	#	11:	6(C)	17(N):	0.893913
#	12:	7(N)	8(C):	1.257891	#	12:	7(N)	8(C):	1.171282
#	13:	8(C)	9(C):	1.445135	#	13:	8(C)	9(C):	1.369162
#	14:	8(C)	27(N):	0.800321	#	14:	8(C)	23(N):	0.910743
#	15:	9(C)	41(N):	0.687665	#	15:	9(C)	45(N):	0.667400
#	16:	10(C)	11(C):	1.409830	#	16:	10(C)	11(C):	1.333156
#	17:	10(C)	38(N):	0.668478	#	17:	10(C)	42(N):	0.665774
#	18:	11(C)	12(N):	1.260110	#	18:	11(C)	12(N):	1.226119

#	19:	11(C)	22(N):	0.819404	#	19:	11(C)	35(N):	0.947544
#	20:	12(N)	13(C):	1.258895	#	20:	12(N)	13(C):	1.204824
#	21:	13(C)	14(C):	1.440522	#	21:	13(C)	14(C):	1.418883
#	22:	13(C)	17(N):	0.783558	#	22:	13(C)	29(N):	0.821136
#	23:	14(C)	44(N):	0.685782	#	23:	14(C)	48(N):	0.710781
#	24:	15(C)	16(N):	1.298126	#	24:	15(C)	16(N):	1.421997
#	25:	15(C)	19(C):	1.274816	#	25:	15(C)	19(C):	1.225368
#	26:	15(C)	47(N):	0.760272	#	26:	15(C)	51(N):	0.747159
#	27:	16(N)	17(N):	0.808705	#	27:	16(N)	17(N):	0.617759
#	28:	17(N)	18(C):	0.935155	#	28:	17(N)	18(C):	0.899476
#	29:	18(C)	19(C):	1.440724	#	29:	18(C)	19(C):	1.371926
#	30:	18(C)	50(N):	0.817179	#	30:	18(C)	20(N):	1.149467
#	31:	19(C)	53(N):	0.732680	#	31:	19(C)	54(N):	0.849047
#	32:	20(C)	21(N):	1.329628	#	32:	20(N)	75(H):	0.678845
#	33:	20(C)	24(C):	1.261232	#	33:	20(N)	76(H):	0.656796
#	34:	20(C)	56(N):	0.754209	#	34:	21(C)	22(N):	1.422075
#	35:	21(N)	22(N):	0.772531	#	35:	21(C)	25(C):	1.228729
#	36:	22(N)	23(C):	0.914449	#	36:	21(C)	57(N):	0.744514
#	37:	23(C)	24(C):	1.454996	#	37:	22(N)	23(N):	0.610665
#	38:	23(C)	59(N):	0.788151	#	38:	23(N)	24(C):	0.882079
#	39:	24(C)	62(N):	0.738829	#	39:	24(C)	25(C):	1.359414
#	40:	25(C)	26(N):	1.311578	#	40:	24(C)	26(N):	1.189178
#	41:	25(C)	29(C):	1.272749	#	41:	25(C)	60(N):	0.859418
#	42:	25(C)	65(N):	0.759579	#	42:	26(N)	77(H):	0.671069
#	43:	26(N)	27(N):	0.792009	#	43:	26(N)	78(H):	0.656696
#	44:	27(N)	28(C):	0.922848	#	44:	27(C)	28(N):	1.437738
#	45:	28(C)	29(C):	1.443925	#	45:	27(C)	31(C):	1.229267
#	46:	28(C)	68(N):	0.802322	#	46:	27(C)	63(N):	0.739589
#	47:	29(C)	71(N):	0.735844	#	47:	28(N)	29(N):	0.585302
#	48:	30(C)	31(N):	1.319073	#	48:	29(N)	30(C):	0.885313
#	49:	30(C)	34(C):	1.267630	#	49:	30(C)	31(C):	1.359642
#	50:	30(C)	74(N):	0.756819	#	50:	30(C)	32(N):	1.187619
#	51:	31(N)	32(N):	0.781373	#	51:	31(C)	66(N):	0.850816
#	52:	32(N)	33(C):	0.919370	#	52:	32(N)	79(H):	0.663018
#	53:	33(C)	34(C):	1.446834	#	53:	32(N)	80(H):	0.658590
#	54:	33(C)	77(N):	0.798430	#	54:	33(C)	34(N):	1.420579
#	55:	34(C)	80(N):	0.734771	#	55:	33(C)	37(C):	1.233121
#	56:	35(N)	36(O):	0.995404	#	56:	33(C)	69(N):	0.746675
#	57:	35(N)	37(O):	0.993324	#	57:	34(N)	35(N):	0.616103
#	58:	38(N)	39(O):	0.985111	#	58:	35(N)	36(C):	0.844598
#	59:	38(N)	40(O):	1.001029	#	59:	36(C)	37(C):	1.355467
#	60:	41(N)	42(O):	0.992856	#	60:	36(C)	38(N):	1.218786
#	61:	41(N)	43(O):	0.971613	#	61:	37(C)	72(N):	0.859076
#	62:	44(N)	45(O):	0.974029	#	62:	38(N)	81(H):	0.658100
#	63:	44(N)	46(O):	0.976911	#	63:	38(N)	82(H):	0.657233

#	64:	47(N)	48(O):	1.001343	#	64:	39(N)	40(O):	0.996387
#	65:	47(N)	49(O):	0.953422	#	65:	39(N)	41(O):	0.991941
#	66:	50(N)	51(O):	0.929196	#	66:	42(N)	43(O):	1.009875
#	67:	50(N)	52(O):	0.988176	#	67:	42(N)	44(O):	1.010742
#	68:	53(N)	54(O):	1.010338	#	68:	45(N)	46(O):	0.991219
#	69:	53(N)	55(O):	1.011356	#	69:	45(N)	47(O):	1.012168
#	70:	56(N)	57(O):	1.006077	#	70:	48(N)	49(O):	0.994662
#	71:	56(N)	58(O):	0.960109	#	71:	48(N)	50(O):	0.931780
#	72:	59(N)	60(O):	0.952357	#	72:	51(N)	52(O):	1.002918
#	73:	59(N)	61(O):	0.985272	#	73:	51(N)	53(O):	0.987410
#	74:	62(N)	63(O):	1.003041	#	74:	54(N)	55(O):	0.858266
#	75:	62(N)	64(O):	1.008582	#	75:	54(N)	56(O):	0.982471
#	76:	65(N)	66(O):	1.007235	#	76:	57(N)	58(O):	0.994314
#	77:	65(N)	67(O):	0.959734	#	77:	57(N)	59(O):	0.992247
#	78:	68(N)	69(O):	0.944488	#	78:	60(N)	61(O):	0.969571
#	79:	68(N)	70(O):	0.985468	#	79:	60(N)	62(O):	0.855726
#	80:	71(N)	72(O):	1.012536	#	80:	63(N)	64(O):	1.009287
#	81:	71(N)	73(O):	1.015738	#	81:	63(N)	65(O):	0.962461
#	82:	74(N)	75(O):	1.008380	#	82:	66(N)	67(O):	0.863756
#	83:	74(N)	76(O):	0.960513	#	83:	66(N)	68(O):	0.965105
#	84:	77(N)	78(O):	0.990146	#	84:	69(N)	70(O):	0.994650
#	85:	77(N)	79(O):	0.947205	#	85:	69(N)	71(O):	0.991286
#	86:	80(N)	81(O):	1.013281	#	86:	72(N)	73(O):	0.960753
#	87:	80(N)	82(O):	1.001638	#	87:	72(N)	74(O):	0.867522
#	17:	10(C)	38(N):	0.668478	#	47:	28(N)	29(N):	0.585302

B11					B12				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	1.444527	#	1:	1(N)	2(N):	1.425156
#	2:	1(N)	3(C):	0.926682	#	2:	1(N)	3(C):	0.924985
#	3:	2(N)	4(C):	0.926686	#	3:	2(N)	4(C):	0.934885
#	4:	3(C)	5(C):	1.354477	#	4:	3(C)	5(C):	1.319410
#	5:	3(C)	9(C):	1.396139	#	5:	3(C)	9(C):	1.406053
#	6:	4(C)	10(C):	1.354487	#	6:	4(C)	10(C):	1.357755
#	7:	4(C)	14(C):	1.396151	#	7:	4(C)	14(C):	1.421964
#	8:	5(C)	6(C):	1.414324	#	8:	5(C)	6(C):	1.390943
#	9:	5(C)	39(N):	0.674611	#	9:	5(C)	39(N):	0.717248
#	10:	6(C)	7(N):	1.248447	#	10:	6(C)	7(N):	1.202990
#	11:	6(C)	17(N):	0.831741	#	11:	6(C)	17(N):	0.847162
#	12:	7(N)	8(C):	1.255510	#	12:	7(N)	8(C):	1.224178
#	13:	8(C)	9(C):	1.410734	#	13:	8(C)	9(C):	1.326572
#	14:	8(C)	23(N):	0.801747	#	14:	8(C)	23(N):	0.971465
#	15:	9(C)	45(N):	0.693290	#	15:	9(C)	45(N):	0.660232
#	16:	10(C)	11(C):	1.414326	#	16:	10(C)	11(C):	1.405704

#	17:	10(C)	42(N):	0.674612	#	17:	10(C)	42(N):	0.679806
#	18:	11(C)	12(N):	1.248452	#	18:	11(C)	12(N):	1.230570
#	19:	11(C)	35(N):	0.831734	#	19:	11(C)	35(N):	0.847112
#	20:	12(N)	13(C):	1.255508	#	20:	12(N)	13(C):	1.234525
#	21:	13(C)	14(C):	1.410726	#	21:	13(C)	14(C):	1.409588
#	22:	13(C)	29(N):	0.801750	#	22:	13(C)	29(N):	0.855351
#	23:	14(C)	48(N):	0.693289	#	23:	14(C)	48(N):	0.682245
#	24:	15(C)	16(N):	1.308504	#	24:	15(C)	16(N):	1.424129
#	25:	15(C)	19(C):	1.210668	#	25:	15(C)	19(N):	1.097430
#	26:	15(C)	51(N):	0.800778	#	26:	15(C)	51(N):	0.744548
#	27:	16(N)	17(N):	0.837349	#	27:	16(N)	17(N):	0.619463
#	28:	17(N)	18(C):	0.837705	#	28:	17(N)	18(C):	0.817562
#	29:	18(C)	19(C):	1.361563	#	29:	18(C)	19(N):	1.277253
#	30:	18(C)	54(N):	0.886698	#	30:	18(C)	20(N):	1.153304
#	31:	19(C)	20(N):	1.163041	#	31:	20(N)	63(H):	0.663127
#	32:	20(N)	75(H):	0.672554	#	32:	20(N)	64(H):	0.678526
#	33:	20(N)	76(H):	0.675040	#	33:	21(C)	22(N):	1.399630
#	34:	21(C)	22(N):	1.306672	#	34:	21(C)	25(N):	1.097850
#	35:	21(C)	25(C):	1.215940	#	35:	21(C)	54(N):	0.732113
#	36:	21(C)	57(N):	0.805174	#	36:	22(N)	23(N):	0.642726
#	37:	22(N)	23(N):	0.854388	#	37:	23(N)	24(C):	0.780935
#	38:	23(N)	24(C):	0.836395	#	38:	24(C)	25(N):	1.275026
#	39:	24(C)	25(C):	1.362546	#	39:	24(C)	26(N):	1.210653
#	40:	24(C)	60(N):	0.920646	#	40:	26(N)	65(H):	0.657378
#	41:	25(C)	26(N):	1.167371	#	41:	26(N)	66(H):	0.675584
#	42:	26(N)	77(H):	0.675193	#	42:	27(C)	28(N):	1.415099
#	43:	26(N)	78(H):	0.677678	#	43:	27(C)	31(N):	1.078220
#	44:	27(C)	28(N):	1.306680	#	44:	27(C)	57(N):	0.738171
#	45:	27(C)	31(C):	1.215943	#	45:	28(N)	29(N):	0.634832
#	46:	27(C)	63(N):	0.805170	#	46:	29(N)	30(C):	0.834284
#	47:	28(N)	29(N):	0.854385	#	47:	30(C)	31(N):	1.286234
#	48:	29(N)	30(C):	0.836392	#	48:	30(C)	32(N):	1.126121
#	49:	30(C)	31(C):	1.362551	#	49:	32(N)	67(H):	0.668302
#	50:	30(C)	66(N):	0.920644	#	50:	32(N)	68(H):	0.674979
#	51:	31(C)	32(N):	1.167372	#	51:	33(C)	34(N):	1.411810
#	52:	32(N)	79(H):	0.675198	#	52:	33(C)	37(N):	1.075028
#	53:	32(N)	80(H):	0.677683	#	53:	33(C)	60(N):	0.738962
#	54:	33(C)	34(N):	1.308498	#	54:	34(N)	35(N):	0.641133
#	55:	33(C)	37(C):	1.210676	#	55:	35(N)	36(C):	0.847287
#	56:	33(C)	69(N):	0.800778	#	56:	36(C)	37(N):	1.289742
#	57:	34(N)	35(N):	0.837354	#	57:	36(C)	38(N):	1.114166
#	58:	35(N)	36(C):	0.837707	#	58:	38(N)	69(H):	0.668557
#	59:	36(C)	37(C):	1.361562	#	59:	38(N)	70(H):	0.678513
#	60:	36(C)	72(N):	0.886702	#	60:	39(N)	40(O):	0.929128
#	61:	37(C)	38(N):	1.163038	#	61:	39(N)	41(O):	0.973968

#	62:	38(N)	81(H):	0.672558	#	62:	42(N)	43(O):	0.952397
#	63:	38(N)	82(H):	0.675041	#	63:	42(N)	44(O):	1.035052
#	64:	39(N)	40(O):	0.988620	#	64:	45(N)	46(O):	0.990860
#	65:	39(N)	41(O):	1.006208	#	65:	45(N)	47(O):	1.021433
#	66:	42(N)	43(O):	1.006207	#	66:	48(N)	49(O):	1.035409
#	67:	42(N)	44(O):	0.988627	#	67:	48(N)	50(O):	0.960207
#	68:	45(N)	46(O):	0.949510	#	68:	51(N)	52(O):	0.995815
#	69:	45(N)	47(O):	0.996683	#	69:	51(N)	53(O):	0.949630
#	70:	48(N)	49(O):	0.949506	#	70:	54(N)	55(O):	0.985128
#	71:	48(N)	50(O):	0.996684	#	71:	54(N)	56(O):	0.969376
#	72:	51(N)	52(O):	1.008130	#	72:	57(N)	58(O):	0.984920
#	73:	51(N)	53(O):	0.884625	#	73:	57(N)	59(O):	0.968844
#	74:	54(N)	55(O):	0.935450	#	74:	60(N)	61(O):	0.983463
#	75:	54(N)	56(O):	0.869383	#	75:	60(N)	62(O):	0.973315
#	76:	57(N)	58(O):	1.001417					
#	77:	57(N)	59(O):	0.878051	#	27:	16(N)	17(N):	0.619463
#	78:	60(N)	61(O):	0.893062					
#	79:	60(N)	62(O):	0.883656					
#	80:	63(N)	64(O):	1.001414					
#	81:	63(N)	65(O):	0.878053					
#	82:	66(N)	67(O):	0.893043					
#	83:	66(N)	68(O):	0.883671					
#	84:	69(N)	70(O):	1.008128					
#	85:	69(N)	71(O):	0.884624					
#	86:	72(N)	73(O):	0.935442					
#	87:	72(N)	74(O):	0.869382					
#	32:	20(N)	75(H):	0.672554					

C1					C2				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	0.667634	#	1:	1(N)	2(N):	0.671968
#	2:	1(N)	3(C):	1.004919	#	2:	1(N)	3(C):	1.006695
#	3:	1(N)	31(H):	0.632053	#	3:	1(N)	33(H):	0.627989
#	4:	2(N)	4(C):	1.004934	#	4:	2(N)	4(C):	1.006646
#	5:	2(N)	32(H):	0.632044	#	5:	2(N)	34(H):	0.627993
#	6:	3(C)	5(C):	1.327820	#	6:	3(C)	5(C):	1.346608
#	7:	3(C)	9(C):	1.301494	#	7:	3(C)	9(C):	1.264437
#	8:	4(C)	10(C):	1.327833	#	8:	4(C)	10(C):	1.346575
#	9:	4(C)	14(C):	1.301531	#	9:	4(C)	14(C):	1.264464
#	10:	5(C)	6(C):	1.398003	#	10:	5(C)	6(C):	1.408289
#	11:	5(C)	19(N):	0.664454	#	11:	5(C)	21(N):	0.653013
#	12:	6(C)	7(N):	1.173072	#	12:	6(C)	7(N):	1.185553
#	13:	6(C)	15(C):	1.253319	#	13:	6(C)	15(N):	0.908840
#	14:	7(N)	8(C):	1.250167	#	14:	7(N)	8(C):	1.233047

#	15:	8(C)	9(C):	1.451437	#	15:	8(C)	9(C):	1.449505
#	16:	8(C)	33(H):	0.856547	#	16:	8(C)	35(H):	0.854756
#	17:	9(C)	22(N):	0.695597	#	17:	9(C)	24(N):	0.716820
#	18:	10(C)	11(C):	1.398016	#	18:	10(C)	11(C):	1.408300
#	19:	10(C)	28(N):	0.664460	#	19:	10(C)	30(N):	0.653012
#	20:	11(C)	12(N):	1.173038	#	20:	11(C)	12(N):	1.185557
#	21:	11(C)	17(C):	1.253321	#	21:	11(C)	18(N):	0.908842
#	22:	12(N)	13(C):	1.250190	#	22:	12(N)	13(C):	1.233049
#	23:	13(C)	14(C):	1.451404	#	23:	13(C)	14(C):	1.449490
#	24:	13(C)	34(H):	0.856547	#	24:	13(C)	36(H):	0.854759
#	25:	14(C)	25(N):	0.695607	#	25:	14(C)	27(N):	0.716802
#	26:	15(C)	16(N):	2.533222	#	26:	15(N)	16(N):	1.129246
#	27:	17(C)	18(N):	2.533226	#	27:	16(N)	17(N):	2.254236
#	28:	19(N)	20(O):	0.972516	#	28:	18(N)	19(N):	1.129239
#	29:	19(N)	21(O):	0.962132	#	29:	19(N)	20(N):	2.254181
#	30:	22(N)	23(O):	1.000274	#	30:	21(N)	22(O):	0.965773
#	31:	22(N)	24(O):	0.893055	#	31:	21(N)	23(O):	0.965276
#	32:	25(N)	26(O):	1.000263	#	32:	24(N)	25(O):	0.975774
#	33:	25(N)	27(O):	0.893063	#	33:	24(N)	26(O):	0.885175
#	34:	28(N)	29(O):	0.972484	#	34:	27(N)	28(O):	0.975773
#	35:	28(N)	30(O):	0.962155	#	35:	27(N)	29(O):	0.885155
					#	36:	30(N)	31(O):	0.965771
					#	37:	30(N)	32(O):	0.965294
#	5:	2(N)	32(H):	0.632044					
					#	3:	1(N)	33(H):	0.627989

