Supplementary Material

Charge Transfer Within Excited States Boron/Nitrogen Doped Polycyclic Aromatic Hydrocarbons

Luan G. F. dos Santos,¹ Julio C. V. Chagas,^{3,4} Reed Nieman,¹ Adelia J. A. Aquino,² Francisco B. C. Machado,^{3,4§} Hans Lischka,^{1*}

* hans.lischka@ttu.edu

§ fmachado@ita.br

¹ Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas 79409, United States.

² Department of Mechanical Engineering, Texas Tech University, Lubbock, Texas 79409, United States.

³ Departamento de Química, Instituto Tecnológico de Aeronáutica, 12228-900, São José dos Campos, SP, Brazil.

⁴ Laboratório de Computação Científica Avançada e Modelamento (Lab – CCAM), Instituto Tecnológico da Aeronáutica, 12228-900, José dos Campos, São Paulo, Brazil.

Table of Contents

Table S2: Excitation energies (eV), oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the pristine periacene. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Table S3: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-zz-B-top. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.7

Table S10: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-edges-line. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity. ... 14

Table S11: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-zz-B-top-line. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.15

Table S12: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-zz-N-top-line. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity. Table S13: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-ac-line. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity. In the Table S14: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-vertical. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity. In the Figure S1: PR_{NTO} values are shown for all computed excited states and all analyzed structures, obtained at ADC(2) (a) and TD-DFT (b) levels of theory.....19 Table S15: Double excitation character values for all computed excited states and all structures, Table S16: Dominant electron configurations and related orbital occupation scheme of the periacene, Table S17: Dominant electron configurations and related orbital occupation scheme of the BN-ac, for the Table S18: Dominant electron configurations and related orbital occupation scheme of the BN-vertical, Table S19: Dominant electron configurations and related orbital excitation with its respective contribution, of the BN-edges-line, with respect to the ground state reference, using MR-CISD(8,8) Figure S2: BN-center NTOs obtained using ADC(2)/def2-SV(P) level of theory, for the first four excited singlet states, relative to the ground state. Molecular orbitals cutoff value for the isosurface of 0.04 e/bohr³. Hole orbitals are printed in red and blue, while electron orbitals are in green and yellow. 22 Figure S3: BN-center NTOs obtained using TD-DFT, at wB97XD/def2-SV(P)) level of theory, for the first four excited singlet states, relative to the ground state. Molecular orbitals cutoff value for the isosurface of 0.04 e/bohr³. Hole orbitals are printed in red and blue, while electron orbitals are in green and yellow.

 Figure S5: BN-vertical NTOs obtained using TD-DFT, at wB97XD/def2-SV(P)) level of theory, for the first four excited singlet states, relative to the ground state. Molecular orbitals cutoff value for the isosurface of 0.04 e/bohr³. Hole orbitals are printed in red and blue, while electron orbitals are in green and yellow.

Figure S7: BN-edges-line NTOs obtained using TD-DFT, at wB97XD/def2-SV(P)) level of theory, for the first four excited singlet states, relative to the ground state. Molecular orbitals cutoff value for the isosurface of 0.04 e/bohr³. Hole orbitals are printed in red and blue, while electron orbitals are in green and yellow.

Figure S9: Character of the first four singlet excited states, obtained at the MR-CISD level, for all the structures not analyzed in detail in the main text, decomposed into contributions of local excitations (LE), charge transfer (between segments) and double excitations (2-el.). The segment division is indicated by numbers in red.

Table S1: Comparison of excitation energies calculated at the MR-CISD level with three different active spaces explained in the text and different basis sets for three selected structures. All excitation energies are given in eV. CI vector sizes in terms of numbers of configuration state functions (CSFs) are also provided.^a

Total CSF counts	2.1 billion	511 million	2.8 billion		
Schemes	CAS(8,8)/6-31G	R(2)CAS(4,4)A(2)/6-31G	R(2)CAS(4,4)A(2)/6-31G*		
		BN-center			
States					
\mathbf{S}_1	2.774	2.715	2.733		
S_2	2.904	2.904	2.812		
S ₃	3.145	3.145	3.214		
S_4	3.187	3.251	3.329		
		BN-vertical			
S_1	0.707	0.709	0.779		
S_2	1.380	1.344	1.237		
S ₃	1.613	1.586	1.536		
S_4	2.009	1.969	1.853		
	BN-edges-line				
S_1	0.455	0.493	0.501		
\mathbf{S}_2	1.081	1.107	1.107		

1.259

S42.3342.319^a R stands for RAS and A for auxiliary space.

1.257

S₃

1.325

2.283

Table S2: Excitation energies (eV), oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the pristine periacene. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4	
		Pristine I	Periacene		
		MR-C	ISD+P		
. –					
ΔE	1.987	2.001	2.227	2.809	
f	0.002	0.000	0.000	0.152	
PRNTO	3.859	3.618	2.003	2.014	
		NEV	PT2		
ΔE	1.269	1.414	1.608	1.614	
f^{a}	0.005	0.000	0.000	0.177	
		ADO	$C(2)^{b}$		
ΔE	-	-	-	-	
f	-	-	-	-	
PRNTO	-	-	-	-	
		TD-	DFT		
ΔE	0.354	0.990	1.122	2.036	
 f	0.268	0.000	0.000	0.000	
PRNTO	1.524	1.390	1.781	1.899	

^{*a*}For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level. ^{*b*}Properties at ADC(2) level were not computed for this structure, due to the elevated D1 diagnostic value.

Properties/States	S_1	S_2	S_3	S_4
		BN-zz	-B-top	
		MR-C	ISD+P	
ΔE	2.665	2.850	2.970	3.257
f	0.261	0.433	0.000	0.000
PRNTO	1.145	1.418	2.533	1.520
		NEV	PT2	
ΔE	2.006	2.415	2.453	2.774
f^{lu}	0.234	0.677	0.000	0.000
		AD	C(2)	
ΔE	1.630	2.239	2.404	2.666
f	0.201	0.374	0.000	0.000
PRNTO	1.000	1.062	1.000	1.000
		TD-	DFT	
ΔE	1.779	2.451	2.598	3.230
f	0.374	0.366	0.000	0.000
PRNTO	1.168	1.301	1.558	1.522

Table S3: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-zz-B-top. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Table S4: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-zz-N-top. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4	
	BN-zz-N-top				
		MR-C	ISD+P		
ΔE	2.879	3.029	3.246	3.426	
f	0.288	0.000	0.277	0.000	
PRNTO	1.147	2.594	1.653	1.343	
		NEV	/PT2		
ΔE	2.007	2.598	2.754	2.814	
f^a	0.274	0.000	0.385	0.000	
		AD	C(2)		
ΔE	1.995	2.655	2.868	3.068	
f	0.233	0.000	0.358	0.000	
PR _{NTO}	1.000	1.000	1.202	1.000	
		TD-	DFT		
ΔE	2.003	2.802	3.017	3.427	
f	0.289	0.000	0.306	0.000	
PRNTO	1.177	1.489	1.494	1.458	

Table S5: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-mixed. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4		
	BN-mixed					
		MR-C	ISD+P			
ΔE	1.981	3.252	3.340	3.543		
f	0.206	0.038	0.080	0.027		
PRNTO	1.072	1.923	1.910	2.078		
		NEV	/PT2			
ΔE	1.589	3.016	3.104	3.366		
f^{a}	0.221	0.106	0.000	0.056		
		AD	C(2)			
ΔE	1.413	2.432	2.636	2.981		
f	0.182	0.002	0.116	0.130		
PR _{NTO}	1.000	1.077	1.000	1.142		
		TD-	DFT			
ΔE	2.070	2.847	3.360	3.430		
f	0.276	0.000	0.002	0.572		
PRNTO	1.144	2.235	1.997	2.094		
	1 (0		1 ~ ~ ~ ~			

Table S6: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-center. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4	
	BN-center				
		MR-C	ISD+P		
ΔE	2.406	2.625	2.741	2.911	
f	0.015	0.380	_ <i>b</i>	0.136	
PRNTO	1.002	1.090	_ <i>b</i>	1.152	
		NEV	PT2		
$\Delta E \ f^{lpha}$	1.104 0.002	1.645 0.541	1.994 0.097	2.233 _ ^b	
		AD	C(2)		
ΔE	1.255	1.728	2.110	2.423	
f PR _{NTO}	$0.001 \\ 1.000$	$0.250 \\ 1.000$	0.159 1.000	0.000 1.999	
		TD-	DFT		
ΔE	2.092	2.175	2.227	2.960	
f	0.370	0.024	0.120	0.022	
PRNTO	1.297	1.053	1.246	1.833	

^{*a*}For the NEVPT2 case, the oscillator strength (f) was computed at CASSCF (8,8) level. ^{*b*}The properties were not computed due to the vanishing of the one-particle transition density matrix in the doubly excited states. Table S7: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-cross. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4		
	BN-cross					
		MR-C	ISD+P			
ΔE	3.321	3.461	3.508	3.744		
f	0.001	0.859	0.017	0.490		
PRNTO	2.016	1.668	1.042	1.230		
	NEVPT2					
ΔE	1.963	2.438	2.464	2.638		
f^a	0.000	0.959	0.004	0.582		
		AD	C(2)			
ΔE	2.120	2.493	2.602	2.676		
f	0.007	0.001	0.440	0.001		
PR _{NTO}	1.000	1.982	1.347	2.065		
		TD-	DFT			
ΔE	2.842	2.871	2.941	2.986		
f	0.001	0.665	0.003	0.142		
PR _{NTO}	3.148	1.687	3.281	1.187		

Table S8: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-ac. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4
		BN	l-ac	
		MR-C	ISD+P	
ΔE	1.821	1.982	2.081	3.530
f	0.051	0.028	0.000	0.003
PRNTO	1.358	1.676	1.001	1.904
		NEV	PT2	
ΔE	1.726	1.857	2.489	2.541
f^{a}	0.017	0.015	0.057	0.000
		ADO	C(2) ^b	
ΔE	-	-	-	_
f	-	-	-	-
PR _{NTO}	-	-	-	-
		TD-	DFT	
ΔE	0.181	0.959	1.139	2.213
f	0.043	0.002	0.000	0.027
PRNTO	1.359	1.610	1.856	1.579

^{*a*}For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level. ^{*b*}Properties at ADC(2) level were not computed for this structure, due to the elevated D1 diagnostic value. Table S9: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-edges. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4	
	BN-edges				
		MR-C	ISD+P		
ΔE	1.771	3.028	3.598	4.556	
ſ	0.040	0.030	0.762	0.478	
PR _{NTO}	1.018	1.796	1.784	1.062	
		NEV	/PT2		
ΔE	1.524	2.840	3.240	4.386	
f^a	0.034	0.011	0.451	0.352	
		AD	C(2)		
ΔE	1.013	2.284	2.554	3.364	
f	0.007	0.000	0.514	0.283	
PRNTO	1.000	1.998	1.998	1.151	
		TD-	DFT		
ΔE	1.978	2.954	3.453	4.055	
f	0.070	0.000	0.762	0.128	
PRNTO	1.035	2.150	2.210	2.415	
1 .11 .	1 (0		1 1		

Properties/States	S_1	S_2	S_3	S_4		
	BN-edges-line					
		MK-C	ISD+P			
ΔE	0.429	1.056	1.179	2.032		
f	0.026	0.036	0.174	0.988		
PRNTO	1.027	1.245	1.222	1.074		
		NEV	/PT2			
ΔE	0.459	0.980	1.110	1.689		
f^a	0.004	0.002	0.254	0.940		
		ADO	C(2) ^b			
ΔE	-	_	-	-		
f	-	-	-	-		
PRNTO	-	-	-	-		
		TD-	DFT			
ΔE	1.356	1.357	1.499	1.865		
f	0.022	0.005	0.145	0.484		
PRNTO	1.452	1.061	1.339	1.302		

Table S10: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-edges-line. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

^{*a*}For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level. ^{*b*}Properties at ADC(2) level were not computed for this structure, due to the elevated D1 diagnostic value. Table S11: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-zz-B-top-line. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4	
	BN-zz-B-top-line				
	MR-CISD+P				
ΔE	1.740	2.090	2.507	2.548	
f	0.141	0.170	0.000	0.140	
PRNTO	1.880	2.176	2.849	2.178	
	NEVPT2				
ΔE	1.095	1.144	1.245	1.258	
f^{a}	0.004	0.031	0.211	0.110	
		AD	C(2)		
ΔE	0.646	0.951	1.160	1.660	
f	0.110	0.196	0.095	0.086	
PR _{NTO}	1.022	1.016	1.087	1.591	
		TD-	DFT		
ΔE	0.564	0.829	1.553	1.845	
f	0.271	0.080	0.078	0.076	
PRNTO	1.234	1.168	1.109	1.219	

Table S12: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-zz-N-top-line. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity. In the NEVPT2 case, the oscillator strengths are at CASSCF (8,8) level.

Properties/States	S_1	S_2	S_3	S_4
	BN-zz-N-top-line			
		MR-C	ISD+P	
ΔE	1.818	1.964	2.119	2.574
f	0.007	0.000	0.080	0.147
PRNTO	2.389	2.486	2.111	2.037
		NEV	PT2	
ΔE	1.299	1.471	1.552	1.662
f^{a}	0.019	0.000	0.076	0.107
		AD	C(2)	
ΔE	0.953	1.109	1.433	1.764
f	0.065	0.330	0.103	0.022
PR _{NTO}	1.069	1.057	1.290	1.149
		TD-	DFT	
ΔE	0.636	0.873	1.840	1.898
f	0.269	0.007	0.000	0.153
PRNTO	1.373	1.091	1.127	1.164

Table S13: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-ac-line. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity. In the NEVPT2 case, the oscillator strengths are at CASSCF (8,8) level.

Properties/States	S_1	S_2	S_3	S_4	
	BN-ac-line				
		MR-C	ISD+P		
ΔE	1.633	2.716	2.941	3.246	
f	0.826	0.540	0.018	0.059	
PRNTO	1.082	1.252	1.062	1.532	
		NEV	PT2		
ΔE	1.205	1.989	2.228	2.239	
f^{a}	0.859	0.034	0.431	0.759	
	ADC(2)				
ΔE	0.733	1.858	1.958	2.021	
f	0.162	0.007	0.138	0.039	
PR _{NTO}	1.000	1.903	1.918	1.142	
		TD-	DFT		
ΔE	1.610	2.509	2.807	2.833	
f	0.599	0.004	0.005	0.147	
PR _{NTO}	1.168	2.217	1.916	2.166	

Table S14: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-vertical. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity. In the NEVPT2 case, the oscillator strengths are at CASSCF (8,8) level.

Properties/States	S_1	S_2	S_3	S_4	
	BN-vertical				
		MR-C	ISD+P		
ΔE	0.770	1.493	1.642	2.021	
f		0.010	1.608	0.089	
PRNTO	_C	1.948	1.847	1.432	
		NEV	PT2		
ΔE	0.535	0.928	1.120	1.174	
f^{a}	_c	0.000	1.105	0.001	
	$ADC(2)^b$				
ΔE	-	-	-	-	
f	-	-	-	-	
PRNTO	-	-	-	-	
	TD-DFT				
ΔE	1.095	1.105	1.631	1.905	
f	0.692	0.003	0.025	0.578	
PRNTO	1.168	2.249	1.967	1.442	

^{*a*}For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level. ^{*b*}Properties at ADC(2) level were not computed for this structure, due to the elevated D1 diagnostic

value.

^cThe properties were not computed due to the vanishing of the one-particle transition density matrix in the doubly excited states.



Figure S1: PR_{NTO} values are shown for all computed excited states and all analyzed structures, obtained at ADC(2) (a) and TD-DFT (b) levels of theory.

^{*a*}The PR_{NTO} values at ADC(2) level of theory were not computed for the periacene, BN-ac, BN-edges-line and BN-vertical, due to large D1 diagnostic values exhibited by these structures.

Structures/States	S_1	S_2	S_3	S_4
Periacene	0.575	0.592	0.600	0.381
BN-zz-B-top	0.195	0.778	0.184	0.486
BN-zz-N-top	0.213	0.773	0.181	0.401
BN-mixed	0.357	0.305	0.241	0.320
BN-center	0.316	0.229	0.986	0.354
BN-cross	0.239	0.196	0.186	0.203
BN-ac	0.575	0.457	0.633	0.691
BN-edges	0.237	0.232	0.235	0.429
BN-edges-line	0.316	0.284	0.273	0.253
BN-zz-B-top-line	0.420	0.517	0.602	0.493
BN-zz-N-top-line	0.684	0.600	0.590	0.528
BN-ac-line	0.363	0.312	0.337	0.286
BN-vertical	0.965	0.320	0.347	0.504

Table S15: Double excitation character values for all computed excited states and all structures, obtained at MR-CISD level of theory.

Table S16: Dominant electron configurations and related orbital occupation scheme of the periacene, for the ground state reference wavefunction, using MR-CISD(8,8) method.

State	Electron Configuration	Contribution %	D1 Diagnostic
	$\frac{(9B_3u)^2(10B_3u)^0(8B_1g)^2(9B_1g)^0}{(9B_2g)^2(10B_2g)^0(7A_u)^2(8A_u)^0}$	31.7	
$1 \ ^1A_g$	$(9B_2g)^2 \rightarrow (10B_3u)^0$	27.4	0.098

Table S17: Dominant electron configurations and related orbital occupation scheme of the BN-ac, for the ground state reference wavefunction, using MR-CISD(8,8) method.

State	Electron Configuration	Contribution %	D1 Diagnostic
$1 {}^{1}A_{1}$	$(17B_1)^2(18B_1)^1(19B_1)^1(20B_1)^0$ $(14A_2)^2(15A_2)^2(16A_2)^0(17A_2)^0$	59.5	0.091

Table S18: Dominant electron configurations and related orbital occupation scheme of the BN-vertical, for the ground state reference wavefunction, using MR-CISD(8,8) method.

State	Electron Configuration	Contribution %	D1 Diagnostic
	$(17B_1)^2(18B_1)^1(19B_1)^1(20B_1)^0$ $(14A_2)^2(15A_2)^2(16A_2)^0(17A_2)^0$	27.9	
$1 {}^{1}A_{1}$	$(19B_1)^1 \rightarrow (18B_1)^1$	11.1	0.161

Table S19: Dominant electron configurations and related orbital excitation with its respective contribution, of the BN-edges-line, with respect to the ground state reference, using MR-CISD(8,8) method.

State	Electron Configuration	Contribution %	D1 Diagnostic
$1 {}^{1}A_{1}$	$\frac{(17B_1)^2(18B_1)^2(19B_1)^0(20B_1)^0}{(14A_2)^2(15A_2)^2(16A_2)^0(17A_2)^0}$	57.2	0.093



Figure S2: BN-center NTOs obtained using ADC(2)/def2-SV(P) level of theory, for the first four excited singlet states, relative to the ground state. Molecular orbitals cutoff value for the isosurface of 0.04 e/bohr³. Hole orbitals are printed in red and blue, while electron orbitals are in green and yellow.



Figure S3: BN-center NTOs obtained using TD-DFT, at wB97XD/def2-SV(P)) level of theory, for the first four excited singlet states, relative to the ground state. Molecular orbitals cutoff value for the isosurface of 0.04 e/bohr³. Hole orbitals are printed in red and blue, while electron orbitals are in green and yellow.



Figure S4: The first four singlet excited states, obtained at ADC(2) and TD-DFT levels, for the BN-center structure decomposed into contributions of local excitations (LE), charge transfer (between segments) and double excitations (2-el.). The segments division is indicated by numbers in red.



