Supporting Information

A coordinatively unsaturated iridium complex with an unsymmetrical redox-active ligand: (Spectro)electrochemical and reactivity studies

Sebastian Sobottka, Margarethe van der Meer, Estelle Glais, Uta Albold, Simon Suhr, Cheng-Yong Su, Biprajit Sarkar

Table of Contents

1		NMR Spectroscopy3				
2		X-ray Crystallography1				
3		Hyd	lrogenation of <i>p</i> -benzoquinone	13		
4		Cycl	lic Voltammetry	17		
5		CV S	Simulation for 1	19		
6		CV S	Simulation for 2	21		
7		EPR	-Spectroelectrochemistry	23		
8		Inte	rconversion of 2 ⁺ to 3 ⁺	24		
	8.2	L	Mass spectrum of 2 ⁺ and Fluoroform	25		
	8.2	2	Mass spectrometry of 2 ⁺ and Chloroform	26		
	8.3	3	Mass spectrometry of 2 ⁺ and Bromoform	27		
	8.4	1	Mass spectrometry of 2 ⁺ and lodoform	28		
9		IR-s	pectroelectrochemistry	29		
	9.1	L	Spectra for 1 and 1 ²⁺ (experimental and calculated)	31		
	9.2	2	IR spectra of 2+	33		
1	9.2 0	2 U	IR spectra of 2+	33		
1	9.2 0 10	2 U	IR spectra of 2+ IV-Vis-NIR-Spectroelectrochemistry Spectra for [2] ⁺	33 38 39		
1	9.2 0 10 10	2 U .1 .2	IR spectra of 2+ IV-Vis-NIR-Spectroelectrochemistry Spectra for [2] ⁺ Spectra for [3] ⁺	33 38 39 42		
1	9.2 0 10 10	2 .1 .2 (T	IR spectra of 2+ IV-Vis-NIR-Spectroelectrochemistry Spectra for [2] ⁺ Spectra for [3] ⁺ ID)DFT	33 38 39 42 43		
1	9.2 0 10 10 1 1	2 .1 .2 .1 .7	IR spectra of 2+ IV-Vis-NIR-Spectroelectrochemistry Spectra for [2] ⁺ Spectra for [3] ⁺ ID)DFT General remarks	33 38 39 42 43 43		
1	9.2 0 10 10 1 1 11	2 .1 .2 .1 .1 .2	IR spectra of 2+ IV-Vis-NIR-Spectroelectrochemistry Spectra for [2] ⁺ Spectra for [3] ⁺ ID)DFT General remarks DFT Calculation for [1] (singlet state)	33 38 42 43 43 43		
1	9.2 0 10 10 1 1 11 11	2 .1 .2 .1 .1 .2 .3	IR spectra of 2+ IV-Vis-NIR-Spectroelectrochemistry Spectra for [2] ⁺ Spectra for [3] ⁺ ID)DFT General remarks DFT Calculation for [1] (singlet state) DFT Calculation [1] ⁺ (doublet state)	33 38 39 42 43 43 44 45		
1	9.2 0 10 10 1 1 11 11 11	2 U .1 .2 (1 .1 .2 .3 .4	IR spectra of 2+ IV-Vis-NIR-Spectroelectrochemistry Spectra for [2] ⁺ Spectra for [3] ⁺ ID)DFT. General remarks DFT Calculation for [1] (singlet state) DFT Calculation [1] ⁺ (doublet state) DFT Calculation [1] ²⁺ (singlet state)	33 38 42 43 43 44 45 50		
1	9.2 0 10 10 11 11 11 11 11	2 U .1 .2 (1 .2 .3 .4 .5	IR spectra of 2+ IV-Vis-NIR-Spectroelectrochemistry Spectra for [2] ⁺ Spectra for [3] ⁺ TD)DFT General remarks DFT Calculation for [1] (singlet state) DFT Calculation [1] ⁺ (doublet state) DFT Calculation [1] ²⁺ (singlet state) DFT Calculation [1] ²⁺ (singlet state)	33 38 39 42 43 43 44 45 50 55		
1	9.2 0 10 10 1 1 11 11 11 11 11	2 U .1 .2 (1 .2 .3 .4 .5 .6	IR spectra of 2+ IV-Vis-NIR-Spectroelectrochemistry Spectra for [2] ⁺ Spectra for [3] ⁺ ID)DFT General remarks DFT Calculation for [1] (singlet state) DFT Calculation for [1] (doublet state) DFT Calculation [1] ⁺ (doublet state) DFT Calculation [1] ²⁺ (singlet state) DFT Calculation for [2] ⁺ (singlet state) DFT Calculation for [2] ⁺ (singlet state)	33 39 42 43 43 44 45 50 55 59		
1	9.3 0 10 10 1 11 11 11 11 11	2 U .1 .2 (1 .2 .3 .4 .5 .6 .7	IR spectra of 2+ IV-Vis-NIR-Spectroelectrochemistry Spectra for [2] ⁺ Spectra for [3] ⁺ TD)DFT General remarks DFT Calculation for [1] (singlet state) DFT Calculation [1] ⁺ (doublet state) DFT Calculation [1] ²⁺ (singlet state) DFT Calculation for [2] ⁺ (singlet state) DFT Calculation for [2] ⁺ (doublet state) DFT Calculation for [2] ⁰ (doublet state) DFT Calculation for [2] ² (doublet state)	33 39 42 43 43 44 45 50 55 59 59 63		
1	9.2 0 10 1 1 11 11 11 11 11 11	2 .1 .2 .1 .2 .3 .4 .5 .6 .7 .8	IR spectra of 2+	33 39 42 43 43 43 45 50 50 55 59 63 67		

1 NMR Spectroscopy



Figure S2:¹H-NMR of 1 in CD_2CI_2 .



Figure S3: ¹³C-NMR of 1 in CD₂Cl₂.



Figure S4: ¹H NMR spectrum of $\car{[2]}BF_4$ in CD_2Cl_2 measured at 283 K.



Figure S5: VT-NMR of [2]BF₄ in CD₂Cl₂.



Figure S6: ¹H-NMR of [3]PF₆ in CD₂Cl₂.



-40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300 -320 -340 -360 -380 -400 -420 -440 -460 -480 -500 -520 Figure S8: ¹⁹F-NMR of [2]BF₄ in CD₂Cl₂ in the presence of Fluoroform, immediately after saturation.



Figure S9: ¹⁹F-NMR of [2]BF₄ in CD_2Cl_2 in the presence of Fluoroform, after three weeks, storage at RT.



2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 Figure S10: ¹H-NMR of 1 in CD₂Cl₂ under an dihydrogen atmosphere as stability test. Red trace: 0 days and blue trace after 5 days. Zoom on the next page.



2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 Figure S11: Zoom in of the ¹H-NMR of 1 in CD_2CI_2 under an dihydrogen atmosphere as stability test. Red trace: 0 days and blue trace after 5 days.



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5Figure S12: Zoom in of the ¹H-NMR of 1 in CD₂Cl₂ under an dihydrogen atmosphere as stability test. Red trace: 0 days and blue trace after 5 days.



Figure S13: ¹H-NMR of 2⁺ in CD₂Cl₂ under an dihydrogen atmosphere as stability test. Blue trace: 0 days and red trace after 3 days. Zoom on the next page.



8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 Figure S14: Zoom-in 1 H-NMR of 2⁺ in CD₂Cl₂ under an dihydrogen atmosphere as stability test. Blue trace: 0 days and red trace after 3 days. Zoom on the next page.



trace after 3 days. Zoom on the next page.

2 X-ray Crystallography



Figure S16: ORTEP representation of [1]. Hydrogen atoms are omitted for clarity.



Figure S17: ORTEP representation of [2]BF₄. Anions and hydrogen atoms are omitted for clarity.



Figure S18: ORTEP representation of [3]OTf. Anions and hydrogen atoms are omitted for clarity.

Table S1 Crystanographic details for [1], [2]BF ₄ and [5]OTT						
	[1]	[2]BF ₄	[3]OTf			
Chemical formula	C ₂₂ H ₂₅ Ir N ₂	$C_{23} H_{27} B F_4 Ir N_2$	$C_{23} H_{25} CI F_3 Ir N_2 O_3 S$			
M _r	509.64	610.47	694.16			
Crystal system	Monoclinic	triclinic	monoclinic			
Space group	P21/c	P-1	P2 ₁ /c			
a (Å)	10.4919(3)	9.8859(17)	14.743(8)			
b (Å)	11.4836(4)	10.6665(19)	11.872(5)			
<i>c</i> (Å)	15.7162(6)	11.563(2)	28.358(15)			
α (°)	90	86.062(4)	90			
в (°)	90.245	72.464(4)	96.077(15)			
γ (°)	90	89.848(4)	90			
V (ų)	1893.55(11)	1159.7(4)	4936(4)			
Ζ	4	2	8			
D _{calc} (g/cm ³)	1.788	1.748	1.868			
Temperature (K)	100	140	100			
μ (mm⁻¹)	7.057	5.800	5.654			
Crystal size (mm)	0.21 x 0.07 x 0.03	0.25 x 0.15 x 0.14	0.35 x 0.16 x 0.14			
Κα	0.71073 (Mo)	0.71073 (Mo)	0.71073 (Mo)			
F(000)	992	594	2704			
meas./ indep. refl.	19851/ 4911	12766/ 4100	67206/ 10057			
obsvd. [/ > 2σ(/)] refl.	4235	3260	8348			
R _{int}	0.0376	0.0290	0.0390			
$R[F^2 > 2\sigma(F^2)]$	0.0229	0.0443	0.0218			
wR (<i>F</i> ²)	0.0432	0.1137	0.0399			
S	1.053	1.102	1.052			
$\Delta \rho_{max}$, $\Delta \rho_{min}$ (e Å ⁻³)	1.371, -1.394	1.439, -1.256	1.116, -0.737			