C3					C4				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	0.674920	#	1:	1(N)	2(N):	0.664476
#	2:	1(N)	3(C):	1.020497	#	2:	1(N)	3(C):	1.049995
#	3:	1(N)	33(H):	0.626484	#	3:	1(N)	29(H):	0.618140
#	4:	2(N)	4(C):	1.020571	#	4:	2(N)	4(C):	1.063291
#	5:	2(N)	34(H):	0.626562	#	5:	2(N)	30(H):	0.615893
#	6:	3(C)	5(C):	1.317256	#	6:	3(C)	5(C):	1.279081
#	7:	3(C)	9(C):	1.282751	#	7:	3(C)	9(C):	1.274380
#	8:	4(C)	10(C):	1.317299	#	8:	4(C)	10(C):	1.306829
#	9:	4(C)	14(C):	1.282631	#	9:	4(C)	14(C):	1.267954
#	10:	5(C)	6(C):	1.393830	#	10:	5(C)	6(C):	1.277801
#	11:	5(C)	21(N):	0.633007	#	11:	5(C)	17(N):	0.712859
#	12:	6(C)	7(N):	1.260721	#	12:	6(C)	7(N):	1.124130
#	13:	6(C)	15(N):	0.851610	#	13:	6(C)	15(N):	1.187459
#	14:	7(N)	8(C):	1.216613	#	14:	7(N)	8(C):	1.288567
#	15:	8(C)	9(C):	1.470923	#	15:	8(C)	9(C):	1.416762
#	16:	8(C)	35(H):	0.856375	#	16:	8(C)	31(H):	0.854957
#	17:	9(C)	24(N):	0.693111	#	17:	9(C)	20(N):	0.737600

#	18:	10(C)	11(C):	1.393849	#	18:	10(C)	11(C):	1.280889
#	19:	10(C)	30(N):	0.633021	#	19:	10(C)	26(N):	0.734073
#	20:	11(C)	12(N):	1.260768	#	20:	11(C)	12(N):	1.117804
#	21:	11(C)	18(N):	0.851637	#	21:	11(C)	16(N):	1.192224
#	22:	12(N)	13(C):	1.216613	#	22:	12(N)	13(C):	1.295672
#	23:	13(C)	14(C):	1.470940	#	23:	13(C)	14(C):	1.410156
#	24:	13(C)	36(H):	0.856361	#	24:	13(C)	32(H):	0.854027
#	25:	14(C)	27(N):	0.693025	#	25:	14(C)	23(N):	0.748490
#	26:	15(N)	16(F):	0.173371	#	26:	15(N)	33(H):	0.682059
#	27:	15(N)	17(F):	0.138407	#	27:	15(N)	34(H):	0.670716
#	28:	18(N)	19(F):	0.173361	#	28:	16(N)	35(H):	0.683349
#	29:	18(N)	20(F):	0.138401	#	29:	16(N)	36(H):	0.668836
#	30:	21(N)	22(O):	0.979721	#	30:	17(N)	18(O):	0.882441
#	31:	21(N)	23(O):	0.985121	#	31:	17(N)	19(O):	0.928155
#	32:	24(N)	25(O):	1.000571	#	32:	20(N)	21(O):	0.952918
#	33:	24(N)	26(O):	0.882310	#	33:	20(N)	22(O):	0.873266
#	34:	27(N)	28(O):	1.000593	#	34:	23(N)	24(O):	0.967091
#	35:	27(N)	29(O):	0.882323	#	35:	23(N)	25(O):	0.831816
#	36:	30(N)	31(O):	0.979747	#	36:	26(N)	27(O):	0.915208
#	37:	30(N)	32(O):	0.985053	#	37:	26(N)	28(O):	0.891974
#	3:	1(N)	33(H):	0.626484	#	5:	2(N)	30(H):	0.615893

C5					C6				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	0.655761	#	1:	1(N)	2(N):	0.671407
#	2:	1(N)	3(C):	1.026918	#	2:	1(N)	3(C):	1.060384
#	3:	1(N)	35(H):	0.629607	#	3:	1(N)	31(H):	0.615438
#	4:	2(N)	4(C):	1.042135	#	4:	2(N)	4(C):	1.069753
#	5:	2(N)	36(H):	0.620574	#	5:	2(N)	32(H):	0.616038
#	6:	3(C)	5(C):	1.307840	#	6:	3(C)	5(C):	1.274227
#	7:	3(C)	9(C):	1.299623	#	7:	3(C)	9(C):	1.263854
#	8:	4(C)	10(C):	1.311480	#	8:	4(C)	10(C):	1.307264
#	9:	4(C)	14(C):	1.288116	#	9:	4(C)	14(C):	1.259772
#	10:	5(C)	6(C):	1.330943	#	10:	5(C)	6(C):	1.232454
#	11:	5(C)	23(N):	0.682698	#	11:	5(C)	19(N):	0.743620
#	12:	6(C)	7(N):	1.207336	#	12:	6(C)	7(N):	1.103680
#	13:	6(C)	15(N):	0.957196	#	13:	6(C)	15(N):	1.163607
#	14:	7(N)	8(C):	1.247477	#	14:	7(N)	8(C):	1.274959
#	15:	8(C)	9(C):	1.437713	#	15:	8(C)	9(C):	1.422138
#	16:	8(C)	37(H):	0.853312	#	16:	8(C)	33(H):	0.854366
#	17:	9(C)	26(N):	0.712075	#	17:	9(C)	22(N):	0.742552
#	18:	10(C)	11(C):	1.311049	#	18:	10(C)	11(C):	1.235867
#	19:	10(C)	32(N):	0.703583	#	19:	10(C)	28(N):	0.752063
#	20:	11(C)	12(N):	1.203906	#	20:	11(C)	12(N):	1.098617

#	21:	11(C)	19(N):	0.972697	#	21:	11(C)	17(N):	1.166086
#	22:	12(N)	13(C):	1.256895	#	22:	12(N)	13(C):	1.280605
#	23:	13(C)	14(C):	1.439770	#	23:	13(C)	14(C):	1.417211
#	24:	13(C)	38(H):	0.854804	#	24:	13(C)	34(H):	0.856387
#	25:	14(C)	29(N):	0.717879	#	25:	14(C)	25(N):	0.750500
#	26:	15(N)	16(N):	0.555869	#	26:	15(N)	16(N):	0.606512
#	27:	15(N)	39(H):	0.654829	#	27:	15(N)	35(H):	0.659602
#	28:	16(N)	17(O):	0.982485	#	28:	16(N)	36(H):	0.691241
#	29:	16(N)	18(O):	1.042880	#	29:	16(N)	37(H):	0.691105
#	30:	19(N)	20(N):	0.563313	#	30:	17(N)	18(N):	0.608764
#	31:	19(N)	40(H):	0.652766	#	31:	17(N)	38(H):	0.663519
#	32:	20(N)	21(O):	0.980368	#	32:	18(N)	39(H):	0.687288
#	33:	20(N)	22(O):	1.037502	#	33:	18(N)	40(H):	0.688231
#	34:	23(N)	24(O):	0.918616	#	34:	19(N)	20(O):	0.868171
#	35:	23(N)	25(O):	0.963801	#	35:	19(N)	21(O):	0.918329
#	36:	26(N)	27(O):	0.982402	#	36:	22(N)	23(O):	0.947551
#	37:	26(N)	28(O):	0.887779	#	37:	22(N)	24(O):	0.881322
#	38:	29(N)	30(O):	0.988991	#	38:	25(N)	26(O):	0.963197
#	39:	29(N)	31(O):	0.863485	#	39:	25(N)	27(O):	0.827933
#	40:	32(N)	33(O):	0.939997	#	40:	28(N)	29(O):	0.899052
#	41:	32(N)	34(O):	0.917879	#	41:	28(N)	30(O):	0.876485
#	26:	15(N)	16(N):	0.555869	#	30:	17(N)	18(N):	0.608764

C7

The bond order >= 0.050000

#	1:	1(N)	2(N):	0.656200
#	2:	1(N)	3(C):	1.033147
#	3:	1(N)	41(H):	0.625314
#	4:	2(N)	4(C):	1.024631
#	5:	2(N)	42(H):	0.635027
#	6:	3(C)	5(C):	1.319531
#	7:	3(C)	9(C):	1.296399
#	8:	4(C)	10(C):	1.315153
#	9:	4(C)	14(C):	1.311556
#	10:	5(C)	6(C):	1.392805
#	11:	5(C)	29(N):	0.681513
#	12:	6(C)	7(N):	1.203102
#	13:	6(C)	15(C):	1.021181
#	14:	7(N)	8(C):	1.228779
#	15:	8(C)	9(C):	1.471011
#	16:	8(C)	43(H):	0.853850
#	17:	9(C)	32(N):	0.692070
#	18:	10(C)	11(C):	1.419233
#	19:	10(C)	38(N):	0.672974

C8

The bond order >= 0.050000

#	1:	1(N)	2(N):	0.646651
#	2:	1(N)	3(C):	0.997410
#	3:	1(N)	47(H):	0.644322
#	4:	2(N)	4(C):	0.996028
#	5:	2(N)	48(H):	0.643817
#	6:	3(C)	5(C):	1.309956
#	7:	3(C)	9(C):	1.314605
#	8:	4(C)	10(C):	1.310325
#	9:	4(C)	14(C):	1.314475
#	10:	5(C)	6(C):	1.373900
#	11:	5(C)	35(N):	0.670889
#	12:	6(C)	7(N):	1.214277
#	13:	6(C)	15(C):	1.004479
#	14:	7(N)	8(C):	1.215126
#	15:	8(C)	9(C):	1.476246
#	16:	8(C)	49(H):	0.855001
#	17:	9(C)	38(N):	0.695276
#	18:	10(C)	11(C):	1.375414
#	19:	10(C)	44(N):	0.672046

#	20:	11(C)	12(N):	1.195520	#	20:	11(C)	12(N):	1.211869
#	21:	11(C)	22(C):	1.045381	#	21:	11(C)	25(C):	1.003996
#	22:	12(N)	13(C):	1.242631	#	22:	12(N)	13(C):	1.215274
#	23:	13(C)	14(C):	1.448732	#	23:	13(C)	14(C):	1.475750
#	24:	13(C)	44(H):	0.855956	#	24:	13(C)	50(H):	0.854949
#	25:	14(C)	35(N):	0.692926	#	25:	14(C)	41(N):	0.695255
#	26:	15(C)	16(N):	0.529885	#	26:	15(C)	16(N):	0.465154
#	27:	15(C)	19(N):	0.557912	#	27:	15(C)	19(N):	0.504847
#	28:	15(C)	45(H):	0.830578	#	28:	15(C)	22(N):	0.463090
#	29:	16(N)	17(O):	0.982843	#	29:	16(N)	17(O):	0.988314
#	30:	16(N)	18(O):	1.022593	#	30:	16(N)	18(O):	1.067253
#	31:	19(N)	20(O):	0.996561	#	31:	19(N)	20(O):	0.974631
#	32:	19(N)	21(O):	1.020696	#	32:	19(N)	21(O):	1.055312
#	33:	22(C)	23(N):	0.531064	#	33:	22(N)	23(O):	1.034717
#	34:	22(C)	26(N):	0.547276	#	34:	22(N)	24(O):	1.041936
#	35:	22(C)	46(H):	0.831323	#	35:	25(C)	26(N):	0.463149
#	36:	23(N)	24(O):	0.999950	#	36:	25(C)	29(N):	0.505189
#	37:	23(N)	25(O):	1.013106	#	37:	25(C)	32(N):	0.460453
#	38:	26(N)	27(O):	0.990909	#	38:	26(N)	27(O):	0.988321
#	39:	26(N)	28(O):	1.033915	#	39:	26(N)	28(O):	1.068024
#	40:	29(N)	30(O):	0.965986	#	40:	29(N)	30(O):	0.973766
#	41:	29(N)	31(O):	0.953408	#	41:	29(N)	31(O):	1.054310
#	42:	32(N)	33(O):	1.006945	#	42:	32(N)	33(O):	1.034425
#	43:	32(N)	34(O):	0.884013	#	43:	32(N)	34(O):	1.041379
#	44:	35(N)	36(O):	0.996467	#	44:	35(N)	36(O):	1.001764
#	45:	35(N)	37(O):	0.904539	#	45:	35(N)	37(O):	0.919962
#	46:	38(N)	39(O):	0.949401	#	46:	38(N)	39(O):	1.006733
#	47:	38(N)	40(O):	0.961426	#	47:	38(N)	40(O):	0.909070
					#	48:	41(N)	42(O):	1.006729
					#	49:	41(N)	43(O):	0.909884
					#	50:	44(N)	45(O):	1.000405
#	26:	15(C)	16(N):	0.529885	#	51:	44(N)	46(O):	0.921124
					#	28:	15(C)	22(N):	0.463090

C9					C10				
The bond order >=			0.050000						
#	1:	1(N)	2(N):	0.675895	The bond order >=			0.050000	
#	2:	1(N)	3(C):	1.026427	#	1:	1(N)	2(N):	0.675484
#	3:	1(N)	55(H):	0.626013	#	2:	1(N)	3(C):	1.020575
#	4:	2(N)	4(C):	1.026422	#	3:	1(N)	51(H):	0.623992
#	5:	2(N)	56(H):	0.626013	#	4:	2(N)	4(C):	1.018262
#	6:	3(C)	5(C):	1.316079	#	5:	2(N)	52(H):	0.624449
#	7:	3(C)	9(C):	1.293096	#	6:	3(C)	5(C):	1.313104
#	8:	4(C)	10(C):	1.316082	#	7:	3(C)	9(C):	1.268950

#	9:	4(C)	14(C):	1.293102	#	8:	4(C)	10(C):	1.310280
#	10:	5(C)	6(C):	1.462239	#	9:	4(C)	14(C):	1.269802
#	11:	5(C)	25(N):	0.649204	#	10:	5(C)	6(C):	1.377511
#	12:	6(C)	7(N):	1.278408	#	11:	5(C)	27(N):	0.642072
#	13:	6(C)	17(N):	0.747410	#	12:	6(C)	7(N):	1.180203
#	14:	7(N)	8(C):	1.214599	#	13:	6(C)	17(N):	0.887534
#	15:	8(C)	9(C):	1.458520	#	14:	7(N)	8(C):	1.215078
#	16:	8(C)	57(H):	0.855765	#	15:	8(C)	9(C):	1.485868
#	17:	9(C)	28(N):	0.683314	#	16:	8(C)	53(H):	0.857148
#	18:	10(C)	11(C):	1.462230	#	17:	9(C)	30(N):	0.697471
#	19:	10(C)	34(N):	0.649201	#	18:	10(C)	11(C):	1.378999
#	20:	11(C)	12(N):	1.278406	#	19:	10(C)	36(N):	0.646866
#	21:	11(C)	22(N):	0.747412	#	20:	11(C)	12(N):	1.181381
#	22:	12(N)	13(C):	1.214597	#	21:	11(C)	23(N):	0.891774
#	23:	13(C)	14(C):	1.458519	#	22:	12(N)	13(C):	1.211364
#	24:	13(C)	58(H):	0.855763	#	23:	13(C)	14(C):	1.484019
#	25:	14(C)	31(N):	0.683312	#	24:	13(C)	54(H):	0.856607
#	26:	15(C)	16(N):	1.305134	#	25:	14(C)	33(N):	0.697922
#	27:	15(C)	19(C):	1.274870	#	26:	15(C)	16(N):	1.417113
#	28:	15(C)	37(N):	0.764849	#	27:	15(C)	19(C):	1.233349
#	29:	16(N)	17(N):	0.809289	#	28:	15(C)	39(N):	0.740299
#	30:	17(N)	18(C):	0.931629	#	29:	16(N)	17(N):	0.624383
#	31:	18(C)	19(C):	1.435643	#	30:	17(N)	18(C):	0.872286
#	32:	18(C)	40(N):	0.806754	#	31:	18(C)	19(C):	1.348000
#	33:	19(C)	43(N):	0.735621	#	32:	18(C)	20(N):	1.219493
#	34:	20(C)	21(N):	1.305137	#	33:	19(C)	42(N):	0.870772
#	35:	20(C)	24(C):	1.274867	#	34:	20(N)	55(H):	0.658965
#	36:	20(C)	46(N):	0.764849	#	35:	20(N)	56(H):	0.659843
#	37:	21(N)	22(N):	0.809284	#	36:	21(C)	22(N):	1.416820
#	38:	22(N)	23(C):	0.931630	#	37:	21(C)	25(C):	1.229348
#	39:	23(C)	24(C):	1.435648	#	38:	21(C)	45(N):	0.743509
#	40:	23(C)	49(N):	0.806752	#	39:	22(N)	23(N):	0.625296
#	41:	24(C)	52(N):	0.735625	#	40:	23(N)	24(C):	0.871022
#	42:	25(N)	26(O):	0.970905	#	41:	24(C)	25(C):	1.348418
#	43:	25(N)	27(O):	0.980586	#	42:	24(C)	26(N):	1.215701
#	44:	28(N)	29(O):	1.009019	#	43:	25(C)	48(N):	0.865473
#	45:	28(N)	30(O):	0.888948	#	44:	26(N)	57(H):	0.659924
#	46:	31(N)	32(O):	1.009013	#	45:	26(N)	58(H):	0.658726
#	47:	31(N)	33(O):	0.888942	#	46:	27(N)	28(O):	0.990501
#	48:	34(N)	35(O):	0.970910	#	47:	27(N)	29(O):	0.970613
#	49:	34(N)	36(O):	0.980596	#	48:	30(N)	31(O):	0.987210
#	50:	37(N)	38(O):	1.004479	#	49:	30(N)	32(O):	0.888475
#	51:	37(N)	39(O):	0.954321	#	50:	33(N)	34(O):	0.989040
#	52:	40(N)	41(O):	0.942647	#	51:	33(N)	35(O):	0.886903
#	53:	40(N)	42(O):	0.982349	#	52:	36(N)	37(O):	0.999012

#	54:	43(N)	44(O):	1.007482	#	53:	36(N)	38(O):	0.965486
#	55:	43(N)	45(O):	1.004207	#	54:	39(N)	40(O):	0.992556
#	56:	46(N)	47(O):	1.004476	#	55:	39(N)	41(O):	0.988314
#	57:	46(N)	48(O):	0.954322	#	56:	42(N)	43(O):	0.857747
#	58:	49(N)	50(O):	0.942645	#	57:	42(N)	44(O):	0.959990
#	59:	49(N)	51(O):	0.982349	#	58:	45(N)	46(O):	0.990281
#	60:	52(N)	53(O):	1.007480	#	59:	45(N)	47(O):	0.986169
#	61:	52(N)	54(O):	1.004214	#	60:	48(N)	49(O):	0.964685
					#	61:	48(N)	50(O):	0.852359
#	5:	2(N)	56(H):	0.626013	#	3:	1(N)	51(H):	0.623992