Figure S5: BN-vertical NTOs obtained using TD-DFT, at wB97XD/def2-SV(P)) level of theory, for the first four excited singlet states, relative to the ground state. Molecular orbitals cutoff value for the isosurface of 0.04 e/bohr³. Hole orbitals are printed in red and blue, while electron orbitals are in green and yellow.



Figure S6: The first four singlet excited states, obtained at TD-DFT level, for the BN-vertical structure decomposed into contributions of local excitations (LE), charge transfer (between segments) and double excitations (2-el.). The segments division is indicated by numbers in red.



Figure S7: BN-edges-line NTOs obtained using TD-DFT, at wB97XD/def2-SV(P)) level of theory, for the first four excited singlet states, relative to the ground state. Molecular orbitals cutoff value for the isosurface of 0.04 e/bohr³. Hole orbitals are printed in red and blue, while electron orbitals are in green and yellow.



Figure S8: The first four singlet excited states, obtained at TD-DFT level, for the BNedges-line structure decomposed into contributions of local excitations (LE), charge transfer (between segments) and double excitations (2-el.). The segments division is indicated by numbers in red.



Figure S9: Character of the first four singlet excited states, obtained at the MR-CISD level, for all the structures not analyzed in detail in the main text, decomposed into contributions of local excitations (LE), charge transfer (between segments) and double excitations (2-el.). The segment division is indicated by numbers in red.

Optimized Geometries:

Cartesian coordinates are in Å and geometries are in the x-y plane:

Pristine,	wB9	7XD/def2-SV(P)	
Н	4.8846600	6.8225330	-0.0000000
Н	2.4410610	6.7890653	-0.0000000
Н	-0.000000	6.7819973	-0.0000000
Н	-2.4410610	6.7890653	-0.0000000
Н	-4.8846600	6.8225330	-0.0000000
С	-6.1004934	5.0477451	-0.0000000
С	-6.1168148	3.6388849	-0.0000000
С	-6.1253238	0.6938557	-0.0000000
С	-6.1253235	-0.6938551	0.0000000
С	-4.9382981	-1.4266169	0.0000000
С	-4.9399855	-2.8948803	0.000000
С	-6.1168155	-3.6388854	0.0000000
С	-6.1004941	-5.0477449	0.000000
С	-4.9080782	-5.7289205	0.000000
С	-2.4487148	-5.6949226	-0.0000000
С	-3.6737445	-5.0189323	0.0000000
С	-3.6906963	-3.5832209	-0.0000000
С	-2.4612866	-2.8629374	-0.0000000
С	-1.2328603	-3.5611080	-0.0000000
С	-1.2259415	-5.0062223	-0.0000000
С	0.000000	-5.6879600	-0.0000000
С	4.9080782	-5.7289205	0.000000
С	3.6737445	-5.0189323	-0.0000000
С	2.4487149	-5.6949226	-0.0000000
С	1.2259415	-5.0062223	-0.000000
С	1.2328603	-3.5611080	-0.0000000
С	2.4612866	-2.8629374	-0.000000
С	3.6906963	-3.5832209	0.000000
С	4.9399855	-2.8948803	0.000000
С	6.1168155	-3.6388854	0.000000
С	6.1253235	-0.6938551	0.000000
С	4.9382981	-1.4266169	0.000000
С	3.7048222	-0.7147112	0.000000
С	2.4618107	-1.4245279	0.000000
С	1.2383407	-0.7200879	-0.0000000
С	0.000000	-1.4256325	-0.0000000
С	-1.2383407	-0.7200879	-0.0000000
С	-2.4618107	-1.4245279	-0.000000
С	-3.7048222	-0.7147112	0.000000
С	0.000000	-2.8522366	-0.000000
С	6.1004941	-5.0477449	0.000000

С	3.7048226	0.7147108	0.000000
С	4.9382978	1.4266159	-0.000000
С	6.1253238	0.6938557	-0.000000
С	-0.0000000	1.4256319	-0.000000
С	1.2383410	0.7200874	-0.000000
С	2.4618106	1.4245270	0.000000
С	-1.2383410	0.7200874	-0.000000
С	-2.4618106	1.4245270	-0.0000000
С	-3.7048226	0.7147108	-0.0000000
С	-4.9382978	1.4266159	-0.0000000
С	-4.9399854	2.8948805	-0.0000000
С	-3.6906963	3.5832206	0.000000
C	-2.4612863	2.8629366	0.000000
C	-1.2328604	3.5611077	0.000000
C	-0.0000000	2.8522354	0.000000
C	1.2328604	3.5611077	0.000000
C	2 4612863	2 8629366	0 0000000
C	3 6906963	3 5832206	0 0000000
C	4 9399854	2 8948805	-0 0000000
C	6 1168148	3 6388849	-0 0000000
C	6 1004934	5 0477451	-0 0000000
C	4 9080783	5 7289214	-0 0000000
C	3 6737439	5 01893214	0 0000000
C	2 4487150	5 6949240	0 0000000
C	1 2259/15	5 0062221	0.0000000
C	_0 000000	5 6879618	0.0000000
C	-1 2259/15	5 0062221	0.0000000
C	-2 //87150	5 69/92/0	0.0000000
C	-3 6737/39	5 0189321	0.0000000
C	-/ 9080783	5 7289217	-0 0000000
с ц	7 0483663	5 59/0211	-0 0000000
и П	7.0403003	-5 59/0208	0.0000000
ц	1 99/6613	-6 9225327	0.0000000
п п	4.0040013	6 7000650	0.0000000
п п	2.4410010	-0.7090030	0.0000000
п II	0.0000000	-0.7019970	0.0000000
п	-2.4410616	-6.7690650	0.0000000
H II	-4.8846613	-0.8223327	0.0000000
H	-7.0483663	5.5940211	-0.0000000
H	-7.0842499	3.1346467	-0.0000000
H	-/.08/9388	1.2072692	-0.0000000
H	-/.08/9389	-1.20/2683	0.0000000
H	-/.0842507	-3.1346469	0.0000000
H	-/.0483671	-5.5940208	0.000000
H	/.0842507	-3.1346469	0.000000
H	7.08/9389	-1.2072683	0.000000
Η	7.0879388	1.2072692	-0.0000000

Н 7.0842500 3.1346467 -0.0000000

BN-	Pri	st	ine.	_

wB97XD/def2-SV(P)

TTTO		WDJ/AD/GEIZ SV	(_)
В	4.9783562	-5.8700126	0.000000
Ν	6.2034018	-5.1409157	-0.000000
Ν	3.7421466	-5.1276109	0.000000
В	6.2486442	-3.7168261	-0.000000
В	3.7580858	-3.6711527	0.000000
Ν	5.0235298	-2.9607807	-0.000000
В	5.0167669	-1.5001437	-0.000000
В	6.2624146	0.6741047	-0.000000
В	3.7732186	0.6905910	-0.000000
Ν	3.7677347	-0.7663817	-0.000000
Ν	6.2335592	-0.7426943	-0.000000
Ν	5.0320116	1.4178572	-0.000000
Н	4.9830987	-7.0832610	-0.000000
В	2.4883973	-5.8338711	0.000000
Ν	2.5097783	-2.9374068	0.000000
В	2.5108122	-1.4839576	0.000000
Ν	2.5160178	1.4117867	-0.000000
В	1.2583553	0.6920514	-0.000000
Ν	1.2569422	-0.7605567	-0.000000
В	1.2527011	-3.6517104	0.000000
Ν	1.2473075	-5.1064894	0.000000
Η	2.4786915	-7.0462364	-0.000000
В	5.0287052	2.8787358	-0.000000
Ν	6.2451805	3.6449412	-0.000000
Ν	3.7691435	3.5916939	-0.000000
В	2.5150837	2.8658470	-0.000000
В	0.000000	-5.8243130	0.000000
В	-0.000000	-1.4786650	0.000000
Ν	0.000000	-2.9297237	0.000000
Ν	-0.000000	1.4105383	-0.000000
Ν	1.2569843	3.5811277	-0.000000
Ν	-1.2473075	-5.1064894	0.000000
В	-1.2527011	-3.6517104	0.000000
В	-0.000000	2.8626032	-0.000000
Ν	-1.2569422	-0.7605567	-0.000000
В	-1.2583553	0.6920514	-0.000000
Н	0.000000	-7.0364236	0.000000
В	-2.4883973	-5.8338711	0.000000
В	-2.5108122	-1.4839576	-0.000000
Ν	-1.2569843	3.5811277	-0.000000
Ν	-2.5160178	1.4117867	-0.000000
Ν	-2.5097783	-2.9374068	0.000000
В	-2.5150837	2.8658470	-0.000000

B -3.7580858 -3.6711527 0.000000 N -3.7421466 -5.1276109 0.000000 N -3.7677347 -0.7663817 -0.000000 H -2.4786915 -7.0462364 -0.000000 B -4.9783562 -5.8700126 -0.0000000 B -5.0167669 -1.5001437 -0.0000000 N -5.0235298 -2.9607807 0.0000000 N -5.0320116 1.4178572 -0.0000000 N -5.0320116 1.4178572 -0.0000000 B -6.2486442 -3.7168261 -0.0000000 B -6.2624146 0.6741047 -0.0000000 N -6.2034018 -5.1409157 -0.0000000 N -6.2335592 -0.7426943 -0.0000000 H -7.0363081 -3.1746384 -0.0000000 H -7.3363081 -3.1746384 -0.0000000 H -7.3466601 1.2245352 -0.0000000 B 3.7674361 5.0457951 -0.000000	В	-3.7732186	0.6905910	-0.000000
N -3.7421466 -5.1276109 0.000000 N -3.7677347 -0.7663817 -0.000000 H -2.4786915 -7.0462364 -0.000000 B -4.9783562 -5.8700126 -0.000000 B -5.0167669 -1.5001437 -0.0000000 N -5.0235298 -2.9607807 0.0000000 N -5.0320116 1.4178572 -0.0000000 N -3.7691435 3.5916939 -0.0000000 B -6.2486442 -3.7168261 -0.0000000 B -6.2634018 -5.1409157 -0.0000000 B -5.0287052 2.8787358 -0.0000000 N -6.2335592 -0.7426943 -0.0000000 H -7.0761784 -5.6551016 -0.0000000 H -7.366601 1.2245352 -0.0000000 H -7.3466601 1.2245352 -0.0000000 B 1.2557418 5.0337713 0.0000000 B -3.7674361 5.0457951 -0.00000000<	В	-3.7580858	-3.6711527	0.000000
N -3.7677347 -0.7663817 -0.000000 H -2.4786915 -7.0462364 -0.000000 B -4.9783562 -5.8700126 -0.000000 N -5.0167669 -1.5001437 -0.000000 N -5.0235298 -2.9607807 0.0000000 N -5.0320116 1.4178572 -0.0000000 N -3.7691435 3.5916939 -0.0000000 B -6.2624146 0.6741047 -0.0000000 B -6.2624146 0.6741047 -0.0000000 N -6.2034018 -5.1409157 -0.0000000 N -6.2335592 -0.7426943 -0.0000000 H -7.363081 -3.1746384 -0.0000000 H -7.3363081 -3.1746384 -0.0000000 H -7.3466601 1.2245352 -0.0000000 B 3.7674361 5.0457951 -0.0000000 B 1.2557418 5.0337713 0.0000000 B -3.7674361 5.0457951 -0.0000000 N 5.0211036 5.7526744 -0.0000000	Ν	-3.7421466	-5.1276109	0.000000
H-2.4786915-7.0462364-0.000000B-4.9783562-5.8700126-0.000000B-5.0167669-1.5001437-0.000000N-5.0235298-2.96078070.0000000N-5.03201161.4178572-0.0000000N-3.76914353.5916939-0.0000000B-6.2486442-3.7168261-0.0000000B-6.26241460.6741047-0.0000000B-5.02870522.8787358-0.0000000N-6.2034018-5.1409157-0.0000000N-6.2335592-0.7426943-0.0000000H-7.0761784-5.6551016-0.0000000H-7.3363081-3.1746384-0.0000000H-7.34666011.2245352-0.0000000B3.76743615.0457951-0.0000000B-1.25574185.0337713-0.0000000B-3.76743615.0457951-0.0000000N5.02110365.7526744-0.0000000N2.50807185.73015350.0000000N-2.50807185.73015350.0000000N-2.50807185.73015350.0000000N-2.50423136.74345380.0000000H-7.12721743.14875250.0000000H-7.32362825.68028090.0000000H-7.32362825.68028090.0000000H-7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.3	Ν	-3.7677347	-0.7663817	-0.000000
B-4.9783562-5.8700126-0.000000B-5.0167669-1.5001437-0.000000N-5.0235298-2.96078070.000000N-5.03201161.4178572-0.0000000N-3.76914353.5916939-0.0000000B-6.2486442-3.7168261-0.0000000B-6.26241460.6741047-0.0000000B-5.02870522.8787358-0.0000000N-6.2034018-5.1409157-0.0000000N-6.2335592-0.7426943-0.0000000H-7.0761784-5.6551016-0.0000000H-7.3363081-3.1746384-0.0000000H-7.33666011.2245352-0.0000000B3.76743615.0457951-0.0000000B3.76743615.0457951-0.0000000B-1.25574185.03377130.0000000B-3.76743615.0457951-0.0000000N5.02110365.7526744-0.0000000N2.50807185.73015350.0000000N-5.02110365.75267440.0000000N-5.02110365.75267440.0000000N-5.02110365.75267440.0000000N-5.02110365.75267440.0000000N-5.02110365.75267440.0000000N-5.02110365.75267440.0000000N-5.02110365.75267440.0000000H-7.32362825.68028090.0000000H-7.32	Η	-2.4786915	-7.0462364	-0.000000
B-5.0167669-1.5001437-0.000000N-5.0235298-2.96078070.000000N-5.03201161.4178572-0.000000N-3.76914353.5916939-0.0000000B-6.2486442-3.7168261-0.0000000B-5.02870522.8787358-0.0000000N-6.2034018-5.1409157-0.0000000N-6.2335592-0.7426943-0.0000000H-7.0761784-5.6551016-0.0000000H-7.3363081-3.1746384-0.0000000H-7.34666011.2245352-0.0000000H-7.34666011.2245352-0.0000000B3.76743615.0457951-0.0000000B-3.76743615.0457951-0.0000000B-3.76743615.0457951-0.0000000N5.02110365.7526744-0.0000000N2.50807185.73015350.0000000N-5.02110365.75267440.0000000N-5.02110365.75267440.0000000N-5.02110365.75267440.0000000N-5.02110365.75267440.0000000N-5.02473416.76542670.0000000H-7.32362825.68028090.0000000H-7.32362825.68028090.0000000H-7.32362825.68028090.0000000H-7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.32362	В	-4.9783562	-5.8700126	-0.000000
N -5.0235298 -2.9607807 0.000000 N -5.0320116 1.4178572 -0.000000 N -3.7691435 3.5916939 -0.000000 B -6.2486442 -3.7168261 -0.000000 B -6.2624146 0.6741047 -0.000000 B -5.0287052 2.8787358 -0.0000000 N -6.2034018 -5.1409157 -0.0000000 N -6.2335592 -0.7426943 -0.0000000 H -7.0761784 -5.6551016 -0.0000000 H -7.3363081 -3.1746384 -0.0000000 H -7.3466601 1.2245352 -0.0000000 B 3.7674361 5.0457951 -0.0000000 B 3.7674361 5.0457951 -0.0000000 B -3.7674361 5.0457951 -0.0000000 N 5.0211036 5.7526744 -0.0000000 N 2.5080718 5.7301535 0.0000000 N -5.0211036 5.7526744 0.00000000	В	-5.0167669	-1.5001437	-0.000000
N -5.0320116 1.4178572 -0.000000 N -3.7691435 3.5916939 -0.000000 B -6.2486442 -3.7168261 -0.000000 B -6.2624146 0.6741047 -0.000000 B -5.0287052 2.8787358 -0.0000000 N -6.2034018 -5.1409157 -0.0000000 N -6.2335592 -0.7426943 -0.0000000 H -4.9830987 -7.0832610 -0.0000000 H -7.0761784 -5.6551016 -0.0000000 H -7.3363081 -3.1746384 -0.0000000 H -7.3466601 1.2245352 -0.0000000 B 3.7674361 5.0457951 -0.0000000 B 1.2557418 5.0337713 0.0000000 N 5.0211036 5.724744 -0.0000000 N 2.5080718 5.7301535 0.0000000 N -2.5080718 5.7301535 0.0000000 N -5.0211036 5.7526744 0.0000000	Ν	-5.0235298	-2.9607807	0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Ν	-5.0320116	1.4178572	-0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Ν	-3.7691435	3.5916939	-0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	В	-6.2486442	-3.7168261	-0.000000
B-5.02870522.8787358-0.000000N-6.2034018-5.1409157-0.000000N-6.2335592-0.7426943-0.000000H-4.9830987-7.0832610-0.0000000H-7.0761784-5.6551016-0.0000000H-7.3363081-3.1746384-0.0000000H-7.34666011.2245352-0.0000000B6.27182035.06918620.0000000B3.76743615.0457951-0.0000000B1.25574185.03377130.0000000B-3.76743615.0457951-0.0000000B-3.76743615.0457951-0.0000000N5.02110365.7526744-0.0000000N2.50807185.73015350.0000000N-2.50807185.73015350.0000000N-5.02110365.75267440.0000000N-6.24518053.6449412-0.0000000N-7.12721743.14875250.0000000H-7.32362825.68028090.0000000H-7.32362825.68028090.0000000H-2.50423136.74345380.0000000H2.50423136.74345380.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.3363081-3.1746384-0.0000000H7.34666011.2245352-0.0000000H7.3466601 <t< td=""><td>В</td><td>-6.2624146</td><td>0.6741047</td><td>-0.000000</td></t<>	В	-6.2624146	0.6741047	-0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	В	-5.0287052	2.8787358	-0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Ν	-6.2034018	-5.1409157	-0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Ν	-6.2335592	-0.7426943	-0.000000
H -7.0761784 -5.6551016 -0.000000 H -7.3363081 -3.1746384 -0.000000 H -7.1163534 -1.2378082 -0.000000 B 6.2718203 5.0691862 0.0000000 B 3.7674361 5.0457951 -0.0000000 B 1.2557418 5.0337713 0.0000000 B -3.7674361 5.0457951 -0.0000000 B -3.7674361 5.0457951 -0.0000000 N 5.0211036 5.7526744 -0.0000000 N 2.5080718 5.7301535 0.0000000 N -2.5080718 5.7301535 0.0000000 N -5.0211036 5.7526744 0.0000000 N -6.2451805 3.6449412 -0.0000000 N -6.2451805 3.6449412 -0.0000000 H -7.1272174 3.1487525 0.0000000 H -7.3236282 5.6802809 0.0000000 H -2.5042313 6.7434538 0.0000000 H 2.5042313 6.7434538 0.0000000 H 7.3236282 5.6802809 0.0000000 H 7.3236282 5.6802809 0.0000000 H 7.3236282 5.6802809 0.0000000 H 7.3363081 -3.1746384 -0.0000000 H 7.3466601 1.2245352 -0.0000000 H 7.1272174 3.1487525 0.0000000	Η	-4.9830987	-7.0832610	-0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	-7.0761784	-5.6551016	-0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	-7.3363081	-3.1746384	-0.000000
H -7.3466601 1.2245352 -0.000000 B 6.2718203 5.0691862 0.000000 B 1.2557418 5.0337713 0.000000 B -1.2557418 5.0337713 -0.0000000 B -1.2557418 5.0337713 -0.0000000 B -3.7674361 5.0457951 -0.0000000 N 5.0211036 5.7526744 -0.0000000 N 2.5080718 5.7301535 0.0000000 N 2.5080718 5.7301535 0.0000000 N -2.5080718 5.7526744 0.0000000 N -2.5080718 5.7301535 0.0000000 N -5.0211036 5.7526744 0.0000000 N -5.0211036 5.7526744 0.0000000 N -6.2451805 3.6449412 -0.0000000 N -6.2718203 5.0691862 0.0000000 H -7.3236282 5.6802809 0.0000000 H -7.3236282 5.6802809 0.0000000 H -2.5042313 6.7434538 0.0000000 H 7.3236282 5.6802809 0.0000000 H 7.3236282 5.6802809 0.0000000 H 7.3236282 5.6802809 0.0000000 H 7.3363081 -3.1746384 -0.0000000 H 7.3466601 1.2245352 -0.0000000 H 7.1272174 3.1487525 0.0000000	Н	-7.1163534	-1.2378082	-0.000000
B6.27182035.06918620.000000B3.76743615.0457951-0.000000B1.25574185.03377130.000000B-1.25574185.0337713-0.000000B-3.76743615.0457951-0.000000N5.02110365.7526744-0.000000N2.50807185.73015350.0000000N-2.50807185.73015350.0000000N-2.50807185.73015350.0000000N-2.50807185.73015350.0000000N-5.02110365.75267440.0000000N-6.24518053.6449412-0.0000000N-6.24518053.6449412-0.0000000H-7.12721743.14875250.0000000H-7.32362825.68028090.0000000H-2.50423136.74345380.0000000H2.50423136.74345380.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.3363081-3.1746384-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	Н	-7.3466601	1.2245352	-0.000000
B3.76743615.0457951-0.000000B1.25574185.03377130.000000B-1.25574185.0337713-0.000000B-3.76743615.0457951-0.000000N5.02110365.7526744-0.000000N2.50807185.73015350.000000N-2.50807185.73015350.0000000N-2.50807185.73015350.0000000N-5.02110365.75267440.0000000N-5.02110365.75267440.0000000N-5.02110365.75267440.0000000N-6.24518053.6449412-0.0000000N-6.24518053.6449412-0.0000000H-7.12721743.14875250.0000000H-7.32362825.68028090.0000000H-2.50423136.74345380.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.3363081-3.1746384-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	В	6.2718203	5.0691862	0.000000
B1.25574185.03377130.000000B-1.25574185.0337713-0.000000B-3.76743615.0457951-0.000000N5.02110365.7526744-0.0000000N2.50807185.73015350.0000000N0.00000005.72426680.0000000N-2.50807185.73015350.0000000N-2.50807185.73015350.0000000N-5.02110365.75267440.0000000N-6.24518053.6449412-0.0000000N-6.24518053.6649412-0.0000000H-7.12721743.14875250.0000000H-7.32362825.68028090.0000000H-2.50423136.74345380.0000000H2.50423136.74345380.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.3363081-3.1746384-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	В	3.7674361	5.0457951	-0.000000
B-1.25574185.0337713-0.0000000B-3.76743615.0457951-0.0000000N5.02110365.7526744-0.0000000N2.50807185.73015350.0000000N0.00000005.72426680.0000000N-2.50807185.73015350.0000000N-2.50807185.73015350.0000000N-5.02110365.75267440.0000000N-6.24518053.6449412-0.0000000B-6.27182035.06918620.0000000H-7.12721743.14875250.0000000H-7.32362825.68028090.0000000H-2.50423136.74345380.0000000H2.50423136.74345380.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.3363081-3.1746384-0.0000000H7.1163534-1.2378082-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	В	1.2557418	5.0337713	0.000000
B-3.76743615.0457951-0.0000000N5.02110365.7526744-0.0000000N2.50807185.73015350.0000000N0.00000005.72426680.0000000N-2.50807185.73015350.0000000N-5.02110365.75267440.0000000N-6.24518053.6449412-0.0000000B-6.27182035.06918620.0000000H-7.12721743.14875250.0000000H-7.32362825.68028090.0000000H-2.50423136.74345380.0000000H2.50423136.74345380.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.3363081-3.1746384-0.0000000H7.34666011.2245352-0.0000000H7.34666011.2245352-0.0000000	В	-1.2557418	5.0337713	-0.000000
N5.02110365.7526744-0.0000000N2.50807185.73015350.0000000N0.00000005.72426680.0000000N-2.50807185.73015350.0000000N-5.02110365.75267440.0000000N-6.24518053.6449412-0.0000000B-6.27182035.06918620.0000000H-7.12721743.14875250.0000000H-7.32362825.68028090.0000000H-2.50423136.74345380.0000000H-0.00000006.73756810.0000000H5.02473416.76542670.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.346601-3.1746384-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	В	-3.7674361	5.0457951	-0.000000
N2.50807185.73015350.0000000N0.00000005.72426680.0000000N-2.50807185.73015350.0000000N-5.02110365.75267440.0000000N-6.24518053.6449412-0.0000000B-6.27182035.06918620.0000000H-7.12721743.14875250.0000000H-7.32362825.68028090.0000000H-2.50423136.74345380.0000000H-0.00000006.73756810.0000000H2.50423136.74345380.0000000H7.32362825.68028090.0000000H7.32362825.6551016-0.0000000H7.32362825.65551016-0.0000000H7.3363081-3.1746384-0.0000000H7.34666011.2245352-0.0000000H7.34666011.2245352-0.0000000	Ν	5.0211036	5.7526744	-0.000000
N0.0000005.72426680.000000N-2.50807185.73015350.0000000N-5.02110365.75267440.0000000N-6.24518053.6449412-0.0000000B-6.27182035.06918620.0000000H-7.12721743.14875250.0000000H-7.32362825.68028090.0000000H-5.02473416.76542670.0000000H-2.50423136.74345380.0000000H2.50423136.74345380.0000000H5.02473416.76542670.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.32362825.68028090.0000000H7.3363081-3.1746384-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	Ν	2.5080718	5.7301535	0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Ν	0.000000	5.7242668	0.000000
N-5.02110365.75267440.0000000N-6.24518053.6449412-0.0000000B-6.27182035.06918620.0000000H-7.12721743.14875250.0000000H-7.32362825.68028090.0000000H-5.02473416.76542670.0000000H-2.50423136.74345380.0000000H-0.00000006.73756810.0000000H2.50423136.74345380.0000000H5.02473416.76542670.0000000H7.32362825.68028090.0000000H7.0761784-5.6551016-0.0000000H7.1163534-1.2378082-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	Ν	-2.5080718	5.7301535	0.000000
N-6.24518053.6449412-0.0000000B-6.27182035.06918620.0000000H-7.12721743.14875250.0000000H-7.32362825.68028090.0000000H-5.02473416.76542670.0000000H-2.50423136.74345380.0000000H-0.00000006.73756810.0000000H2.50423136.76542670.0000000H5.02473416.76542670.0000000H7.32362825.68028090.0000000H7.0761784-5.6551016-0.0000000H7.3363081-3.1746384-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	Ν	-5.0211036	5.7526744	0.000000
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Ν	-6.2451805	3.6449412	-0.000000
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	В	-6.2718203	5.0691862	0.000000
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Н	-7.1272174	3.1487525	0.000000
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Н	-7.3236282	5.6802809	0.000000
H-2.50423136.74345380.0000000H-0.0000006.73756810.0000000H2.50423136.74345380.0000000H5.02473416.76542670.0000000H7.32362825.68028090.0000000H7.0761784-5.6551016-0.0000000H7.1163534-1.2378082-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	Н	-5.0247341	6.7654267	0.000000
H-0.0000006.73756810.000000H2.50423136.74345380.000000H5.02473416.76542670.0000000H7.32362825.68028090.0000000H7.0761784-5.6551016-0.0000000H7.3363081-3.1746384-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	Н	-2.5042313	6.7434538	0.000000
H2.50423136.74345380.000000H5.02473416.76542670.000000H7.32362825.68028090.0000000H7.0761784-5.6551016-0.0000000H7.3363081-3.1746384-0.0000000H7.1163534-1.2378082-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	Н	-0.0000000	6.7375681	0.000000
H5.02473416.76542670.000000H7.32362825.68028090.0000000H7.0761784-5.6551016-0.0000000H7.3363081-3.1746384-0.0000000H7.1163534-1.2378082-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	Н	2.5042313	6.7434538	0.000000
H7.32362825.68028090.0000000H7.0761784-5.6551016-0.0000000H7.3363081-3.1746384-0.0000000H7.1163534-1.2378082-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	Н	5.0247341	6.7654267	0.000000
H7.0761784-5.6551016-0.000000H7.3363081-3.1746384-0.0000000H7.1163534-1.2378082-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	Н	7.3236282	5.6802809	0.000000
H7.3363081-3.1746384-0.000000H7.1163534-1.2378082-0.0000000H7.34666011.2245352-0.0000000H7.12721743.14875250.0000000	Н	7.0761784	-5.6551016	-0.0000000
H 7.1163534 -1.2378082 -0.0000000 H 7.3466601 1.2245352 -0.0000000 H 7.1272174 3.1487525 0.0000000	Н	7.3363081	-3.1746384	-0.0000000
H 7.3466601 1.2245352 -0.0000000 H 7.1272174 3.1487525 0.0000000	Н	7.1163534	-1.2378082	-0.0000000
Н 7.1272174 3.1487525 0.000000	Н	7.3466601	1.2245352	-0.000000
	Н	7.1272174	3.1487525	0.000000