Table S1	Crystallogra	phic details	for [1].	[2]BF ₄	and [3]OTf
	Joundary	phile accuits	101 1119		

3 Hydrogenation of *p*-benzoquinone

To monitor the reaction of $[1]^+$ with dihydrogen by ¹H NMR, dry THF-d₈ was saturated with H₂ by the freeze and pump method. **1** (9.5 mg, 19 µmol, 1eq) was dissolved in THF-d₈ (0.5 mL). A ¹H NMR spectrum was measured (Figure SS14). FcBArF (19.5 mg, 19 µmol, 1 eq) was added and after 30 min a second ¹H NMR spectrum was recorded. Although no hydride signal was detected, the formation of a new complex was observed (Figure SS15). *p*-Benzoquinone (2 mg, 19 µmol, 1 eq) was added three times. After every addition a ¹H NMR spectrum was recorded (Figure SS16). The formation of 1,4-hydroxy benzene was observed.



Figure S20: ¹H NMR of **1** after the addition of 1 eq of FcBArF. Signals at 4.11, 7.58 and 7.79 ppm correspond to ferrocene and BArF⁻, signals at 1.70, 6.44, 6.75, 7.18, 7.21 7.30 and 7.51 ppm correspond to the formed iridium complex.

4.5

7.25

4.0

3.5

3.0

2.5

15.00-

1.5

2.0

6.75 6.44

1.88 0.88

6.5

6.0

5.5

5.0

1.19

7.0

7.5

8.0



Figure S21:¹H NMR after the addition of 1 eq (1,2) and 2 eq (3, 4) and 3 eq (5, 6) of *p*-benzoquinone. Full conversion to 1,4 dihydroxy benzene was observed.

The solvent (THF) was saturated with dihydrogen before by the freeze and pump method. The reaction was carried out under H₂-atmosphere. **1** (4.0 mg, 7.9 μ mol, 5 mol%) was dissolved in THF (2 mL) and FcBArF (8.2 mg, 7.9 μ mol, 5 mol%) was added. After the addition of *p*-benzoquinone (17 mg, 0.16 mmol, 1 eq) the reaction mixture was stirred for 20 h at room temperature. The solvent was remove *in vacuum*, the residue was dissolved in CDCl₃ and filtrated of cotton, to remove the residue of the complex. 42 % conversion from *p*-benzoquinone to 1,4-dihydroxy benzene was reached. The conversion was calculated from the NMR integrals.



Figure S22: To confirm that [1] is necessary for the hydration of p-benzoquinone, the reaction was repeated in the absence of [1]. No dihydroxy benzene was detected by 1 H NMR.

4 Cyclic Voltammetry

	$E_{1/2}$ (1 st Red)	$E_{1/2}(2^{nd}Ox)$	E _{1/2} (2 nd Red)
[1]		-0.07 ^[c]	
[2]+	-1.04 ^[d]		-1.98 ^[d]
[3]+	0.64	-0.15	

Table S1: Redoxpotentials ($E_{1/2}$) vs Fc/Fc⁺ measured in CH₂Cl₂ at 100 mVs⁻¹ with 0.1 M Bu₄NPF₆ at room temperature.

^[a]Measured with a gold electrode. ^[b]Potential of the peak current. [c]Two electron process as determined by Baranski method.[d] First process one electron process, second two electron process as determined by differential pulse voltammety.



Figure S23: Cyclic voltammogram of **1**. Conditions: THF, glassy carbon working electrode, 0.1 M Bu₄NPF₆, room temperature 1and scan rate 100 mVs⁻¹.



Figure S24: Cyclic voltammograms of $[2]^+$ measured with different working electrodes (gold, platinum, glassy carbon) in $CH_2Cl_2/0.1 \text{ M Bu}_4\text{NPF}_6$. Different peak currents arise from differences in the surface area of the electrode.



Figure S25: Differential PulseVoltammogram of $[2]^+$ measured with a gold working electrode in $CH_2Cl_2/0.1$ M Bu_4NPF_6 . The numbers show the normalized areas and correspond to the transferred electrons in the process.



Figure S26: Cyclic voltammogram of 3^+ . Conditions: DCM, glassy carbon working electrode, 0.1 M Bu₄NPF₆, room temperature and scan rate 100 mVs⁻¹.



Figure S27: Cyclic voltammograms of $[3]^+$ measured with different working electrodes (gold, platinum, glassy carbon) in $CH_2Cl_2/0.1$ M Bu₄NPF6. Different peak currents arise from differences in the surface area of the electrode.

5 CV Simulation for 1



Figure S28. Scan rate dependent CVs of 1 (1.3 mM) and $CoCp_2 PF_6$ (1.4 mM) in 0.1 $NBu_4 PF_6$ / DCM.



Figure S29. Comparison of the experimental CV at 100 mV/s and the CV simulation for two consectutive one-electron transfers.



Figure S30. Comparison of the experimental CV at 100 mV/s and the CV simulation for a concerted two-electron transfer.



Figure S32. Plot of the anodic and cathodic peak currents over the square root of the scan rate. The slope yieled the diffusion coefficient for the iridium complex 1 and 1^{2+} respectively.



Figure S31. Comparison of the experimental CV at 100 mV/s and the CV simulation for a one-electron transfer.



Figure S33. Plot of the anodic and cathodic peak currents over the square root of the scan rate. The slope yieled the diffusion coefficient for $CoCp_2^+$ and $CoCp_2$ respectively.

The peak for the oxidation of 1 splits into two close lying waves during the re-reduction in the CV at high scan rates (e.g. 5 V/s) indicating two one-electron steps (see Fig. S28).

The diffusion coefficients have been determined by literature known procedures [A] and yielded the values, which have been used for the CV simulation. It has to be noted that these are only approximations, since the measurements have been conducted in dichloromethane and and evaporation of the solvent certainly had a detrimental effect on the accuracy of the measurement (room temperature>30°C). However the values are in agreement with the expected values (see figures S32+S33).

For comparative purposes three mechanisms have been simulated, one for two succesive but very close one-electron oxidations of complex 1, a one-electron oxidation of complex 1 and a concerted two-electron oxidation of 1. It can clearly be seen, that the process matches best with two succesive one-electron oxidations.

The cyclic voltammogram of **1** was simulated in three segments from -0.30 V to 0.15 V, from 0.15 V to -1.92 V and from -1.92 V to 0.15 V with the software DigiElch Professional [B] by using the Butler-Volmer equation. The surface area of the working electrode was set to 0.07 cm² and the starting concentration of **1** was set to 1.3 mM and of $CoCp_2PF_6$ to 1.4 mM. The charge transfer coefficients α were left at their initial value of 0.5 and the heterogeneous rate constants k_s were calculated from the peak-to-peak separation[C] and consequently set to 0.005 cm/s . The diffusion coefficients were set to values of 8x10^-6 cm² s⁻¹ for **1** and 1x10^-5 cm² s⁻¹ for CoCp₂PF₆. The simulated charge-transfer reactions are described by the following equations for the mechanisms (1)-(3), the E⁰ values for 1 was set to -0.07 V and for CoCp₂PF₆ to -1.33 V. The electrochemical reactions are denoted with (E).

Mechanism	Reaction
(1) Sim. 1e ⁻ 1e ⁻	$1^+ + e^- \rightleftharpoons 1^0$ (E)
	$1^{2+} + e^- \rightleftharpoons 1^+$ (E)
	$CoCp_2^+ \rightleftarrows CoCp_2$ (E)
(2) Sim. 2e ⁻	$1^{2+} + 2 e^- \rightleftharpoons 1^0 (E)$
	$CoCp_2^+ \rightleftarrows CoCp_2$ (E)
(3) Sim. 1e ⁻	$1^+ + e^- \rightleftharpoons 1^0$ (E)
	$CoCp_2^+ \rightleftarrows CoCp_2$ (E)

A N. Elgrishi, K. J. Rountree, B. D. McCarthy, E. S. Rountree, T. T. Eisenhart, J. L. Dempsey, *J. Chem. Educ.* **2018**, *95,* 197–206.

B DigiElch Professional Version 7.FD 2006, ElchSoft GbR, Kleinromstedt, Germany. C (a) R. S. Nicholson, I. Shain, *Anal. Chem.*, **1965**, *37*, 1351. (b) A. S. N. Murthy, K. S. Reddy, *Electrochim. Acta*, **1983**, *28*, 1677.



Figure S34: Comparison of experiment and simulation with two consecutive one electron transfer steps (=1e1e) and no chemical reactions.



Figure S35: Comparison of experiment and simulation for two consecutive electron transfers, of which the first one is a one electron transfer and the second one is a true two electron transfer (=1e2e).



Figure S36: Comparison of experiment and simulation with three one electron transfer steps, of which the two have the same redox potential (=1e1e1e). Rate constant for heterogeneous charge transfer was set to $k_s = 0.02$ cm/s.