C11					C12				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	0.679191	#	1:	1(N)	2(N):	0.671808
#	2:	1(N)	3(C):	1.025859	#	2:	1(N)	3(C):	1.009645
#	3:	1(N)	51(H):	0.628898	#	3:	1(N)	45(H):	0.624550
#	4:	2(N)	4(C):	1.025853	#	4:	2(N)	4(C):	1.009635
#	5:	2(N)	52(H):	0.628903	#	5:	2(N)	46(H):	0.624594
#	6:	3(C)	5(C):	1.317432	#	6:	3(C)	5(C):	1.308825
#	7:	3(C)	9(C):	1.290754	#	7:	3(C)	9(C):	1.297421
#	8:	4(C)	10(C):	1.317429	#	8:	4(C)	10(C):	1.308803
#	9:	4(C)	14(C):	1.290740	#	9:	4(C)	14(C):	1.297247
#	10:	5(C)	6(C):	1.454819	#	10:	5(C)	6(C):	1.421912
#	11:	5(C)	27(N):	0.648310	#	11:	5(C)	27(N):	0.652379
#	12:	6(C)	7(N):	1.257755	#	12:	6(C)	7(N):	1.245293
#	13:	6(C)	17(N):	0.781297	#	13:	6(C)	17(N):	0.822372
#	14:	7(N)	8(C):	1.226444	#	14:	7(N)	8(C):	1.232047
#	15:	8(C)	9(C):	1.448999	#	15:	8(C)	9(C):	1.452206
#	16:	8(C)	53(H):	0.855240	#	16:	8(C)	47(H):	0.855737
#	17:	9(C)	30(N):	0.695014	#	17:	9(C)	30(N):	0.693803
#	18:	10(C)	11(C):	1.454823	#	18:	10(C)	11(C):	1.421958
#	19:	10(C)	36(N):	0.648308	#	19:	10(C)	36(N):	0.652453
#	20:	11(C)	12(N):	1.257760	#	20:	11(C)	12(N):	1.245354
#	21:	11(C)	23(N):	0.781297	#	21:	11(C)	23(N):	0.822323
#	22:	12(N)	13(C):	1.226447	#	22:	12(N)	13(C):	1.232068
#	23:	13(C)	14(C):	1.449002	#	23:	13(C)	14(C):	1.452249
#	24:	13(C)	54(H):	0.855242	#	24:	13(C)	48(H):	0.855734
#	25:	14(C)	33(N):	0.695013	#	25:	14(C)	33(N):	0.693713
#	26:	15(C)	16(N):	1.277853	#	26:	15(C)	16(N):	1.405541
#	27:	15(C)	19(C):	1.217776	#	27:	15(C)	19(N):	1.074840
#	28:	15(C)	39(N):	0.803450	#	28:	15(C)	39(N):	0.741629
#	29:	16(N)	17(N):	0.845028	#	29:	16(N)	17(N):	0.651948
#	30:	17(N)	18(C):	0.853151	#	30:	17(N)	18(C):	0.867633
#	31:	18(C)	19(C):	1.355207	#	31:	18(C)	19(N):	1.293854

#	32:	18(C)	42(N):	0.899277	#	32:	18(C)	20(N):	1.085701
#	33:	19(C)	20(N):	1.158325	#	33:	20(N)	49(H):	0.665617
#	34:	20(N)	55(H):	0.674658	#	34:	20(N)	50(H):	0.675538
#	35:	20(N)	56(H):	0.677655	#	35:	21(C)	22(N):	1.405461
#	36:	21(C)	22(N):	1.277855	#	36:	21(C)	25(N):	1.074916
#	37:	21(C)	25(C):	1.217777	#	37:	21(C)	42(N):	0.741643
#	38:	21(C)	45(N):	0.803453	#	38:	22(N)	23(N):	0.651988
#	39:	22(N)	23(N):	0.845028	#	39:	23(N)	24(C):	0.867683
#	40:	23(N)	24(C):	0.853148	#	40:	24(C)	25(N):	1.293809
#	41:	24(C)	25(C):	1.355207	#	41:	24(C)	26(N):	1.085974
#	42:	24(C)	48(N):	0.899275	#	42:	26(N)	51(H):	0.665620
#	43:	25(C)	26(N):	1.158325	#	43:	26(N)	52(H):	0.675511
#	44:	26(N)	57(H):	0.674659	#	44:	27(N)	28(O):	1.018992
#	45:	26(N)	58(H):	0.677654	#	45:	27(N)	29(O):	0.916672
#	46:	27(N)	28(O):	0.970542	#	46:	30(N)	31(O):	1.000817
#	47:	27(N)	29(O):	0.982226	#	47:	30(N)	32(O):	0.888508
#	48:	30(N)	31(O):	0.997558	#	48:	33(N)	34(O):	1.000856
#	49:	30(N)	32(O):	0.885935	#	49:	33(N)	35(O):	0.888518
#	50:	33(N)	34(O):	0.997565	#	50:	36(N)	37(O):	1.019047
#	51:	33(N)	35(O):	0.885937	#	51:	36(N)	38(O):	0.916710
#	52:	36(N)	37(O):	0.970546	#	52:	39(N)	40(O):	0.980228
#	53:	36(N)	38(O):	0.982244	#	53:	39(N)	41(O):	0.970141
#	54:	39(N)	40(O):	0.999244	#	54:	42(N)	43(O):	0.980303
#	55:	39(N)	41(O):	0.870018	#	55:	42(N)	44(O):	0.970073
#	56:	42(N)	43(O):	0.920878					
#	57:	42(N)	44(O):	0.870114	#	3:	1(N)	45(H):	0.624550
#	58:	45(N)	46(O):	0.999242					
#	59:	45(N)	47(O):	0.870018					
#	60:	48(N)	49(O):	0.920881					
#	61:	48(N)	50(O):	0.870111					
#	3:	1(N)	51(H):	0.628898					

D1

The bond order >= 0.050000

#	1:	1(N)	2(N):	0.666524
#	2:	1(N)	3(C):	0.997023
#	3:	1(N)	35(H):	0.633172
#	4:	2(N)	4(C):	1.015247
#	5:	2(N)	36(H):	0.623871
#	6:	3(C)	5(C):	1.345671
#	7:	3(C)	9(C):	1.294997
#	8:	4(C)	10(C):	1.331882
#	9:	4(C)	14(C):	1.289943
#	10:	5(C)	6(C):	1.406543

D2

The total bond order >= 0.050000

#	1:	1(N)	2(N)	1.27609110
#	2:	1(N)	3(C)	1.31279477
#	8:	1(N)	39(H)	0.70236608
#	10:	2(N)	4(C)	1.32291334
#	15:	2(N)	40(H)	0.68747391
#	16:	3(C)	5(C)	1.27918663
#	20:	3(C)	9(C)	1.22634077
#	23:	4(C)	10(C)	1.27354282
#	27:	4(C)	14(C)	1.22504346
#	30:	5(C)	6(C)	1.28626258

#	11:	5(C)	15(N):	0.662144	#	34:	5(C)	15(N)	0.94985307
#	12:	6(C)	7(N):	1.193975	#	38:	6(C)	7(N)	1.44406184
#	13:	6(C)	29(C):	1.254980	#	42:	6(C)	30(N)	1.20174609
#	14:	7(N)	8(C):	1.199510	#	45:	7(N)	8(C)	1.44447676
#	15:	8(C)	9(C):	1.371650	#	46:	7(N)	9(C)	0.08994708
#	16:	8(C)	27(C):	1.256281	#	47:	7(N)	27(N)	0.11205020
#	17:	9(C)	21(N):	0.694235	#	48:	7(N)	28(N)	0.08721032
#	18:	10(C)	11(C):	1.412176	#	49:	7(N)	30(N)	0.10598665
#	19:	10(C)	18(N):	0.664454	#	50:	7(N)	31(N)	0.07896348
#	20:	11(C)	12(N):	1.190016	#	51:	8(C)	9(C)	1.26695473
#	21:	11(C)	31(C):	1.254276	#	52:	8(C)	21(N)	0.05668652
#	22:	12(N)	13(C):	1.202089	#	53:	8(C)	27(N)	1.21177884
#	23:	13(C)	14(C):	1.362069	#	54:	8(C)	28(N)	0.10885265
#	24:	13(C)	33(C):	1.253879	#	55:	8(C)	29(N)	0.06751844
#	25:	14(C)	24(N):	0.687779	#	56:	9(C)	21(N)	1.02415311
#	26:	15(N)	16(O):	0.981566	#	57:	9(C)	22(O)	0.13403788
#	27:	15(N)	17(O):	0.967661	#	58:	9(C)	23(O)	0.13024740
#	28:	18(N)	19(O):	0.977217	#	59:	9(C)	27(N)	0.08182754
#	29:	18(N)	20(O):	0.965545	#	60:	10(C)	11(C)	1.28645283
#	30:	21(N)	22(O):	1.025817	#	61:	10(C)	12(N)	0.09257508
#	31:	21(N)	23(O):	0.884840	#	62:	10(C)	13(C)	0.05791237
#	32:	24(N)	25(O):	1.020289	#	63:	10(C)	14(C)	0.07640062
#	33:	24(N)	26(O):	0.888722	#	64:	10(C)	18(N)	0.95468325
#	34:	27(C)	28(N):	2.535490	#	65:	10(C)	19(O)	0.13516799
#	35:	29(C)	30(N):	2.538983	#	66:	10(C)	20(O)	0.12855789
#	36:	31(C)	32(N):	2.539549	#	67:	10(C)	33(N)	0.08625500
#	37:	33(C)	34(N):	2.532869	#	68:	11(C)	12(N)	1.44197091
					#	69:	11(C)	13(C)	0.10403030
					#	70:	11(C)	14(C)	0.05623125
#	5:	2(N)	36(H):	0.623871	#	71:	11(C)	18(N)	0.05666548
					#	72:	11(C)	33(N)	1.20307159
					#	73:	11(C)	34(N)	0.10785317
					#	74:	11(C)	35(N)	0.06601538
					#	75:	12(N)	13(C)	1.44630832
					#	76:	12(N)	14(C)	0.09017373
					#	77:	12(N)	33(N)	0.10614926
					#	78:	12(N)	34(N)	0.07943112
					#	79:	12(N)	36(N)	0.11281519
					#	80:	12(N)	37(N)	0.08846393
					#	81:	13(C)	14(C)	1.26267541
					#	82:	13(C)	24(N)	0.05770163
					#	83:	13(C)	36(N)	1.21374235
					#	84:	13(C)	37(N)	0.10905675
					#	85:	13(C)	38(N)	0.06785652
					#	86:	14(C)	24(N)	1.03454965

#	87:	14(C)	25(O)	0.13720640
#	88:	14(C)	26(O)	0.12800161
#	89:	14(C)	36(N)	0.08108851
#	90:	15(N)	16(O)	1.84459401
#	91:	15(N)	17(O)	1.83703220
#	92:	16(O)	17(O)	0.43404599
#	93:	18(N)	19(O)	1.83828002
#	94:	18(N)	20(O)	1.83398279
#	95:	19(O)	20(O)	0.43218472
#	96:	21(N)	22(O)	1.86324266
#	97:	21(N)	23(O)	1.76021961
#	98:	22(O)	23(O)	0.40906540
#	99:	22(O)	27(N)	0.10846874
#	100:	23(O)	39(H)	0.07064729
#	101:	24(N)	25(O)	1.85519994
#	102:	24(N)	26(O)	1.75989813
#	103:	25(O)	26(O)	0.40686012
#	104:	25(O)	36(N)	0.11472374
#	105:	26(O)	40(H)	0.07770926
#	106:	27(N)	28(N)	1.67397052
#	107:	27(N)	29(N)	0.40605626
#	108:	28(N)	29(N)	2.56175831
#	109:	30(N)	31(N)	1.67522454
#	110:	30(N)	32(N)	0.40571957
#	111:	31(N)	32(N)	2.56759490
#	112:	33(N)	34(N)	1.67373737
#	113:	33(N)	35(N)	0.40480211
#	114:	34(N)	35(N)	2.56788238
#	115:	36(N)	37(N)	1.67149410
#	116:	36(N)	38(N)	0.40475763
#	117:	37(N)	38(N)	2.56247032
#	15:	2(N)	40(H)	0.68747391

D3

The bond order >= 0.050000

#	1:	1(N)	2(N):	0.672250
#	2:	1(N)	3(C):	0.984381
#	3:	1(N)	39(H):	0.642351
#	4:	2(N)	4(C):	1.003155
#	5:	2(N)	40(H):	0.634647
#	6:	3(C)	5(C):	1.338140
#	7:	3(C)	9(C):	1.287983
#	8:	4(C)	10(C):	1.324693
#	9:	4(C)	14(C):	1.281109

D4

The bond order >= 0.050000

#	1:	1(N)	2(N):	0.672861
#	2:	1(N)	3(C):	1.054687
#	3:	1(N)	31(H):	0.610916
#	4:	2(N)	4(C):	1.070347
#	5:	2(N)	32(H):	0.604794
#	6:	3(C)	5(C):	1.277965
#	7:	3(C)	9(C):	1.242196
#	8:	4(C)	10(C):	1.309337
#	9:	4(C)	14(C):	1.227982

#	10:	5(C)	6(C):	1.393313	#	10:	5(C)	6(C):	1.252976
#	11:	5(C)	15(N):	0.641852	#	11:	5(C)	19(N):	0.749478
#	12:	6(C)	7(N):	1.258840	#	12:	6(C)	7(N):	1.178905
#	13:	6(C)	30(N):	0.859248	#	13:	6(C)	16(N):	1.179148
#	14:	7(N)	8(C):	1.255437	#	14:	7(N)	8(C):	1.175541
#	15:	8(C)	9(C):	1.409566	#	15:	8(C)	9(C):	1.217496
#	16:	8(C)	27(N):	0.830183	#	16:	8(C)	15(N):	1.187854
#	17:	9(C)	21(N):	0.675325	#	17:	9(C)	25(N):	0.787731
#	18:	10(C)	11(C):	1.398283	#	18:	10(C)	11(C):	1.252142
#	19:	10(C)	18(N):	0.643106	#	19:	10(C)	22(N):	0.764634
#	20:	11(C)	12(N):	1.243882	#	20:	11(C)	12(N):	1.177271
#	21:	11(C)	33(N):	0.864640	#	21:	11(C)	17(N):	1.187155
#	22:	12(N)	13(C):	1.258053	#	22:	12(N)	13(C):	1.185306
#	23:	13(C)	14(C):	1.401634	#	23:	13(C)	14(C):	1.217658
#	24:	13(C)	36(N):	0.829491	#	24:	13(C)	18(N):	1.186605
#	25:	14(C)	24(N):	0.684070	#	25:	14(C)	28(N):	0.801798
#	26:	15(N)	16(O):	0.976870	#	26:	15(N)	33(H):	0.661374
#	27:	15(N)	17(O):	0.982057	#	27:	15(N)	34(H):	0.683727
#	28:	18(N)	19(O):	0.987909	#	28:	16(N)	35(H):	0.682788
#	29:	18(N)	20(O):	0.977986	#	29:	16(N)	36(H):	0.666858
#	30:	21(N)	22(O):	1.044788	#	30:	17(N)	37(H):	0.684723
#	31:	21(N)	23(O):	0.896059	#	31:	17(N)	38(H):	0.667329
#	32:	24(N)	25(O):	1.027007	#	32:	18(N)	39(H):	0.663469
#	33:	24(N)	26(O):	0.896472	#	33:	18(N)	40(H):	0.687295
#	34:	27(N)	28(F):	0.145374	#	34:	19(N)	20(O):	0.855665
#	35:	27(N)	29(F):	0.153082	#	35:	19(N)	21(O):	0.913335
#	36:	30(N)	31(F):	0.175521	#	36:	22(N)	23(O):	0.884102
#	37:	30(N)	32(F):	0.140017	#	37:	22(N)	24(O):	0.866622
#	38:	33(N)	34(F):	0.176742	#	38:	25(N)	26(O):	0.861250
#	39:	33(N)	35(F):	0.139845	#	39:	25(N)	27(O):	0.874833
#	40:	36(N)	37(F):	0.150736	#	40:	28(N)	29(O):	0.871623
#	41:	36(N)	38(F):	0.149687	#	41:	28(N)	30(O):	0.818579

#	39:	33(N)	35(F):	0.139845	#	5:	2(N)	32(H):	0.604794

D5					D6				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	0.662897	#	1:	1(N)	2(N):	0.673893
#	2:	1(N)	3(C):	1.032068	#	2:	1(N)	3(C):	1.059377
#	3:	1(N)	43(H):	0.618647	#	3:	1(N)	35(H):	0.606219
#	4:	2(N)	4(C):	1.052951	#	4:	2(N)	4(C):	1.074314
#	5:	2(N)	44(H):	0.614765	#	5:	2(N)	36(H):	0.602676
#	6:	3(C)	5(C):	1.304598	#	6:	3(C)	5(C):	1.269859
#	7:	3(C)	9(C):	1.262178	#	7:	3(C)	9(C):	1.242272
#	8:	4(C)	10(C):	1.310448	#	8:	4(C)	10(C):	1.304688