BN-zz-B-to	op,	wB97XD/def2-SV	7(P)
Н	4.9500835	6.9840559	0.000000
Н	2.4616248	6.9445923	0.000000
Н	0.000000	6.9354485	0.000000
Н	-2.4616248	6.9445923	0.000000
Н	-4.9500835	6.9840559	0.000000
С	-6.1249021	0.7078182	0.000000
С	-6.1249018	-0.7078183	-0.0000000
С	-4.9696340	-1.4340531	0.000000
С	6.1249019	-0.7078182	-0.0000000
С	4.9696339	-1.4340532	0.000000
С	3.6984863	-0.7276631	-0.0000000
С	2.4849533	-1.4199297	0.000000
С	1.2339054	-0.7228285	-0.0000000
С	0.000000	-1.4164242	0.000000
С	-1.2339054	-0.7228285	-0.0000000
С	-2.4849533	-1.4199297	0.000000
С	-3.6984863	-0.7276631	-0.0000000
С	3.6984863	0.7276631	0.000000
С	4.9696338	1.4340532	-0.0000000
С	6.1249019	0.7078182	0.000000
С	-0.0000000	1.4164242	-0.0000000
С	1.2339054	0.7228285	0.000000
С	2.4849533	1.4199297	-0.0000000
С	-1.2339054	0.7228285	0.000000
C	-2.4849533	1.4199297	-0.0000000
С	-3.6984863	0.7276631	0.000000
С	-4.9696337	1.4340532	-0.0000000
Н	7.0469188	5.5442262	0.000000
Н	7.0469188	-5.5442262	0.000000
Н	4.9500835	-6.9840559	-0.0000000
Н	2.4616248	-6.9445923	-0.0000000
Н	-0.0000000	-6.9354485	-0.0000000
Н	-2.4616248	-6.9445923	-0.0000000
Н	-4.9500835	-6.9840559	-0.0000000
Н	-7.0469188	5.5442262	0.000000
Н	-7.3021901	3.0903165	-0.0000000
Н	-7.0907593	1.2071512	-0.0000000
Н	-7.0907594	-1.2071512	-0.0000000
Н	-7.3021901	-3.0903165	-0.0000000
Н	-7.0469188	-5.5442262	-0.0000000
H	7.3021901	-3.0903165	-0.0000000
H	7.0907593	-1.2071512	-0.0000000
H	7.0907593	1.2071512	-0.0000000
Н	7.3021901	3.0903165	0.000000
В	4.9520159	5.7721398	-0.0000000

В	2.4748552	5.7336343	-0.000000
В	0.0000000	5.7248691	-0.000000
В	-2.4748552	5.7336343	-0.000000
В	-4.9520159	5.7721398	-0.000000
В	6.2168561	3.6160488	-0.000000
В	3.7340977	3.5703137	0.000000
В	1.2438208	3.5531032	0.000000
В	-1.2438208	3.5531032	0.000000
В	-3.7340977	3.5703137	0.000000
В	-6.2168561	3.6160488	-0.000000
В	4.9520159	-5.7721398	0.000000
В	2.4748552	-5.7336343	0.000000
В	0.0000000	-5.7248691	0.000000
В	-2.4748552	-5.7336343	0.000000
В	-4.9520159	-5.7721398	0.000000
В	6.2168561	-3.6160488	0.000000
В	3.7340977	-3.5703137	-0.000000
В	1.2438208	-3.5531032	-0.000000
В	-1.2438208	-3.5531032	-0.000000
В	-3.7340977	-3.5703137	-0.000000
В	-6.2168561	-3.6160488	0.000000
N	6.1684511	5.0396543	-0.000000
N	4.9849554	2.8601213	0.000000
N	3.7198897	5.0226408	-0.000000
N	2.4869085	2.8358710	0.000000
N	1.2393011	5.0017324	-0.000000
N	0.000000	2.8285886	0.000000
N	-1.2393011	5.0017324	-0.0000000
N	-2.4869085	2.8358710	0.000000
N	-3.7198897	5.0226408	-0.0000000
N	-4.9849554	2.8601213	0.000000
N	-6.1684511	5.0396543	-0.0000000
N	4.9849554	-2.8601213	-0.0000000
N	3.7198897	-5.0226408	-0.0000000
N	6.1684511	-5.0396543	0.0000000
N	1.2393011	-5.001/324	0.0000000
N	-1.2393011	-5.001/324	0.000000
N	-3.7198897	-5.0226408	-0.0000000
N	-6.1684511	-5.0396543	0.000000
N	-4.9849554	-2.8601214	-0.0000000
N	-2.4869085	-2.8358710	-0.000000
N	-0.000000	-2.8285886	-0.000000
Ν	2.4869085	-2.8358710	-0.0000000
BN-zz-N-to	, ac	wB97XD/def2-SV	7(P)

•		00P/		(=)
	Н	5.0511228	6.8898833	0.000000

Η	2.5073613	6.8999657	-0.000000
Н	0.000000	6.8991826	-0.000000
Н	-2.5073613	6.8999657	-0.000000
Н	-5.0511228	6.8898833	-0.000000
С	-6.1166454	0.7112981	0.000000
С	-6.1166454	-0.7112981	0.000000
С	-4.9533309	-1.4366137	0.000000
С	6.1166454	-0.7112981	-0.0000000
C	4.9533310	-1.4366137	-0.000000
C	3.6862086	-0.7242077	-0.000000
C	2 4767713	-1 4347342	-0 0000000
C	1 2300594	-0 7246100	-0 0000000
C		-1 4339922	-0 0000000
C	-1 2300594	-0.7246100	-0 0000000
C	-2 4767713	-1 4347342	-0 0000000
C	-3 6862086	-0 7242077	-0 0000000
C	3 6862086	0 72/2077	0 0000000
C	J.0002000 / 9533309	1 /366137	0.0000000
C	6 1166454	0 7112081	0.0000000
C	0.1100404	1 1330022	0.0000000
C	1 2200504	1.4333922	0.0000000
C	1.2300J94 2.4767712	1 4240100	0.0000000
C	2.4/0//13	1.434/342	0.0000000
C	-1.2300394	1 4247240	0.0000000
	-2.4/6//13	1.434/342	0.0000000
C	-3.6862086	0./2420//	0.0000000
C	-4.9533310	1.4366137	0.0000000
H	7.3297750	5.7681962	0.0000000
H	7.3297750	-5./681962	0.0000000
H	5.0511228	-6.8898833	0.0000000
H	2.50/3613	-6.8999657	0.0000000
H	-0.0000000	-6.8991826	-0.0000000
Н	-2.50/3613	-6.899965/	-0.0000000
Н	-5.0511228	-6.8898833	-0.0000000
Η	-7.3297750	5.7681962	-0.0000000
Η	-7.0977654	3.2450922	0.000000
Η	-7.0881323	1.2187898	0.000000
Η	-7.0881323	-1.2187898	-0.0000000
Η	-7.0977654	-3.2450922	-0.0000000
Η	-7.3297750	-5.7681962	-0.0000000
Η	7.0977654	-3.2450922	0.000000
Η	7.0881323	-1.2187898	0.000000
Η	7.0881323	1.2187898	0.000000
Η	7.0977654	3.2450922	0.000000
Ν	5.0286578	5.8771274	-0.000000
Ν	6.2186822	3.7475182	-0.000000
Ν	3.7462951	3.7389333	-0.0000000

Ν	1.2488691	3.7373181	0.000000
Ν	-1.2488691	3.7373181	0.000000
Ν	-3.7462951	3.7389333	-0.0000000
N	-6.2186822	3.7475182	0.000000
Ν	-5.0286578	5.8771274	0.000000
Ν	-2.5083039	5.8864961	-0.0000000
Ν	-0.0000000	5.8857666	-0.0000000
N	2.5083039	5.8864961	-0.0000000
N	3 7462951	-3 7389333	0 0000000
N	5 0286578	-5 8771274	0 0000000
N	2 5083039	-5 8864961	0 0000000
N	1 2488691	-3 7373181	0 0000000
N	-0 000000	-5 8857666	0 0000000
N	-1 2/88691	-3 7373181	-0 0000000
N	-2 5083039	-5 886/961	0.0000000
N	-3 7/62951	-3 7389333	0.0000000
IN NT	5 0206570	5 0771071	0.0000000
IN	-5.0200570	-J.0//12/4 2 7/75102	0.0000000
IN D	-0.2100022	-3.7473102	0.0000000
B	0.2000005	2.000(027	-0.0000000
В	4.9886005	5.0086827	-0.0000000
В	3.7609799	5.1924066	-0.0000000
В	2.4939608	3.0100127	0.0000000
В	1.2533323	5.1922662	-0.0000000
В	-0.0000000	3.0082917	0.0000000
В	-1.2533323	5.1922662	-0.0000000
В	-2.4939608	3.0100127	0.000000
В	-3.7609799	5.1924066	-0.0000000
В	-4.9886005	3.0086827	0.000000
В	-6.2680063	5.1750120	0.000000
В	6.2680063	-5.1750120	0.000000
В	3.7609799	-5.1924066	0.000000
В	4.9886005	-3.0086827	-0.000000
В	1.2533323	-5.1922662	0.000000
В	-1.2533323	-5.1922662	0.000000
В	-3.7609799	-5.1924066	0.000000
В	-6.2680063	-5.1750120	0.000000
В	-4.9886005	-3.0086827	-0.0000000
В	-2.4939608	-3.0100127	-0.0000000
В	-0.0000000	-3.0082917	-0.000000
В	2.4939608	-3.0100127	-0.000000
Ν	6.2186822	-3.7475182	0.000000
BN-mixed,	wB91	7XD/def2-SV(P)	
H	4.9515196	-7.0516982	-0.000000
Н	2.4643756	-7.0115267	-0.0000000
Н	-0.0000000	-7.0039586	0.000000