Figure S38: Comparison of all the various simulations.



Figure S37: Comparison of experiment and simulation with three one electron transfer steps, of which the two have the same redox potential (=1e1e1e). Rate constant for heterogeneous charge transfer was set to $k_s = 0.002$ cm/s.



Figure S39: Comparison of experiment and simulation for two consecutive electron transfers, of which the first one is a one electron transfer and the second one is a true two electron transfer and two coupled chemical reaction as shown below (=1e2eRxn).

In order to gain a deeper understanding for the redox processes the the cyclic voltammogram of [2]⁺ was simulated in two segments from -0.20 V to -2.5 V and from -2.5 V to -0.20 V with the software DigiElch Professional [A] by using the Butler-Volmer equation. The surface area of the working electrode was set to 0.07 cm² and the starting concentration of [2]⁺ was set to 0.21 mM. The charge transfer coefficients α were left at their initial value of 0.5 and the heterogeneous rate constants k_s were calculated from the peak-to-peak separation[B] (1st red.: 0.001 cm/s and 2nd red.: 0.015) and used as starting values. The shown simulations are above used a k_s of 0.02 cm/s or 0.02 cm/s, where is is indicated. The diffusion coefficients were left at their initial values of 1x10^-5 cm² s⁻¹. The simulated charge-transfer reactions are described by the following equations for the mechanisms (1)-(4), the E⁰ values for [2]⁺ was set the values shown below. The electrochemical reactions are denoted with (E) and the coupled chemical reactions with (C), which are characterized by the equilibrium constant K_{eq}, and the rate constants for the forward and back reaction k_f and k_b. The asterisk denotes a rearrangement:

Mechanism	Reaction
(1) 1e1e	$[2]^{+} + e^{-} \rightleftharpoons [2]^{0}$ (E) $E_{1/2} = -1.04 \text{ V}$
	$[2]^+ + e^- ightarrow [2]^-$ (E) $E_{1/2} = -1.95 V$
(2) 1e1e1e	$[2]^{+} + e^{-} \rightleftharpoons [2]^{0}$ (E) $E_{1/2} = -1.04 \text{ V}$
	$[2]^{0}$ + e ⁻ \rightleftharpoons $[2]^{-}$ (E) E _{1/2} = -1.95 V
	$[2]^{-} + e^{-} \rightleftharpoons [2]^{2-}$ (E) $E_{1/2} = -1.95 V$
(3) 1e2e	$[2]^{+} + e^{-} \rightleftharpoons [2]^{0}$ (E) $E_{1/2} = -1.10 \text{ V}$
	$[2]^{0}$ + 2 e ⁻ \rightleftharpoons $[2]^{2-}$ (E) E _{1/2} = -1.95 V
(4) 1e2eRxn	$[2]^{+} + e^{-} \rightleftharpoons [2]^{0}$ (E) $E_{1/2} = -1.10 \text{ V}$
	$[2]^{0^{\bullet}} + 2 e^{-} \rightleftharpoons [2]^{2-}$ (E) $E_{1/2} = -1.95 V$
	$[2]^{0\bullet} \rightleftharpoons [2]^{0\bullet*}$ (C) K _{eq} = 8; k _f =10 ³ ; k _b =125
	$[2]^{2-} \rightleftharpoons [2]^{2-*}$ (C) K _{eq} = 5; k _f = 20; k _b = 4

[A] DigiElch Professional Version 7.FD 2006, ElchSoft GbR, Kleinromstedt, Germany.[B] R. S. Nicholson, I. Shain, Anal. Chem., 1965, 37, 1351.

7 EPR-Spectroelectrochemistry



Figure S40: EPR spectrum of [1]+, generated in-situ in CH2Cl2 / 0.1 M NBu4PF6 at a platinum working electrode. [1]+ shows a g-value of 2.056 at 9.46 GHz.

Table S2: Loewdin spin populations [%] for selected compounds from B3LYP/def2-TZVP level of theory.

Compound	ρ_{Ir}	$\rho_{N1(NH)}$	ρ _{N2(NPhN)}	ρ_{Me}	ρ _{Cl}
1+•	7	10	14		
20•	19	21	18	4	
22-	36	2	2	1	
30•	12	22	20		5



Figure S41: Loewdin spin density population for $[1]^+$, iso value = 0,005.





Figure S43: Loewdin spin density of $[2]^{2-}$ Iso value = 0.01



8 Interconversion of 2⁺ to 3⁺



Scheme S1: Proposed mechanism for the interconversion of [2]+ into [3]+. References: K. Reimer, F. Tiemann, Ber. Dtsch. Chem. Ges. **1876**, 9, 1268. H. Wynberg, Chem. Rev. **1960**, 60, 169.



Figure S45: Haloform activation with [2]BF₄.

8.1 Mass spectrum of 2⁺ and Fluoroform



Figure S46: Mass spectrum (simulation and experiment) of [2]BF₄ in MeCN solution in the presence of Fluoroform.







Chemical Formula: C₂₄H₃₀IrN₂

Exact Mass: 539,2038

С

Chemical Formula: C₂₂H₂₅IrN₂ Exact Mass: 510,1647





Chemical Formula: C₂₃H₂₉FIrN₂ Exact Mass: 545,1944





в





Chemical Formula: C₂₃H₂₆F₂IrN₂ Exact Mass: 561,1693

Figure S47: Proposed intermediates for the reaction of [2]BF4 and Fluoroform.

Mass spectrometry of 2⁺ and Chloroform 8.2



Figure S48: Mass spectrum (simulation and experiment) of [2]BF₄ in Chloroform solution.





Exact Mass: 525,1882



Exact Mass: 539,2038

Chemical Formula: C₂₂H₂₅IrN₂ Exact Mass: 510,1647





Chemical Formula: C₂₂H₂₅CllrN₂ Exact Mass: 545,1336

Chemical Formula: C23H22Cl2IrN2 Exact Mass: 589,0789

Figure S49: Proposed intermediates for the reaction of [2]BF4 and Chloroform.

8.3 Mass spectrometry of 2⁺ and Bromoform



Figure S50: Mass spectrum (simulation and experiment) of [2]BF₄ in Bromoform solution.



 $\label{eq:chemical-Formula: C22H25IN2} Chemical Formula: C_{23}H_{28}IN_2 \ Chemical Formula: C_{24}H_{30}IrN_2$ Exact Mass: 510,1647







Exact Mass: 525,1882



Exact Mass: 539,2038



Chemical Formula: C23H27BrIrN2 Exact Mass: 603,0987



Chemical Formula: C23H22Br2IrN2 Exact Mass: 676,9779

Figure S51: Proposed intermediates for the reaction of [2]BF4 and Bromoform.

8.4 Mass spectrometry of 2⁺ and Iodoform



Figure S52: Zoom-in of the mass spectrum (simulation and experiment) of [2]BF₄ in MeCN solution in the presence of lodoform.



Chemical Formula: C₂₂H₂₅IrN₂ Exact Mass: 510,1647



Chemical Formula: C₂₂H₂₅IIrN₂ Exact Mass: 637,0692



Chemical Formula: C₂₃H₂₈IrN₂ Exact Mass: 525,1882



Chemical Formula: C₂₂H₂₅IIrN₂O Exact Mass: 653,0641



Chemical Formula: C₂₂H₂₅IIrN₂O₂ Exact Mass: 669,0590

Figure S53: Proposed intermediates for the reaction of [2]BF4 and Iodoform.

9 IR-spectroelectrochemistry

Table S3: IR data for compounds [1] and [2]⁺ from OTTLE-spectroelectrochemistry in DCM with 0.1 NBu_4PF_6 measured with a gold mesh working electrode.

Compound	Peaks / cm ⁻¹
1	1591 w, 1577 w, 1483 s, 1461 sh, 1382m, 1361 m, 1324 s, 1228 m, 1191 w,
	1147w, 1095 s, 1024s
1^{2+}	1591 w, 1486 m, 1454 m, 1382m, 1361w, 1324 w, 1095 s, 1024s
2+	1483m, 1469m, 1459m, 1423s, 1382 w, 1274s, 1255s,
2 ²⁻	1483m,. 1469m, 1459m, 1423m, 1382w, 1272m, 1253m

Table S4: Comparison of calculated and experimental peaks for the IR spectra of various species. Calculated at the RI-BP86/def2-TZVP level of DFT.