#	9:	4(C)	14(C):	1.241420	#	9:	4(C)	14(C):	1.227828
#	10:	5(C)	6(C):	1.311945	#	10:	5(C)	6(C):	1.236387
#	11:	5(C)	15(N):	0.698910	#	11:	5(C)	15(N):	0.750663
#	12:	6(C)	7(N):	1.226028	#	12:	6(C)	7(N):	1.161124
#	13:	6(C)	31(N):	0.981853	#	13:	6(C)	29(N):	1.136236
#	14:	7(N)	8(C):	1.229017	#	14:	7(N)	8(C):	1.161273
#	15:	8(C)	9(C):	1.231721	#	15:	8(C)	9(C):	1.200101
#	16:	8(C)	27(N):	1.012174	#	16:	8(C)	27(N):	1.138269
#	17:	9(C)	21(N):	0.747196	#	17:	9(C)	21(N):	0.791702
#	18:	10(C)	11(C):	1.294969	#	18:	10(C)	11(C):	1.235591
#	19:	10(C)	18(N):	0.730315	#	19:	10(C)	18(N):	0.772068
#	20:	11(C)	12(N):	1.229901	#	20:	11(C)	12(N):	1.159651
#	21:	11(C)	35(N):	1.000827	#	21:	11(C)	31(N):	1.146952
#	22:	12(N)	13(C):	1.244694	#	22:	12(N)	13(C):	1.170258
#	23:	13(C)	14(C):	1.220722	#	23:	13(C)	14(C):	1.197520
#	24:	13(C)	39(N):	1.013390	#	24:	13(C)	33(N):	1.136794
#	25:	14(C)	24(N):	0.754465	#	25:	14(C)	24(N):	0.809165
#	26:	15(N)	16(O):	0.898961	#	26:	15(N)	16(O):	0.852752
#	27:	15(N)	17(O):	0.952295	#	27:	15(N)	17(O):	0.900834
#	28:	18(N)	19(O):	0.917486	#	28:	18(N)	19(O):	0.883001
#	29:	18(N)	20(O):	0.902440	#	29:	18(N)	20(O):	0.861829
#	30:	21(N)	22(O):	0.901811	#	30:	21(N)	22(O):	0.857616
#	31:	21(N)	23(O):	0.906722	#	31:	21(N)	23(O):	0.870530
#	32:	24(N)	25(O):	0.902759	#	32:	24(N)	25(O):	0.871234
#	33:	24(N)	26(O):	0.861444	#	33:	24(N)	26(O):	0.811770
#	34:	27(N)	28(N):	0.542486	#	34:	27(N)	28(N):	0.615317
#	35:	27(N)	45(H):	0.638113	#	35:	27(N)	37(H):	0.658145
#	36:	28(N)	29(O):	0.982883	#	36:	28(N)	38(H):	0.690135
#	37:	28(N)	30(O):	1.062426	#	37:	28(N)	39(H):	0.690447
#	38:	31(N)	32(N):	0.532041	#	38:	29(N)	30(N):	0.624704
#	39:	31(N)	46(H):	0.655015	#	39:	29(N)	40(H):	0.663371
#	40:	32(N)	33(O):	0.990457	#	40:	30(N)	41(H):	0.692765
#	41:	32(N)	34(O):	1.057446	#	41:	30(N)	42(H):	0.693440
#	42:	35(N)	36(N):	0.544582	#	42:	31(N)	32(N):	0.618488
#	43:	35(N)	47(H):	0.644354	#	43:	31(N)	43(H):	0.663910
#	44:	36(N)	37(O):	0.988359	#	44:	32(N)	44(H):	0.693492
#	45:	36(N)	38(O):	1.045883	#	45:	32(N)	45(H):	0.695301
#	46:	39(N)	40(N):	0.530515	#	46:	33(N)	34(N):	0.619259
#	47:	39(N)	48(H):	0.638951	#	47:	33(N)	46(H):	0.658259
#	48:	40(N)	41(O):	0.975925	#	48:	34(N)	47(H):	0.690190
#	49:	40(N)	42(O):	1.063994	#	49:	34(N)	48(H):	0.692957
#	46:	39(N)	40(N):	0.530515	#	5:	2(N)	36(H):	0.602676
D7					D8				

The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	0.651558	#	1:	1(N)	2(N):	0.689911
#	2:	1(N)	3(C):	1.017481	#	2:	1(N)	3(C):	1.029439
#	3:	1(N)	55(H):	0.631824	#	3:	1(N)	67(H):	0.618802
#	4:	2(N)	4(C):	1.018531	#	4:	2(N)	4(C):	1.029445
#	5:	2(N)	56(H):	0.639469	#	5:	2(N)	68(H):	0.618800
#	6:	3(C)	5(C):	1.338826	#	6:	3(C)	5(C):	1.295882
#	7:	3(C)	9(C):	1.278588	#	7:	3(C)	9(C):	1.276190
#	8:	4(C)	10(C):	1.325282	#	8:	4(C)	10(C):	1.295889
#	9:	4(C)	14(C):	1.289369	#	9:	4(C)	14(C):	1.276189
#	10:	5(C)	6(C):	1.412544	#	10:	5(C)	6(C):	1.406223
#	11:	5(C)	15(N):	0.685670	#	11:	5(C)	15(N):	0.668630
#	12:	6(C)	7(N):	1.205647	#	12:	6(C)	7(N):	1.187610
#	13:	6(C)	34(C):	1.025124	#	13:	6(C)	37(C):	0.993905
#	14:	7(N)	8(C):	1.214831	#	14:	7(N)	8(C):	1.214016
#	15:	8(C)	9(C):	1.386362	#	15:	8(C)	9(C):	1.377713
#	16:	8(C)	27(C):	1.030299	#	16:	8(C)	27(C):	0.998210
#	17:	9(C)	21(N):	0.697502	#	17:	9(C)	21(N):	0.699445
#	18:	10(C)	11(C):	1.443097	#	18:	10(C)	11(C):	1.406227
#	19:	10(C)	18(N):	0.675587	#	19:	10(C)	18(N):	0.668632
#	20:	11(C)	12(N):	1.197792	#	20:	11(C)	12(N):	1.187611
#	21:	11(C)	41(C):	1.044985	#	21:	11(C)	47(C):	0.993913
#	22:	12(N)	13(C):	1.221152	#	22:	12(N)	13(C):	1.214010
#	23:	13(C)	14(C):	1.357277	#	23:	13(C)	14(C):	1.377714
#	24:	13(C)	48(C):	1.022739	#	24:	13(C)	57(C):	0.998209
#	25:	14(C)	24(N):	0.687801	#	25:	14(C)	24(N):	0.699442
#	26:	15(N)	16(O):	0.975977	#	26:	15(N)	16(O):	1.002891
#	27:	15(N)	17(O):	0.959952	#	27:	15(N)	17(O):	0.952013
#	28:	18(N)	19(O):	0.944869	#	28:	18(N)	19(O):	1.002888
#	29:	18(N)	20(O):	0.964023	#	29:	18(N)	20(O):	0.952013
#	30:	21(N)	22(O):	0.979962	#	30:	21(N)	22(O):	0.987297
#	31:	21(N)	23(O):	0.909069	#	31:	21(N)	23(O):	0.915541
#	32:	24(N)	25(O):	0.977770	#	32:	24(N)	25(O):	0.987299
#	33:	24(N)	26(O):	0.919370	#	33:	24(N)	26(O):	0.915541
#	34:	27(C)	28(N):	0.537938	#	34:	27(C)	28(N):	0.447731
#	35:	27(C)	31(N):	0.544669	#	35:	27(C)	31(N):	0.477637
#	36:	27(C)	57(H):	0.836516	#	36:	27(C)	34(N):	0.516419
#	37:	28(N)	29(O):	0.988263	#	37:	28(N)	29(O):	1.028678
#	38:	28(N)	30(O):	1.027233	#	38:	28(N)	30(O):	1.050200
#	39:	31(N)	32(O):	0.987569	#	39:	31(N)	32(O):	0.997153
#	40:	31(N)	33(O):	1.031226	#	40:	31(N)	33(O):	1.077773
#	41:	34(C)	35(N):	0.525927	#	41:	34(N)	35(O):	1.047626
#	42:	34(C)	38(N):	0.552746	#	42:	34(N)	36(O):	0.975308
#	43:	34(C)	58(H):	0.830037	#	43:	37(C)	38(N):	0.456829
#	44:	35(N)	36(O):	0.979904					

#	45:	35(N)	37(O):	1.033070	#	44:	37(C)	41(N):	0.530701
#	46:	38(N)	39(O):	1.004179	#	45:	37(C)	44(N):	0.450752
#	47:	38(N)	40(O):	1.014376	#	46:	38(N)	39(O):	0.992789
#	48:	41(C)	42(N):	0.529233	#	47:	38(N)	40(O):	1.072050
#	49:	41(C)	45(N):	0.543283	#	48:	41(N)	42(O):	0.982580
#	50:	41(C)	59(H):	0.832047	#	49:	41(N)	43(O):	1.048642
#	51:	42(N)	43(O):	0.992927	#	50:	44(N)	45(O):	1.025825
#	52:	42(N)	44(O):	1.028189	#	51:	44(N)	46(O):	1.041989
#	53:	45(N)	46(O):	0.992753	#	52:	47(C)	48(N):	0.456834
#	54:	45(N)	47(O):	1.038829	#	53:	47(C)	51(N):	0.530703
#	55:	48(C)	49(N):	0.541644	#	54:	47(C)	54(N):	0.450751
#	56:	48(C)	52(N):	0.543245	#	55:	48(N)	49(O):	0.992785
#	57:	48(C)	60(H):	0.835832	#	56:	48(N)	50(O):	1.072054
#	58:	49(N)	50(O):	0.987258	#	57:	51(N)	52(O):	0.982582
#	59:	49(N)	51(O):	1.023343	#	58:	51(N)	53(O):	1.048640
#	60:	52(N)	53(O):	0.991917	#	59:	54(N)	55(O):	1.025834
#	61:	52(N)	54(O):	1.024470	#	60:	54(N)	56(O):	1.042006
					#	61:	57(C)	58(N):	0.447736
#	41:	34(C)	35(N):	0.525927	#	62:	57(C)	61(N):	0.477633
					#	63:	57(C)	64(N):	0.516421
					#	64:	58(N)	59(O):	1.028680
					#	65:	58(N)	60(O):	1.050198
					#	66:	61(N)	62(O):	0.997149
					#	67:	61(N)	63(O):	1.077776
					#	68:	64(N)	65(O):	1.047623
					#	69:	64(N)	66(O):	0.975313
					#	34:	27(C)	28(N):	0.447731

D9

The bond order >= 0.050000

#	1:	1(N)	2(N):	0.659003
#	2:	1(N)	3(C):	1.046953
#	3:	1(N)	83(H):	0.626190
#	4:	2(N)	4(C):	1.022771
#	5:	2(N)	84(H):	0.636855
#	6:	3(C)	5(C):	1.316108
#	7:	3(C)	9(C):	1.278518
#	8:	4(C)	10(C):	1.324314
#	9:	4(C)	14(C):	1.291913
#	10:	5(C)	6(C):	1.461135
#	11:	5(C)	35(N):	0.679244
#	12:	6(C)	7(N):	1.251951
#	13:	6(C)	17(N):	0.762216
#	14:	7(N)	8(C):	1.267755

D10

The bond order >= 0.050000

#	1:	1(N)	2(N):	0.676390
#	2:	1(N)	3(C):	1.013252
#	3:	1(N)	75(H):	0.629141
#	4:	2(N)	4(C):	0.993110
#	5:	2(N)	76(H):	0.636911
#	6:	3(C)	5(C):	1.309098
#	7:	3(C)	9(C):	1.268415
#	8:	4(C)	10(C):	1.327219
#	9:	4(C)	14(C):	1.237896
#	10:	5(C)	6(C):	1.395694
#	11:	5(C)	39(N):	0.652285
#	12:	6(C)	7(N):	1.176806
#	13:	6(C)	17(N):	0.887331
#	14:	7(N)	8(C):	1.181259

#	15:	8(C)	9(C):	1.420275	#	15:	8(C)	9(C):	1.409520
#	16:	8(C)	27(N):	0.794772	#	16:	8(C)	29(N):	0.905421
#	17:	9(C)	41(N):	0.676302	#	17:	9(C)	45(N):	0.690926
#	18:	10(C)	11(C):	1.460829	#	18:	10(C)	11(C):	1.369314
#	19:	10(C)	38(N):	0.668147	#	19:	10(C)	42(N):	0.646102
#	20:	11(C)	12(N):	1.258833	#	20:	11(C)	12(N):	1.194238
#	21:	11(C)	32(N):	0.774414	#	21:	11(C)	35(N):	0.926167
#	22:	12(N)	13(C):	1.268010	#	22:	12(N)	13(C):	1.247561
#	23:	13(C)	14(C):	1.418414	#	23:	13(C)	14(C):	1.392265
#	24:	13(C)	22(N):	0.805098	#	24:	13(C)	23(N):	0.857015
#	25:	14(C)	44(N):	0.689130	#	25:	14(C)	48(N):	0.685545
#	26:	15(C)	16(N):	1.312038	#	26:	15(C)	16(N):	1.412256
#	27:	15(C)	19(C):	1.276327	#	27:	15(C)	19(C):	1.228899
#	28:	15(C)	47(N):	0.760552	#	28:	15(C)	51(N):	0.742176
#	29:	16(N)	17(N):	0.812566	#	29:	16(N)	17(N):	0.623000
#	30:	17(N)	18(C):	0.910700	#	30:	17(N)	18(C):	0.887761
#	31:	18(C)	19(C):	1.436380	#	31:	18(C)	19(C):	1.363686
#	32:	18(C)	50(N):	0.811027	#	32:	18(C)	20(N):	1.176741
#	33:	19(C)	53(N):	0.728324	#	33:	19(C)	54(N):	0.856023
#	34:	20(C)	21(N):	1.311286	#	34:	20(N)	77(H):	0.676541
#	35:	20(C)	24(C):	1.266109	#	35:	20(N)	78(H):	0.655414
#	36:	20(C)	56(N):	0.758954	#	36:	21(C)	22(N):	1.417703
#	37:	21(N)	22(N):	0.797768	#	37:	21(C)	25(C):	1.228619
#	38:	22(N)	23(C):	0.929873	#	38:	21(C)	57(N):	0.743824
#	39:	23(C)	24(C):	1.445448	#	39:	22(N)	23(N):	0.611513
#	40:	23(C)	59(N):	0.802085	#	40:	23(N)	24(C):	0.923775
#	41:	24(C)	62(N):	0.734819	#	41:	24(C)	25(C):	1.357153
#	42:	25(C)	26(N):	1.308380	#	42:	24(C)	26(N):	1.157929
#	43:	25(C)	29(C):	1.270264	#	43:	25(C)	60(N):	0.857447
#	44:	25(C)	65(N):	0.757833	#	44:	26(N)	79(H):	0.679468
#	45:	26(N)	27(N):	0.805423	#	45:	26(N)	80(H):	0.652734
#	46:	27(N)	28(C):	0.935151	#	46:	27(C)	28(N):	1.426652
#	47:	28(C)	29(C):	1.439049	#	47:	27(C)	31(C):	1.219336
#	48:	28(C)	68(N):	0.805210	#	48:	27(C)	63(N):	0.745251
#	49:	29(C)	71(N):	0.733699	#	49:	28(N)	29(N):	0.616290
#	50:	30(C)	31(N):	1.307339	#	50:	29(N)	30(C):	0.892268
#	51:	30(C)	34(C):	1.271668	#	51:	30(C)	31(C):	1.364025
#	52:	30(C)	74(N):	0.760561	#	52:	30(C)	32(N):	1.183872
#	53:	31(N)	32(N):	0.792783	#	53:	31(C)	66(N):	0.859050
#	54:	32(N)	33(C):	0.915571	#	54:	32(N)	81(H):	0.675493
#	55:	33(C)	34(C):	1.443099	#	55:	32(N)	82(H):	0.655997
#	56:	33(C)	77(N):	0.812000	#	56:	33(C)	34(N):	1.418038
#	57:	34(C)	80(N):	0.729958	#	57:	33(C)	37(C):	1.234988
#	58:	35(N)	36(O):	0.945336	#	58:	33(C)	69(N):	0.744594
#	59:	35(N)	37(O):	0.996171	#	59:	34(N)	35(N):	0.619090

#	60:	38(N)	39(O):	0.971708	#	60:	35(N)	36(C):	0.855752
#	61:	38(N)	40(O):	0.964404	#	61:	36(C)	37(C):	1.345618
#	62:	41(N)	42(O):	1.016323	#	62:	36(C)	38(N):	1.224046
#	63:	41(N)	43(O):	0.893602	#	63:	37(C)	72(N):	0.866183
#	64:	44(N)	45(O):	1.004689	#	64:	38(N)	83(H):	0.656592
#	65:	44(N)	46(O):	0.924043	#	65:	38(N)	84(H):	0.662889
#	66:	47(N)	48(O):	1.006962	#	66:	39(N)	40(O):	0.983340
#	67:	47(N)	49(O):	0.955211	#	67:	39(N)	41(O):	0.967988
#	68:	50(N)	51(O):	0.923713	#	68:	42(N)	43(O):	1.002862
#	69:	50(N)	52(O):	0.992697	#	69:	42(N)	44(O):	0.965978
#	70:	53(N)	54(O):	1.013990	#	70:	45(N)	46(O):	1.010573
#	71:	53(N)	55(O):	1.011765	#	71:	45(N)	47(O):	0.902349
#	72:	56(N)	57(O):	1.005547	#	72:	48(N)	49(O):	1.029378
#	73:	56(N)	58(O):	0.963198	#	73:	48(N)	50(O):	0.877880
#	74:	59(N)	60(O):	0.938595	#	74:	51(N)	52(O):	0.999597
#	75:	59(N)	61(O):	0.986311	#	75:	51(N)	53(O):	0.990994
#	76:	62(N)	63(O):	1.010811	#	76:	54(N)	55(O):	0.857726
#	77:	62(N)	64(O):	1.004215	#	77:	54(N)	56(O):	0.979459
#	78:	65(N)	66(O):	1.002569	#	78:	57(N)	58(O):	0.991314
#	79:	65(N)	67(O):	0.957393	#	79:	57(N)	59(O):	0.981554
#	80:	68(N)	69(O):	0.943932	#	80:	60(N)	61(O):	0.858512
#	81:	68(N)	70(O):	0.985635	#	81:	60(N)	62(O):	0.977001
#	82:	71(N)	72(O):	1.005420	#	82:	63(N)	64(O):	0.997165
#	83:	71(N)	73(O):	1.005128	#	83:	63(N)	65(O):	0.987599
#	84:	74(N)	75(O):	1.004667	#	84:	66(N)	67(O):	0.968086
#	85:	74(N)	76(O):	0.952729	#	85:	66(N)	68(O):	0.852971
#	86:	77(N)	78(O):	0.930094	#	86:	69(N)	70(O):	1.003465
#	87:	77(N)	79(O):	0.995631	#	87:	69(N)	71(O):	0.991073
#	88:	80(N)	81(O):	1.018942	#	88:	72(N)	73(O):	0.957091
#	89:	80(N)	82(O):	1.010522	#	89:	72(N)	74(O):	0.867287
#	5:	2(N)	84(H):	0.636855	#	39:	22(N)	23(N):	0.611513

D11					D12				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(N)	2(N):	0.677090	#	1:	1(N)	2(N):	0.675806
#	2:	1(N)	3(C):	1.027756	#	2:	1(N)	3(C):	0.994185
#	3:	1(N)	75(H):	0.624677	#	3:	1(N)	63(H):	0.635493
#	4:	2(N)	4(C):	1.010781	#	4:	2(N)	4(C):	0.994177
#	5:	2(N)	76(H):	0.623698	#	5:	2(N)	64(H):	0.635463
#	6:	3(C)	5(C):	1.313979	#	6:	3(C)	5(C):	1.302676
#	7:	3(C)	9(C):	1.270068	#	7:	3(C)	9(C):	1.311017
#	8:	4(C)	10(C):	1.319790	#	8:	4(C)	10(C):	1.302598
#	9:	4(C)	14(C):	1.282035	#	9:	4(C)	14(C):	1.311065
#	10:	5(C)	6(C):	1.442829	#	10:	5(C)	6(C):	1.426465