Η	-2.4643756	-7.0115267	-0.000000
Н	-4.9515196	-7.0516982	-0.000000
С	-6.1464144	-0.7810334	0.000000
С	-6.1142912	0.6269687	0.000000
С	-4.9498704	1.3568245	0.000000
С	6.1142912	0.6269687	0.000000
С	4.9498704	1.3568245	0.000000
С	3.6941860	0.6384055	0.000000
С	2.4777234	1.3514128	-0.0000000
С	1.2338831	0.6492883	-0.0000000
С	-0.0000000	1.3542363	-0.0000000
С	-1.2338831	0.6492883	-0.0000000
С	-2.4777234	1.3514128	-0.0000000
C	-3.6941860	0.6384055	-0.0000000
C	3.7109046	-0.8086855	-0.0000000
C	4.9766904	-1.5078087	0.000000
C	6 1464144	-0 7810334	-0 0000000
C	0 0000000	-1 4987432	0 0000000
C	1 2389265	-0 8011158	-0 0000000
C	2 4834471	-1 5029803	0 0000000
C	-1 2389265	-0 8011158	-0 0000000
C	-2 4834471	-1 5029803	0 0000000
C	-3 7109046	-0 8086855	-0 0000000
C	-4 9766904	-1 5078087	-0 0000000
н	7 0492161	-5 6147188	-0 0000000
н	7 3286615	5 6885426	0 0000000
H	5 0463123	6 8050103	0 0000000
H	2.5034288	6.8091442	0.000000
H	-0.0000000	6.8046737	-0.000000
H	-2.5034288	6.8091442	-0.000000
H	-5.0463123	6.8050103	0.000000
H	-7.0492161	-5.6147188	-0.0000000
H	-7.3103094	-3.1622424	-0.000000
H	-7.1123654	-1.2788749	-0.0000000
H	-7.0828015	1.1405661	-0.0000000
H	-7.1034421	3.1671587	0.000000
Н	-7.3286615	5.6885426	0.000000
H	7.1034421	3.1671587	0.000000
H	7.0828015	1.1405661	-0.0000000
H	7.1123654	-1.2788749	0.000000
H	7.3103094	-3.1622424	-0.000000
B	4.9549384	-5.8406588	-0.0000000
B	2.4775264	-5.8016488	-0.0000000
– B	0.0000000	-5.7946780	0.0000000
– B	-2.4775264	-5.8016488	0.0000000
В	-4.9549384	-5.8406588	-0.0000000

В	6.2264812	-3.6869980	-0.000000
В	3.7425122	-3.6399327	0.000000
В	1.2460601	-3.6258108	0.000000
В	-1.2460601	-3.6258108	0.000000
В	-3.7425122	-3.6399327	0.000000
В	-6.2264812	-3.6869980	-0.000000
Ν	6.1715060	-5.1082576	-0.000000
Ν	4.9905604	-2.9277521	-0.0000000
N	3.7221421	-5.0895790	-0.0000000
N	2.4879235	-2.9041688	-0.000000
N	1.2396341	-5.0702773	0.000000
N	-0.000000	-2.8950398	0.000000
N	-1 2396341	-5 0702773	0 0000000
N	-2 4879235	-2 9041688	0 0000000
N	-3 7221421	-5 0895790	0 0000000
N	-4 9905604	-2 9277521	0 0000000
N	-6 1715060	-5 1082576	-0 0000000
N	5 0271804	5 7921084	0 0000000
N	6.2220995	3.6653360	-0.0000000
N	3.7485943	3.6506458	-0.0000000
N	2.5070827	5.7956078	-0.0000000
N	1.2503035	3.6430613	0.0000000
N	0.0000000	5.7912326	-0.0000000
Ν	-1.2503035	3.6430613	0.000000
Ν	-2.5070827	5.7956078	-0.000000
Ν	-3.7485943	3.6506458	-0.000000
Ν	-6.2220995	3.6653360	-0.000000
Ν	-5.0271804	5.7921084	0.000000
В	6.2676256	5.0915473	0.000000
В	3.7602914	5.1027224	-0.000000
В	4.9883222	2.9222384	-0.000000
В	1.2533016	5.0960318	-0.000000
В	2.4944168	2.9141347	-0.000000
В	-0.000000	2.9108930	0.000000
В	-1.2533016	5.0960318	-0.000000
В	-2.4944168	2.9141347	-0.000000
В	-3.7602914	5.1027224	-0.000000
В	-4.9883222	2.9222384	-0.000000
В	-6.2676256	5.0915473	-0.000000
BN-center,	wE	97XD/def2-SV(P)
Н	4.8767766	-6.9390689	-0.000000
Н	2.4343880	-6.8970865	-0.000000
Н	-0.000000	-6.8841106	-0.000000
Н	-2.4343880	-6.8970865	-0.000000
Н	-4.8767766	-6.9390689	-0.000000

С	-6.0913392	-5.1724328	-0.000000
С	-6.0975643	-3.7427977	0.000000
С	-4.9762619	2.9213672	-0.000000
С	-6.1266864	3.6730182	0.000000
С	-6.0807008	5.0969544	0.000000
С	-4.8962235	5.7655123	0.000000
С	-2.4483507	5.7081476	-0.0000000
С	-3.6596270	5.0394962	0.000000
C	-3 6936842	3 5929441	-0 0000000
C	-2 4826767	2 8873895	-0 0000000
C	-1.2317022	3.5749072	0.000000
C	-1.2196278	5.0184699	0.000000
C		5 6986840	-0 0000000
C	4 8962235	5 7655123	-0 0000000
C	3 6596270	5 0394962	-0 0000000
C	2 4483507	5 7081476	-0 0000000
C	1 2196278	5 0184699	-0 0000000
C	1 2317022	3 5749072	-0 0000000
C	2 4826767	2 8873895	-0 0000000
C	3 6936842	3 5929441	-0 0000000
C	1 9762619	2 9213672	-0 0000000
C	4.J70201J	3 6730182	0.0000000
C	0.1200004	2 8781780	-0 0000000
C	6 0807008	5 0969511	-0 0000000
C	-1 9452034	-2 99/705/	0.0000000
C	-3 6722124	-3 6856/18	0.0000000
C	-2 1711613	-2 96/92/5	0.0000000
C	-1 2252445	-3 6602204	0 0000000
C	-0 0000000	-2 9555984	0 0000000
C	1 2252445	-3 6602204	0 0000000
C	2 4714643	-2 9649245	0 0000000
C	3 6722124	-3 6856418	0 0000000
C	4 9452034	-2 9947054	-0 0000000
C	6 0975643	-3 7427977	-0 0000000
C	6 0913392	-5 1724328	-0 0000000
C	4 9061241	-5 8449656	-0 0000000
C	3 6607532	-5 131/393	0.0000000
C	2 1186298	-5 8021/1/1	0.0000000
C	1 2203387	-5 10/8186	0.0000000
C		-5 7891//2	-0.0000000
C	-1 2203387	-5 10/91442	0.0000000
C	-2 1186298	-5.2040100	0.0000000
C	-2.4400230 -3 6607530	-J.0021441 _5 131/303	0.0000000
C	-3.000/JJZ _/ QA612/1	-J.IJI4393 _5 8110656	
U U	7 0301697	_5 7166062	
л II	1.UJY402/ 7.0010560	-J./100003 5 6500707	-0.0000000
п	1.0248366	5.0500/9/	0.0000000

Н	4.8551765	6.8583114	0.000000
Н	2.4365225	6.8015594	0.000000
Н	-0.0000000	6.7919161	0.000000
Н	-2.4365225	6.8015594	0.000000
Н	-4.8551765	6.8583114	0.000000
Н	-7.0394627	-5.7166863	-0.0000000
Н	-7.0730190	-3.2430497	-0.0000000
Н	-7.0725701	-1.1553675	-0.0000000
Н	-7.3103790	1.2806527	-0.0000000
Н	-7.1000152	3.1885500	0.000000
Н	-7.0248566	5.6500797	0.000000
Н	7.1000152	3.1885500	0.000000
Н	7.3103790	1.2806527	0.000000
Н	7.0725701	-1.1553675	-0.0000000
Н	7.0730190	-3.2430497	-0.0000000
В	4.9699104	-1.4252189	0.000000
В	2.4882706	-1.4059768	0.000000
В	0.000000	-1.4042268	0.000000
В	-2.4882706	-1.4059768	0.000000
В	-4.9699104	-1.4252189	0.000000
В	-3.7493744	0.7694603	0.000000
В	-6.2289752	0.7477611	-0.0000000
В	-1.2489701	0.7612726	0.000000
В	1.2489701	0.7612726	0.000000
В	3.7493744	0.7694603	0.000000
В	6.2289752	0.7477611	0.000000
N	6.1831380	-0.6714061	0.000000
Ν	4.9938235	1.4986622	0.000000
Ν	2.4901356	1.4867462	-0.0000000
Ν	0.0000000	1.4828294	-0.0000000
Ν	-2.4901356	1.4867462	-0.0000000
Ν	-4.9938235	1.4986622	-0.0000000
Ν	-3.7355992	-0.6769658	0.000000
Ν	-6.1831380	-0.6714061	-0.0000000
Ν	-1.2455294	-0.6759734	0.000000
Ν	1.2455294	-0.6759734	0.000000
N	3.7355992	-0.6769658	0.000000
BN-cross,	wB9	7XD/def2-SV(P)	
Н	4.8629704	-6.9614034	-0.0000000
Н	2.4007367	-6.8646993	0.000000
Н	-0.000000	-7.0708785	0.000000
Н	-2.4007367	-6.8646993	0.000000
Н	-4.8629704	-6.9614034	-0.000000
С	-6.0967528	-5.2141099	-0.000000
С	-6.1407238	-3.7774132	-0.0000000

С	-5.0102022	2.9211069	0.000000
С	-6.1777441	3.6422789	0.000000
С	-6.1757770	5.0675629	0.000000
С	-5.0108411	5.7586223	0.000000
С	-2.5710212	5.7884225	-0.0000000
С	-3.7422576	5.0712144	0.000000
C	-3.7249478	3.6072404	-0.0000000
C	-2.5056717	2.9089379	-0.0000000
C	5 0108411	5 7586223	-0 0000000
C	3 7422576	5 0712144	-0 0000000
C	2 5710212	5 788/225	-0.0000000
C	2.5710212	2 9089379	-0.0000000
C	2.3030717	2.9009579	0.0000000
C	5.1249470	3.0072404	-0.0000000
C	5.0102022	2.9211069	-0.0000000
C	0.177441	5.0422709	-0.0000000
C	6.1/5///1	5.06/5629	-0.0000000
C	-5.009/208	-3.0004318	-0.0000000
С	-3./22/858	-3.6/15389	0.0000000
С	-2.5528512	-2.9348967	0.0000000
С	2.5528512	-2.9348967	0.0000000
С	3.7227858	-3.6715389	0.000000
С	5.0097208	-3.0004318	-0.0000000
С	6.1407238	-3.7774132	-0.0000000
С	6.0967528	-5.2141099	0.000000
С	4.9007527	-5.8668326	0.000000
С	3.6657904	-5.1251067	0.000000
С	2.4437770	-5.7700010	0.000000
С	-2.4437770	-5.7700010	0.000000
С	-3.6657904	-5.1251067	0.000000
С	-4.9007527	-5.8668326	-0.0000000
Н	7.0339463	-5.7779970	-0.0000000
Н	7.1356565	5.5948090	0.000000
Н	4.9951023	6.8522626	0.000000
Н	2.6436072	6.8828081	0.000000
Н	-0.0000000	6.7051594	0.000000
Н	-2.6436072	6.8828081	0.000000
н	-4.9951023	6.8522626	0.000000
н	-7 0339463	-5 7779970	-0 0000000
н	-7 1327198	-3 3089374	-0 0000000
н	-7 1169624	-1 1444428	-0 0000000
и П	-7 3/18039	1 2808356	-0.0000000
и П	-7 1376/29	3 13//091	0.0000000
ц	-7 1256565	5.1344091 5.50/0000	
л U	7 1276420	J.JJ40UJU 2 1211001	_0_0000000
n 11	1.13/0429 7 3/10030	J. LJ44U9L 1. JOAAJEC	-0.0000000
п	1.3418U39	1.20U0356	-0.0000000
Н	/.1169624	-1.1444428	-0.0000000

$\begin{array}{llllllllllllllllllllllllllllllllllll$
$\begin{array}{llllllllllllllllllllllllllllllllllll$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
$\begin{array}{llllllllllllllllllllllllllllllllllll$
$\begin{array}{llllllllllllllllllllllllllllllllllll$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$
B -1.2544595 0.7397257 -0.0000000 B 1.2544595 0.7397257 -0.0000000 B 3.7734003 0.7840419 -0.0000000 B 6.2592961 0.7517002 -0.0000000 N 6.2240428 -0.6661524 -0.0000000 N 5.0202181 1.5017712 -0.0000000 N 2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5017712 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -3.7764064 -0.6661524 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 1.2882979 3.5745640 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2885916 -5.1192359 0.0000000
B 1.2544595 0.7397257 -0.0000000 B 3.7734003 0.7840419 -0.0000000 B 6.2592961 0.7517002 -0.0000000 N 6.2240428 -0.6661524 -0.0000000 N 5.0202181 1.5017712 -0.0000000 N 2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -3.7764064 -0.6661524 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 1.2882979 3.5745640 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -1.2885916 -5.1192359 0.00000000 <t< td=""></t<>
B 3.7734003 0.7840419 -0.0000000 B 6.2592961 0.7517002 -0.0000000 N 6.2240428 -0.6661524 -0.0000000 N 5.0202181 1.5017712 -0.0000000 N 2.4984356 1.5027791 -0.0000000 N -0.0000000 1.4464524 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -3.7764064 -0.6661524 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2882979 3.5745640 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.2385916 -5.1192359 0.0000000 <t< td=""></t<>
B 6.2592961 0.7517002 -0.0000000 N 6.2240428 -0.6661524 -0.0000000 N 5.0202181 1.5017712 -0.0000000 N 2.4984356 1.5027791 -0.0000000 N -0.0000000 1.4464524 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -3.7764064 -0.6661524 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 1.2882979 3.5745640 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.2385916 -5.1192359 0.00000000 <
N 6.2240428 -0.6661524 -0.0000000 N 5.0202181 1.5017712 -0.0000000 N 2.4984356 1.5027791 -0.0000000 N -0.0000000 1.4464524 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -3.7764064 -0.6661524 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 1.2882979 3.5745640 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -1.2885916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 N -1.2678319 5.0550201 0.0000000
N 5.0202181 1.5017712 -0.0000000 N 2.4984356 1.5027791 -0.0000000 N -0.0000000 1.4464524 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -3.7764064 -0.6606254 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 1.2882979 3.5745640 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 -5.923853 0.0000000 N -0.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.00000000
N 2.4984356 1.5027791 -0.0000000 N -0.0000000 1.4464524 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -3.7764064 -0.6661524 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 1.2882979 3.5745640 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 N -1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.00000000 <t< td=""></t<>
N -0.0000000 1.4464524 -0.0000000 N -2.4984356 1.5027791 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -3.7764064 -0.6606254 -0.0000000 N -6.2240428 -0.6661524 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 N -1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B -0.263815 -3.6426494 0.0000000
N -2.4984356 1.5027791 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -3.7764064 -0.6606254 -0.0000000 N -6.2240428 -0.6661524 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 B 1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B -0.263815 -3.6426494 0.0000000
N -2.4984336 1.3027791 -0.0000000 N -5.0202181 1.5017712 -0.0000000 N -3.7764064 -0.6606254 -0.0000000 N -6.2240428 -0.6661524 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 1.2882979 3.5745640 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.2385916 -5.1192359 0.0000000 N 1.2385916 -5.1192359 0.0000000 N -1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B -0.2363815 -3.6426494 0.0000000
N -3.0202181 1.3017712 -0.0000000 N -3.7764064 -0.6606254 -0.0000000 N -6.2240428 -0.6661524 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 3.7764064 -0.6606254 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.0000000 -2.9107791 0.0000000 N -1.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 B 1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -1.2363815 -3.6426494 0.0000000
N -3.7764064 -0.66605234 -0.0000000 N -6.2240428 -0.6661524 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 3.7764064 -0.6606254 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.0000000 -2.9107791 0.0000000 N -0.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 N -1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
N -0.2240428 -0.0000000 N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 3.7764064 -0.6606254 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.0000000 -2.9107791 0.0000000 N -1.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 B 1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
N -1.2613512 -0.7025060 0.0000000 N 1.2613512 -0.7025060 0.0000000 N 3.7764064 -0.6606254 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.0000000 -2.9107791 0.0000000 N -1.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 N -1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
N 1.2613512 -0.7025060 0.0000000 N 3.7764064 -0.6606254 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.0000000 -2.9107791 0.0000000 N -0.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 N -1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
N 3.7764064 -0.6606234 -0.0000000 N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.0000000 -2.9107791 0.0000000 N 1.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 B 1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
N 1.2882979 3.5745640 -0.0000000 N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.0000000 -2.9107791 0.0000000 N 1.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 B 1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
N -1.2882979 3.5745640 -0.0000000 N -0.0000000 5.6923853 0.0000000 N -0.0000000 -2.9107791 0.0000000 N 1.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 B 1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
N -0.0000000 5.6923853 0.0000000 N -0.0000000 -2.9107791 0.0000000 N 1.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 B 1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
N -0.0000000 -2.9107791 0.0000000 N 1.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 B 1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
N 1.2385916 -5.1192359 0.0000000 N -1.2385916 -5.1192359 0.0000000 B 1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
N -1.2385916 -5.1192359 0.0000000 B 1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
B 1.2678319 5.0550201 0.0000000 B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
B -1.2678319 5.0550201 0.0000000 B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000 D 1.2363815 -3.6426494 0.0000000
B -0.0000000 2.8707464 -0.0000000 B 1.2363815 -3.6426494 0.0000000
B 1.2363815 -3.6426494 0.0000000
B -1.2363815 -3.6426494 0.0000000
B 0.0000000 -5.8585958 0.0000000
BN-ac, wB97XD/def2-SV(P)
н 5.0273516 6.7437537 0.0000000
н 2.3872304 6.9019186 0.0000000
н 0.000000 6.8632268 0.0000000
н -2.3872304 6.9019186 0.0000000
н -5.0273516 6.7437537 0.0000000
C -2.4178268 -5.6773807 0.0000000
C -2.4349626 -2.8120697 -0.0000000
C -1.2264196 -3.5006305 -0.0000000
C -1.2213052 -4.9601077 0.0000000

С	-0.0000001	-5.6523718	0.000000
С	2.4178267	-5.6773807	0.000000
С	1.2213054	-4.9601077	0.000000
С	1.2264192	-3.5006305	-0.0000000
С	2.4349629	-2.8120696	-0.0000000
С	2.4580101	-1.3855118	-0.0000000
С	1.2488127	-0.6552343	-0.0000000
С	-0.0000002	-1.3671050	-0.0000000
С	-1.2488124	-0.6552343	-0.0000000
C	-2.4580102	-1.3855119	0.000000
C	0.0000003	-2.7928172	-0.0000000
C	0.000002	1.5048635	0.000000
C	1 2399311	0 8033191	-0 0000000
C	2.4517458	1.5008665	-0.0000000
C	-1,2399314	0.8033191	-0.0000000
C	-2.4517457	1.5008665	-0.0000000
C	-2 4726770	2 9330798	-0 0000000
C	-1 2522540	3 6460251	-0 0000000
C	-0 0000001	2 9323561	-0 0000000
C	1 2522541	3 6460251	-0 0000000
C	2 4726770	2 9330799	-0 0000000
C	2.4720770	5 8055393	0.0000000
C	1 2390156	5 1131026	-0 0000000
C	0 000000	5 7685102	0 0000000
C	-1 2390157	5 1131026	-0 0000000
C	-2 4494615	5 8055393	0 0000000
н	6 9394406	-5 7344570	0 0000000
Н	2.4005395	-6.7726745	0.000000
н	0 0000000	-6 7476941	0 0000000
Н	-2.4005395	-6.7726744	0.000000
Н	-7.0672467	3.0971606	0.000000
Н	-7.0533053	-1.2634942	0.000000
H	-6.9394406	-5.7344570	0.000000
Н	7.0533053	-1.2634941	0.000000
н	7 0672467	3 0971606	0 0000000
B	-4 8556880	-5 8906259	0 0000000
н	-4 7790625	-7 0992149	-0 0000000
B	-6 1935789	-3 7579876	0 0000000
н	-7 3017967	-3 2679692	0 0000000
B	-3 7211545	-3 6165405	-0 0000000
B	-4 9644737	-1 4994827	-0 0000000
B	-6 2388988	0 6678346	-0 0000000
— Н	-7.3355942	1.1878971	0.000000
B	-3.7583732	0.7096708	-0.0000000
– B	-4.9777245	2.8737306	-0.000000
B	-6.2695382	5.0470164	0.000000
	0.200000	0.01/0101	