Compound	Peak(exp.)	Peak(calc.)	Assignment
1	1483	1474.21	Methyl groups of Cp* mostly, bit of C-N and
			Aromativ
		1474.84	Asym C-N stretch; quite a bit of Cp*, aromatic
			C=C
	1361	1388.93	Symmetric c-n stretch; Cp* frame deformation;
			C=C of aromatic ring
	1324	1326.8	asymmetric C-N stretch; N-H deformation; C=C
			of aromatic rings
		1334.93	Symmetric C-N stretch; N-H deformation; C=C of
			aromatic rings
1^{2+}	1486 &	1462.47	Sym C=N and aromatic C=C stretch,
	1454	1453.34	Cp* Me; bit aromatic rings
		1464.18	Cp* Me; bit aromatic rings
		1479.2	Cp* Me Deformation
		1491.62	Asym. C=N stretch; C=C stretch; bit of Cp*
	1384	1383.41	Cp*Me deform; bit C=N; C-H deform
		1386.01	Sym. C=N; C=C stretch, bit of Cp*; C-H deform.
		1381.7	More deform, less C=N/C=C
2+	1483-1423	1487.23	Asym C=N; C=C stretch MeCp* deform
		1485.36	Same
		1480.34	IrMe deform, MeCp*deform
		1466.36	Sym C=N; C=C, bit MeCp* deform
		1415.37	Various MeCp* deform; and IrMe
		till1461.87	
	1274+1255	1292.28	C=N sym; C=C stretch; IrMe derform, NH deform
		1280.01	IrMe deform
		1274.96	IrMe leicht deform,C=N, NH deform
		1234.7	NH deform, N=C stretch asym
22-	1483	1538.64	C=N asym stretch; C=C
			Phenylenediamindebenzene stretch asym
		1516.01	
	1420	1490.84	C=N sym stretch; sym benzeneNN sym stretch;
			Cp* deform
	1276	1344.06	C=NPh stretch with benzene strech
	1253	1313.55	C=NH stretch with benzene stretch



9.1 Spectra for 1 and 1²⁺ (experimental and calculated)

Figure S54: Changes in the IR spectrum of 1 during OTTLE-spectroelectrochemistry in CH₂Cl₂/0.1 M NBu₄PF₆.



Figure S55: Zoom-in of the changes of the IR spectrum of 1 during OTTLE-spectroelectrochemistry in CH₂Cl₂/0.1 M NBu₄PF₆..



Figure S56: Comparison of the calculated (red) and experimental (black) IR spectrum of 1.



Figure S57: Comparison of the calculated (red) and experimental (black) IR spectrum of 1²⁺.



Figure S58: Comparison of the IR spectra of 1 and 1²⁺, asterisks indicate region of strong solvent absorptivity during the electrolysis.



9.2 IR spectra of 2+

Figure S59: Changes of the IR spectrum of 2⁺ during OTTLE-spectroelectrochemistry in CH₂Cl₂/0.1 M NBu₄PF₆.



Figure S60: IR spectra of 2⁺ before and after electrolysis and 2²⁻ OTTLE-spectroelectrochemistry in CH₂Cl₂/0.1 M NBu₄PF₆.



Figure S61: IR spectra of 1, 1^{2+} , 2^+ and 2^{2-} during OTTLE-spectroelectrochemistry in CH₂Cl₂/0.1 M NBu₄PF₆.



Figure S62: Comparison of the experimental (black) and calculated (red) IR spectra of [2]⁺.



Figure S63: Comparison of the experimental (black) of [2]²⁻ and calculated (red) IR spectrum of [2]⁻.



Figure S64: Comparison of the experimental (black) of [2]²⁻ and scaled calculated (red) IR spectrum of [2]⁻.



Figure S65: Comparison of the experimental (black) and calculated (red) IR spectra of [2]²⁻.



Figure S66: Comparison of the experimental (black) and scaled calculated (red) IR spectra of [2]⁺.



Figure S67: Comparison of the calculated IR spectra of 1, 1²⁺ and 2⁺ at the RI-BP86/def2-TZVP level of theory.

10 UV-Vis-NIR-Spectroelectrochemistry

Table S5: (UV-)Vis-NIR data for compounds [1], [2]⁺ and [3]⁺ from OTTLE-spectroelectrochemistry in DCM with 0.1 NBu₄PF₆ measured with agold or platinum mesh working electrode.

	$\lambda [nm] (e [10^3 M^{-1} \cdot cm^{-1}])$					
[1]	304 (4.2), 434 (9.4), 504 (1.7) sh					
[1]+	424 (4.4) br, 504 (1.7) sh, 638 (0.9) sh, 1044 (0.3) br					
$[1]^{2+}$	341 (1.9), 449 (3.7), 513 (1.9) sh, 663 (0.3) br , 955 (0.2) br					
[2]+	315 (3.9), 486 (12.9), 608 (1.6) sh					
$[2]^{0}$	308 (4.5), 443 (9.5), 486 (10.7), 608 (1.4) sh					
[2] ²⁻	307 (5.5), 437 (9.9), 568 (4.0), 842 (0.6) br					
[3]-	308 (2.5), 469 (2.5), 776 br (2.1)					
[3]2-	See [1]					
Obtai	ned from spectroelectrochemical measurements using an OTTLE-cell with a gold working					
electr	ode in $CH_2CL_2/0.1$ M NBu ₄ PF ₆ at 295K.					

10.1 Spectra for [2]⁺



Figure S68: UV-Vis-NIR spectra of 2⁺, 2[•] and 2⁻.



Figure S69: Changes in the UV-Vis-NIR spectrum of 2⁺ during OTTLE-spectroelectrochemistry in CH₂Cl₂/0.1 M NBu₄PF₆.



Figure S70: Changes in the UV-Vis-NIR spectrum of 2^{0} during OTTLE-spectroelectrochemistry in $CH_{2}Cl_{2}/0.1$ M NBu₄PF₆.



Figure S71: Comparison of the UV-Vis-NIR spectrum of 2 before and after oxidative OTTLE spectroelectrochemistry.



Figure S72: Changes in the UV-Vis-NIR spectrum of 2 during OTTLE spectroelectrochemistry in CH₂Cl₂ / 0.1 M NBu₄PF₆.



Figure S73: Comparison of the UV/Vis-NIR spectrum of [1] in the absence of the middle UV part of the spectrum and the spectrum of [2]⁺ after electrochemical reduction.

10.2 Spectra for [3]⁺



Figure S74: Changes in the UV-Vis-NIR spectrum of 3 during OTTLE spectroelectrochemistry in CH₂Cl₂ / 0.1 M NBu₄PF₆.



Figure S75: Comparison of the UV-Vis-NIR spectrum of 3 before and after reductive OTTLE spectroelectrochemistry.

11 (TD)DFT





Figure S76: Comparison of frontier orbitals and main contributions to transitions observed in (UV-)Vis-NIR spectroscopy. HOMO and LUMO marked in red.

11.2 DFT Calculation for [1] (singlet state)



Figure S77: Calculated TD-DFT spectrum with discrete transitions (left), experimental spectrum with discrete calculated transitions (middle) and experimental (black) and calculated TD-DFT spectrum (red) (left).

Table S6: TD-DFT transitions for 1

Stat	Difference	Transiti	Transiti	Calculat	Oscillat	Experimen	Molar
e	density (iso	on	on	ed	or	tal	absorpti
	value 0.004)		homo	Transitio	strengt	transition	on
			lumo	n energy	h	energy	coefficie
							nt 10^3
	-					434	9.3
	Conservation of the second sec	123->					
		124	номо				
	200	(0.89)	\rightarrow	363.9	0.5171		
3			LUMO				

Table S7: Selected molecular orbitals for 1.

HOMO-1	НОМО	LUMO	LUMO+1

Table S8: Selected molecular orbital energies for 1.

Orbital	HOMO/LUMO	Energy	Energy
No.		(Eh)	(eV)
122	HOMO-1	-0.191448	-5.2096
123	НОМО	-0.180974	-4.9245
124	LUMO	-0.048281	-1.3138
125	LUMO+1	-0.014316	-0.3896

11.3 DFT Calculation [1]⁺(doublet state)



Figure S78: Calculated TD-DFT spectrum with discrete transitions (left), experimental spectrum with discrete calculated transitions (middle) and experimental (black) and calculated TD-DFT spectrum (red) (left).

Table S9: TD-DFT transitions for [1]⁺ (doublet state) (raw data) iso 0.004

State		Transition	Transition homo lumo	Calculated	Oscillator	Experimental	Molar
				Transition	strength	transition	absorption
				energy		energy	coefficient
							10^3
	Jone of					424	4.4
	and a set of the set o						
	and the second s	123a -> 124a (0.25)	ΗΟΜΟα -> LUMOα (0.25)				
		115b -> 123b (0.42)	ΗΟΜΟβ-7 -> LUMOβ (0.42)				
11	R	122b -> 124b (0.16)	ΗΟΜΟβ -> LUMOβ+1 (0.16)	388.9	0.2633		
	and all						
		122a -> 124a (0.14)	ΗΟΜΟα-1 -> LUΜΟα (0.14)				
	No. of the second se	$123a \rightarrow 124a (0.10)$	HOMOQ \rightarrow LUMOQ (0.10)				
	X	$115b \rightarrow 123b(0.11)$	HOMOB-7 -> IUMOB(0.11)				
12	\mathcal{H}°	$122b \rightarrow 122b$ (0.11)	HOMOB \rightarrow LUMOB+1 (0.47)	380.1	0.1197		
						638	0.9
	and all						
	Sector Se						
		$117h_{->}123h(0/13)$					
1		1170 > 1230 (0.43) 110h > 123h (0.42)	$HOMOB_3 > LUMOB (0.43)$	626.8	0.0072		
4	9			020.8	0.0072	-	
	San of						
		117b -> 123b (0.35)	ΗΟΜΟβ-5 -> LUΜΟβ (0.35)				
6	~~~ <u>~</u> ~	119b -> 123b (0.56)	ΗΟΜΟβ-3 -> LUMOβ (0.56)	652.6	0.0006		

1	122b -> 123b (0.97)	ΗΟΜΟβ -> LUMOβ (0.97)	1652.6	0.0007	1044	0.3
2	120b -> 123b (0.64) 121b -> 123b (0.29)	ΗΟΜΟβ-2 -> LUΜΟβ (0.64) ΗΟΜΟβ-1 -> LUΜΟβ (0.29)	890.4	0.0017		

Table S10: Selected molecular orbitals for [2]⁺.