#	11:	5(C)	39(N):	0.642243	#	11:	5(C)	39(N):	0.642458
#	12:	6(C)	7(N):	1.222712	#	12:	6(C)	7(N):	1.221258
#	13:	6(C)	17(N):	0.825418	#	13:	6(C)	17(N):	0.828553
#	14:	7(N)	8(C):	1.291839	#	14:	7(N)	8(C):	1.209452
#	15:	8(C)	9(C):	1.405879	#	15:	8(C)	9(C):	1.369581
#	16:	8(C)	29(N):	0.789313	#	16:	8(C)	35(N):	0.941598
#	17:	9(C)	45(N):	0.695417	#	17:	9(C)	45(N):	0.683496
#	18:	10(C)	11(C):	1.449368	#	18:	10(C)	11(C):	1.426479
#	19:	10(C)	42(N):	0.647384	#	19:	10(C)	42(N):	0.642460
#	20:	11(C)	12(N):	1.242227	#	20:	11(C)	12(N):	1.221260
#	21:	11(C)	35(N):	0.812866	#	21:	11(C)	29(N):	0.828549
#	22:	12(N)	13(C):	1.268623	#	22:	12(N)	13(C):	1.209451
#	23:	13(C)	14(C):	1.388414	#	23:	13(C)	14(C):	1.369597
#	24:	13(C)	23(N):	0.791524	#	24:	13(C)	23(N):	0.941599
#	25:	14(C)	48(N):	0.703331	#	25:	14(C)	48(N):	0.683521
#	26:	15(C)	16(N):	1.310759	#	26:	15(C)	16(N):	1.411249
#	27:	15(C)	19(C):	1.209459	#	27:	15(C)	19(N):	1.094151
#	28:	15(C)	51(N):	0.796204	#	28:	15(C)	51(N):	0.742807
#	29:	16(N)	17(N):	0.831366	#	29:	16(N)	17(N):	0.628657
#	30:	17(N)	18(C):	0.835243	#	30:	17(N)	18(C):	0.838404
#	31:	18(C)	19(C):	1.363914	#	31:	18(C)	19(N):	1.270690
#	32:	18(C)	54(N):	0.882494	#	32:	18(C)	20(N):	1.137594
#	33:	19(C)	20(N):	1.167271	#	33:	20(N)	65(H):	0.666179
#	34:	20(N)	77(H):	0.675683	#	34:	20(N)	66(H):	0.675927
#	35:	20(N)	78(H):	0.674968	#	35:	21(C)	22(N):	1.398060
#	36:	21(C)	22(N):	1.309617	#	36:	21(C)	25(N):	1.087278
#	37:	21(C)	25(C):	1.218128	#	37:	21(C)	54(N):	0.733258
#	38:	21(C)	57(N):	0.800937	#	38:	22(N)	23(N):	0.642578
#	39:	22(N)	23(N):	0.861825	#	39:	23(N)	24(C):	0.816923
#	40:	23(N)	24(C):	0.833183	#	40:	24(C)	25(N):	1.271414
#	41:	24(C)	25(C):	1.356406	#	41:	24(C)	26(N):	1.189270
#	42:	24(C)	60(N):	0.920970	#	42:	26(N)	67(H):	0.660830
#	43:	25(C)	26(N):	1.168343	#	43:	26(N)	68(H):	0.675660
#	44:	26(N)	79(H):	0.673627	#	44:	27(C)	28(N):	1.411246
#	45:	26(N)	80(H):	0.675373	#	45:	27(C)	31(N):	1.094139
#	46:	27(C)	28(N):	1.258165	#	46:	27(C)	57(N):	0.742803
#	47:	27(C)	31(C):	1.220971	#	47:	28(N)	29(N):	0.628642
#	48:	27(C)	63(N):	0.810946	#	48:	29(N)	30(C):	0.838413
#	49:	28(N)	29(N):	0.876811	#	49:	30(C)	31(N):	1.270690
#	50:	29(N)	30(C):	0.867864	#	50:	30(C)	32(N):	1.137608
#	51:	30(C)	31(C):	1.353485	#	51:	32(N)	69(H):	0.666165
#	52:	30(C)	66(N):	0.921096	#	52:	32(N)	70(H):	0.675931
#	53:	31(C)	32(N):	1.149844	#	53:	33(C)	34(N):	1.398064
#	54:	32(N)	81(H):	0.677584	#	54:	33(C)	37(N):	1.087288
#	55:	32(N)	82(H):	0.672445	#	55:	33(C)	60(N):	0.733257

#	56:	33(C)	34(N):	1.306927	#	56:	34(N)	35(N):	0.642572
#	57:	33(C)	37(C):	1.212269	#	57:	35(N)	36(C):	0.816921
#	58:	33(C)	69(N):	0.798942	#	58:	36(C)	37(N):	1.271407
#	59:	34(N)	35(N):	0.839781	#	59:	36(C)	38(N):	1.189272
#	60:	35(N)	36(C):	0.841654	#	60:	38(N)	71(H):	0.660832
#	61:	36(C)	37(C):	1.359549	#	61:	38(N)	72(H):	0.675665
#	62:	36(C)	72(N):	0.889327	#	62:	39(N)	40(O):	0.926666
#	63:	37(C)	38(N):	1.165452	#	63:	39(N)	41(O):	1.007964
#	64:	38(N)	83(H):	0.672780	#	64:	42(N)	43(O):	0.926703
#	65:	38(N)	84(H):	0.675556	#	65:	42(N)	44(O):	1.007937
#	66:	39(N)	40(O):	0.978564	#	66:	45(N)	46(O):	1.044369
#	67:	39(N)	41(O):	0.989999	#	67:	45(N)	47(O):	0.896609
#	68:	42(N)	43(O):	0.974230	#	68:	48(N)	49(O):	1.044359
#	69:	42(N)	44(O):	0.987950	#	69:	48(N)	50(O):	0.896602
#	70:	45(N)	46(O):	1.001794	#	70:	51(N)	52(O):	0.989928
#	71:	45(N)	47(O):	0.889549	#	71:	51(N)	53(O):	0.956971
#	72:	48(N)	49(O):	0.983654	#	72:	54(N)	55(O):	0.979338
#	73:	48(N)	50(O):	0.897926	#	73:	54(N)	56(O):	0.966628
#	74:	51(N)	52(O):	1.011489	#	74:	57(N)	58(O):	0.989898
#	75:	51(N)	53(O):	0.880086	#	75:	57(N)	59(O):	0.956997
#	76:	54(N)	55(O):	0.938792	#	76:	60(N)	61(O):	0.979348
#	77:	54(N)	56(O):	0.863990	#	77:	60(N)	62(O):	0.966622
#	78:	57(N)	58(O):	1.006839					
#	79:	57(N)	59(O):	0.876480					
#	80:	60(N)	61(O):	0.891445	#	47:	28(N)	29(N):	0.628642
#	81:	60(N)	62(O):	0.873663					
#	82:	63(N)	64(O):	0.998452					
#	83:	63(N)	65(O):	0.872268					
#	84:	66(N)	67(O):	0.907825					
#	85:	66(N)	68(O):	0.875030					
#	86:	69(N)	70(O):	1.007770					
#	87:	69(N)	71(O):	0.885758					
#	88:	72(N)	73(O):	0.930210					
#	89:	72(N)	74(O):	0.869913					
#	5:	2(N)	76(H):	0.623698					

E1					E2				
The bond order >=			0.050000		The bond order >=			0.050000	
#	1:	1(C)	2(C):	1.695560	#	1:	1(C)	2(C):	1.715096
#	2:	1(C)	3(C):	1.109632	#	2:	1(C)	3(C):	1.115638
#	3:	1(C)	27(H):	0.834378	#	3:	1(C)	27(H):	0.833663
#	4:	2(C)	4(C):	1.109632	#	4:	2(C)	4(C):	1.115705
#	5:	2(C)	28(H):	0.834378	#	5:	2(C)	28(H):	0.833683
#	6:	3(C)	5(C):	1.363796	#	6:	3(C)	5(C):	1.364004

#	7:	3(C)	9(C):	1.364856	#	7:	3(C)	9(C):	1.338130
#	8:	4(C)	10(C):	1.363796	#	8:	4(C)	10(C):	1.364051
#	9:	4(C)	14(C):	1.364856	#	9:	4(C)	14(C):	1.338140
#	10:	5(C)	6(C):	1.397135	#	10:	5(C)	6(C):	1.450126
#	11:	5(C)	15(N):	0.678121	#	11:	5(C)	15(N):	0.683305
#	12:	6(C)	7(N):	1.185844	#	12:	6(C)	7(N):	1.250407
#	13:	6(C)	31(C):	1.254216	#	13:	6(C)	29(H):	0.852612
#	14:	7(N)	8(C):	1.234071	#	14:	7(N)	8(C):	1.210986
#	15:	8(C)	9(C):	1.460992	#	15:	8(C)	9(C):	1.325666
#	16:	8(C)	29(H):	0.853280	#	16:	8(C)	30(N):	0.884937
#	17:	9(C)	18(N):	0.667120	#	17:	9(C)	18(N):	0.673069
#	18:	10(C)	11(C):	1.397135	#	18:	10(C)	11(C):	1.450080
#	19:	10(C)	24(N):	0.678121	#	19:	10(C)	24(N):	0.683360
#	20:	11(C)	12(N):	1.185844	#	20:	11(C)	12(N):	1.250294
#	21:	11(C)	33(C):	1.254216	#	21:	11(C)	36(H):	0.852628
#	22:	12(N)	13(C):	1.234071	#	22:	12(N)	13(C):	1.211044
#	23:	13(C)	14(C):	1.460992	#	23:	13(C)	14(C):	1.325655
#	24:	13(C)	30(H):	0.853280	#	24:	13(C)	34(N):	0.884912
#	25:	14(C)	21(N):	0.667120	#	25:	14(C)	21(N):	0.673010
#	26:	15(N)	16(O):	0.963156	#	26:	15(N)	16(O):	0.942907
#	27:	15(N)	17(O):	1.000376	#	27:	15(N)	17(O):	0.978034
#	28:	18(N)	19(O):	0.973960	#	28:	18(N)	19(O):	0.944439
#	29:	18(N)	20(O):	0.957712	#	29:	18(N)	20(O):	0.961903
#	30:	21(N)	22(O):	0.973960	#	30:	21(N)	22(O):	0.944486
#	31:	21(N)	23(O):	0.957712	#	31:	21(N)	23(O):	0.961884
#	32:	24(N)	25(O):	0.963156	#	32:	24(N)	25(O):	0.978135
#	33:	24(N)	26(O):	1.000376	#	33:	24(N)	26(O):	0.942791
#	34:	31(C)	32(N):	2.535011	#	34:	30(N)	31(N):	1.149040
#	35:	33(C)	34(N):	2.535011	#	35:	31(N)	32(N):	2.201061
					#	36:	33(N)	35(N):	2.201122
					#	37:	34(N)	35(N):	1.148954
#	17:	9(C)	18(N):	0.667120					
					#	25:	14(C)	21(N):	0.673010

E3					E4				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(C)	2(C):	1.715117	#	1:	1(C)	2(C):	1.741112
#	2:	1(C)	3(C):	1.126386	#	2:	1(C)	3(C):	1.082658
#	3:	1(C)	27(H):	0.833543	#	3:	1(C)	35(H):	0.828670
#	4:	2(C)	4(C):	1.126386	#	4:	2(C)	4(C):	1.082714
#	5:	2(C)	28(H):	0.833543	#	5:	2(C)	36(H):	0.828634
#	6:	3(C)	5(C):	1.368145	#	6:	3(C)	5(C):	1.322392
#	7:	3(C)	9(C):	1.354326	#	7:	3(C)	9(C):	1.354021
#	8:	4(C)	10(C):	1.368145	#	8:	4(C)	10(C):	1.322014
#	9:	4(C)	14(C):	1.354326	#	9:	4(C)	14(C):	1.354100

#	10:	5(C)	6(C):	1.453123	#	10:	5(C)	6(C):	1.280449
#	11:	5(C)	15(N):	0.682880	#	11:	5(C)	15(N):	0.702892
#	12:	6(C)	7(N):	1.212301	#	12:	6(C)	7(N):	1.127788
#	13:	6(C)	29(H):	0.852652	#	13:	6(C)	29(N):	1.176347
#	14:	7(N)	8(C):	1.268539	#	14:	7(N)	8(C):	1.286916
#	15:	8(C)	9(C):	1.439141	#	15:	8(C)	9(C):	1.422511
#	16:	8(C)	32(N):	0.855712	#	16:	8(C)	27(H):	0.851316
#	17:	9(C)	18(N):	0.680203	#	17:	9(C)	18(N):	0.698444
#	18:	10(C)	11(C):	1.453123	#	18:	10(C)	11(C):	1.280507
#	19:	10(C)	24(N):	0.682880	#	19:	10(C)	24(N):	0.702995
#	20:	11(C)	12(N):	1.212301	#	20:	11(C)	12(N):	1.127652
#	21:	11(C)	30(H):	0.852652	#	21:	11(C)	32(N):	1.176458
#	22:	12(N)	13(C):	1.268539	#	22:	12(N)	13(C):	1.287071
#	23:	13(C)	14(C):	1.439141	#	23:	13(C)	14(C):	1.422447
#	24:	13(C)	31(N):	0.855712	#	24:	13(C)	28(H):	0.851345
#	25:	14(C)	21(N):	0.680203	#	25:	14(C)	21(N):	0.698396
#	26:	15(N)	16(O):	0.958009	#	26:	15(N)	16(O):	0.887762
#	27:	15(N)	17(O):	0.984857	#	27:	15(N)	17(O):	0.956514
#	28:	18(N)	19(O):	0.991479	#	28:	18(N)	19(O):	0.949949
#	29:	18(N)	20(O):	0.966518	#	29:	18(N)	20(O):	0.948516
#	30:	21(N)	22(O):	0.991479	#	30:	21(N)	22(O):	0.950103
#	31:	21(N)	23(O):	0.966518	#	31:	21(N)	23(O):	0.948682
#	32:	24(N)	25(O):	0.958009	#	32:	24(N)	25(O):	0.887621
#	33:	24(N)	26(O):	0.984857	#	33:	24(N)	26(O):	0.956713
#	34:	31(N)	33(F):	0.142371	#	34:	29(N)	30(H):	0.681924
#	35:	31(N)	36(F):	0.153541	#	35:	29(N)	31(H):	0.671230
#	36:	32(N)	34(F):	0.142371	#	36:	32(N)	33(H):	0.681936
#	37:	32(N)	35(F):	0.153541	#	37:	32(N)	34(H):	0.671190
#	34:	31(N)	33(F):	0.142371	#	37:	32(N)	34(H):	0.671190

E5

The bond order >= 0.050000

#	1:	1(C)	2(C):	1.728707
#	2:	1(C)	3(C):	1.070016
#	3:	1(C)	35(H):	0.827669
#	4:	2(C)	4(C):	1.070024
#	5:	2(C)	36(H):	0.827667
#	6:	3(C)	5(C):	1.369229
#	7:	3(C)	9(C):	1.385060
#	8:	4(C)	10(C):	1.369221
#	9:	4(C)	14(C):	1.385071
#	10:	5(C)	6(C):	1.308623
#	11:	5(C)	23(N):	0.674273
#	12:	6(C)	7(N):	1.215356

E6

The bond order >= 0.050000

#	1:	1(C)	2(C):	1.727605
#	2:	1(C)	3(C):	1.067567
#	3:	1(C)	27(H):	0.827392
#	4:	2(C)	4(C):	1.067579
#	5:	2(C)	28(H):	0.827392
#	6:	3(C)	5(C):	1.377482
#	7:	3(C)	9(C):	1.370302
#	8:	4(C)	10(C):	1.377522
#	9:	4(C)	14(C):	1.370267
#	10:	5(C)	6(C):	1.248555
#	11:	5(C)	15(N):	0.683836
#	12:	6(C)	7(N):	1.152405

#	13:	6(C)	15(N):	0.963414	#	13:	6(C)	31(N):	1.122837
#	14:	7(N)	8(C):	1.237307	#	14:	7(N)	8(C):	1.270734
#	15:	8(C)	9(C):	1.454611	#	15:	8(C)	9(C):	1.428359
#	16:	8(C)	37(H):	0.853482	#	16:	8(C)	29(H):	0.851703
#	17:	9(C)	26(N):	0.688512	#	17:	9(C)	18(N):	0.712453
#	18:	10(C)	11(C):	1.308649	#	18:	10(C)	11(C):	1.248604
#	19:	10(C)	32(N):	0.674265	#	19:	10(C)	24(N):	0.683841
#	20:	11(C)	12(N):	1.215351	#	20:	11(C)	12(N):	1.152417
#	21:	11(C)	19(N):	0.963395	#	21:	11(C)	33(N):	1.122826
#	22:	12(N)	13(C):	1.237320	#	22:	12(N)	13(C):	1.270718
#	23:	13(C)	14(C):	1.454604	#	23:	13(C)	14(C):	1.428365
#	24:	13(C)	38(H):	0.853479	#	24:	13(C)	30(H):	0.851705
#	25:	14(C)	29(N):	0.688505	#	25:	14(C)	21(N):	0.712451
#	26:	15(N)	16(N):	0.568525	#	26:	15(N)	16(O):	0.977330
#	27:	15(N)	39(H):	0.649152	#	27:	15(N)	17(O):	0.891096
#	28:	16(N)	17(O):	0.983690	#	28:	18(N)	19(O):	0.944883
#	29:	16(N)	18(O):	1.033952	#	29:	18(N)	20(O):	0.934433
#	30:	19(N)	20(N):	0.568453	#	30:	21(N)	22(O):	0.944879
#	31:	19(N)	40(H):	0.649161	#	31:	21(N)	23(O):	0.934441
#	32:	20(N)	21(O):	0.983698	#	32:	24(N)	25(O):	0.891076
#	33:	20(N)	22(O):	1.033942	#	33:	24(N)	26(O):	0.977333
#	34:	23(N)	24(O):	0.990506	#	34:	31(N)	32(H):	0.660006
#	35:	23(N)	25(O):	0.919833	#	35:	31(N)	35(N):	0.626331
#	36:	26(N)	27(O):	0.970807	#	36:	33(N)	34(H):	0.660006
#	37:	26(N)	28(O):	0.943352	#	37:	33(N)	38(N):	0.626341
#	38:	29(N)	30(O):	0.970807	#	38:	35(N)	36(H):	0.695875
#	39:	29(N)	31(O):	0.943358	#	39:	35(N)	37(H):	0.694307
#	40:	32(N)	33(O):	0.919833	#	40:	38(N)	39(H):	0.694305
#	41:	32(N)	34(O):	0.990511	#	41:	38(N)	40(H):	0.695876
#	30:	19(N)	20(N):	0.568453	#	35:	31(N)	35(N):	0.626331