Н	-7.3450208	5.6194136	0.000000
В	-3.7461897	5.0697502	0.000000
В	4.8556880	-5.8906259	0.000000
Н	4.7790625	-7.0992149	-0.000000
В	6.1935789	-3.7579876	0.000000
Н	7.3017967	-3.2679692	0.000000
В	3.7211545	-3.6165405	-0.000000
В	4.9644737	-1.4994827	-0.000000
В	3.7583732	0.7096708	-0.0000000
В	6.2388988	0.6678346	0.000000
Н	7.3355942	1.1878971	0.000000
В	4.9777245	2.8737306	-0.0000000
В	3.7461897	5.0697502	0.000000
В	6.2695382	5.0470164	0.000000
Н	7.3450208	5.6194136	0.000000
Ν	-3.6311420	-5.0884476	0.000000
Ν	-4.9963330	-2.9699771	0.000000
Ν	-6.0811987	-5.1940462	0.000000
Ν	-6.1769239	-0.7564086	-0.000000
Ν	-3.7058877	-0.7542846	-0.000000
Ν	-5.0175453	1.4058013	-0.000000
N	-3.7101296	3.5887479	-0.000000
N	-5.0409338	5.7311024	0.000000
N	-6.1990981	3.6157888	0.000000
N	5.0409338	5.7311024	0.000000
N	6.1990981	3.6157888	-0.000000
N	3.7101297	3.5887479	0.000000
N	5.0175453	1.4058013	-0.000000
N	3.7058877	-0.7542847	-0.000000
N	6.1769239	-0.7564086	-0.000000
N	4.9963330	-2.9699771	0.000000
N	3.6311420	-5.0884476	0.000000
Ν	6.0811987	-5.1940462	0.000000
BN-edges,	wB9	7XD/def2-SV(P)	
Н	4.9178923	-7.0744632	-0.000000
Н	2.4285619	-7.0036774	-0.000000
Н	-0.000000	-6.9683996	-0.000000
Н	-2.4285619	-7.0036774	-0.000000
Н	-4.9178923	-7.0744632	-0.000000
С	2.4463464	1.4000856	-0.000000
С	1.2334992	0.6939813	0.000000
С	-0.000000	1.3873165	-0.000000
С	-1.2334992	0.6939813	-0.000000
С	-2.4463464	1.4000856	0.000000
С	0.0000000	-1.4755684	0.000000

С	1.2492167	-0.7769188	0.000000
С	2.4922570	-1.4744389	0.000000
С	-1.2492167	-0.7769188	0.000000
С	-2.4922570	-1.4744389	0.000000
Η	7.0411722	-5.6834159	-0.000000
Η	7.3505634	5.6409551	0.000000
Н	5.0775625	6.7759221	0.000000
Н	2.5583394	6.8084177	0.000000
Н	-0.0000000	6.8441519	0.000000
Н	-2.5583394	6.8084177	0.000000
Н	-5.0775625	6.7759221	0.000000
Н	-7.0411722	-5.6834159	-0.0000000
Н	-7.3235644	-3.1944149	-0.0000000
Н	-7.0544309	-1.2630337	-0.0000000
Н	-7.3288185	1.1832839	-0.0000000
Н	-7.1115411	3.1223173	0.000000
Н	-7.3505633	5.6409551	0.000000
Н	7.1115411	3.1223173	0.000000
Н	7.3288185	1.1832839	-0.0000000
Н	7.0544309	-1.2630337	-0.0000000
Н	7.3235644	-3.1944149	-0.0000000
В	4.9419469	-5.8636232	-0.0000000
B	2.4619599	-5.7949748	0.000000
В	0.000000	-5.7599759	0.000000
В	-2.4619599	-5.7949748	0.000000
В	-4.9419469	-5.8636232	-0.0000000
В	6.2392266	-3.7354644	-0.0000000
В	3.7528180	-3.6529988	-0.000000
В	1.2510989	-3.5944636	0.000000
В	-1.2510989	-3.5944636	0.000000
В	-3.7528180	-3.6529988	0.000000
В	-6.2392266	-3.7354644	-0.0000000
Ν	6.1757094	-5.1563247	-0.0000000
Ν	5.0105120	-2.9775741	0.000000
Ν	3.7117078	-5.0995393	0.000000
Ν	2.5026831	-2.8735442	0.000000
Ν	1.2393078	-5.0381257	0.000000
Ν	-0.0000000	-2.8660202	0.000000
Ν	-1.2393078	-5.0381257	0.000000
Ν	-2.5026831	-2.8735442	0.000000
Ν	-3.7117078	-5.0995393	0.000000
Ν	-5.0105120	-2.9775741	0.000000
Ν	-6.1757094	-5.1563247	-0.0000000
Ν	5.0513356	5.7634390	-0.0000000
Ν	6.2346329	3.6266085	-0.0000000
Ν	3.7645779	3.6263679	-0.0000000

Ν	2.5324285	5.7950686	-0.0000000
Ν	1.2466293	3.6817031	-0.000000
Ν	-0.0000000	5.8305494	-0.0000000
Ν	-1.2466293	3.6817031	-0.0000000
Ν	-2.5324285	5.7950686	-0.0000000
Ν	-3.7645779	3.6263679	-0.0000000
N	-6.2346329	3.6266085	-0.0000000
N	-5.0513356	5.7634390	-0.0000000
B	6 2840965	5 0514913	-0 0000000
B	3 7796560	5 0782273	-0 0000000
B	5 0001/92	2 8793377	-0 0000000
B	1 2565379	5 1281023	-0.0000000
D	1.2J0JJ79	2.1201023	0.0000000
D	2.4775591	2.9311773	-0.0000000
В	-0.0000000	Z.9430279	0.0000000
В	-1.2363379	J.1281U23	-0.0000000
В	-2.4//5391	2.9311//3	-0.0000000
В	-3.//96560	5.0782273	0.0000000
В	-5.0001492	2.8/933//	0.0000000
В	-6.2840965	5.0514913	-0.0000000
В	6.2279185	0.6676311	-0.0000000
В	4.9829121	-1.5278874	-0.0000000
В	3.7364516	0.6784463	-0.0000000
В	-6.2279185	0.6676311	-0.0000000
В	-4.9829121	-1.5278874	-0.0000000
В	-3.7364516	0.6784463	-0.0000000
Ν	-5.0136891	1.3992752	-0.0000000
Ν	-3.6955668	-0.8256783	0.000000
Ν	-6.1741439	-0.7635225	-0.0000000
Ν	5.0136891	1.3992752	-0.0000000
Ν	6.1741439	-0.7635225	-0.0000000
Ν	3.6955668	-0.8256783	0.000000
BN-edges-	line,	wB97XD/def2	-SV(P)
H	4.7871573	-7.0181844	0.000000
Н	2.4128258	-6.9140816	0.000000
Н	0.000000	-6.9007249	-0.0000000
Н	-2.4128258	-6.9140816	0.000000
Н	-4.7871573	-7.0181844	-0.0000000
С	-3.6899081	3.5923083	0.000000
C	-2.4723684	2.9011235	0.000000
C	-1 2304418	3 5956748	0 0000000
C	1 2304418	3 5956748	
C	2 4723681	2 9011225	
C	3 6800081	2,5071233	
C	3 6070601	0 710/57C	_0_0000000
	3.09/2021	U./L040/0 1 /2E0EC2	-0.0000000
C	2.4003001	1.4339303	-0.0000000

С	1.2356260	0.7213912	-0.0000000
С	-0.0000000	1.4319666	-0.0000000
С	-1.2356260	0.7213912	-0.0000000
С	-2.4853661	1.4359563	0.000000
С	-3.6972621	0.7184576	0.000000
С	0.0000000	2.8966328	-0.0000000
C	3 6707930	-0 7172505	0 0000000
C		-1 4182626	-0 0000000
C	1 2241669	-0 7148495	-0 0000000
C	2 /670173	-1 /19/180	-0 0000000
C	-1 22/1669	-0 71/8/95	-0.0000000
C	-2 1670173	_1 /19/180	-0.0000000
C	-2.40/01/3	-1.4194100	-0.0000000
C	-3.0707930	-0.7172303	0.0000000
C	-3.0009422	-3.0110070	-0.0000000
	-2.4//40/8	-2.8844990	-0.0000000
C	-1.2298202	-3.5/39595	-0.0000000
C	0.0000000	-2.8/22154	-0.0000000
С	1.2298202	-3.5739595	0.0000000
С	2.4774078	-2.8844990	0.0000000
С	3.6869422	-3.6110676	-0.0000000
Η	6.9910661	-5.6669450	0.000000
Н	7.3341021	5.6002168	0.000000
Н	5.1098215	6.7769711	0.000000
Н	2.4991117	6.8706145	0.000000
Н	-0.0000000	6.8681089	0.000000
Н	-2.4991117	6.8706145	0.000000
Н	-5.1098215	6.7769711	0.000000
Н	-6.9910661	-5.6669450	-0.0000000
Н	-7.2122500	-3.1519096	-0.0000000
Н	-7.0955586	-1.2490941	-0.0000000
Н	-7.2367938	1.2045551	0.000000
Н	-7.1226298	3.1145382	0.000000
Н	-7.3341021	5.6002168	0.000000
Н	7.1226298	3.1145382	0.000000
Н	7.2367938	1.2045551	0.000000
Н	7.0955586	-1.2490941	-0.0000000
н	7 2122500	-3 1519096	-0 0000000
R	4 8875144	-5 8174221	0 0000000
B	6 1557083	-3 7275635	-0 0000000
B	A 9691799	-1 5053523	-0 0000000
D D	6 1721108	0 6313884	_0_0000000
D D	V. I / Z I I VO	0.0313004	-0.0000000
D D	4.7704708	2.0404004 5.0016540	0.0000000
D D	0.2000000	J.UZ10348 5 1202007	-0.0000000
Ъ	3./3/9880	J.12838U/	-0.0000000
В	1.2485140	5.14960/2	0.0000000
В	-1.2485140	5.1496072	0.0000000

В	-3.7379880	5.1283807	0.000000
В	-6.2580088	5.0216548	0.000000
В	-4.9904958	2.8464054	0.000000
В	-6.1721108	0.6313884	-0.0000000
В	-4.9691499	-1.5053523	-0.0000000
В	-6.1557083	-3.7275635	-0.0000000
В	-4.8875144	-5.8174221	0.000000
В	-2.4416065	-5.7134812	0.000000
В	-0.0000000	-5.6996819	0.000000
В	2.4416065	-5.7134812	0.000000
N	6.1236094	-5.1436004	0.000000
N	4.9085638	-2.9862560	-0.0000000
N	6.1922337	-0.7954127	-0.0000000
N	4.9428727	1.3605041	0.000000
N	6.2299153	3.5890957	0.000000
N	5.0441005	5.7653308	-0.0000000
N	2.5048978	5.8547072	-0.0000000
N	-0.0000000	5.8522060	0.000000
N	-2.5048978	5.8547072	0.000000
N	-5.0441005	5.7653308	0.000000
N	-6.2299153	3.5890957	0.000000
N	-4.9428727	1.3605041	0.000000
N	-6.1922337	-0.7954127	-0.0000000
N	-4.9085638	-2.9862560	-0.0000000
N	-3.6784228	-5.0043627	0.000000
N	-6.1236094	-5.1436004	-0.0000000
N	-1.2232534	-4.9640655	0.000000
N	1.2232534	-4.9640655	0.000000
Ν	3.6784228	-5.0043627	0.000000
BN-zz-B-t	op-line,	wB97XD/de	ef2-SV(P)
Н	-4.9103946	6.9507733	-0.0000000
Н	-2.4155474	6.9160417	-0.0000000
Н	0.0368956	6.9018724	-0.0000000
Н	2.4720479	6.9021166	-0.0000000
Н	4.8501061	6.9771591	-0.0000000
С	6.1283095	0.6987579	-0.0000000
С	6.1283081	-0.6987606	-0.0000000
С	4.9520219	-1.4334846	-0.0000000
С	-6.1043008	-0.6977744	-0.000000
С	-4.9249612	-1.4263384	-0.000000
С	-3.6809771	-0.7174261	0.000000
С	-2.4494900	-1.4269422	-0.0000000
С	-1.2231887	-0.7212107	0.000000
С	0.0171136	-1.4249063	-0.000000
С	1.2460540	-0.7220201	0.000000