LUMOa+3	LUMOa+2	LUMOa+1	LUMOa	ΗΟΜΟα
ΗΟΜΟα-1	ΗΟΜΟα-2	ΗΟΜΟα-3		

Table S11: Selected molecular orbitals for [2]⁺.

LUMOβ+3	LUMOβ+2	LUMOβ+1	LUMOβ	ΗΟΜΟβ
ΗΟΜΟβ-1	ΗΟΜΟβ-2	ΗΟΜΟβ-3	ΗΟΜΟβ-4	ΗΟΜΟβ-5
ΗΟΜΟβ-6	ΗΟΜΟβ-7			

Spin up Orbi	itals alpha			Spin down c	orbitals beta		
Orbital No.	Orbital	Energy (Eh)	Energy (eV)	Orbital No.	Orbital	Energy (Eh)	Energy (eV)
114	ΗΟΜΟα-9	-0.355101	-9.6628	114	ΗΟΜΟβ-8	-0.344884	-9.3848
115	ΗΟΜΟα-8	-0.321275	-8.7423	115	ΗΟΜΟβ-7	-0.313018	-8.5177
116	ΗΟΜΟα-7	-0.299267	-8.1435	116	ΗΟΜΟβ-6	-0.298623	-8.1259
117	ΗΟΜΟα-6	-0.295000	-8.0274	117	ΗΟΜΟβ-5	-0.291469	-7.9313
118	ΗΟΜΟα-5	-0.290216	-7.8972	118	ΗΟΜΟβ-4	-0.289554	-7.8792
119	ΗΟΜΟα-4	-0.278126	-7.5682	119	ΗΟΜΟβ-3	-0.277392	-7.5482
120	ΗΟΜΟα-3	-0.271645	-7.3918	120	ΗΟΜΟβ-2	-0.270393	-7.3578
121	ΗΟΜΟα-2	-0.263343	-7.1659	121	ΗΟΜΟβ-1	-0.262364	-7.1393
122	ΗΟΜΟα-1	-0.246584	-6.7099	122	ΗΟΜΟβ	-0.239958	-6.5296
123	ΗΟΜΟα	-0.229292	-6.2394	123	LUMOβ	-0.172193	-4.6856
124	LUMOα	-0.094578	-2.5736	124	LUMOβ+	-0.083993	-2.2856
125	LUMOα+1	-0.044587	-1.2133	125	LUMOβ+	-0.044150	-1.2014

Table S12: Orbital energies for [1]⁺ (doublet state)

11.4 DFT Calculation [1]²⁺(singlet state)



Figure S79: Calculated TD-DFT spectrum with discrete transitions (left), experimental spectrum with discrete calculated transitions (middle) and experimental (black) and calculated TD-DFT spectrum (red) (left).

State		Transition	Transition homo lumo	Calculated	Oscillator	Experimental	Molar
				Transition	strength	transition	absorption
				energy		energy	coefficient
							10^3
	-					341	1.9
		119a -> 124a (0.19)	HOMO-3 -> LUMO+1 (0.19)				
		121a -> 124a (0.40)	HOMO-1 -> LUMO+1 (0.40)				
11	A second	122a -> 124a (0.17)	HOMO -> LUMO+1 (0.17)	346.6	0.1407		
						449	3.7
		115a -> 123a (0.74)	HOMO-7 -> LUMO (0.74)				
9	200 0 P	121a -> 124a (0.16)	HOMO-1 -> LUMO+1 (0.16)	389.8	0.0850		
8		122a -> 124a (0.63)	HOMO -> LUMO+1 (0.63)	393.2	0.0718	_	
		116a -> 123a (0.38)	HOMO-6 -> LUMO (0.38)				
7	5° 8	118a -> 123a (0.42)	HOMO-4 -> LUMO (0.42)	481.9	0.0951		

Table S13: TD-DFT transitions for [1]²⁺ (singlet state) (raw data)

	117a -> 123a (0.76)	HOMO-5 -> LUMO (0.76)					
5	118a -> 123a (0.14)	HOMO-4 -> LUMO (0.14)	523.9	0.0489			
					663sh	1.9	
	121a -> 123a (0.67)	HOMO-1 -> LUMO (0.67)					
3	122a -> 123a (0.11)	HOMO -> LUMO (0.11)	663.9	0.0999			
4	119a -> 123a (0.16) 120a -> 123a (0.78)	HOMO-3 -> LUMO (0.16) HOMO-2 -> LUMO (0.78)	737.4	0.0098			
1	121a -> 123a (0.17) 122a -> 123a (0.75)	HOMO-1 -> LUMO (0.17) HOMO -> LUMO (0.75)	990.7	0.0181	995	0.2	

Table S14: Selected molecular orbitals for [2].

LUMO+3	LUMO+2	LUMO+1	LUMO	НОМО
HOMO-1	НОМО-2	НОМО-3	HOMO-4	НОМО-5
HOMO-6	HOMO-7			

Table S15: Selected molecular orbital energies for [2].

Orbital No.	HOMO/LUMO	Energy (Eh)	Energy (eV)
115	HOMO-7	-0.358431	-9.7534
116	HOMO-6	-0.340761	-9.2726
117	HOMO-5	-0.335119	-9.1191
118	HOMO-4	-0.333889	-9.0856
119	HOMO-3	-0.316401	-8.6097
120	HOMO-2	-0.313341	-8.5265
121	HOMO-1	-0.303275	-8.2525
122	НОМО	-0.283697	-7.7198
123	LUMO	-0.216146	-5.8816
124	LUMO+1	-0.138525	-3.7695
125	LUMO+2	-0.092869	-2.5271

11.5 DFT Calculation for [2]⁺ (singlet state)



Figure S80: Calculated TD-DFT spectrum with discrete transitions (left), experimental spectrum with discrete calculated transitions (middle) and experimental (black) and calculated TD-DFT spectrum (red) (left).

Table S16: TD-DFT transitions for [2]⁺ (singlet state).k

State	Difference densities	Transition	Transition homo lumo	Calculated	Oscillator	Experimental	Molar
	(iso 0,004; red			Transition	strength	transition	absorption
	negative, blue			energy		energy	coefficient
	positive)						10^3
						593	1.0
1	, 19	127a -> 128a (0.81)	HOMO -> LUMO (0.81)	613.3	0.0267		
						486	6.4
	marke	122a -> 128a (0.40)	HOMO-5 -> LUMO (0.40)				
		123a -> 128a (0.13)	HOMO-4 -> LUMO (0.13)				
		124a -> 128a (0.11)	HOMO-3 -> LUMO (0.11)				
2	9	126a -> 128a (0.25)	HOMO-1 -> LUMO (0.25)	438.9	0.1135		
		124a -> 128a (0.38) 125a -> 128a (0.10)	HOMO-3 -> LUMO (0.38) HOMO-2 -> LUMO (0.10)				
3	Jan .	126a -> 128a (0.39)	HOMO-1 -> LUMO (0.39)	436.5	0.1710		
						413	3.1
4		125a -> 128a (0.72)	HOMO-2 -> LUMO (0.72)	409.1	0.0255		

		122a -> 128a (0.42)	HOMO-5 -> LUMO (0.42)			
6	2000 - Contra - Contr	123a -> 128a (0.44)	HOMO-4 -> LUMO (0.44)	392.9	0.0450	
		123a -> 128a (0.37)	HOMO-4 -> LUMO (0.37)			
	and po	124a -> 128a (0.29)	HOMO-3 -> LUMO (0.29)			
5		126a -> 128a (0.14)	HOMO-1 -> LUMO (0.14)	387.2	0.1439	

Table S17: Selected molecular orbitals for [2]⁺.

LUMO+3	LUMO+2	LUMO+1	LUMO	НОМО	HOMO-1
HOMO-2	HOMO-3	HOMO-4	HOMO-5	HOMO-6	HOMO-7

Orbital	HOMO/LUMO	Energy	Energy
No.		(Eh)	(eV)
120	HOMO-7	-0.311020	-8.4633
121	HOMO-6	-0.305476	-8.3124
122	HOMO-5	-0.293880	-7.9969
123	HOMO-4	-0.283206	-7.7064
124	HOMO-3	-0.281052	-7.6478
125	HOMO-2	-0.271251	-7.3811
126	HOMO-1	-0.243830	-6.6349
127	НОМО	-0.240521	-6.5449
128	LUMO	-0.136344	-3.7101
129	LUMO+1	-0.054350	-1.4790
130	LUMO+2	-0.042796	-1.1645
131	LUMO+3	-0.037464	-1.0195

Table S18: Selected molecular orbital energies for [1]²⁺.

11.6 DFT Calculation for [2]⁰ (doublet state)



Figure S81: Calculated TD-DFT spectrum with discrete transitions (left), experimental spectrum with discrete calculated transitions (middle) and experimental (black) and calculated TD-DFT spectrum (red) (left).