E7					E8				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(C)	3(C):	1.369684	#	1:	1(C)	2(C):	1.731188
#	2:	1(C)	7(C):	1.397455	#	2:	1(C)	3(C):	1.064195
#	3:	1(C)	46(C):	1.071459	#	3:	1(C)	47(H):	0.820143
#	4:	2(C)	8(C):	1.377434	#	4:	2(C)	4(C):	1.064195
#	5:	2(C)	12(C):	1.388959	#	5:	2(C)	48(H):	0.820143
#	6:	2(C)	45(C):	1.070562	#	6:	3(C)	5(C):	1.381994
#	7:	3(C)	4(C):	1.394759	#	7:	3(C)	9(C):	1.387987
#	8:	3(C)	27(N):	0.676198	#	8:	4(C)	10(C):	1.381986
#	9:	4(C)	5(N):	1.207722	#	9:	4(C)	14(C):	1.387987
#	10:	4(C)	13(C):	1.044805	#	10:	5(C)	6(C):	1.368985
#	11:	5(N)	6(C):	1.227721	#	11:	5(C)	35(N):	0.677740

#	12:	6(C)	7(C):	1.462894	#	12:	6(C)	7(N):	1.214378
#	13:	6(C)	41(H):	0.854353	#	13:	6(C)	15(C):	1.011501
#	14:	7(C)	30(N):	0.679054	#	14:	7(N)	8(C):	1.215554
#	15:	8(C)	9(C):	1.380982	#	15:	8(C)	9(C):	1.486401
#	16:	8(C)	36(N):	0.670538	#	16:	8(C)	49(H):	0.852932
#	17:	9(C)	10(N):	1.210323	#	17:	9(C)	38(N):	0.679944
#	18:	9(C)	20(C):	1.027136	#	18:	10(C)	11(C):	1.369006
#	19:	10(N)	11(C):	1.217434	#	19:	10(C)	44(N):	0.677753
#	20:	11(C)	12(C):	1.475782	#	20:	11(C)	12(N):	1.214373
#	21:	11(C)	42(H):	0.853921	#	21:	11(C)	25(C):	1.011512
#	22:	12(C)	33(N):	0.680709	#	22:	12(N)	13(C):	1.215550
#	23:	13(C)	14(N):	0.536952	#	23:	13(C)	14(C):	1.486394
#	24:	13(C)	17(N):	0.546964	#	24:	13(C)	50(H):	0.852928
#	25:	13(C)	43(H):	0.835002	#	25:	14(C)	41(N):	0.679954
#	26:	14(N)	15(O):	0.998601	#	26:	15(C)	16(N):	0.462907
#	27:	14(N)	16(O):	1.015829	#	27:	15(C)	19(N):	0.519349
#	28:	17(N)	18(O):	0.988834	#	28:	15(C)	22(N):	0.465836
#	29:	17(N)	19(O):	1.029643	#	29:	16(N)	17(O):	0.997897
#	30:	20(C)	21(N):	0.524263	#	30:	16(N)	18(O):	1.072185
#	31:	20(C)	24(N):	0.559620	#	31:	19(N)	20(O):	0.981333
#	32:	20(C)	44(H):	0.830721	#	32:	19(N)	21(O):	1.044017
#	33:	21(N)	22(O):	0.982102	#	33:	22(N)	23(O):	1.023122
#	34:	21(N)	23(O):	1.028144	#	34:	22(N)	24(O):	1.042178
#	35:	24(N)	25(O):	1.005021	#	35:	25(C)	26(N):	0.519347
#	36:	24(N)	26(O):	1.019140	#	36:	25(C)	29(N):	0.462892
#	37:	27(N)	28(O):	0.948244	#	37:	25(C)	32(N):	0.465842
#	38:	27(N)	29(O):	0.981250	#	38:	26(N)	27(O):	0.981335
#	39:	30(N)	31(O):	0.983284	#	39:	26(N)	28(O):	1.044017
#	40:	30(N)	32(O):	0.950906	#	40:	29(N)	30(O):	0.997844
#	41:	33(N)	34(O):	0.978063	#	41:	29(N)	31(O):	1.072179
#	42:	33(N)	35(O):	0.954064	#	42:	32(N)	33(O):	1.042175
#	43:	36(N)	37(O):	1.000276	#	43:	32(N)	34(O):	1.023127
#	44:	36(N)	38(O):	0.946173	#	44:	35(N)	36(O):	1.007210
#	45:	39(H)	46(C):	0.824420	#	45:	35(N)	37(O):	0.952765
#	46:	40(H)	45(C):	0.824070	#	46:	38(N)	39(O):	0.983791
#	47:	45(C)	46(C):	1.733080	#	47:	38(N)	40(O):	0.958237
					#	48:	41(N)	42(O):	0.983797
					#	49:	41(N)	43(O):	0.958241
#	30:	20(C)	21(N):	0.524263	#	50:	44(N)	45(O):	0.952764
					#	51:	44(N)	46(O):	1.007207
					#	36:	25(C)	29(N):	0.462892

E9	E10
The bond order >= 0.050000	The bond order >= 0.050000

#	1:	1(C)	2(C):	1.707677	#	1:	1(C)	2(C):	1.707568
#	2:	1(C)	3(C):	1.109864	#	2:	1(C)	3(C):	1.087919
#	3:	1(C)	27(H):	0.838118	#	3:	1(C)	27(H):	0.834493
#	4:	2(C)	4(C):	1.093002	#	4:	2(C)	4(C):	1.087924
#	5:	2(C)	28(H):	0.825727	#	5:	2(C)	28(H):	0.834490
#	6:	3(C)	5(C):	1.357527	#	6:	3(C)	5(C):	1.367321
#	7:	3(C)	9(C):	1.368714	#	7:	3(C)	9(C):	1.345989
#	8:	4(C)	10(C):	1.346280	#	8:	4(C)	10(C):	1.367341
#	9:	4(C)	14(C):	1.356168	#	9:	4(C)	14(C):	1.345977
#	10:	5(C)	6(C):	1.443252	#	10:	5(C)	6(C):	1.353055
#	11:	5(C)	15(N):	0.673058	#	11:	5(C)	15(N):	0.657111
#	12:	6(C)	7(N):	1.299267	#	12:	6(C)	7(N):	1.195592
#	13:	6(C)	31(N):	0.751833	#	13:	6(C)	31(N):	0.897268
#	14:	7(N)	8(C):	1.204002	#	14:	7(N)	8(C):	1.196443
#	15:	8(C)	9(C):	1.474507	#	15:	8(C)	9(C):	1.490673
#	16:	8(C)	29(H):	0.856315	#	16:	8(C)	29(H):	0.857848
#	17:	9(C)	18(N):	0.665121	#	17:	9(C)	18(N):	0.682235
#	18:	10(C)	11(C):	1.432825	#	18:	10(C)	11(C):	1.353063
#	19:	10(C)	24(N):	0.679557	#	19:	10(C)	24(N):	0.657122
#	20:	11(C)	12(N):	1.293876	#	20:	11(C)	12(N):	1.195592
#	21:	11(C)	45(N):	0.760068	#	21:	11(C)	43(N):	0.897256
#	22:	12(N)	13(C):	1.206473	#	22:	12(N)	13(C):	1.196444
#	23:	13(C)	14(C):	1.474493	#	23:	13(C)	14(C):	1.490676
#	24:	13(C)	30(H):	0.856579	#	24:	13(C)	30(H):	0.857855
#	25:	14(C)	21(N):	0.673956	#	25:	14(C)	21(N):	0.682247
#	26:	15(N)	16(O):	0.952197	#	26:	15(N)	16(O):	0.981342
#	27:	15(N)	17(O):	0.998061	#	27:	15(N)	17(O):	1.017076
#	28:	18(N)	19(O):	0.978184	#	28:	18(N)	19(O):	0.963833
#	29:	18(N)	20(O):	0.960624	#	29:	18(N)	20(O):	0.956578
#	30:	21(N)	22(O):	0.978983	#	30:	21(N)	22(O):	0.963800
#	31:	21(N)	23(O):	0.967247	#	31:	21(N)	23(O):	0.956593
#	32:	24(N)	25(O):	0.983339	#	32:	24(N)	25(O):	0.981345
#	33:	24(N)	26(O):	0.985957	#	33:	24(N)	26(O):	1.017075
#	34:	31(N)	32(C):	0.935581	#	34:	31(N)	32(C):	0.868660
#	35:	31(N)	33(N):	0.809965	#	35:	31(N)	33(N):	0.618197
#	36:	32(C)	34(C):	1.435067	#	36:	32(C)	34(C):	1.353572
#	37:	32(C)	35(N):	0.814035	#	37:	32(C)	35(N):	1.217350
#	38:	33(N)	36(C):	1.300674	#	38:	33(N)	36(C):	1.422637
#	39:	34(C)	36(C):	1.278307	#	39:	34(C)	36(C):	1.228149
#	40:	34(C)	37(N):	0.727136	#	40:	34(C)	37(N):	0.867142
#	41:	35(N)	38(O):	0.940898	#	41:	35(N)	55(H):	0.660850
#	42:	35(N)	39(O):	0.984979	#	42:	35(N)	58(H):	0.660983
#	43:	36(C)	40(N):	0.764832	#	43:	36(C)	38(N):	0.746581
#	44:	37(N)	41(O):	1.007826	#	44:	37(N)	39(O):	0.855204
#	45:	37(N)	42(O):	1.010094	#	45:	37(N)	40(O):	0.961820

#	46:	40(N)	43(O):	0.999556	#	46:	38(N)	41(O):	0.997445
#	47:	40(N)	44(O):	0.952830	#	47:	38(N)	42(O):	0.991038
#	48:	45(N)	46(C):	0.932197	#	48:	43(N)	44(C):	0.868634
#	49:	45(N)	47(N):	0.802998	#	49:	43(N)	45(N):	0.618196
#	50:	46(C)	48(C):	1.439548	#	50:	44(C)	46(C):	1.353570
#	51:	46(C)	49(N):	0.801414	#	51:	44(C)	47(N):	1.217350
#	52:	47(N)	50(C):	1.304153	#	52:	45(N)	48(C):	1.422632
#	53:	48(C)	50(C):	1.273506	#	53:	46(C)	48(C):	1.228148
#	54:	48(C)	51(N):	0.731874	#	54:	46(C)	49(N):	0.867134
#	55:	49(N)	52(O):	0.949222	#	55:	47(N)	56(H):	0.660856
#	56:	49(N)	53(O):	0.982610	#	56:	47(N)	57(H):	0.660982
#	57:	50(C)	54(N):	0.761920	#	57:	48(C)	50(N):	0.746579
#	58:	51(N)	55(O):	1.000972	#	58:	49(N)	51(O):	0.855215
#	59:	51(N)	56(O):	1.003599	#	59:	49(N)	52(O):	0.961813
#	60:	54(N)	57(O):	1.004503	#	60:	50(N)	53(O):	0.997449
#	61:	54(N)	58(O):	0.950970	#	61:	50(N)	54(O):	0.991048
#	17:	9(C)	18(N):	0.665121	#	49:	43(N)	45(N):	0.618196

E11

The bond order >= 0.050000

#	1:	1(C)	2(C):	1.708936
#	2:	1(C)	3(C):	1.105868
#	3:	1(C)	27(H):	0.835804
#	4:	2(C)	4(C):	1.091825
#	5:	2(C)	28(H):	0.828191
#	6:	3(C)	5(C):	1.353860
#	7:	3(C)	9(C):	1.362090
#	8:	4(C)	10(C):	1.351166
#	9:	4(C)	14(C):	1.348922
#	10:	5(C)	6(C):	1.429433
#	11:	5(C)	15(N):	0.669727
#	12:	6(C)	7(N):	1.273570
#	13:	6(C)	31(N):	0.806562
#	14:	7(N)	8(C):	1.214206
#	15:	8(C)	9(C):	1.467393
#	16:	8(C)	29(H):	0.853893
#	17:	9(C)	18(N):	0.671805
#	18:	10(C)	11(C):	1.424554
#	19:	10(C)	24(N):	0.672557
#	20:	11(C)	12(N):	1.282125
#	21:	11(C)	42(N):	0.797620
#	22:	12(N)	13(C):	1.212846
#	23:	13(C)	14(C):	1.469986
#	24:	13(C)	30(H):	0.854534

E12

The bond order >= 0.050000

#	1:	1(C)	2(C):	1.722912
#	2:	1(C)	3(C):	1.071509
#	3:	1(C)	27(H):	0.822823
#	4:	2(C)	4(C):	1.071248
#	5:	2(C)	28(H):	0.822713
#	6:	3(C)	5(C):	1.383452
#	7:	3(C)	9(C):	1.347068
#	8:	4(C)	10(C):	1.383356
#	9:	4(C)	14(C):	1.347306
#	10:	5(C)	6(C):	1.359488
#	11:	5(C)	15(N):	0.668206
#	12:	6(C)	7(N):	1.200971
#	13:	6(C)	31(N):	0.908449
#	14:	7(N)	8(C):	1.196514
#	15:	8(C)	9(C):	1.487595
#	16:	8(C)	29(H):	0.853630
#	17:	9(C)	18(N):	0.694130
#	18:	10(C)	11(C):	1.359505
#	19:	10(C)	24(N):	0.668479
#	20:	11(C)	12(N):	1.200735
#	21:	11(C)	39(N):	0.908795
#	22:	12(N)	13(C):	1.196353
#	23:	13(C)	14(C):	1.487488
#	24:	13(C)	30(H):	0.853456

#	25:	14(C)	21(N):	0.676166	#	25:	14(C)	21(N):	0.694539
#	26:	15(N)	16(O):	0.958555	#	26:	15(N)	16(O):	0.991194
#	27:	15(N)	17(O):	1.002012	#	27:	15(N)	17(O):	0.991519
#	28:	18(N)	19(O):	0.967630	#	28:	18(N)	19(O):	0.967755
#	29:	18(N)	20(O):	0.954743	#	29:	18(N)	20(O):	0.966217
#	30:	21(N)	22(O):	0.972511	#	30:	21(N)	22(O):	0.967757
#	31:	21(N)	23(O):	0.964083	#	31:	21(N)	23(O):	0.966513
#	32:	24(N)	25(O):	0.978954	#	32:	24(N)	25(O):	0.991346
#	33:	24(N)	26(O):	0.983929	#	33:	24(N)	26(O):	0.991319
#	34:	31(N)	32(C):	0.856664	#	34:	31(N)	32(C):	0.835219
#	35:	31(N)	33(N):	0.844965	#	35:	31(N)	33(N):	0.649374
#	36:	32(C)	34(C):	1.354763	#	36:	32(C)	34(N):	1.173099
#	37:	32(C)	35(N):	0.893721	#	37:	32(C)	49(N):	1.280396
#	38:	33(N)	36(C):	1.285619	#	38:	33(N)	35(C):	1.402874
#	39:	34(C)	36(C):	1.217352	#	39:	34(N)	47(H):	0.668011
#	40:	34(C)	53(N):	1.161056	#	40:	34(N)	48(H):	0.680273
#	41:	35(N)	37(O):	0.926274	#	41:	35(C)	36(N):	0.739726
#	42:	35(N)	38(O):	0.866944	#	42:	35(C)	49(N):	1.083440
#	43:	36(C)	39(N):	0.804217	#	43:	36(N)	37(O):	0.970943
#	44:	39(N)	40(O):	1.005497	#	44:	36(N)	38(O):	0.975877
#	45:	39(N)	41(O):	0.879127	#	45:	39(N)	40(C):	0.835443
#	46:	42(N)	43(C):	0.855770	#	46:	39(N)	41(N):	0.649497
#	47:	42(N)	44(N):	0.850203	#	47:	40(C)	42(N):	1.173389
#	48:	43(C)	45(C):	1.356629	#	48:	40(C)	52(N):	1.280464
#	49:	43(C)	46(N):	0.896568	#	49:	41(N)	43(C):	1.402992
#	50:	44(N)	47(C):	1.280742	#	50:	42(N)	50(H):	0.680253
#	51:	45(C)	47(C):	1.219273	#	51:	42(N)	51(H):	0.667971
#	52:	45(C)	56(N):	1.156858	#	52:	43(C)	44(N):	0.739988
#	53:	46(N)	48(O):	0.926390	#	53:	43(C)	52(N):	1.083192
#	54:	46(N)	49(O):	0.872303	#	54:	44(N)	45(O):	0.971205
#	55:	47(C)	50(N):	0.806359	#	55:	44(N)	46(O):	0.976584
#	56:	50(N)	51(O):	1.002134					
#	57:	50(N)	52(O):	0.875566					
#	58:	53(N)	54(H):	0.674943	#	35:	31(N)	33(N):	0.649374
#	59:	53(N)	55(H):	0.674741					
#	60:	56(N)	57(H):	0.675129					
#	61:	56(N)	58(H):	0.674889					
#	11:	5(C)	15(N):	0.669727					

F1

The bond order >= 0.050000

#	1:	1(C)	2(C):	1.700569
#	2:	1(C)	3(C):	1.111234

F2

The bond order >= 0.050000

#	1:	1(C)	2(C):	1.702270
#	2:	1(C)	3(C):	1.104033
#	3:	1(C)	33(H):	0.833238

#	3:	1(C)	31(H):	0.833592	#	4:	2(C)	4(C):	1.104026
#	4:	2(C)	4(C):	1.111234	#	5:	2(C)	34(H):	0.833193
#	5:	2(C)	32(H):	0.833592	#	6:	3(C)	5(C):	1.406543
#	6:	3(C)	5(C):	1.377112	#	7:	3(C)	9(C):	1.305131
#	7:	3(C)	9(C):	1.373422	#	8:	4(C)	10(C):	1.406532
#	8:	4(C)	10(C):	1.377112	#	9:	4(C)	14(C):	1.305080
#	9:	4(C)	14(C):	1.373422	#	10:	5(C)	6(C):	1.392215
#	10:	5(C)	6(C):	1.391285	#	11:	5(C)	15(N):	0.675047
#	11:	5(C)	15(N):	0.685037	#	12:	6(C)	7(N):	1.230431
#	12:	6(C)	7(N):	1.199116	#	13:	6(C)	27(N):	0.908433
#	13:	6(C)	27(C):	1.257213	#	14:	7(N)	8(C):	1.186216
#	14:	7(N)	8(C):	1.183598	#	15:	8(C)	9(C):	1.324554
#	15:	8(C)	9(C):	1.382793	#	16:	8(C)	39(N):	0.889450
#	16:	8(C)	33(C):	1.257807	#	17:	9(C)	21(N):	0.694912
#	17:	9(C)	21(N):	0.681675	#	18:	10(C)	11(C):	1.392194
#	18:	10(C)	11(C):	1.391285	#	19:	10(C)	18(N):	0.674975
#	19:	10(C)	18(N):	0.685037	#	20:	11(C)	12(N):	1.230467
#	20:	11(C)	12(N):	1.199116	#	21:	11(C)	30(N):	0.908411
#	21:	11(C)	29(C):	1.257213	#	22:	12(N)	13(C):	1.186168
#	22:	12(N)	13(C):	1.183598	#	23:	13(C)	14(C):	1.324596
#	23:	13(C)	14(C):	1.382793	#	24:	13(C)	38(N):	0.889402
#	24:	13(C)	35(C):	1.257807	#	25:	14(C)	24(N):	0.694912
#	25:	14(C)	24(N):	0.681675	#	26:	15(N)	16(O):	0.960436
#	26:	15(N)	16(O):	0.967808	#	27:	15(N)	17(O):	1.001399
#	27:	15(N)	17(O):	1.000915	#	28:	18(N)	19(O):	0.960269
#	28:	18(N)	19(O):	0.967808	#	29:	18(N)	20(O):	1.001661
#	29:	18(N)	20(O):	1.000915	#	30:	21(N)	22(O):	0.928110
#	30:	21(N)	22(O):	0.988737	#	31:	21(N)	23(O):	0.953534
#	31:	21(N)	23(O):	0.952852	#	32:	24(N)	25(O):	0.928100
#	32:	24(N)	25(O):	0.988737	#	33:	24(N)	26(O):	0.953521
#	33:	24(N)	26(O):	0.952852	#	34:	27(N)	28(N):	1.129668
#	34:	27(C)	28(N):	2.538581	#	35:	28(N)	29(N):	2.259476
#	35:	29(C)	30(N):	2.538581	#	36:	30(N)	31(N):	1.129693
#	36:	33(C)	34(N):	2.537639	#	37:	31(N)	32(N):	2.259468
#	37:	35(C)	36(N):	2.537639	#	38:	35(N)	40(N):	2.208448
					#	39:	36(N)	37(N):	2.208427
					#	40:	37(N)	38(N):	1.155296
					#	41:	39(N)	40(N):	1.155272
#	17:	9(C)	21(N):	0.681675	#	19:	10(C)	18(N):	0.674975