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С	2.4824699	-1.4282814	-0.0000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	С	3.7073973	-0.7196553	0.000000
C -4.9249647 1.4263256 0.000000 C -6.1043029 0.6977639 -0.000000 C 0.0171187 1.4248957 0.0000000 C -1.2231859 0.7211957 -0.0000000 C -2.4494883 1.4269284 -0.0000000 C 1.2460577 0.7220092 0.0000000 C 2.4824743 1.4282755 0.0000000 C 3.7074000 0.7196492 0.0000000 C 4.9520240 1.4334816 0.0000000 H -7.0118767 5.4492381 -0.0000000 H -7.0118540 -5.4492287 0.0000000 H -4.9103913 -6.9507513 0.0000000 H -2.4155478 -6.9021084 0.0000000 H 2.4720465 -6.9021084 0.0000000 H 7.0974113 1.1985437 -0.0000000 H 7.0974113 1.985434 0.0000000 H 7.0656490 -3.1371151 -0.0000000 <	С	-3.6809761	0.7174102	-0.000000
C -6.1043029 0.6977639 -0.000000 C 0.0171187 1.4248957 0.000000 C -1.2231859 0.7211957 -0.000000 C -2.4494883 1.4269284 -0.000000 C 1.2460577 0.7220092 0.0000000 C 1.4482755 0.0000000 C 2.4824743 1.4282755 0.0000000 C 3.7074000 0.7196492 0.0000000 C 4.9520240 1.4334816 0.0000000 H -7.0118767 5.4492287 0.0000000 H -7.0118540 -5.4492287 0.0000000 H -7.018547 -6.9160201 0.0000000 H -2.4155478 -6.9160201 0.0000000 H 2.4720465 -6.9021084 0.0000000 H 7.0374113 1.1985437 -0.0000000 H 7.143309 3.0549819 0.0000000 H 7.0974113 1.1985437 -0.0000000 H <t< td=""><td>С</td><td>-4.9249647</td><td>1.4263256</td><td>0.000000</td></t<>	С	-4.9249647	1.4263256	0.000000
C 0.0171187 1.4248957 0.000000 C -1.2231859 0.7211957 -0.000000 C -2.4494883 1.4269284 -0.000000 C 1.2460577 0.7220092 0.0000000 C 2.4824743 1.4282755 0.0000000 C 3.7074000 0.7196492 0.0000000 C 3.7074000 0.7196492 0.0000000 H -7.0118540 -5.4492287 0.0000000 H -7.0118540 -5.4492287 0.0000000 H -7.0118547 -6.9160201 0.0000000 H -7.0118547 -6.9102084 0.0000000 H -2.4155478 -6.9021084 0.0000000 H 2.4720465 -6.9021084 0.0000000 H 7.0532145 -4653209 0.0000000 H 7.143309 3.0549834 -0.0000000 H 7.0974105 -1.1985437 -0.0000000 H 7.0556693 3.1371151 -0.0000000 <tr< td=""><td>С</td><td>-6.1043029</td><td>0.6977639</td><td>-0.0000000</td></tr<>	С	-6.1043029	0.6977639	-0.0000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	С	0.0171187	1.4248957	0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	С	-1.2231859	0.7211957	-0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	С	-2.4494883	1.4269284	-0.000000
C 2.4824743 1.4282755 0.000000 C 3.7074000 0.7196492 0.000000 C 4.9520240 1.4334816 0.0000000 H -7.0118767 5.4492381 -0.0000000 H -7.0118767 5.4492287 0.0000000 H -7.0118540 -5.4492287 0.0000000 H -2.4155478 -6.9160201 0.0000000 H -2.4155478 -6.9160201 0.0000000 H -2.4155478 -6.9018569 0.0000000 H 2.4720465 -6.9021084 0.0000000 H 2.4720465 -6.9021084 0.0000000 H 7.0532214 5.4653209 0.0000000 H 7.0974105 -1.1985448 0.0000000 H 7.0974105 -1.1985437 -0.0000000 H 7.0556490 -3.1371151 -0.0000000 H -7.0656693 3.1371044 -0.0000000 H -7.0656693 3.1371044 -0.0000000	С	1.2460577	0.7220092	0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	С	2.4824743	1.4282755	0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	С	3.7074000	0.7196492	0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	С	4.9520240	1.4334816	0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	-7.0118767	5.4492381	-0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	-7.0118540	-5.4492287	0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	-4.9103913	-6.9507513	0.000000
H0.0368940-6.90185690.000000H2.4720465-6.90210840.000000H4.8501049-6.9771557-0.0000000H7.25322145.46532090.0000000H7.09741131.1985437-0.0000000H7.0974105-1.19854480.0000000H7.2532186-5.4653206-0.0000000H7.2532186-5.4653206-0.0000000H7.0656490-3.1371151-0.0000000H-7.0717745-1.2034289-0.0000000H-7.06566933.1371044-0.0000000H-7.06566933.1371044-0.0000000B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B2.49489485.69882570.0000000B-2.4279851-5.71118030.0000000B-2.4279851-5.7716384-0.0000000B-2.494883-5.6988207-0.0000000B-2.4948883-5.6988207-0.0000000B-2.4948883-5.6988207-0.0000000B-2.4948883-5.6988207-0.0000000N-3.66912674.9991155-0.0000000N-3.66912674.9991155-0.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Н	-2.4155478	-6.9160201	0.000000
H2.4720465-6.90210840.000000H4.8501049-6.9771557-0.000000H7.25322145.46532090.000000H7.09741131.1985437-0.0000000H7.0974105-1.19854480.0000000H7.2532186-5.4653206-0.0000000H7.2532186-5.4653206-0.0000000H7.0656490-3.1371151-0.0000000H-7.0717745-1.2034299-0.0000000H-7.06566933.1371044-0.0000000H-7.06566933.1371044-0.0000000B-4.90268045.7448723-0.0000000B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B2.49489485.69882570.0000000B-2.4279851-5.71118030.0000000B-2.4279851-5.7716384-0.0000000B-2.494883-5.6988207-0.0000000B-2.4948883-5.6988207-0.0000000B-2.4279851-5.7716384-0.0000000N-3.66912674.9991155-0.0000000N-3.66912674.9769207-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Н	0.0368940	-6.9018569	0.000000
H4.8501049-6.9771557-0.000000H7.25322145.46532090.000000H7.09741131.1985437-0.000000H7.0974105-1.19854480.000000H7.1143280-3.0549834-0.0000000H7.2532186-5.4653206-0.0000000H-7.0656490-3.1371151-0.0000000H-7.0717745-1.2034299-0.0000000H-7.06566933.1371044-0.0000000H-7.06566933.1371044-0.0000000B-4.90268045.7448723-0.0000000B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B2.49489485.69882570.0000000B-2.4279851-5.71118030.0000000B-2.4279851-5.69772330.0000000B-2.4279851-5.018271-0.0000000B-2.494883-5.6988207-0.0000000B-3.66912674.9991155-0.0000000N-3.66912674.9769207-0.0000000N-3.66912674.96894720.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Н	2.4720465	-6.9021084	0.000000
H7.25322145.46532090.000000H7.01433093.05498190.000000H7.09741131.1985437-0.000000H7.0974105-1.19854480.000000H7.1143280-3.0549834-0.000000H7.2532186-5.4653206-0.000000H-7.0656490-3.1371151-0.0000000H-7.0717745-1.2034299-0.0000000H-7.06566933.1371044-0.0000000H-7.06566933.1371044-0.0000000B-4.90268045.7448723-0.0000000B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B2.49489485.69882570.0000000B-2.4279851-5.7118030.0000000B-2.4279851-5.69772330.0000000B2.4948883-5.6988207-0.0000000B2.4948883-5.6988207-0.0000000B2.4948883-5.6988207-0.0000000N-3.66912674.9991155-0.0000000N-3.66912674.96894720.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Н	4.8501049	-6.9771557	-0.000000
H7.11433093.05498190.000000H7.09741131.1985437-0.000000H7.0974105-1.19854480.000000H7.1143280-3.0549834-0.0000000H7.2532186-5.4653206-0.0000000H-7.0656490-3.1371151-0.0000000H-7.0717745-1.2034299-0.0000000H-7.07177791.2034289-0.0000000H-7.06566933.1371044-0.0000000B-4.90268045.7448723-0.0000000B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B2.49489485.69882570.0000000B-4.9026658-5.74485840.0000000B-2.4279851-5.71118030.0000000B-2.4279851-5.69772330.0000000B-2.4948883-5.6988207-0.0000000B-2.4948883-5.6988207-0.0000000B-2.4279851-5.7716384-0.0000000N-3.66912674.9991155-0.0000000N-3.66912674.9769207-0.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Н	7.2532214	5.4653209	0.000000
H7.09741131.1985437-0.000000H7.0974105-1.19854480.000000H7.1143280-3.0549834-0.000000H7.2532186-5.4653206-0.0000000H-7.0656490-3.1371151-0.0000000H-7.0717745-1.2034299-0.0000000H-7.06566933.1371044-0.0000000H-7.06566933.1371044-0.0000000B-4.90268045.7448723-0.0000000B-2.42798645.7111941-0.0000000B2.49489485.69882570.0000000B4.96303035.7716405-0.0000000B-2.4279851-5.71118030.0000000B-2.4279851-5.69772330.0000000B-2.4948883-5.6988207-0.0000000B2.4948883-5.6988207-0.0000000B-2.4219851-5.7716384-0.0000000B-2.4219851-5.018271-0.0000000N-3.66912674.99991155-0.0000000N-3.66912674.9769207-0.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Н	7.1143309	3.0549819	0.000000
H7.0974105-1.19854480.000000H7.1143280-3.0549834-0.000000H7.2532186-5.4653206-0.000000H-7.0656490-3.1371151-0.000000H-7.0717745-1.2034299-0.0000000H-7.07177791.2034289-0.0000000H-7.06566933.1371044-0.0000000B-4.90268045.7448723-0.0000000B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B4.96303035.7716405-0.0000000B-2.4279851-5.71118030.0000000B-2.4279851-5.7716384-0.0000000B2.4948883-5.6988207-0.0000000B2.4948883-5.6988207-0.0000000B2.4948883-5.6988207-0.0000000N-3.66912674.99991155-0.0000000N-3.66912674.9769207-0.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Н	7.0974113	1.1985437	-0.000000
H7.1143280-3.0549834-0.0000000H7.2532186-5.4653206-0.0000000H-7.0656490-3.1371151-0.0000000H-7.0717745-1.2034299-0.0000000H-7.06566933.1371044-0.0000000B-4.90268045.7448723-0.0000000B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B2.49489485.69882570.0000000B4.96303035.7716405-0.0000000B-2.4279851-5.71118030.0000000B-2.4279851-5.69772330.0000000B-2.4279851-5.6988207-0.0000000B-2.4279851-5.69772330.0000000B-2.4279851-5.0018271-0.0000000N-6.10456675.0018271-0.0000000N-1.20107364.9769207-0.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Н	7.0974105	-1.1985448	0.000000
H7.2532186-5.4653206-0.0000000H-7.0656490-3.1371151-0.0000000H-7.0717745-1.2034299-0.0000000H-7.06566933.1371044-0.0000000B-4.90268045.7448723-0.0000000B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B2.49489485.69882570.0000000B4.96303035.7716405-0.0000000B-2.4279851-5.71118030.0000000B-2.4279851-5.69772330.0000000B-2.4279851-5.6988207-0.0000000B2.4948883-5.6988207-0.0000000B2.4948883-5.69872330.0000000B1.26468884.96894720.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Η	7.1143280	-3.0549834	-0.0000000
H-7.0656490-3.1371151-0.000000H-7.0717745-1.2034299-0.0000000H-7.06566933.1371044-0.0000000B-4.90268045.7448723-0.0000000B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B2.49489485.69882570.0000000B4.96303035.7716405-0.0000000B-2.4279851-5.71118030.0000000B2.49489485.6988207-0.0000000B-2.4279851-5.7716384-0.0000000B-2.4948883-5.6988207-0.0000000B-2.4279851-5.7716384-0.0000000B-3.66912674.9991155-0.0000000N-3.66912674.9769207-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Н	7.2532186	-5.4653206	-0.000000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	-7.0656490	-3.1371151	-0.000000
H-7.07177791.2034289-0.0000000H-7.06566933.1371044-0.0000000B-4.90268045.7448723-0.0000000B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B2.49489485.69882570.0000000B4.96303035.7716405-0.0000000B-4.9026658-5.74485840.0000000B-2.4279851-5.71118030.0000000B0.0349162-5.69772330.0000000B2.4948883-5.6988207-0.0000000B4.9630256-5.7716384-0.0000000B4.9630256-5.7716384-0.0000000N-3.66912674.9991155-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Н	-7.0717745	-1.2034299	-0.000000
H-7.06566933.1371044-0.0000000B-4.90268045.7448723-0.0000000B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B2.49489485.69882570.0000000B4.96303035.7716405-0.0000000B-4.9026658-5.74485840.0000000B-2.4279851-5.71118030.0000000B0.0349162-5.69772330.0000000B2.4948883-5.6988207-0.0000000B2.4948883-5.6988207-0.0000000B2.4948883-5.6988207-0.0000000N-6.10456675.0018271-0.0000000N-3.66912674.9991155-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Н	-7.0717779	1.2034289	-0.000000
B-4.90268045.7448723-0.0000000B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B2.49489485.69882570.0000000B4.96303035.7716405-0.0000000B-4.9026658-5.74485840.0000000B-2.4279851-5.71118030.0000000B0.0349162-5.69772330.0000000B2.4948883-5.6988207-0.0000000B4.9630256-5.7716384-0.0000000B4.9630256-5.7716384-0.0000000N-6.10456675.0018271-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	Η	-7.0656693	3.1371044	-0.0000000
B-2.42798645.7111941-0.0000000B0.03492195.69773290.0000000B2.49489485.69882570.0000000B4.96303035.7716405-0.0000000B-4.9026658-5.74485840.0000000B-2.4279851-5.71118030.0000000B0.0349162-5.69772330.0000000B2.4948883-5.6988207-0.0000000B4.9630256-5.7716384-0.0000000N-6.10456675.0018271-0.0000000N-3.66912674.9991155-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	В	-4.9026804	5.7448723	-0.0000000
B0.03492195.69773290.0000000B2.49489485.69882570.0000000B4.96303035.7716405-0.0000000B-4.9026658-5.74485840.0000000B-2.4279851-5.71118030.0000000B0.0349162-5.69772330.0000000B2.4948883-5.6988207-0.0000000B4.9630256-5.7716384-0.0000000N-6.10456675.0018271-0.0000000N-3.66912674.9991155-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	В	-2.4279864	5.7111941	-0.000000
B2.49489485.69882570.0000000B4.96303035.7716405-0.0000000B-4.9026658-5.74485840.0000000B-2.4279851-5.71118030.0000000B0.0349162-5.69772330.0000000B2.4948883-5.6988207-0.0000000B4.9630256-5.7716384-0.0000000N-6.10456675.0018271-0.0000000N-3.66912674.9991155-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	В	0.0349219	5.6977329	0.000000
B4.96303035.7716405-0.0000000B-4.9026658-5.74485840.0000000B-2.4279851-5.71118030.0000000B0.0349162-5.69772330.0000000B2.4948883-5.6988207-0.0000000B4.9630256-5.7716384-0.0000000N-6.10456675.0018271-0.0000000N-3.66912674.9991155-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	В	2.4948948	5.6988257	0.000000
B-4.9026658-5.74485840.000000B-2.4279851-5.71118030.000000B0.0349162-5.69772330.0000000B2.4948883-5.6988207-0.0000000B4.9630256-5.7716384-0.0000000N-6.10456675.0018271-0.0000000N-3.66912674.9991155-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-6.1045499-5.00182110.0000000	В	4.9630303	5.7716405	-0.000000
B-2.4279851-5.71118030.000000B0.0349162-5.69772330.0000000B2.4948883-5.6988207-0.0000000B4.9630256-5.7716384-0.0000000N-6.10456675.0018271-0.0000000N-3.66912674.9991155-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-3.6691200-4.99910580.0000000	В	-4.9026658	-5.7448584	0.000000
B0.0349162-5.69772330.000000B2.4948883-5.6988207-0.000000B4.9630256-5.7716384-0.000000N-6.10456675.0018271-0.0000000N-3.66912674.9991155-0.0000000N-1.20107364.9769207-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-6.1045499-5.00182110.0000000	В	-2.4279851	-5.7111803	0.000000
B2.4948883-5.6988207-0.000000B4.9630256-5.7716384-0.0000000N-6.10456675.0018271-0.0000000N-3.66912674.99991155-0.0000000N-1.20107364.9769207-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-6.1045499-5.00182110.0000000	В	0.0349162	-5.6977233	0.000000
B4.9630256-5.7716384-0.0000000N-6.10456675.0018271-0.0000000N-3.66912674.9991155-0.0000000N-1.20107364.9769207-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-6.1045499-5.00182110.0000000	В	2.4948883	-5.6988207	-0.000000
N-6.10456675.0018271-0.0000000N-3.66912674.9991155-0.0000000N-1.20107364.9769207-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-6.1045499-5.00182110.0000000	В	4.9630256	-5.7716384	-0.000000
N-3.66912674.9991155-0.000000N-1.20107364.9769207-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-6.1045499-5.00182110.0000000	Ν	-6.1045667	5.0018271	-0.000000
N-1.20107364.9769207-0.0000000N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-6.1045499-5.00182110.0000000	Ν	-3.6691267	4.9991155	-0.000000
N1.26468884.96894720.0000000N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-6.1045499-5.00182110.0000000	Ν	-1.2010736	4.9769207	-0.0000000
N3.74044104.98646870.0000000N-3.6691200-4.99910580.0000000N-6.1045499-5.00182110.0000000	Ν	1.2646888	4.9689472	0.000000
N -3.6691200 -4.9991058 0.0000000 N -6.1045499 -5.0018211 0.0000000	Ν	3.7404410	4.9864687	0.000000
N -6.1045499 -5.0018211 0.000000	Ν	-3.6691200	-4.9991058	0.000000
	Ν	-6.1045499	-5.0018211	0.000000

Ν	-1.2010759	-4.9769146	0.000000
Ν	1.2646829	-4.9689443	-0.0000000
Ν	3.7404356	-4.9864678	-0.0000000
С	-6.0891681	3.6211762	-0.0000000
С	-4.9269118	2.8995912	-0.0000000
С	-3.6562470	3.5862619	-0.0000000
С	-2.4551384	2.8832116	-0.0000000
С	-1.1941760	3.5667957	-0.0000000
С	0.0112518	2.8701702	-0.0000000
С	1.2746255	3.5628752	0.000000
С	2.4781941	2.8784807	0.000000
С	3.7476681	3.5904737	0.000000
С	4.9524457	2.9004849	0.000000
С	6.2617188	4.9993172	-0.0000000
С	6.1871394	3.6347198	0.000000
С	-6.0891524	-3.6211793	0.000000
С	-4.9269048	-2.8995966	0.000000
С	-3.6562444	-3.5862625	0.000000
С	-2.4551405	-2.8832167	0.000000
С	-1.1941833	-3.5667972	0.000000
С	0.0112436	-2.8701753	0.000000
С	1.2746160	-3.5628761	-0.0000000
С	2.4781858	-2.8784837	-0.0000000
С	3.7476616	-3.5904739	-0.0000000
С	4.9524411	-2.9004872	-0.0000000
С	6.1871360	-3.6347208	-0.0000000
С	6.2617155	-4.9993181	-0.000000
BN-zz-N-t	op-line,	wB97XD/de	ef2-SV(P)
Н	5.0053940	6.8814756	-0.0000000
Н	2.4899685	6.8780695	-0.0000000
Н	0.0076530	6.8686492	-0.0000000
Н	-2.4867593	6.8675884	-0.0000000
Н	-5.1231563	6.7503923	-0.0000000
С	-6.0721874	0.6973981	0.000000
С	-6.0721928	-0.6973921	-0.0000000
С	-4.8907186	-1.4281646	0.000000
С	6.1605916	-0.6967710	0.000000
С	4.9834782	-1.4285283	0.000000
С	3.7427428	-0.7171760	0.000000
С	2.5120374	-1.4296517	-0.000000
С	1.2858585	-0.7221888	-0.000000
С	0.0491970	-1.4322984	-0.000000
С	-1.1792708	-0.7213262	0.000000
С	-2.4130728	-1.4253270	-0.000000
С	-3.6455247	-0.7175726	-0.000000

С	3.7427449	0.7171710	0.000000
С	4.9834721	1.4285301	-0.000000
С	6.1605975	0.6967764	0.000000
С	0.0491937	1.4322988	0.000000
С	1.2858569	0.7221858	0.000000
С	2.5120329	1.4296502	0.000000
C	-1.1792706	0.7213262	-0.0000000
C	-2.4130764	1,4253283	0.000000
C	-3 6455202	0 7175756	0 0000000
C	-4 8907209	1 4281657	-0 0000000
н	7 2783374	5 7874093	-0 0000000
н	7 2783499	-5 7874101	0 0000000
и Ц	5 005/090	-6 8814766	0.0000000
и П	2 1899723	-6 8780707	0.0000000
и П	0 0076486	-6 8686502	0.0000000
и П	-2 4867664	-6 9675992	0.0000000
п	-2.4007004 5 1001626	-0.0073002	0.0000000
л тт	-3.1231030	-0./JUJ0/1	0.0000000
П II	-7.0944409	3.3511943 2.1257070	-0.0000000
H	-7.0912368	3.1257078	-0.0000000
H	-7.0356912	1.2083837	0.0000000
H	-7.0356930	-1.2083765	-0.0000000
H	-7.0912468	-3.125/03/	0.0000000
H	-/.094458/	-5.5511934	0.0000000
Н	7.1207622	-3.069993/	0.0000000
Н	7.1243911	-1.2069171	-0.0000000
Н	7.1243897	1.2069314	0.0000000
H	7.1207556	3.0699868	-0.0000000
Ν	4.9954152	5.8665896	-0.0000000
Ν	-5.0062633	5.7431508	-0.0000000
Ν	-2.4876097	5.8525344	0.000000
Ν	0.0053646	5.8531596	0.000000
Ν	2.4938750	5.8625247	0.000000
Ν	4.9954269	-5.8665906	-0.0000000
Ν	2.4938816	-5.8625260	-0.0000000
Ν	0.0053658	-5.8531606	-0.0000000
Ν	-2.4876132	-5.8525356	-0.0000000
Ν	-5.0062673	-5.7431582	0.000000
В	6.2301010	5.1673531	-0.0000000
В	3.7391487	5.1671092	-0.0000000
В	1.2522105	5.1572353	-0.0000000
В	-1.2375225	5.1526955	-0.000000
В	-3.7100326	5.1184747	-0.000000
В	6.2301101	-5.1673547	-0.0000000
В	3.7391578	-5.1671140	-0.0000000
В	1.2522152	-5.1572386	-0.0000000
В	-1.2375219	-5.1526964	0.000000