Table S19: TD-DFT transitions for [2]⁰ (doublet state) (raw data)

State	Difference	Transition	Transition homo lumo	Calculated	Oscillator	Experimental	Molar
	densities			Transition	strength	transition	absorption
				energy		energy	coefficient
							10^3
	A Contraction of the second se				0.0545	443	9.5
7		128a -> 131a (0.59)	ΗΟΜΟα -> LUMOα+2 (0.59)	411.2			
	CONTRACTOR DO	128a -> 132a (0.25)	HOMOα -> LUMOα+3 (0.25)				
11		128a -> 133a (0.30)	HOMOα -> LUMOα+4 (0.30)	358.0	0.0575		
	and the second					486	10.7
2		126b -> 128b (0.82)	ΗΟΜΟβ-1 -> LUMOβ (0.82)	533.4	0.0984		
						608	1.4
1	<u> </u>	127b -> 128b (0.93)	HOMOβ -> LUMOβ (0.93)	768.9	0.0168		

Table S20: Composition of selected spin up and spin down molecular orbitals of [2]⁰.

LUMOa+5	LUMOa+4	LUMOa+3	LUMOa+2	LUMO _{β+5}	LUMO _{β+4}	
LUMOa+1	LUMOa	ΗΟΜΟα	ΗΟΜΟα-1	LUMO _{β+3}	LUMOβ+2	LUMO _{β+1}
ΗΟΜΟα-2	ΗΟΜΟα-3			LUMOβ	ΗΟΜΟβ	ΗΟΜΟβ-1

Spin up Orbi	itals alpha			Spin down orbitals beta			
Orbital No.	Orbital	Energy (Eh)	Energy (eV)	Orbital No.	Orbital	Energy (Eh)	Energy (eV)
126	ΗΟΜΟα-2	-0.212939	-5.7944	126	ΗΟΜΟβ-1	-0.199963	-5.4413
127	ΗΟΜΟα-	-0.194693	-5.2979	127	ΗΟΜΟβ	-0.183648	-4.9973
128	ΗΟΜΟα	-0.146421	-3.9843	128	LUMOβ	-0.086230	-2.3464
129	LUMOα	-0.020399	-0.5551	129	LUMOβ+1	-0.018420	-0.5012
130	LUMOa+1	-0.014510	-0.3948	130	LUMOβ+2	-0.013372	-0.3639
131	LUMOα+2	0.002959	0.0805	131	LUMOβ+3	0.007712	0.2099
132	LUMOa+3	0.012268	0.3338	132	LUMOβ+4	0.019694	0.5359
133	LUMOα+4	0.017902	0.4871	133	LUMOβ+5	0.021276	0.5789
134	LUMOa+5	0.023008	0.6261	134	LUMOβ+6	0.027368	0.7447

Table S21: Orbital energies of [2]⁰ from DFT-calculation

11.7 DFT Calculation for [2]²⁻ (doublet state)



Figure S82: Calculated TD-DFT spectrum with discrete transitions (left), experimental spectrum with discrete calculated transitions (right) and experimental (black) and calculated TD-DFT spectrum (red) (below).

Table S22: TD-DFT transitions for [2]²⁻ (doublet state)

State	Difference densities	Transition	Transition homo lumo	Calculated	Oscillator	Experimental	Molar absorption
				Transition energy	strength	transition energy	coefficient 10^3
	9- 9- 0		ΗΟΜΟα-1 -> LUΜΟα			437	9.9
			(0.20)				
	all the second		ΗΟΜΟβ -> LUMOβ+2				
		128a -> 130a	(0.25)				
		(0.20)					
		128b -> 131b					
14	8	(0.25)		509.8	0.1409		
	8a 🔓 D		HOMOα-1 -> LUMOα+3				
			(0.21)				
	···	128a -> 133a	HOMOβ -> LUMOβ+4				
		(0.21)	(0.14) mixed				
		128b -> 133b	IIIXed				
		(0.14)					
31	0 8	mixed		378.7	0.0663		
	SR 📥 🚺 🖉					568	4.0
	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~						
		129a -> 133a					
		(0.25)	HOMO $\alpha$ -> LUMO $\alpha$ +3				
	**	128b -> 129b	(0.25)	C 1 9 C	0.0651		
5		(0.34)		648.6	0.0651		
	A A A A A A A A A A A A A A A A A A A		(0.41)				
	C C C C C C C C C C C C C C C C C C C						
	CONTRACT OF A						
		129a -> 133a					
7	8	(0.41)		629.4	0.0143		

	8		ΗΟΜΟα -> LUMOα+2			842	0.6
			(0.88)				
	X	129a -> 132a					
3	**	(0.88)		748.6	0.0073		
	Se a store R			1752.9	0.0080		
	C 4 4 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5						
		129a -> 130a					
		(0.69)	HOMOα -> LUMOα (0.69)				
		129a -> 131a	HOMOα -> LUMOα+1				
1	9 2	(0.28)	(0.28)				
	Se _ Lo R			1455.4	0.0173		
	Contraction of the contraction o						
		129a -> 130a					
		(0.26)	HOMOα -> LUMOα (0.26)				
		129a -> 131a	HOMO $\alpha$ -> LUMO $\alpha$ +1				
2		(0.69)	(0.69)				

Table S23: Selected molecular orbitals fo	r [2] ²⁻ .
-------------------------------------------	-----------------------

LUMOa+3	LUMOa+2	LUMOa+1
LUMOα	ΗΟΜΟα	ΗΟΜΟα-1

Table S24: Selected molecular orbitals for [2]²⁻.

LUMOβ+4	LUMOβ+3	LUMOβ+2	LUMOβ+1
LUMOβ	ΗΟΜΟβ	ΗΟΜΟβ-1	

Table S25. Orbital energies of [2]²⁻ for selected molecular orbitals.

Spin up Orbitals alpha					Spin down o	orbitals beta	
Orbital No.	Orbital	Energy (Eh)	Energy (eV)	Orbital No.	Orbital	Energy (Eh)	Energy (eV)
127	ΗΟΜΟα-2	-0.094693	-2.5767	127	ΗΟΜΟβ-1	-0.089895	-2.4462
128	ΗΟΜΟα-	-0.070057	-1.9063	128	ΗΟΜΟβ	-0.065503	-1.7824
129	ΗΟΜΟα	-0.022785	-0.6200	129	lumoβ	0.035628	0.9695
130	LUMOα	0.039168	1.0658	130	LUMOβ+1	0.042805	1.1648
131	LUMOα+1	0.042582	1.1587	131	LUMOβ+2	0.050174	1.3653
132	LUMOα+2	0.066167	1.8005	132	LUMOβ+3	0.068563	1.8657
133	LUMOα+3	0.075235	2.0473	133	LUMOβ+4	0.078047	2.1238
134	LUMOα+4	0.084832	2.3084	134	LUMOβ+5	0.085907	2.3377
135	LUMOα+5	0.085475	2.3259	135	LUMOβ+6	0.086927	2.3654

## **11.8 DFT Calculation for [3]**⁺ (singlet state)



Figure S83: Calculated TD-DFT spectrum with discrete transitions (left), experimental spectrum with discrete calculated transitions (middle) and experimental (black) and calculated TD-DFT spectrum (red) (left).

State	Difference densities (iso-	Transition	Transition homo lumo	Calculated	Oscillator	Experim	Molar
	value of 0.004)			Transition	strength	ental	absorption
				energy		transitio	coefficient
						n energy	10^3
						776 br	2.1
1	J.	131a -> 132a (0.90)	HOMO -> LUMO (0.81)	885.3	0.009		
		129a -> 132a (0.30)	HOMO-2 -> LUMO (0.30)	511.7		469	2.5
3	300	130a -> 132a (0.30)	HOMO-1 -> LUMO (0.30)		0.069		
		126a -> 132a (0.35)	HOMO-5 -> LUMO (0.35)	441.5			
5		129a -> 132a (0.29)	HOMO-2 -> LUMO (0.29)		0.053		
6		130a -> 132a (0.29)	HOMO-1 -> LUMO (0.29)	431.3	0.132		

Table S26: TD-DFT calculated eletronic transistions and difference densities of [3]⁺. (Including raw data)

Table S27: Composition of selected molecular orbitals of [3]⁺.

HOMO-5	HOMO-4	НОМО-3	НОМО-2
HOMO-1	НОМО	LUMO	LUMO+1

Table S28: Selected molecular orbital energies for [3]⁺.