F3					F4				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(C)	2(C):	1.711936	#	1:	1(C)	2(C):	1.725343
#	2:	1(C)	3(C):	1.107848	#	2:	1(C)	3(C):	1.054876

#	3:	1(C)	33(H):	0.833210	#	3:	1(C)	29(H):	0.822738
#	4:	2(C)	4(C):	1.090982	#	4:	2(C)	4(C):	1.054872
#	5:	2(C)	34(H):	0.827853	#	5:	2(C)	30(H):	0.822737
#	6:	3(C)	5(C):	1.379980	#	6:	3(C)	5(C):	1.370892
#	7:	3(C)	9(C):	1.350987	#	7:	3(C)	9(C):	1.370611
#	8:	4(C)	10(C):	1.375456	#	8:	4(C)	10(C):	1.370614
#	9:	4(C)	14(C):	1.336051	#	9:	4(C)	14(C):	1.370838
#	10:	5(C)	6(C):	1.370149	#	10:	5(C)	6(C):	1.252326
#	11:	5(C)	15(N):	0.671342	#	11:	5(C)	17(N):	0.724295
#	12:	6(C)	7(N):	1.270266	#	12:	6(C)	7(N):	1.173974
#	13:	6(C)	27(N):	0.874613	#	13:	6(C)	15(N):	1.168607
#	14:	7(N)	8(C):	1.226719	#	14:	7(N)	8(C):	1.173885
#	15:	8(C)	9(C):	1.456872	#	15:	8(C)	9(C):	1.252221
#	16:	8(C)	35(N):	0.858324	#	16:	8(C)	35(N):	1.168706
#	17:	9(C)	21(N):	0.684515	#	17:	9(C)	23(N):	0.724495
#	18:	10(C)	11(C):	1.363755	#	18:	10(C)	11(C):	1.252128
#	19:	10(C)	18(N):	0.674324	#	19:	10(C)	20(N):	0.724557
#	20:	11(C)	12(N):	1.273644	#	20:	11(C)	12(N):	1.173980
#	21:	11(C)	30(N):	0.866584	#	21:	11(C)	16(N):	1.168682
#	22:	12(N)	13(C):	1.229737	#	22:	12(N)	13(C):	1.173882
#	23:	13(C)	14(C):	1.462200	#	23:	13(C)	14(C):	1.252431
#	24:	13(C)	36(N):	0.859265	#	24:	13(C)	38(N):	1.168683
#	25:	14(C)	24(N):	0.688782	#	25:	14(C)	26(N):	0.724270
#	26:	15(N)	16(O):	0.974583	#	26:	15(N)	31(H):	0.683844
#	27:	15(N)	17(O):	1.003769	#	27:	15(N)	32(H):	0.668866
#	28:	18(N)	19(O):	0.972823	#	28:	16(N)	33(H):	0.683847
#	29:	18(N)	20(O):	1.008744	#	29:	16(N)	34(H):	0.668758
#	30:	21(N)	22(O):	0.999312	#	30:	17(N)	18(O):	0.874294
#	31:	21(N)	23(O):	0.958773	#	31:	17(N)	19(O):	0.953098
#	32:	24(N)	25(O):	1.010441	#	32:	20(N)	21(O):	0.873856
#	33:	24(N)	26(O):	0.961047	#	33:	20(N)	22(O):	0.952849
#	34:	27(N)	28(F):	0.176781	#	34:	23(N)	24(O):	0.874037
#	35:	27(N)	29(F):	0.138466	#	35:	23(N)	25(O):	0.952882
#	36:	30(N)	31(F):	0.176657	#	36:	26(N)	27(O):	0.874407
#	37:	30(N)	32(F):	0.138046	#	37:	26(N)	28(O):	0.953077
#	38:	35(N)	37(F):	0.155117	#	38:	35(N)	36(H):	0.683870
#	39:	35(N)	38(F):	0.144773	#	39:	35(N)	37(H):	0.668764
#	40:	36(N)	39(F):	0.146237	#	40:	38(N)	39(H):	0.683868
#	41:	36(N)	40(F):	0.153786	#	41:	38(N)	40(H):	0.668840

#	37:	30(N)	32(F):	0.138046	#	39:	35(N)	37(H):	0.668764

F5	F6

The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(C)	2(C):	1.729899	#	1:	1(C)	2(C):	1.719865

#	2:	1(C)	3(C):	1.053127	#	2:	1(C)	3(C):	1.051040
#	3:	1(C)	35(H):	0.822212	#	3:	1(C)	31(H):	0.821633
#	4:	2(C)	4(C):	1.053126	#	4:	2(C)	4(C):	1.051040
#	5:	2(C)	36(H):	0.822212	#	5:	2(C)	32(H):	0.821633
#	6:	3(C)	5(C):	1.375891	#	6:	3(C)	5(C):	1.369679
#	7:	3(C)	9(C):	1.376399	#	7:	3(C)	9(C):	1.369679
#	8:	4(C)	10(C):	1.375846	#	8:	4(C)	10(C):	1.369679
#	9:	4(C)	14(C):	1.376436	#	9:	4(C)	14(C):	1.369679
#	10:	5(C)	6(C):	1.282340	#	10:	5(C)	6(C):	1.236470
#	11:	5(C)	15(N):	0.700305	#	11:	5(C)	15(N):	0.728782
#	12:	6(C)	7(N):	1.220285	#	12:	6(C)	7(N):	1.153883
#	13:	6(C)	27(N):	0.992977	#	13:	6(C)	27(N):	1.124833
#	14:	7(N)	8(C):	1.220707	#	14:	7(N)	8(C):	1.153883
#	15:	8(C)	9(C):	1.281955	#	15:	8(C)	9(C):	1.236470
#	16:	8(C)	43(N):	0.992974	#	16:	8(C)	47(N):	1.124833
#	17:	9(C)	21(N):	0.700212	#	17:	9(C)	21(N):	0.728782
#	18:	10(C)	11(C):	1.282358	#	18:	10(C)	11(C):	1.236470
#	19:	10(C)	18(N):	0.700314	#	19:	10(C)	18(N):	0.728782
#	20:	11(C)	12(N):	1.220271	#	20:	11(C)	12(N):	1.153883
#	21:	11(C)	31(N):	0.992993	#	21:	11(C)	29(N):	1.124833
#	22:	12(N)	13(C):	1.220728	#	22:	12(N)	13(C):	1.153883
#	23:	13(C)	14(C):	1.281887	#	23:	13(C)	14(C):	1.236470
#	24:	13(C)	41(N):	0.992985	#	24:	13(C)	46(N):	1.124833
#	25:	14(C)	24(N):	0.700201	#	25:	14(C)	24(N):	0.728782
#	26:	15(N)	16(O):	0.974266	#	26:	15(N)	16(O):	0.875235
#	27:	15(N)	17(O):	0.909273	#	27:	15(N)	17(O):	0.951809
#	28:	18(N)	19(O):	0.909249	#	28:	18(N)	19(O):	0.875235
#	29:	18(N)	20(O):	0.974267	#	29:	18(N)	20(O):	0.951809
#	30:	21(N)	22(O):	0.909489	#	30:	21(N)	22(O):	0.875235
#	31:	21(N)	23(O):	0.974371	#	31:	21(N)	23(O):	0.951809
#	32:	24(N)	25(O):	0.909509	#	32:	24(N)	25(O):	0.875235
#	33:	24(N)	26(O):	0.974377	#	33:	24(N)	26(O):	0.951809
#	34:	27(N)	28(N):	0.559340	#	34:	27(N)	28(N):	0.620174
#	35:	27(N)	37(H):	0.642370	#	35:	27(N)	33(H):	0.668351
#	36:	28(N)	29(O):	0.983741	#	36:	28(N)	34(H):	0.694936
#	37:	28(N)	30(O):	1.052411	#	37:	28(N)	35(H):	0.691669
#	38:	31(N)	32(N):	0.559298	#	38:	29(N)	30(N):	0.620174
#	39:	31(N)	38(H):	0.642373	#	39:	29(N)	36(H):	0.668351
#	40:	32(N)	33(O):	0.983742	#	40:	30(N)	37(H):	0.691669
#	41:	32(N)	34(O):	1.052405	#	41:	30(N)	38(H):	0.694936
#	42:	39(H)	43(N):	0.642298	#	42:	39(H)	47(N):	0.668351
#	43:	40(H)	41(N):	0.642302	#	43:	40(H)	48(N):	0.694936
#	44:	41(N)	42(N):	0.559866	#	44:	41(H)	48(N):	0.691669
#	45:	42(N)	45(O):	0.983804	#	45:	42(H)	46(N):	0.668351
#	46:	42(N)	46(O):	1.052757	#	46:	43(H)	45(N):	0.694936

#	47:	43(N)	44(N):	0.559868	#	47:	44(H)	45(N):	0.691669
#	48:	44(N)	47(O):	1.052733	#	48:	45(N)	46(N):	0.620174
#	49:	44(N)	48(O):	0.983796	#	49:	47(N)	48(N):	0.620174
#	38:	31(N)	32(N):	0.559298	#	34:	27(N)	28(N):	0.620174

F7					F8				
The bond order >= 0.050000					The bond order >= 0.050000				
#	1:	1(C)	2(C):	1.703525	#	1:	1(C)	2(C):	1.728006
#	2:	1(C)	3(C):	1.069575	#	2:	1(C)	3(C):	1.053762
#	3:	1(C)	41(H):	0.822075	#	3:	1(C)	40(H):	0.819206
#	4:	2(C)	4(C):	1.086192	#	4:	2(C)	4(C):	1.053762
#	5:	2(C)	42(H):	0.826493	#	5:	2(C)	41(H):	0.819203
#	6:	3(C)	5(C):	1.367611	#	6:	3(C)	5(C):	1.386820
#	7:	3(C)	9(C):	1.366320	#	7:	3(C)	9(C):	1.386644
#	8:	4(C)	10(C):	1.373993	#	8:	4(C)	10(C):	1.386852
#	9:	4(C)	14(C):	1.357222	#	9:	4(C)	14(C):	1.386652
#	10:	5(C)	6(C):	1.407266	#	10:	5(C)	6(C):	1.388729
#	11:	5(C)	15(N):	0.663770	#	11:	5(C)	15(N):	0.684379
#	12:	6(C)	7(N):	1.206899	#	12:	6(C)	7(N):	1.199851
#	13:	6(C)	27(C):	1.026398	#	13:	6(C)	26(C):	1.014739
#	14:	7(N)	8(C):	1.204532	#	14:	7(N)	8(C):	1.199666
#	15:	8(C)	9(C):	1.385726	#	15:	8(C)	9(C):	1.388692
#	16:	8(C)	45(C):	1.022667	#	16:	8(C)	42(C):	1.014689
#	17:	9(C)	21(N):	0.674804	#	17:	9(C)	21(N):	0.684478
#	18:	10(C)	11(C):	1.416215	#	18:	10(C)	11(C):	1.388645
#	19:	10(C)	18(N):	0.678100	#	19:	10(C)	18(N):	0.684417
#	20:	11(C)	12(N):	1.218262	#	20:	11(C)	12(N):	1.199880
#	21:	11(C)	34(C):	1.042516	#	21:	11(C)	33(C):	1.014717
#	22:	12(N)	13(C):	1.209118	#	22:	12(N)	13(C):	1.199639
#	23:	13(C)	14(C):	1.386398	#	23:	13(C)	14(C):	1.388714
#	24:	13(C)	47(C):	1.031790	#	24:	13(C)	43(C):	1.014724
#	25:	14(C)	24(N):	0.672972	#	25:	14(C)	23(N):	0.684489
#	26:	15(N)	16(O):	1.010808	#	26:	15(N)	16(O):	0.966859
#	27:	15(N)	17(O):	0.949450	#	27:	15(N)	17(O):	1.000460
#	28:	18(N)	19(O):	1.005643	#	28:	18(N)	19(O):	1.000470
#	29:	18(N)	20(O):	0.946288	#	29:	18(N)	20(O):	0.966921
#	30:	21(N)	22(O):	0.951739	#	30:	21(N)	22(O):	1.000500
#	31:	21(N)	23(O):	1.002007	#	31:	21(N)	66(O):	0.966865
#	32:	24(N)	25(O):	0.951667	#	32:	23(N)	24(O):	0.966773
#	33:	24(N)	26(O):	0.978290	#	33:	23(N)	25(O):	1.000493
#	34:	27(C)	28(N):	0.526888	#	34:	26(C)	27(N):	0.455244
#	35:	27(C)	31(N):	0.555687	#	35:	26(C)	30(N):	0.525118
#	36:	27(C)	43(H):	0.832737	#	36:	26(C)	57(N):	0.464653
#	37:	28(N)	29(O):	0.970702	#	37:	27(N)	28(O):	1.045385

#	38:	28(N)	30(O):	1.040155	#	38:	27(N)	29(O):	1.028001
#	39:	31(N)	32(O):	1.004669	#	39:	30(N)	31(O):	0.978472
#	40:	31(N)	33(O):	1.022690	#	40:	30(N)	32(O):	1.046703
#	41:	34(C)	35(N):	0.531606	#	41:	33(C)	34(N):	0.455302
#	42:	34(C)	38(N):	0.546871	#	42:	33(C)	37(N):	0.525099
#	43:	34(C)	44(H):	0.832234	#	43:	33(C)	59(N):	0.464594
#	44:	35(N)	36(O):	0.990093	#	44:	34(N)	35(O):	1.045396
#	45:	35(N)	37(O):	1.024759	#	45:	34(N)	36(O):	1.028000
#	46:	38(N)	39(O):	0.993515	#	46:	37(N)	38(O):	0.978485
#	47:	38(N)	40(O):	1.029422	#	47:	37(N)	39(O):	1.046695
#	48:	45(C)	46(H):	0.832593	#	48:	42(C)	44(N):	0.455155
#	49:	45(C)	49(N):	0.548356	#	49:	42(C)	45(N):	0.526164
#	50:	45(C)	50(N):	0.524957	#	50:	42(C)	56(N):	0.463491
#	51:	47(C)	48(H):	0.836113	#	51:	43(C)	46(N):	0.526239
#	52:	47(C)	51(N):	0.542762	#	52:	43(C)	47(N):	0.455337
#	53:	47(C)	52(N):	0.539924	#	53:	43(C)	58(N):	0.463318
#	54:	49(N)	57(O):	1.014971	#	54:	44(N)	52(O):	1.028111
#	55:	49(N)	58(O):	1.007334	#	55:	44(N)	53(O):	1.045582
#	56:	50(N)	59(O):	0.982578	#	56:	45(N)	54(O):	0.978195
#	57:	50(N)	60(O):	1.033493	#	57:	45(N)	55(O):	1.046495
#	58:	51(N)	53(O):	1.024654	#	58:	46(N)	48(O):	1.046417
#	59:	51(N)	54(O):	0.987176	#	59:	46(N)	49(O):	0.978242
#	60:	52(N)	55(O):	1.030871	#	60:	47(N)	50(O):	1.027963
#	61:	52(N)	56(O):	0.994093	#	61:	47(N)	51(O):	1.045679
					#	62:	56(N)	67(O):	0.989487
					#	63:	56(N)	68(O):	1.080007
					#	64:	57(N)	60(O):	0.988897
#	50:	45(C)	50(N):	0.524957	#	65:	57(N)	61(O):	1.079834
					#	66:	58(N)	62(O):	1.080055
					#	67:	58(N)	63(O):	0.989451
					#	68:	59(N)	64(O):	0.988870
					#	69:	59(N)	65(O):	1.079984
					#	48:	42(C)	44(N):	0.455155

F9

The bond order >= 0.050000

#	1:	1(C)	2(C):	1.711518
#	2:	1(C)	3(C):	1.109726
#	3:	1(C)	83(H):	0.838729
#	4:	2(C)	4(C):	1.100017
#	5:	2(C)	84(H):	0.824301
#	6:	3(C)	5(C):	1.366765
#	7:	3(C)	9(C):	1.358344
#	8:	4(C)	10(C):	1.355694

F10

The bond order >= 0.050000

#	1:	1(C)	2(C):	1.713778
#	2:	1(C)	3(C):	1.096758
#	3:	1(C)	75(H):	0.831536
#	4:	2(C)	4(C):	1.085831
#	5:	2(C)	76(H):	0.823207
#	6:	3(C)	5(C):	1.362756
#	7:	3(C)	9(C):	1.358602
#	8:	4(C)	10(C):	1.330719