$ \begin{array}{cccccc} -6.1496684 & 4.9992909 & 0.000000 \\ c & -6.1296330 & 3.6373608 & 0.000000 \\ c & -3.6860004 & 3.5804627 & -0.000000 \\ c & -2.4151961 & 2.8728360 & 0.000000 \\ c & -1.2175804 & 3.5843253 & 0.000000 \\ c & 0.0473482 & 2.8802408 & 0.000000 \\ c & 1.2594978 & 3.5883843 & 0.000000 \\ c & 2.5172212 & 2.8874429 & 0.000000 \\ c & 3.7281131 & 3.5991591 & 0.000000 \\ c & 4.9979570 & 2.9053347 & -0.000000 \\ c & 6.1772185 & 3.6232245 & 0.000000 \\ c & 6.1772185 & 3.6232245 & 0.000000 \\ c & 6.1772185 & 3.6232247 & -0.000000 \\ c & 4.9979678 & -2.9053347 & -0.000000 \\ c & 3.7281200 & -3.5991612 & -0.000000 \\ c & 3.7281200 & -3.5991612 & -0.000000 \\ c & 1.2595013 & -3.5883851 & -0.000000 \\ c & 1.2595013 & -3.5843250 & -0.000000 \\ c & -2.4151969 & -2.8728361 & -0.000000 \\ c & -2.4151969 & -2.8728361 & -0.000000 \\ c & -3.6860009 & -3.5804644 & 0.000000 \\ c & -4.8926350 & -2.8959658 & 0.000000 \\ c & -6.1296360 & -3.6373710 & -0.000000 \\ c & -6.1296360 & -3.6373710 & -0.000000 \\ c & -6.1496750 & -4.9992762 & -0.000000 \\ c & -2.4619528 & 5.7167553 & -0.000000 \\ H & -2.4183951 & -6.7926508 & 0.000000 \\ H & -2.4619528 & 5.7167553 & -0.000000 \\ c & -3.6686493 & 3.5982390 & -0.000000 \\ c & -3.6686493 & 3.5982390 & -0.000000 \\ c & -1.2217960 & 3.5813767 & 0.000000 \\ c & -1.2217970 & 5.0184219 & 0.000000 \\ c & 2.4619528 & 5.7167553 & 0.000000 \\ c & -1.2217970 & 5.0184219 & 0.000000 \\ c & -1.2217970 & 5.0184219 & 0.000000 \\ c & -2.4619528 & 5.7167553 & 0.000000 \\ c & -1.2217970 & 5.0184219 & 0.000000 \\ c & -2.4619528 & 5.7167553 & 0.0000000 \\ c & -2.4619528$	В	-3.7100369	-5.1184718	0.000000
C -6.1296330 3.6373608 0.000000 C -4.8926308 2.8959738 -0.000000 C -3.6860004 3.5804627 -0.0000000 C -2.4151961 2.8728360 0.000000 C 0.0473482 2.8802408 0.0000000 C 1.2594978 3.5883843 0.0000000 C 2.5172212 2.8874429 0.0000000 C 3.7281131 3.5991591 0.0000000 C 4.9979570 2.9053347 -0.0000000 C 6.1772185 3.6232245 0.0000000 C 4.9979678 -2.9053437 -0.0000000 C 4.9979678 -2.9053437 -0.0000000 C 3.7281200 -3.5991612 -0.0000000 C 1.2595013 -3.5883851 -0.0000000 C 0.0473538 -2.8802435 -0.0000000 C -1.2175801 -3.5843250 -0.0000000 C -3.6860009 -3.5804644 0.0000000 C -3.6860099 -3.5804644 0.0000000 C -4.8926350 -2.8959658 0.0000000 C -6.1296360 -3.6373710 -0.0000000 C -6.1296360 -3.6373710 -0.0000000 C -4.8926350 -2.8959658 0.0000000 C -4.8926350 -2.8959658 0.0000000 C -4.8926350 -2.8959658 0.0000000 C -4.8926350 -2.8959658 0.0000000 C -6.1296360 -3.6373710 -0.0000000 C -6.1296360 -3.6373710 -0.0000000 C -6.1296360 -3.6373710 -0.0000000 C -2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 C -2.4619528 5.7167553 -0.0000000 C -3.668493 3.5982390 -0.0000000 C -1.2217970 5.0184219 0.0000000 C -1.2217970 5.0184219 0.0000000 C -1.2217970 5.0184219 0.0000000 C 1.2217970 5.0184219 0.0000000 C 1.2217970 5.0184219 0.0000000	С	-6.1496684	4.9992909	0.000000
C -4.8926308 2.8959738 -0.000000 C -3.686004 3.5804627 -0.000000 C -2.4151961 2.8728360 0.000000 C -1.2175804 3.5843253 0.000000 C 0.0473482 2.8802408 0.000000 C 1.2594978 3.5883843 0.000000 C 2.5172212 2.8874429 0.000000 C 3.7281131 3.5991591 0.000000 C 4.9979570 2.9053347 -0.000000 C 6.1772185 3.6232245 0.000000 C 6.1772185 3.6232247 -0.000000 C 3.7281200 -3.5991612 -0.000000 C 3.7281200 -3.5991612 -0.000000 C 1.2595013 -3.5883851 -0.000000 C 1.2595013 -3.5883851 -0.000000 C -1.2175801 -3.5843250 -0.000000 C -1.2175801 -3.5843250 -0.000000 C -3.6860099 -3.5804644 0.000000 C -3.6860099 -3.5804644 0.000000 C -4.8926350 -2.8959658 0.000000 C -6.1296360 -3.6373710 -0.000000 C -6.1296360 -3.6373710 -0.000000 C -6.1496750 -4.9992762 -0.000000 H 2.4183951 -6.7926508 0.000000 H -2.4183951 -6.7926508 0.000000 H -2.4183951 -6.7926508 0.000000 C -3.6686493 3.5982390 -0.000000 C -3.668493 3.5982390 -0.000000 C -3.668493 3.5982390 -0.000000 C -1.2217970 5.0184219 0.000000 C -1.2217970 5.0184219 0.000000 C 1.2217970 5.0184219 0.000000	С	-6.1296330	3.6373608	0.000000
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	-4.8926308	2.8959738	-0.000000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С	-3.6860004	3.5804627	-0.000000
$ \begin{array}{cccccc} -1.2175804 & 3.5843253 & 0.0000000 \\ C & 0.0473482 & 2.8802408 & 0.0000000 \\ C & 1.2594978 & 3.5883843 & 0.0000000 \\ C & 2.5172212 & 2.8874429 & 0.0000000 \\ C & 3.7281131 & 3.5991591 & 0.0000000 \\ C & 4.9979570 & 2.9053347 & -0.0000000 \\ C & 6.1772185 & 3.6232245 & 0.0000000 \\ C & 6.1772185 & 3.6232247 & -0.0000000 \\ C & 4.9979678 & -2.9053437 & -0.0000000 \\ C & 3.7281200 & -3.5991612 & -0.0000000 \\ C & 2.5172295 & -2.8874497 & -0.0000000 \\ C & 1.2595013 & -3.5883851 & -0.0000000 \\ C & 0.0473538 & -2.8802435 & -0.0000000 \\ C & -1.2175801 & -3.5843250 & -0.0000000 \\ C & -2.4151969 & -2.8728361 & -0.0000000 \\ C & -3.6860009 & -3.5804644 & 0.0000000 \\ C & -4.8926350 & -2.8959658 & 0.0000000 \\ C & -6.1296360 & -3.6373710 & -0.0000000 \\ C & -6.1296360 & -3.6373710 & -0.0000000 \\ C & -6.1496750 & -4.9992762 & -0.0000000 \\ H & 2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4619528 & 5.7167553 & -0.0000000 \\ C & -3.6686493 & 3.5982390 & -0.0000000 \\ C & -1.2217060 & 3.5813767 & 0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & 2.4619528 & 5.7167553 & 0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217960 & 3.5813767 & 0.0000000 \\ C & 1.2217970 & 5.0184219 & 0.00$	С	-2.4151961	2.8728360	0.000000
C 0.0473482 2.8802408 0.000000 C 1.2594978 3.5883843 0.000000 C 2.5172212 2.8874429 0.0000000 C 3.7281131 3.5991591 0.0000000 C 4.9979570 2.9053347 -0.0000000 C 6.1772185 3.6232245 0.0000000 C 6.177232 -3.6232247 -0.0000000 C 4.9979678 -2.9053437 -0.0000000 C 3.7281200 -3.5991612 -0.0000000 C 2.5172295 -2.8874497 -0.0000000 C 1.2595013 -3.5883851 -0.0000000 C 0.0473538 -2.8802435 -0.0000000 C -1.2175801 -3.5843250 -0.0000000 C -2.4151969 -2.8728361 -0.0000000 C -3.6860009 -3.5804644 0.0000000 C -4.8926350 -2.8959658 0.0000000 C -6.1296360 -3.6373710 -0.0000000 C -6.1496750 -4.9992762 -0.0000000 H 2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 C -3.6547308 5.0302693 -0.0000000 C -3.6547308 5.0302693 -0.0000000 C -3.6547308 5.0302693 -0.0000000 C -1.2217960 3.5813767 0.0000000 C -1.2217970 5.0184219 0.0000000 C -1.2217970 5.0184219 0.0000000 C -1.2217970 5.0184219 0.0000000	С	-1.2175804	3.5843253	0.000000
C 1.2594978 3.5883843 0.0000000 C 2.5172212 2.8874429 0.0000000 C 3.7281131 3.5991591 0.0000000 C 4.9979570 2.9053347 -0.0000000 C 6.1772185 3.6232245 0.0000000 C 6.1772232 -3.6232247 -0.0000000 C 4.9979678 -2.9053437 -0.0000000 C 4.9979678 -2.9053437 -0.0000000 C 2.5172295 -2.8874497 -0.0000000 C 1.2595013 -3.5883851 -0.0000000 C 0.0473538 -2.8802435 -0.0000000 C -1.2175801 -3.5843250 -0.0000000 C -2.4151969 -2.8728361 -0.0000000 C -3.6860009 -3.5804644 0.0000000 C -4.8926350 -2.8959658 0.0000000 C -6.1296360 -3.6373710 -0.0000000 C -6.1496750 -4.9992762 -0.0000000 H 2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 C -3.6547308 5.0302693 -0.0000000 C -3.6547308 5.0302693 -0.0000000 C -1.2217970 5.0184219 0.0000000 C -1.2217970 5.0184219 0.0000000	С	0.0473482	2.8802408	0.000000
C 2.5172212 2.8874429 0.000000 C 3.7281131 3.5991591 0.0000000 C 4.9979570 2.9053347 -0.0000000 C 6.1772185 3.6232245 0.0000000 C 6.1772232 -3.6232247 -0.0000000 C 4.9979678 -2.9053437 -0.0000000 C 2.5172295 -2.8874497 -0.0000000 C 1.2595013 -3.5991612 -0.0000000 C 0.0473538 -2.802435 -0.0000000 C -1.2175801 -3.5843250 -0.0000000 C -2.4151969 -2.8728361 -0.0000000 C -3.6860009 -3.5804644 0.0000000 C -4.8926350 -2.8959658 0.0000000 C -6.1296360 -3.6373710 -0.0000000 C -6.1296360 -3.6373710 -0.0000000 C -6.1496750 -4.9992762 -0.0000000 H 2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 H -2.4619528 5.7167553 -0.0000000 C -3.6686493 3.5982390 -0.0000000 C -3.6686493 3.5982390 -0.0000000 C -1.2217060 3.5813767 0.0000000 C -1.2217970 5.0184219 0.0000000 C -1.2217970 5.0184219 0.0000000 C -1.2217970 5.0184219 0.0000000	С	1.2594978	3.5883843	0.000000
$ \begin{array}{cccccc} C & 3.7281131 & 3.5991591 & 0.000000 \\ C & 4.9979570 & 2.9053347 & -0.000000 \\ C & 6.1772185 & 3.6232245 & 0.0000000 \\ C & 4.9979678 & -2.9053437 & -0.0000000 \\ C & 4.9979678 & -2.9053437 & -0.0000000 \\ C & 3.7281200 & -3.5991612 & -0.0000000 \\ C & 2.5172295 & -2.8874497 & -0.0000000 \\ C & 1.2595013 & -3.5883851 & -0.0000000 \\ C & 0.0473538 & -2.8802435 & -0.0000000 \\ C & -1.2175801 & -3.5843250 & -0.0000000 \\ C & -2.4151969 & -2.8728361 & -0.0000000 \\ C & -3.6860009 & -3.5804644 & 0.0000000 \\ C & -3.6860009 & -3.5804644 & 0.0000000 \\ C & -4.8926350 & -2.8959658 & 0.0000000 \\ C & -6.1296360 & -3.6373710 & -0.0000000 \\ C & -6.1496750 & -4.9992762 & -0.0000000 \\ H & 2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4619528 & 5.7167553 & -0.0000000 \\ C & -3.6686493 & 3.5982390 & -0.0000000 \\ C & -3.6686493 & 3.5982390 & -0.0000000 \\ C & -1.2217060 & 3.5813767 & 0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217970 & 5.0184219 & 0.0000000 \\ C & 2.4619528 & 5.7167553 & -0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217970 & 5.0184219 & 0.0000000 \\ \end{array}$	С	2.5172212	2.8874429	0.000000
$\begin{array}{cccccc} C & 4.9979570 & 2.9053347 & -0.0000000 \\ C & 6.1772185 & 3.6232245 & 0.0000000 \\ C & 4.9979678 & -2.9053437 & -0.0000000 \\ C & 3.7281200 & -3.5991612 & -0.0000000 \\ C & 2.5172295 & -2.8874497 & -0.0000000 \\ C & 1.2595013 & -3.5883851 & -0.0000000 \\ C & 0.0473538 & -2.8802435 & -0.0000000 \\ C & -1.2175801 & -3.5843250 & -0.0000000 \\ C & -2.4151969 & -2.8728361 & -0.0000000 \\ C & -3.6860009 & -3.5804644 & 0.0000000 \\ C & -4.8926350 & -2.8959658 & 0.0000000 \\ C & -6.1296360 & -3.6373710 & -0.0000000 \\ C & -6.1296360 & -3.6373710 & -0.0000000 \\ C & -6.1496750 & -4.9992762 & -0.0000000 \\ C & -6.1496750 & -4.9992762 & -0.0000000 \\ H & 2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4619528 & 5.7167553 & -0.0000000 \\ C & -3.6547308 & 5.0302693 & -0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & 2.4619528 & 5.7167553 & 0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217970 & 5.0184219 & 0.000000000 \\ C & 1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217970 & 5.0184219 & 0.00000000 \\ C & 1.2217970 & 5.0184219 & 0.00000000 \\ C & 1.2217970 & 5.0184219 $	С	3.7281131	3.5991591	0.000000
$ \begin{array}{ccccc} & 6.1772185 & 3.6232245 & 0.000000 \\ C & 6.1772232 & -3.6232247 & -0.0000000 \\ C & 4.9979678 & -2.9053437 & -0.0000000 \\ C & 3.7281200 & -3.5991612 & -0.0000000 \\ C & 2.5172295 & -2.8874497 & -0.0000000 \\ C & 1.2595013 & -3.5883851 & -0.0000000 \\ C & 0.0473538 & -2.8802435 & -0.0000000 \\ C & -1.2175801 & -3.5843250 & -0.0000000 \\ C & -2.4151969 & -2.8728361 & -0.0000000 \\ C & -3.6860009 & -3.5804644 & 0.0000000 \\ C & -4.8926350 & -2.8959658 & 0.0000000 \\ C & -6.1296360 & -3.6373710 & -0.0000000 \\ C & -6.1296360 & -3.6373710 & -0.0000000 \\ C & -6.1496750 & -4.9992762 & -0.0000000 \\ \end{array} $	С	4.9979570	2.9053347	-0.000000
C 6.1772232 -3.6232247 -0.0000000 C 4.9979678 -2.9053437 -0.0000000 C 3.7281200 -3.5991612 -0.0000000 C 2.5172295 -2.8874497 -0.0000000 C 1.2595013 -3.5883851 -0.0000000 C 0.0473538 -2.8802435 -0.0000000 C -1.2175801 -3.5843250 -0.0000000 C -2.4151969 -2.8728361 -0.0000000 C -3.6860009 -3.5804644 0.0000000 C -4.8926350 -2.8959658 0.0000000 C -6.1296360 -3.6373710 -0.0000000 C -6.1496750 -4.9992762 -0.0000000 H 2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 C -3.6547308 5.0302693 -0.0000000 C -3.6547308 5.0302693 -0.0000000 C -1.2217970 5.0184219 0.0000000 C 2.4619528 5.7167553 0.0000000 C -1.2217970 5.0184219 0.0000000 C -1.2217970 5.0184219 0.0000000 C 2.4619528 5.7167553 0.0000000 C -1.2217970 5.0184219	С	6.1772185	3.6232245	0.000000
$ \begin{array}{cccccc} C & 4.9979678 & -2.9053437 & -0.000000 \\ C & 3.7281200 & -3.5991612 & -0.0000000 \\ C & 2.5172295 & -2.8874497 & -0.0000000 \\ C & 1.2595013 & -3.5883851 & -0.0000000 \\ C & 0.0473538 & -2.8802435 & -0.0000000 \\ C & -1.2175801 & -3.5843250 & -0.0000000 \\ C & -2.4151969 & -2.8728361 & -0.0000000 \\ C & -3.6860009 & -3.5804644 & 0.0000000 \\ C & -4.8926350 & -2.8959658 & 0.0000000 \\ C & -6.1296360 & -3.6373710 & -0.0000000 \\ C & -6.1496750 & -4.9992762 & -0.0000000 \\ C & -6.1496750 & -4.9992762 & -0.0000000 \\ H & 2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4183951 & -6.7926508 & 0.0000000 \\ H & -4.9501247 & -7.0944891 & 0.0000000 \\ C & -3.6547308 & 5.0302693 & -0.0000000 \\ C & -3.6686493 & 3.5982390 & -0.0000000 \\ C & -1.2217960 & 3.5813767 & 0.0000000 \\ C & 0.000000 & 5.6998658 & 0.0000000 \\ C & 3.6547308 & 5.0302693 & -0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & 2.4619528 & 5.7167553 & 0.0000000 \\ C & 0.000000 & 5.6998658 & 0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217960 & 3.5813767 & 0.0000000 \\ \end{array}$	С	6.1772232	-3.6232247	-0.000000
C $3.7281200 -3.5991612 -0.0000000$ C $2.5172295 -2.8874497 -0.0000000$ C $1.2595013 -3.5883851 -0.0000000$ C $0.0473538 -2.8802435 -0.0000000$ C $-1.2175801 -3.5843250 -0.0000000$ C $-2.4151969 -2.8728361 -0.0000000$ C $-3.6860009 -3.5804644 0.0000000$ C $-4.8926350 -2.8959658 0.0000000$ C $-6.1296360 -3.6373710 -0.0000000$ C $-6.1496750 -4.9992762 -0.0000000$ H $2.4183951 -6.7926508 0.0000000$ H $-0.0000000 -6.7768626 -0.0000000$ H $-2.4183951 -6.7926508 0.0000000$ H $-2.4183951 -6.7926508 0.0000000$ H $-2.4183951 -6.7926508 0.0000000$ H $-2.4183951 -6.7926508 0.0000000$ C $-3.6547308 5.0302693 -0.0000000$ C $-3.6686493 3.5982390 -0.0000000$ C $-1.2217060 3.5813767 0.0000000$ C $-1.2217970 5.0184219 0.0000000$ C $2.4619528 5.7167553 -0.0000000$ C $-1.2217970 5.0184219 0.0000000$ C $-1.2217970 5.0184219 0.0000000$ C $1.2217970 5.0184219 0.0000000$	С	4.9979678	-2.9053437	-0.000000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С	3.7281200	-3.5991612	-0.000000
$\begin{array}{cccccc} C & 1.2595013 & -3.5883851 & -0.0000000 \\ C & 0.0473538 & -2.8802435 & -0.0000000 \\ C & -1.2175801 & -3.5843250 & -0.0000000 \\ C & -2.4151969 & -2.8728361 & -0.0000000 \\ C & -3.6860009 & -3.5804644 & 0.0000000 \\ C & -4.8926350 & -2.8959658 & 0.0000000 \\ C & -6.1296360 & -3.6373710 & -0.0000000 \\ C & -6.1496750 & -4.9992762 & -0.0000000 \\ C & -6.1496750 & -4.9992762 & -0.0000000 \\ H & 2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4183951 & -6.7926508 & 0.0000000 \\ H & -2.4619528 & 5.7167553 & -0.0000000 \\ C & -3.6547308 & 5.0302693 & -0.0000000 \\ C & -3.6686493 & 3.5982390 & -0.0000000 \\ C & -1.2217060 & 3.5813767 & 0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & 3.6547308 & 5.0302693 & -0.0000000 \\ C & -1.2217970 & 5.0184219 & 0.0000000 \\ C & 1.2217970 & 5.0184219 & 0.0000000 \\ \end{array}$	С	2.5172295	-2.8874497	-0.000000
$\begin{array}{ccccccc} C & 0.0473538 & -2.8802435 & -0.0000000\\ C & -1.2175801 & -3.5843250 & -0.0000000\\ C & -2.4151969 & -2.8728361 & -0.0000000\\ C & -3.6860009 & -3.5804644 & 0.0000000\\ C & -4.8926350 & -2.8959658 & 0.00000000\\ C & -6.1296360 & -3.6373710 & -0.0000000\\ C & -6.1496750 & -4.9992762 & -0.0000000\\ C & -6.1496750 & -4.9992762 & -0.0000000\\ H & 2.4183951 & -6.7926508 & 0.0000000\\ H & -0.0000000 & -6.7768626 & -0.0000000\\ H & -2.4183951 & -6.7926508 & 0.0000000\\ H & -2.4183951 & -6.7926508 & 0.0000000\\ H & -2.4183951 & -6.7926508 & 0.0000000\\ C & -2.4619528 & 5.7167553 & -0.0000000\\ C & -3.6547308 & 5.0302693 & -0.0000000\\ C & -3.6686493 & 3.5982390 & -0.0000000\\ C & -1.2217060 & 3.5813767 & 0.0000000\\ C & -1.2217970 & 5.0184219 & 0.0000000\\ C & 3.6547308 & 5.0302693 & -0.0000000\\ C & -1.2217970 & 5.0184219 & 0.0000000\\ C & 1.2217970 & 5.0184219 & 0.000000\\ C & 1.2217970 & 5.0184219 & 0.000000\\ C & 1.2217970 & 5.0184219 & 0.000000\\ \end{array}$	С	1.2595013	-3.5883851	-0.000000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С	0.0473538	-2.8802435	-0.000000
C -2.4151969 -2.8728361 -0.000000 C -3.6860009 -3.5804644 0.0000000 C -4.8926350 -2.8959658 0.0000000 C -6.1296360 -3.6373710 -0.0000000 C -6.1496750 -4.9992762 -0.0000000 H 4.9501247 -7.0944891 0.0000000 H 2.4183951 -6.7926508 0.0000000 H -0.0000000 -6.7768626 -0.0000000 H -2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 C -2.4619528 5.7167553 -0.0000000 C -3.6686493 3.5982390 -0.0000000 C -1.2217060 3.5813767 0.0000000 C -1.2217970 5.0184219 0.000000 C 3.6547308 5.0302693 -0.0000000 C -1.2217970 5.0184219 0.000000 C -1.2217970 5.0184219 0.000000 C 1.2217970 5.0184219 0.000000 C 1.2217970 5.0184219 0.000000 C 1.2217970 5.0184219 0.000000 C 1.2217970 5.0184219 0.0000000 C 1.2217060 3.5813767 0.0000000 C 1.2217060 3.5813767 0.0000000 C 1.2217060 3.5813767 0.0000000 C 1.2217970 5.0184219 0.0000000 C 1.2217970 5.0184219 0.0000000 C 1.2217970 5.0184219 0.000000000000000 C 1.2217970 5.0184219 0.0000000000	С	-1.2175801	-3.5843250	-0.000000
C -3.6860009 -3.5804644 0.000000 C -4.8926350 -2.8959658 0.0000000 C -6.1296360 -3.6373710 -0.0000000 C -6.1496750 -4.9992762 -0.0000000 BN-ac-line, wB97XD/def2-SV(P) H 4.9501247 -7.0944891 0.0000000 H 2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 H -2.4183951 -6.7926508 0.0000000 C -2.4619528 5.7167553 -0.0000000 C -3.6547308 5.0302693 -0.0000000 C -3.6686493 3.5982390 -0.0000000 C -1.2217960 3.5813767 0.0000000 C -1.2217970 5.0184219 0.0000000 C 2.4619528 5.7167553 -0.0000000 C -1.2217970 5.0184219 0.0000000 C -2.4619528 5.7167553 0.0000000 C -1.2217970 5.0184219 0.0000000 C 1.2217970 5.0184219 0.0000000 C 1.2217960 3.5813767 0.0000000 C 1.2217960 3.5813767 0.0000000 C 1.2217970 5.0184219 0.0000000 C 1.2217960 3.5813767 0.0000000 C 1.2217970 5.0184219 0.0000000 C 1.2217960 3.5813767 0.0000000 C 1.2217970 5.0184219 0.0000000 C 1.2217970 5.0184219 0.0000000 C 1.2217970 5.0184219 0.000000000000 C 1.2217970 5.0184219 0.000000000000	С	-2.4151969	-2.8728361	-0.000000
C -4.8926350 -2.8959658 0.000000 C -6.1296360 -3.6373710 -0.0000000 C -6.1496750 -4.9992762 -0.0000000 BN-ac-line, wB97XD/def2-SV(P) H 4.9501247 -7.0944891 0.0000000 H 2.4183951 -6.7926508 0.0000000 H -0.0000000 -6.7768626 -0.0000000 H -2.4183951 -6.7926508 0.0000000 H -4.9501247 -7.0944891 0.0000000 C -2.4619528 5.7167553 -0.0000000 C -3.6547308 5.0302693 -0.0000000 C -3.6686493 3.5982390 -0.0000000 C -1.2217060 3.5813767 0.0000000 C -1.2217970 5.0184219 0.0000000 C 2.4619528 5.7167553 -0.0000000 C -1.2217970 5.0184219 0.0000000 C 2.4619528 5.7167553 0.0000000 C 1.2217970 5.0184219 0.0000000 C 1.2217960 3.5813767 0.0000000	С	-3.6860009	-3.5804644	0.000000
C -6.1296360 -3.6373710 -0.000000 C -6.1496750 -4.9992762 -0.0000000 BN-ac-line, wB97XD/def2-SV(P) H 4.9501247 -7.0944891 0.0000000 H 2.4183951 -6.7926508 0.0000000 H -0.0000000 -6.7768626 -0.0000000 H -2.4183951 -6.7926508 0.0000000 H -4.9501247 -7.0944891 0.0000000 C -2.4619528 5.7167553 -0.0000000 C -3.6547308 5.0302693 -0.0000000 C -3.6686493 3.5982390 -0.0000000 C -1.2217060 3.5813767 0.0000000 C -1.2217970 5.0184219 0.0000000 C 3.6547308 5.0302693 -0.0000000 C 1.2217970 5.0184219 0.0000000 C 1.2217970 5.0184219 0.0000000	С	-4.8926350	-2.8959658	0.000000
C -6.1496750 -4.9992762 -0.0000000 BN-ac-line, wB97XD/def2-SV(P) H 4.9501247 -7.0944891 0.0000000 H 2.4183951 -6.7926508 0.0000000 H -0.0000000 -6.7768626 -0.0000000 H -2.4183951 -6.7926508 0.0000000 H -4.9501247 -7.0944891 0.0000000 C -2.4619528 5.7167553 -0.0000000 C -3.6547308 5.0302693 -0.0000000 C -3.6686493 3.5982390 -0.0000000 C -1.2217060 3.5813767 0.0000000 C -1.2217970 5.0184219 0.0000000 C 3.6547308 5.0302693 -0.0000000 C -1.2217970 5.0184219 0.0000000 C 2.4619528 5.7167553 0.0000000 C 1.2217970 5.0184219 0.0000000	С	-6.1296360	-3.6373710	-0.000000
BN-ac-line, wB97XD/def2-SV(P) H 4.9501247 -7.0944891 0.0000000 H 2.4183951 -6.7926508 0.0000000 H -0.0000000 -6.7768626 -0.0000000 H -2.4183951 -6.7926508 0.0000000 H -4.9501247 -7.0944891 0.0000000 C -2.4619528 5.7167553 -0.0000000 C -3.6547308 5.0302693 -0.0000000 C -3.6686493 3.5982390 -0.0000000 C -1.2217060 3.5813767 0.0000000 C -1.2217970 5.0184219 0.0000000 C 3.6547308 5.0302693 -0.0000000 C 3.6547308 5.0302693 -0.0000000 C 1.2217970 5.0184219 0.0000000 C 2.4619528 5.7167553 0.0000000 C 1.2217970 5.0184219 0.0000000	С	-6.1496750	-4.9992762	-0.000000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	BN-ac-lin	e, wł	397XD/def2-SV	(P)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	4.9501247	-7.0944891	0.000000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	2.4183951	-6.7926508	0.000000
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Н	-0.0000000	-6.7768626	-0.000000
H-4.9501247-7.09448910.0000000C-2.46195285.7167553-0.0000000C-3.65473085.0302693-0.0000000C-3.66864933.5982390-0.0000000C-2.46709562.88702900.0000000C-1.22170603.58137670.0000000C-1.22179705.01842190.0000000C3.65473085.0302693-0.0000000C2.46195285.71675530.0000000C1.22179705.01842190.0000000C3.58137670.0000000	Н	-2.4183951	-6.7926508	0.000000
C-2.46195285.7167553-0.000000C-3.65473085.0302693-0.0000000C-3.66864933.5982390-0.0000000C-2.46709562.88702900.0000000C-1.22170603.58137670.0000000C-1.22179705.01842190.0000000C0.00000005.69986580.0000000C3.65473085.0302693-0.0000000C2.46195285.71675530.0000000C1.22179705.01842190.0000000C1.22179603.58137670.0000000	Н	-4.9501247	-7.0944891	0.000000
C-3.65473085.0302693-0.000000C-3.66864933.5982390-0.0000000C-2.46709562.88702900.0000000C-1.22170603.58137670.0000000C-1.22179705.01842190.0000000C0.00000005.69986580.0000000C3.65473085.0302693-0.0000000C2.46195285.71675530.0000000C1.22179705.01842190.0000000C1.22179603.58137670.0000000	С	-2.4619528	5.7167553	-0.000000
C-3.66864933.5982390-0.0000000C-2.46709562.88702900.0000000C-1.22170603.58137670.0000000C-1.22179705.01842190.0000000C0.00000005.69986580.0000000C3.65473085.0302693-0.0000000C2.46195285.71675530.0000000C1.22179705.01842190.0000000C1.22179603.58137670.0000000	С	-3.6547308	5.0302693	-0.000000
C-2.46709562.88702900.0000000C-1.22170603.58137670.0000000C-1.22179705.01842190.0000000C0.00000005.69986580.0000000C3.65473085.0302693-0.0000000C2.46195285.71675530.0000000C1.22179705.01842190.0000000C1.22179603.58137670.0000000	С	-3.6686493	3.5982390	-0.000000
C-1.22170603.58137670.0000000C-1.22179705.01842190.0000000C0.00000005.69986580.0000000C3.65473085.0302693-0.0000000C2.46195285.71675530.0000000C1.22179705.01842190.0000000C1.22170603.58137670.0000000	С	-2.4670956	2.8870290	0.000000
C-1.22179705.01842190.0000000C0.00000005.69986580.0000000C3.65473085.0302693-0.0000000C2.46195285.71675530.0000000C1.22179705.01842190.0000000C1.22170603.58137670.0000000	С	-1.2217060	3.5813767	0.000000
C0.0000005.69986580.000000C3.65473085.0302693-0.0000000C2.46195285.71675530.0000000C1.22179705.01842190.0000000C1.22170603.58137670.0000000	С	-1.2217970	5.0184219	0.000000
C3.65473085.0302693-0.000000C2.46195285.71675530.0000000C1.22179705.01842190.0000000C1.22170603.58137670.0000000	С	0.000000	5.6998658	0.000000
C2.46195285.71675530.000000C1.22179705.01842190.0000000C1.22170603.58137670.0000000	С	3.6547308	5.0302693	-0.000000
C 1.2217970 5.0184219 0.0000000 C 1.2217060 3.5813767 0.0000000	С	2.4619528	5.7167553	0.000000
C 1.2217060 3.5813767 0.0000000	C	1.2217970	5.0184219	0.000000
	C	1.2217060	3.5813767	0.000000
C 2.4670956 2.8870290 0.000000	C	2.4670956	2.8870290	0.000000
C 3.6686493 3.5982390 -0.0000000	Ċ	3.6686493	3.5982390	-0.000000
C 3.6974321 0.7186730 0.0000000	C	3.6974321	0.7186730	0.000000