Orbital No.	HOMO/LUMO	Energy (Eh)	Energy (eV)
126	HOMO-5	-0.287293	-7.8176
127	HOMO-4	-0.284895	-7.7524
128	HOMO-3	-0.281419	-7.6578
129	HOMO-2	-0.273177	-7.4335
130	HOMO-1	-0.266413	-7.2495
131	НОМО	-0.244328	-6.6485
132	LUMO	-0.156737	-4.2650
133	LUMO+1	-0.075974	-2.0674

#### **11.9** Coordinates of optimized structures

#### IrNPhH native [1]

Ir	-0.67726332572944	-0.06303930746490	-0.20961079613236
Ν	-1.44850661327445	-0.14203345029253	1.59457938145844
Ν	0.93080986225125	0.01677503658800	0.94545155610124
C	-0.01879792299984	-0.01044501572778	-2.32322165362881
c	-0.86579877026948	1.11989347722544	-2.02573388985032
C	-0.//69893/51525/	-1.20934108459474	-2.0561838/222021
c	-2.1/381603536422	0.01840043781833	-1.62/644844/4/85
c	-2.11978105991778	-0.82000502140050	2 67878010687102
ĉ	0.75430661867054	-0.00877728239247	2 31127124621120
c	2,23725631614573	0.12387899921584	0.40603223913086
č	1.36096908329263	0.05473313546414	-2.88083260080010
c	-0.46588098658997	2.55514255715373	-2.13519012428338
С	-0.28322861182809	-2.61135770149051	-2.20456678317452
С	-3.38212699762713	1.44620414105091	-1.34639478605504
С	-3.26449471052481	-1.73568428231291	-1.36731581269857
С	-0.98346353484205	-0.14840587364541	4.03644578649556
С	1.74589724149025	0.04467365223607	3.30661884273137
С	2.92407582847282	-1.02830535158292	0.00639030968967
С	2.83055599550450	1.38156570325692	0.23295557605071
C	0.00787420545610	-0.08679465983188	5.01065626801953
c	1.30445132429304	0.00896309171305	4.64529128422554
c	4.09303991209334	-0 92545201248773	-0.5710220470507
c	4 77812989751392	0.33038223077483	-0.75402023050052
н	-2.44465551234042	-0.20308806536354	1.78981465155919
н	1.32704578339177	0.03825215448394	-3.98151035613549
н	1.97804949173057	-0.78913596931217	-2.55154821379096
н	1.88419532425479	0.97190368359504	-2.57670696094996
н	0.62659405234956	2.63531701768904	-2.09873325333918
н	-0.86888140071683	3.15337897507138	-1.30602079793356
Н	-0.80580615533250	3.01266807409281	-3.08012300234442
H	-4.07311291146733	1.44098942098675	-2.20739716141411
H	-5.121148/0006827	2.494/2808722491	-1.150/4635102265
Н	-3.95158341/65063	1.07881483099942	-0.48023695049160
н	2.80020904080234	0.10708489109065	5.03622500159645
н	-0 25431516268949	-0 12060659533703	6 06822833964000
н	-2 03937087925956	-0 23330617919503	4 30070897735319
н	2.28557984926393	2.26449264807051	0.56933236944033
н	2.43818112916572	-1.99576971398581	0.13794034067351
н	0.81230716323648	-2.64770895057452	-2.15191329925188
н	-0.67107477602675	-3.25663432648346	-1.40443754427702
н	-0.58083296915433	-3.05856072619873	-3.16927043774552
н	-3.96581534417808	-1.76117117288059	-2.21909719242004
н	-2.93186792397718	-2.76697786985699	-1.19337741358102
н	-3.83919178771601	-1.40904921297580	-0.48963622216534
н	5.//10809/44/552	0.41338100577736	-1.20042946625942
н	4.55790120655501	-1 82455266093749	-0.47541226457092
	4.72011501025770	1.02455200055745	0.07505002205754
		• • • • • • • • • • • • • • • • • • • •	
h	rNPhH 2ox	sing [1] ²⁺	
lı Ir	NPhH 20x 1.41088720406001	sing [1] ²⁺	-0.52084122656546
lr N	1.41088720406001 0.62432480600080	2.92029272859950 3.30440555846520	-0.52084122656546 1.29673240746397
lr N N	NPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197	2.92029272859950 3.30440555846520 2.72989865799167	-0.52084122656546 1.29673240746397 0.75419368039073
Ir N N C	NPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.85368850960539	x sing [1] ²⁺ 2.92029272859950           3.30440555846520           2.72989865799167           2.63628272149615	-0.52084122656546 1.29673240746397 0.75419368039073 -2.69992582522569
	NPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.85368850960539 0.93557082828671	c sing [1] ²⁺ 2.92029272859950 3.30440555846520 2.72989865799167 2.63628272149615 3.74889930123350	-0.52084122656546 1.29673240746397 0.75419368039073 -2.69992582522569 -2.46983366371063
	NPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.85368850960539 0.93557082828671 1.2515594328491 0.309051476475	<b>x sing [1]</b> ²⁺ 2.92029272859950 3.30440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 2.24920467350158	-0.52084122656546 1.29673240746397 0.75419368039073 -2.69992582522569 -2.46983366371063 -2.14575757648773
	NPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.85368850960539 0.935570828288671 1.25155943428491 -0.28096142664570 -0.0831023903284	c sing [1] ²⁺ 2.92029272859950 3.30440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829198623914 1.8447092423000	-0.52084122656546 1.29673240746397 0.75419368039073 -2.69992582525569 -2.46983366371063 -2.14575757648773 -1.86401549550671 -1.6166980240457
	NPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.85368850960539 0.93557082828671 1.25155943428491 -0.28096142664570 -0.08310238093284 1.34422020966979	c sing [1] ²⁺ 2.92029272859950 3.30440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829198623914 1.84479292423000 2.96550884009903	-0.52084122656546 1.29673240746397 0.75419368039073 -2.69992582522569 -2.46983366371063 -2.14575757648773 -1.86401549550671 -1.6166898249457 2.3596188607230
Ir N C C C C C C C C	CNPhH 200X 1.41088720406001 0.6243248060080 3.05758138251197 1.83368850960539 0.93557082828671 1.25155943428491 0.28096142664570 0.08310238093284 1.3442020966579 2.76259611423955	<pre>\$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$</pre>	-0.52084122656546 1.29673240746397 -2.69992582522569 -2.46983366371063 -2.14575757648773 -1.86401549550671 -1.61668989249457 2.35996188697230 2.05640688505471
Ir N N C C C C C C C C	CNPhH 200X 1.41088720406001 0.62432480600080 0.305788138251197 1.85368850960539 0.93557082828671 1.2515594328491 -0.28096142664570 0.08310238093284 1.34422020966979 2.76259611423955 1.34428200966979	<pre>2.5cing [1]²⁺ 2.92029272859950 3.30440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829198623914 1.84479292423000 2.96595884009903 2.69116592484193 2.69116592484193</pre>	-0.52084122555546 1.29673240746397 0.75419386039073 -2.69992582522569 -2.46983366371063 -2.14575757648773 -1.86401549550671 1.61666898249457 2.35996188697230 2.05640688505471 0.30662255176950
Ir N N C C C C C C C C C C	CNPhH 200X 1.41088720406001 0.6243248060080 0.3057818251197 1.85368850960539 0.9355708228671 1.25155943428491 -0.28096142664570 -0.08310238093284 1.3422202066979 2.76259611423955 4.37389129862140 3.12577478091566	<pre>C sing [1]²⁺ 2.9202972859950 3.30440555846520 2.72989865799167 2.63628272149615 3.7489930123350 3.24829198623914 1.84479292423000 2.6951582409903 2.6951582409903 2.6951582484193 2.89163356801305</pre>	-0.52084122656546 1.29673240746397 -2.69992582522569 -2.46983366371063 -1.86401549550671 -1.61668988249457 2.35996188697230 2.05640688505471 0.36622255176950
Ir N N C C C C C C C C C C C C C C C C C	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.83368850960539 0.9355708228671 1.25155943428491 -0.28096142664570 -0.831023093284 1.34422020966979 2.76259611423955 4.37389129862140 3.12577478091566 1.19637833768494	C sing [1] ²⁺ 2.92029272859950 3.30440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829198623914 1.84479292423000 2.956595884009903 2.69116592484139 2.89163356801307 2.73543220819863 5.168962538161046	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 -2.14575757648773 -1.86401549550671 -1.6166889249457 2.35996188697230 0.30622255176950 3.47023587115834 -2.81626636277268
Ir N N C C C C C C C C C C C C C C C C C	CNPhH 200X 1.41088720406001 0.62432480600080 0.30578138251197 1.85368850960539 0.93557082828671 1.25155943428491 -0.28096142664570 -0.08310238093284 1.34422020966979 2.76259611423955 4.37389129862140 3.12577478091566 1.19637833768494 1.76648168687959	<pre>c sing [1]²⁺ 2.92029272859950 3.30440555846520 2.72989865799167 2.63628272149615 1.46608667350958 3.24829198623914 1.84479292423000 2.96595884009903 2.69116592484193 2.691659288610307 2.73543220819863 5.16896258161046 0.07430718160776</pre>	-0.52084122656546 1.29673240746397 0.75419368039073 -2.69992582522569 -2.46983366371063 -2.14573757648773 -1.86401549550671 1.6166898249457 2.35996188697230 2.0564068850547 2.35996188697230 2.0564068850547 -3.47023587115834 -2.81264636277268 -2.18214431496753
Ir N N C C C C C C C C C C C C C C C C C	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758188251197 1.83368850960532 0.93557082828671 1.25155943428491 0.28096142645470 -0.8310238093284 1.3442202086979 1.342422020869747 1.250472491369747	c sing [1] ²⁺ 2.92029772859950 3.0440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.74889930423300 2.96595884009903 2.669116592484193 2.89163356801307 2.73543220819863 5.16896258161046 0.07430718160776 4.04625860850845	0.52084122656546 1.29673240746397 0.75419368039073 -2.69992582522569 -2.46983366371063 -2.14575757648773 -1.84601549550671 -1.61668989249457 2.3599618869724 -3.05540688505471 0.30622255176950 -3.47023587115834 -2.8126636277268 -2.18214431496753 -1.58261367385847