#	9:	4(C)	14(C):	1.341455	#	9:	4(C)	14(C):	1.383557
#	10:	5(C)	6(C):	1.435121	#	10:	5(C)	6(C):	1.380031
#	11:	5(C)	35(N):	0.674053	#	11:	5(C)	39(N):	0.668786
#	12:	6(C)	7(N):	1.262639	#	12:	6(C)	7(N):	1.174907
#	13:	6(C)	17(N):	0.796935	#	13:	6(C)	35(N):	0.901924
#	14:	7(N)	8(C):	1.263671	#	14:	7(N)	8(C):	1.181193
#	15:	8(C)	9(C):	1.435450	#	15:	8(C)	9(C):	1.404059
#	16:	8(C)	21(N):	0.790152	#	16:	8(C)	16(N):	0.897312
#	17:	9(C)	41(N):	0.674589	#	17:	9(C)	45(N):	0.681232
#	18:	10(C)	11(C):	1.390528	#	18:	10(C)	11(C):	1.434463
#	19:	10(C)	38(N):	0.674721	#	19:	10(C)	42(N):	0.673878
#	20:	11(C)	12(N):	1.245425	#	20:	11(C)	12(N):	1.211487
#	21:	11(C)	32(N):	0.835879	#	21:	11(C)	29(N):	0.820680
#	22:	12(N)	13(C):	1.256142	#	22:	12(N)	13(C):	1.212612
#	23:	13(C)	14(C):	1.453275	#	23:	13(C)	14(C):	1.361509
#	24:	13(C)	26(N):	0.790911	#	24:	13(C)	22(N):	0.930526
#	25:	14(C)	44(N):	0.676119	#	25:	14(C)	48(N):	0.672473
#	26:	15(C)	16(N):	1.314633	#	26:	15(C)	16(N):	0.902323
#	27:	15(C)	19(C):	1.267782	#	27:	15(C)	19(C):	1.367969
#	28:	15(C)	47(N):	0.754647	#	28:	15(C)	20(N):	1.162163
#	29:	16(N)	17(N):	0.790990	#	29:	16(N)	17(N):	0.615450
#	30:	17(N)	18(C):	0.922506	#	30:	17(N)	18(C):	1.423116
#	31:	18(C)	19(C):	1.446167	#	31:	18(C)	19(C):	1.225614
#	32:	18(C)	50(N):	0.796292	#	32:	18(C)	51(N):	0.741900
#	33:	19(C)	53(N):	0.739558	#	33:	19(C)	54(N):	0.856082
#	34:	20(C)	21(N):	0.930858	#	34:	20(N)	77(H):	0.677183
#	35:	20(C)	24(C):	1.438734	#	35:	20(N)	78(H):	0.654224
#	36:	20(C)	56(N):	0.810110	#	36:	21(C)	22(N):	0.872296
#	37:	21(N)	22(N):	0.800148	#	37:	21(C)	25(C):	1.353796
#	38:	22(N)	23(C):	1.305924	#	38:	21(C)	26(N):	1.211118
#	39:	23(C)	24(C):	1.276271	#	39:	22(N)	23(N):	0.604928
#	40:	23(C)	59(N):	0.758565	#	40:	23(N)	24(C):	1.419174
#	41:	24(C)	62(N):	0.733363	#	41:	24(C)	25(C):	1.230905
#	42:	25(C)	26(N):	0.934579	#	42:	24(C)	57(N):	0.748125
#	43:	25(C)	29(C):	1.440216	#	43:	25(C)	60(N):	0.861226
#	44:	25(C)	65(N):	0.810470	#	44:	26(N)	79(H):	0.667740
#	45:	26(N)	27(N):	0.804600	#	45:	26(N)	80(H):	0.656773
#	46:	27(N)	28(C):	1.300933	#	46:	27(C)	28(N):	1.416777
#	47:	28(C)	29(C):	1.274049	#	47:	27(C)	31(C):	1.233027
#	48:	28(C)	68(N):	0.758688	#	48:	27(C)	63(N):	0.744285
#	49:	29(C)	71(N):	0.734671	#	49:	28(N)	29(N):	0.590586
#	50:	30(C)	31(N):	1.365785	#	50:	29(N)	30(C):	0.897784
#	51:	30(C)	34(C):	1.236267	#	51:	30(C)	31(C):	1.354725
#	52:	30(C)	74(N):	0.744672	#	52:	30(C)	32(N):	1.170971
#	53:	31(N)	32(N):	0.728987	#	53:	31(C)	66(N):	0.852316

#	54:	32(N)	33(C):	0.935675	#	54:	32(N)	81(H):	0.663284
#	55:	33(C)	34(C):	1.459910	#	55:	32(N)	82(H):	0.655163
#	56:	33(C)	77(N):	0.749729	#	56:	33(C)	34(N):	1.417972
#	57:	34(C)	80(N):	0.775258	#	57:	33(C)	37(C):	1.228016
#	58:	35(N)	36(O):	0.963028	#	58:	33(C)	69(N):	0.744731
#	59:	35(N)	37(O):	1.013995	#	59:	34(N)	35(N):	0.615171
#	60:	38(N)	39(O):	1.012053	#	60:	35(N)	36(C):	0.880311
#	61:	38(N)	40(O):	0.990422	#	61:	36(C)	37(C):	1.360006
#	62:	41(N)	42(O):	0.975846	#	62:	36(C)	38(N):	1.183717
#	63:	41(N)	43(O):	0.980771	#	63:	37(C)	72(N):	0.852684
#	64:	44(N)	45(O):	0.975089	#	64:	38(N)	83(H):	0.673021
#	65:	44(N)	46(O):	0.975886	#	65:	38(N)	84(H):	0.656656
#	66:	47(N)	48(O):	1.007465	#	66:	39(N)	40(O):	0.974846
#	67:	47(N)	49(O):	0.960739	#	67:	39(N)	41(O):	1.009702
#	68:	50(N)	51(O):	0.944164	#	68:	42(N)	43(O):	0.958660
#	69:	50(N)	52(O):	0.985450	#	69:	42(N)	44(O):	1.001116
#	70:	53(N)	54(O):	1.009427	#	70:	45(N)	46(O):	0.986587
#	71:	53(N)	55(O):	1.011912	#	71:	45(N)	47(O):	0.980381
#	72:	56(N)	57(O):	0.934078	#	72:	48(N)	49(O):	0.973838
#	73:	56(N)	58(O):	0.986947	#	73:	48(N)	50(O):	1.010363
#	74:	59(N)	60(O):	1.003759	#	74:	51(N)	52(O):	0.997419
#	75:	59(N)	61(O):	0.956429	#	75:	51(N)	53(O):	0.992768
#	76:	62(N)	63(O):	1.011120	#	76:	54(N)	55(O):	0.977803
#	77:	62(N)	64(O):	1.010296	#	77:	54(N)	56(O):	0.856443
#	78:	65(N)	66(O):	0.928527	#	78:	57(N)	58(O):	0.997893
#	79:	65(N)	67(O):	0.994661	#	79:	57(N)	59(O):	0.987265
#	80:	68(N)	69(O):	1.005858	#	80:	60(N)	61(O):	0.967898
#	81:	68(N)	70(O):	0.955807	#	81:	60(N)	62(O):	0.859663
#	82:	71(N)	72(O):	1.012993	#	82:	63(N)	64(O):	0.997274
#	83:	71(N)	73(O):	1.009068	#	83:	63(N)	65(O):	0.985045
#	84:	74(N)	75(O):	0.997339	#	84:	66(N)	67(O):	0.862602
#	85:	74(N)	76(O):	0.979687	#	85:	66(N)	68(O):	0.964622
#	86:	77(N)	78(O):	0.983506	#	86:	69(N)	70(O):	0.996115
#	87:	77(N)	79(O):	1.018117	#	87:	69(N)	71(O):	0.994713
#	88:	80(N)	81(O):	0.987309	#	88:	72(N)	73(O):	0.856582
#	89:	80(N)	82(O):	0.961836	#	89:	72(N)	74(O):	0.971190
#	11:	5(C)	35(N):	0.674053	#	49:	28(N)	29(N):	0.590586

F11

The bond order >= 0.050000

#	1:	1(C)	2(C):	1.739258
#	2:	1(C)	3(C):	1.076188
#	3:	1(C)	67(H):	0.823895
#	4:	2(C)	4(C):	1.073874

F12

The bond order >= 0.050000

#	1:	1(C)	2(C):	1.719727
#	2:	1(C)	3(C):	1.071928
#	3:	1(C)	63(H):	0.829017
#	4:	2(C)	4(C):	1.075082

#	5:	2(C)	68(H):	0.827847	#	5:	2(C)	64(H):	0.820408
#	6:	3(C)	5(C):	1.361358	#	6:	3(C)	5(C):	1.299082
#	7:	3(C)	9(C):	1.355547	#	7:	3(C)	9(C):	1.403296
#	8:	4(C)	10(C):	1.362019	#	8:	4(C)	10(C):	1.337665
#	9:	4(C)	14(C):	1.353719	#	9:	4(C)	14(C):	1.392137
#	10:	5(C)	6(C):	1.406094	#	10:	5(C)	6(C):	1.362037
#	11:	5(C)	39(N):	0.681508	#	11:	5(C)	39(N):	0.725782
#	12:	6(C)	7(N):	1.260925	#	12:	6(C)	7(N):	1.224178
#	13:	6(C)	35(N):	0.826840	#	13:	6(C)	17(N):	0.827582
#	14:	7(N)	8(C):	1.256184	#	14:	7(N)	8(C):	1.222245
#	15:	8(C)	9(C):	1.418781	#	15:	8(C)	9(C):	1.347955
#	16:	8(C)	16(N):	0.823552	#	16:	8(C)	29(N):	0.969155
#	17:	9(C)	45(N):	0.683212	#	17:	9(C)	45(N):	0.665416
#	18:	10(C)	11(C):	1.393993	#	18:	10(C)	11(C):	1.421484
#	19:	10(C)	42(N):	0.687141	#	19:	10(C)	42(N):	0.670043
#	20:	11(C)	12(N):	1.255616	#	20:	11(C)	12(N):	1.215857
#	21:	11(C)	29(N):	0.797810	#	21:	11(C)	35(N):	0.835559
#	22:	12(N)	13(C):	1.259201	#	22:	12(N)	13(C):	1.212544
#	23:	13(C)	14(C):	1.422421	#	23:	13(C)	14(C):	1.360611
#	24:	13(C)	22(N):	0.827971	#	24:	13(C)	23(N):	0.937826
#	25:	14(C)	48(N):	0.679764	#	25:	14(C)	48(N):	0.678665
#	26:	15(C)	16(N):	0.849193	#	26:	15(C)	16(N):	1.422587
#	27:	15(C)	19(C):	1.356412	#	27:	15(C)	19(N):	1.105446
#	28:	15(C)	20(N):	0.890774	#	28:	15(C)	51(N):	0.742895
#	29:	16(N)	17(N):	0.851823	#	29:	16(N)	17(N):	0.656378
#	30:	17(N)	18(C):	1.296036	#	30:	17(N)	18(C):	0.832825
#	31:	18(C)	19(C):	1.215576	#	31:	18(C)	19(N):	1.287073
#	32:	18(C)	51(N):	0.806610	#	32:	18(C)	20(N):	1.101817
#	33:	19(C)	54(N):	1.165061	#	33:	20(N)	65(H):	0.653651
#	34:	20(N)	75(O):	0.928044	#	34:	20(N)	66(H):	0.680501
#	35:	20(N)	76(O):	0.869660	#	35:	21(C)	22(N):	1.395872
#	36:	21(C)	22(N):	0.841546	#	36:	21(C)	25(N):	1.092441
#	37:	21(C)	25(C):	1.358854	#	37:	21(C)	54(N):	0.734988
#	38:	21(C)	26(N):	0.887573	#	38:	22(N)	23(N):	0.644448
#	39:	22(N)	23(N):	0.836418	#	39:	23(N)	24(C):	0.820072
#	40:	23(N)	24(C):	1.304561	#	40:	24(C)	25(N):	1.271907
#	41:	24(C)	25(C):	1.212062	#	41:	24(C)	26(N):	1.188651
#	42:	24(C)	55(N):	0.801840	#	42:	26(N)	67(H):	0.661596
#	43:	25(C)	58(N):	1.164606	#	43:	26(N)	68(H):	0.679762
#	44:	26(N)	71(O):	0.869808	#	44:	27(C)	28(N):	1.394349
#	45:	26(N)	72(O):	0.935007	#	45:	27(C)	31(N):	1.105713
#	46:	27(C)	28(N):	1.312851	#	46:	27(C)	57(N):	0.734037
#	47:	27(C)	31(C):	1.214883	#	47:	28(N)	29(N):	0.642837
#	48:	27(C)	59(N):	0.802396	#	48:	29(N)	30(C):	0.786051
#	49:	28(N)	29(N):	0.850765	#	49:	30(C)	31(N):	1.261333

#	50:	29(N)	30(C):	0.834173	#	50:	30(C)	32(N):	1.213613
#	51:	30(C)	31(C):	1.358681	#	51:	32(N)	69(H):	0.648977
#	52:	30(C)	32(N):	0.920731	#	52:	32(N)	70(H):	0.677322
#	53:	31(C)	62(N):	1.168497	#	53:	33(C)	34(N):	1.411200
#	54:	32(N)	73(O):	0.883712	#	54:	33(C)	37(N):	1.099262
#	55:	32(N)	74(O):	0.888752	#	55:	33(C)	60(N):	0.742219
#	56:	33(C)	34(N):	1.300824	#	56:	34(N)	35(N):	0.629286
#	57:	33(C)	37(C):	1.210638	#	57:	35(N)	36(C):	0.837570
#	58:	33(C)	63(N):	0.802172	#	58:	36(C)	37(N):	1.263359
#	59:	34(N)	35(N):	0.836733	#	59:	36(C)	38(N):	1.147040
#	60:	35(N)	36(C):	0.842455	#	60:	38(N)	71(H):	0.661331
#	61:	36(C)	37(C):	1.358243	#	61:	38(N)	72(H):	0.675864
#	62:	36(C)	38(N):	0.888024	#	62:	39(N)	40(O):	0.966159
#	63:	37(C)	66(N):	1.163019	#	63:	39(N)	41(O):	0.911122
#	64:	38(N)	69(O):	0.867964	#	64:	42(N)	43(O):	1.003085
#	65:	38(N)	70(O):	0.932321	#	65:	42(N)	44(O):	0.953652
#	66:	39(N)	40(O):	0.984188	#	66:	45(N)	46(O):	0.982627
#	67:	39(N)	41(O):	0.979643	#	67:	45(N)	47(O):	1.010111
#	68:	42(N)	43(O):	0.973731	#	68:	48(N)	49(O):	0.979462
#	69:	42(N)	44(O):	0.958923	#	69:	48(N)	50(O):	1.003386
#	70:	45(N)	46(O):	0.984684	#	70:	51(N)	52(O):	0.993658
#	71:	45(N)	47(O):	0.969581	#	71:	51(N)	53(O):	0.953260
#	72:	48(N)	49(O):	0.984389	#	72:	54(N)	55(O):	0.979939
#	73:	48(N)	50(O):	0.982634	#	73:	54(N)	56(O):	0.971699
#	74:	51(N)	52(O):	1.005725	#	74:	57(N)	58(O):	0.983181
#	75:	51(N)	53(O):	0.883704	#	75:	57(N)	59(O):	0.968645
#	76:	54(N)	83(H):	0.675180	#	76:	60(N)	61(O):	0.986216
#	77:	54(N)	84(H):	0.677139	#	77:	60(N)	62(O):	0.951808
#	78:	55(N)	56(O):	1.002114					
#	79:	55(N)	57(O):	0.881884	#	56:	34(N)	35(N):	0.629286
#	80:	58(N)	79(H):	0.672358					
#	81:	58(N)	80(H):	0.674319					
#	82:	59(N)	60(O):	1.002855					
#	83:	59(N)	61(O):	0.878625					
#	84:	62(N)	77(H):	0.673495					
#	85:	62(N)	78(H):	0.672189					
#	86:	63(N)	64(O):	1.008426					
#	87:	63(N)	65(O):	0.876652					
#	88:	66(N)	81(H):	0.671659					
#	89:	66(N)	82(H):	0.672527					

#	88:	66(N)	81(H):	0.671659

Table S4. Specific data of $C_{p,m}^{\theta}$, S_m^{θ} and H_m^{θ}, just for A1 and A2

T/K	A1			A2		
	H_m^{θ} (kJ mol^{-1})	S_m^{θ} (J mol^{-1}K^{-1})	$C_{p,m}^{\theta}$ (J mol^{-1}K^{-1})	H_m^{θ} (kJ mol^{-1})	S_m^{θ} (J mol^{-1}K^{-1})	$C_{p,m}^{\theta}$ (J mol^{-1}K^{-1})
200	35.4127	612.9644	291.4536	37.70777	640.3654	309.7545
210	38.34014	627.2109	301.1438	40.81898	655.5073	320.0136
220	41.36471	641.2357	310.7042	44.0326	670.4107	330.1431
230	44.48118	655.0554	320.135	47.34598	685.0923	340.147
240	47.69217	668.6785	329.4276	50.7565	699.5648	350.0087
250	50.99242	682.1133	338.5864	54.26417	713.8406	359.7365
260	54.38457	695.3766	347.6029	57.86636	727.9323	369.3221
270	57.86335	708.4725	356.4772	61.56306	741.8483	378.7654
280	61.43141	721.4053	365.2092	65.35428	755.5886	388.058
290	65.08348	734.1874	373.7948	69.23477	769.1698	397.2042
300	68.82219	746.8231	382.2381	73.20715	782.5963	406.1998
310	72.64229	759.3123	390.5308	77.26618	795.8679	415.0448
320	76.54379	771.6635	398.6728	81.41184	808.9973	423.7308
330	80.52405	783.885	406.6685	85.64415	821.9845	432.2662
340	84.58569	795.9725	414.5093	89.96047	834.8335	440.6425
350	88.72348	807.9346	422.2036	94.35818	847.5487	448.8599
360	92.93478	819.7711	429.7432	98.83728	860.1342	456.9183
370	97.22223	831.4863	437.1322	103.3952	872.5899	464.8177

380	101.5832	843.0844	444.3663	108.0318	884.9202	472.5581
390	106.015	854.5653	451.4498	112.7446	897.1333	480.1353
400	110.5178	865.9332	458.3785	117.5335	909.2209	487.5535
410	115.0861	877.1923	465.1608	122.3933	921.1913	494.8128
420	119.7228	888.3385	471.7882	127.3266	933.0487	501.913
430	124.425	899.3759	478.2692	132.3282	944.789	508.8543
440	129.1929	910.3045	484.6038	137.4006	956.4206	515.6366
450	134.0212	921.1327	490.7878	142.5387	967.9391	522.264
460	138.9125	931.8563	496.8295	147.7425	979.3489	528.7408
470	143.8616	942.4753	502.7331	153.0092	990.654	535.0629
480	148.8711	952.9939	508.4903	158.339	1001.85	541.2343
490	153.9357	963.4162	514.1136	163.7318	1012.938	547.2592
500	159.058	973.7381	519.5988	169.1823	1023.929	553.1377
510	164.2329	983.968	524.9501	174.6932	1034.816	558.874
520	169.4602	994.0975	530.1676	180.2593	1045.598	564.468
530	174.7427	1004.135	535.2595	185.8805	1056.284	569.9281
540	180.0725	1014.08	540.2259	191.5568	1066.874	575.2502
550	185.4522	1023.929	545.071	197.2857	1077.363	580.4383
560	190.8817	1033.691	549.7947	203.067	1087.756	585.501
570	196.3585	1043.364	554.4013	208.8982	1098.057	590.4339
580	201.8799	1052.945	558.8907	214.7767	1108.262	595.2455
590	207.4433	1062.443	563.2672	220.7051	1118.379	599.9358

600	213.054	1071.853	567.5391	226.6808	1128.4	604.5089