С	2.4820691	1.4348464	0.000000
С	1.2363977	0.7207616	0.000000
С	0.000000	1.4251321	0.000000
С	-1.2363977	0.7207616	0.000000
С	-2.4820691	1.4348464	0.000000
С	-3.6974321	0.7186730	0.000000
C	-0.0000000	2.8711053	0.000000
C	3 6803924	-0 7109107	-0 0000000
C		-1 4139835	0 0000000
C	1 2279080	-0 7097289	-0 0000000
C	2 1715161	-1 /136/89	-0 0000000
C	-1 2279080	-0 7097289	0.0000000
C	1.2279000	1 1126100	0.0000000
C	-2.4/10104	-1.4130409	0.0000000
C	-3.6603924	-0.7109107	-0.0000000
	-3.6828034	-3.608/154	-0.0000000
C	-2.481/292	-2.8686357	-0.0000000
C	-1.2301133	-3.5649131	-0.0000000
С	0.0000000	-2.85/4230	-0.0000000
С	1.2301133	-3.5649131	-0.0000000
С	2.481/292	-2.8686357	-0.0000000
С	3.6828034	-3.6087154	0.000000
С	3.6560475	-5.0492563	0.000000
С	2.4442551	-5.6980118	0.000000
С	1.2137803	-4.9963827	-0.0000000
С	-0.000000	-5.6822501	-0.000000
С	-1.2137803	-4.9963827	-0.000000
С	-2.4442551	-5.6980119	0.000000
С	-3.6560475	-5.0492563	0.000000
Η	7.0643637	-5.6240824	0.000000
Н	7.1594783	5.7137346	-0.000000
Η	4.8279437	6.6968012	-0.000000
Η	2.4470987	6.8113935	-0.000000
Н	-0.0000000	6.7943280	0.000000
Н	-2.4470987	6.8113935	-0.0000000
Н	-4.8279437	6.6968012	-0.0000000
H	-7.0643637	-5.6240824	0.000000
н	-7 2206578	-3 1385223	0 0000000
н	-7 1023159	-1 2314665	0 0000000
н	-7 2332392	1 2384668	-0 0000000
н	-7 1037740	3 1633537	-0 0000000
и П	-7 159/783	5 7137346	-0 0000000
ц П	1.1J94/0J 7 10277/0	J. 1 L J / J 4 U J 1 L J 7 L J 7	
п u	7 000000	J. 1 030/660	-0.0000000
л тт	1.2332372 7 1000150	1 0011665	-0.0000000
п	7.1023139	-1.2314003	0.0000000
Н	1.22065/8	-3.1385223	0.0000000
В	4.958/488	-5.8804345	0.0000000

Ν	6.1705464	-5.1454746	0.000000
В	6.1631845	-3.7241671	0.000000
В	4.9807962	-1.5105787	-0.000000
В	6.1799185	0.6426534	-0.000000
В	4.9872562	2.8419200	-0.000000
В	6.1501255	5.0393332	-0.000000
Ν	4.9259233	-2.9706681	-0.000000
Ν	6.2022699	-0.7690341	-0.000000
Ν	4.9354603	1.3785564	-0.000000
Ν	6.1977298	3.6136816	-0.0000000
Ν	4.8826480	5.6860049	-0.0000000
В	-4.9587488	-5.8804345	0.000000
В	-6.1631845	-3.7241671	-0.000000
В	-4.9807962	-1.5105787	-0.000000
В	-6.1799185	0.6426534	-0.000000
В	-4.9872562	2.8419200	-0.000000
В	-6.1501255	5.0393332	-0.000000
Ν	-4.8826480	5.6860049	-0.000000
Ν	-6.1977298	3.6136816	-0.000000
Ν	-4.9354603	1.3785564	0.000000
Ν	-6.2022699	-0.7690341	-0.000000
Ν	-4.9259233	-2.9706681	-0.0000000
Ν	-6.1705464	-5.1454746	0.000000

BN-vertical, wB97XD/def2-SV(P)

	•		
Η	-4.8735713	6.8499324	0.000000
Η	-2.4416012	6.7954756	-0.000000
Н	-0.0000000	7.0160369	-0.000000
Н	2.4416012	6.7954756	-0.000000
Η	4.8735713	6.8499323	0.000000
С	6.0945531	5.0880924	0.000000
С	6.1336227	3.6651862	0.000000
С	6.1530840	0.7002440	-0.000000
С	6.1675989	-0.6991994	-0.000000
С	5.0023407	-1.4505749	-0.000000
С	4.9989394	-2.9199108	-0.000000
С	6.1847437	-3.6339902	-0.000000
С	6.2022342	-5.0531510	0.000000
С	5.0363168	-5.7578221	0.000000
С	2.5778969	-5.7960565	0.000000
С	3.7608529	-5.0882018	-0.000000
С	3.7383222	-3.6337841	-0.000000
С	2.5195443	-2.9208696	-0.000000
С	-5.0363164	-5.7578224	0.000000
С	-3.7608531	-5.0882017	-0.0000000

С	-2.5778969	-5.7960565	0.000000
С	-2.5195443	-2.9208696	-0.000000
С	-3.7383220	-3.6337841	-0.000000
С	-4.9989397	-2.9199108	-0.000000
С	-6.1847434	-3.6339902	-0.0000000
С	-6.1675991	-0.6991994	-0.0000000
C	-5.0023404	-1.4505749	-0.000000
C	-3 7466982	-0 7582684	-0 0000000
C	-2 5426705	-1 4792127	-0 0000000
C	2 5426706	-1 4792126	-0 0000000
C	3 7/66980	-0.7582681	-0 0000000
C	-6 2022348	-5 0531508	-0 0000000
C	0.2022540 2 7244251	0 6000222	0.0000000
C	-J./2442JI	1 4227021	0.0000000
C	-4.9701197	1.4237931	0.0000000
	-0.1000000	0.7002440	0.0000000
C	-2.503/490	1.4047666	-0.0000000
C	2.503/490	1.404/666	0.0000000
С	3.7244253	0.6909222	-0.0000000
С	4.9701194	1.4237931	-0.0000000
С	4.9833416	2.8960256	0.0000000
С	3.7153829	3.5715503	0.000000
С	2.5268970	2.8436104	0.000000
С	-2.5268968	2.8436104	0.000000
С	-3.7153832	3.5715503	-0.0000000
С	-4.9833413	2.8960255	-0.000000
С	-6.1336231	3.6651862	0.000000
С	-6.0945526	5.0880926	0.000000
С	-4.9036807	5.7561207	0.000000
С	-3.6680373	5.0246555	0.000000
С	-2.4597637	5.7011860	0.000000
С	2.4597636	5.7011861	-0.000000
С	3.6680376	5.0246554	0.000000
С	4.9036803	5.7561210	0.000000
Н	-7.0370390	5.6430451	0.000000
Н	-7.1648213	-5.5750970	0.000000
Н	-5.0394073	-6.8522152	0.000000
H	-2 6404460	-6 8918721	0 0000000
н	0 0000000	-6 7129204	0 0000000
н	2 6404460	-6 8918721	0 0000000
и Ц	5 039/073	-6 8522153	0.0000000
ц П	7 0370380	5 6430451	0.0000000
п u	7 11/7521	J.04304JL 3 1950000	0.0000000
л II	7 1147001	3.1000000	0.0000000
п тт	/.140441 7 1401500	1.1042001	-0.0000000
н	/.14U1382	-1.1943991	-0.0000000
H	/.1434012	-3.1132200	-0.0000000
Н	/.1648214	-5.5/50971	0.0000000

-7.1434012	-3.1132199	-0.000000
-7.1401582	-1.1943991	0.000000
-7.1140441	1.2178724	0.000000
-7.1147531	3.1859001	0.000000
0.000000	5.8052383	0.000000
1.2368201	3.6079735	0.000000
-1.2368201	3.6079734	0.000000
-0.0000000	1.4744323	-0.0000000
1.2510549	-0.7121205	-0.000000
-1.2510549	-0.7121205	-0.000000
-0.0000000	-2.8514096	-0.000000
1.2661725	-5.0522051	0.000000
-1.2661725	-5.0522051	0.000000
-1.2454960	5.0688458	-0.0000000
1.2454960	5.0688458	0.000000
-0.0000000	2.9051748	-0.0000000
1.2760786	0.7486829	-0.000000
-1.2760786	0.7486829	-0.000000
0.000000	-1.4117355	-0.000000
1.2858523	-3.5785808	-0.000000
-0.0000000	-5.7001446	0.000000
-1.2858523	-3.5785808	-0.0000000
	-7.1434012 -7.1401582 -7.1140441 -7.1147531 0.0000000 1.2368201 -1.2368201 -0.0000000 1.2510549 -1.2510549 -0.0000000 1.2661725 -1.2661725 -1.2454960 1.2454960 1.2454960 -0.0000000 1.2760786 -1.2760786 0.0000000 1.2858523 -0.0000000 -1.2858523	-7.1434012 -3.1132199 -7.1401582 -1.1943991 -7.1140441 1.2178724 -7.1147531 3.1859001 0.000000 5.8052383 1.2368201 3.6079735 -1.2368201 3.6079734 -0.0000000 1.4744323 1.2510549 -0.7121205 -1.2510549 -0.7121205 -0.0000000 -2.8514096 1.2661725 -5.0522051 -1.2454960 5.0688458 1.2454960 5.0688458 1.2760786 0.7486829 -1.2760786 0.7486829 0.000000 -1.4117355 1.2858523 -3.5785808 -0.000000 -5.7001446 -1.2858523 -3.5785808