	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.83368850960539 0.9355708228671 1.25155943428491 -0.28096142664570 0.0831023093284 1.344220209669378 4.37389129862140 3.12577478091566 1.1963783786494 1.76648168687959 -1.50547241369747 -1.0761874704031	c sing [1] ²⁺ 2.9202972859950 3.30440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829198623914 1.8447929423000 2.95595884009903 2.89163356801307 2.7543220819863 5.16896258161046 0.07430718160776 4.04625860850845 0.91137435326223	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 -2.14575757648773 1.86401549550671 -1.6166889249457 2.35996188697230 0.30622255176950 3.47023587115834 -2.81626636777268 -2.8162663677768 -1.8262167385847 -1.9267385247 -1.9267385247 -1.9267385247 -1.92673822128828
	CNPhH 200X 1.41088720406001 0.62432480600080 0.30578182851197 1.85368850960539 0.93557082828671 1.25155943428491 -0.28096142664570 -0.8310238093284 1.34422020966979 2.76259611423955 4.37389129862140 3.12577478091566 1.19637833768494 1.76648168687959 -1.0516474740431 0.89340556586150 0.89340556586150	<pre>c sing [1]²⁺ 2.92029272859950 3.30440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829198623914 1.84479292423000 2.956595884009903 2.69116592484193 2.89163356801307 2.73543220819863 5.16896258161046 0.07430718160776 4.04625860850845 5.16896258161046 0.07430718160776 4.04625860850845 2.92564786992273 2.92564786992273</pre>	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.8640154955067 2.05640688505471 0.30622255176950 3.47023587115834 2.81626636277268 2.1821441496753 1.58261367385847 1.02673822128828 3.70943539344579
	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.83368859060532 0.93557082828671 1.25155943428491 0.2809614264570 -0.08310238093284 1.344202006697 1.3432020864570 -0.08310238093284 1.34420209667 1.19637833768494 1.76648168687959 -1.50547241369747 -1.07161874704031 0.89340455658150 3.6594424000055	c sing [1] ²⁺ 2.9202972859950 3.0440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.74889930423300 2.96595884009903 2.669116592484193 2.89163356801307 2.7354322018963 5.16896258161046 0.07430718160776 4.04625860850845 0.91137435326203 2.92564786092273 2.40700973243855	0.52084122656546 1.29673240746397 0.75419368039073 -2.69992582522569 -2.46983366371063 -2.14575757648773 -1.84601549550671 -1.61668989249457 2.3599618869724 -2.8126636277268 -2.18214431496753 -1.58261367385247 -1.02673822128828 -2.18214431496753 -1.58261367385847 -1.02673822128828
	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.83368850960539 0.9355708228671 1.25155943428491 -0.28096142664570 0.0831023093284 1.3442202096693284 1.3442202096093284 1.34422020961429355 4.37389129862140 3.12577478091566 1.1963783768494 1.76648168687959 -1.50547241369747 -1.07161874704031 0.83940556586150 0.83940556586150 0.83940556586150 0.83940556586150 0.83940556586150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055686150 0.8394055586150 0.8394055586150 0.8394055586150 0.8394055586150 0.8394055586150 0.8394055586150 0.8394055586150 0.8394055586150 0.8394055586150 0.8394055586150 0.8394040055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.83940400055 0.8394040005 0.839400005 0.839400005 0.839400005 0.839400005 0.839400005 0.839400005 0.839400005 0.839400005 0.839400005 0.839400005 0.839400005 0.839400005 0.839400005 0.839400005 0.8394000000000000000000000000000000000000	C Sing [1] ²⁺ 2.9202972859950 3.0440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829198623914 1.84479292423000 2.95595884009903 2.6911659284193 2.8916356801307 2.73543220819863 5.168962583161046 0.07430718160776 4.04625860850845 0.91137435326203 2.925647669922433 2.92564766992243358 2.08965253718889	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 -2.14575757648773 -1.86401549550671 -1.6166889249457 2.35996188697230 0.30622255176950 -3.47023587115834 -2.81626636277268 -2.18214431496753 -1.5261367385847 -1.02673822128828 3.70943539344579 3.12224522490416 0.75581657003833 3.12224522490416 0.9992611343830
	CNPhH 200X 1.41088720406001 0.62432480600080 0.30578138251197 1.85368850960539 0.93557082828671 1.2515594328491 -0.28096142664570 0.08310238093284 1.34422020966979 2.76259611423955 4.37389129862140 3.12577478091566 1.1953783768494 1.76648168687959 -1.50547241369747 -1.07618474704031 0.89340556586150 3.66948424000655 4.83313265882764 5.23240034303841 -17998968332496	C Sing [1] ²⁺ 2.92029272859950 3.30440555846520 2.72983865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.2482919862310 1.84479292423100 2.956595884009903 2.69116592484193 2.89163356801307 2.73543220819863 2.89163356801307 2.73543220819863 2.89163356801307 2.73543220819863 2.891633526203 2.92564786992273 2.40700973243585 2.08965253718889 3.84156367577506	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 -1.8640154955067 2.35996188697230 0.36620255176950 3.47023587115834 2.81526636277268 2.18214431496753 -1.8261367385847 -1.026738227128828 3.70943539344579 3.12224522490416 0.75681657603833 0.90976113438303
	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.83368850960539 0.9355708282671 1.25155943428491 0.28096142664570 -0.08310238093284 1.3442020966597 2.76259611423955 4.37389129862140 1.12637433768494 1.76648168687959 1.50547241369747 -1.07161874704031 1.7664816887959 3.66948424000055 4.83313265885150 3.66948424000055 4.83313265882764 -2.3240034303841 1.7998968332496	c sing [1] ²⁺ 2.9202972859950 2.9202972859950 2.63628272149615 2.63628272149615 2.63628272149615 3.74889930123350 1.46608667350958 2.950386823914 1.84479292423000 2.950386823914 2.85163356801307 2.73543220189633 5.16896258161046 0.0743071816077 2.92564786092273 2.04070973243585 2.08965253718889 3.8415636757506 2.64100817506740 1.76472040177	0.52084122656546 1.296732.40746397 0.75419368039073 -2.69992582522569 -2.46983366371063 -2.14575757648773 -1.86401549550671 -1.8640549550671 -0.30622255176950 0.30622255176950 -3.47023587115834 -2.81626636277268 -2.18214431496753 -1.58261367385847 -1.02673822128828 3.7094353934579 3.122245224904163 -0.75681657603834579 3.122245224904163 -0.90976113438303 4.69629285053729
	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.83368850960539 0.9355708228671 1.25155943428491 -0.28096142664570 0.0381028093284 1.34422020966903284 1.3442202096142 2.7625961142395 4.37389129862140 3.12577478091566 1.1963783768494 1.76648168687959 -1.05164874704031 0.83940556586150 0.83940456586150 0.8394056586150 0.83940400055 4.83313265882764 5.23240034303841 1.79989683832496 3.18729739898977 -1.379739898977	C Sing [1] ²⁺ 2.9202972859950 3.0440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829198623914 1.84479292423000 2.95595884009903 2.8916356801307 2.7554220819863 5.168962583161046 0.07430718160776 4.04625860850845 0.91137435326203 2.92564786992273 2.92564786992273 2.92564786992273 2.92564786992273 2.9256478692273 2.935478692273 2.935478692273 2.935478692273 2.935478692273 2.935478692273 2.935478692273	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 -2.14575757648773 1.86401549550671 -1.6166889249457 2.35996188697230 0.30622255176950 3.47023587115834 -2.8162663677268 -2.8162663677268 -2.816266377268 -3.8261367385247 -1.02673822128828 3.70943533344579 -1.02673822128828 3.70943533344579 3.12224522490416 -0.75681657603833 0.9097611348303 4.69629285053729 4.40046011698177 0.45275317639583
Ir N N C C C C C C C C C C C C C C C C C	CNPhH 200X 1.41088720406001 0.62432480600080 0.305781828251197 1.85368850960539 0.93557082828671 1.2515594328491 -0.28096142664570 -0.8310238093284 1.34422020966979 2.76259611423955 1.036142805742801566 1.1963783768494 1.76648168687959 -1.50547241369747 1.0761874704031 0.89340556586150 3.66948424000055 4.83313265882754 5.23240034303841 .1799896832496 3.18729739898977 6.5369748330488	C Sing [1] ²⁺ 2.920297285950 3.0440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829188623914 1.84479292423000 2.6951884009903 2.6951884009903 2.695186409903 2.695186409903 2.695186409903 2.695186409903 2.73543220618963 5.16896258161046 0.9113743532605 4.04625860850845 0.911374353267 4.04625860850845 0.911374353267 2.92564786992273 2.40700973243585 2.64100817506740 2.36847714904177 3.96277981679329	0.52084122656546 1.29673240746397 0.75419368039073 2.699925822263 2.46983366371063 2.14575757648773 1.36401549550671 -1.61668989249457 2.35996188697230 2.056440688505471 0.30622255176950 3.47023827115834 -2.8126636277268 2.1821443149673 -1.82661367385247 -1.026738221288228 2.1821443149673 3.1224522490416 0.75581657603833 0.90976113438303 4.6962928053729 4.40046011698177 0.45275317639583
Ir N N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.83368850960539 0.9355708282671 1.25155943428491 1.25155943428491 1.3442202066570 -0.08310238093284 1.3442202096571 1.3454202096571 1.3547478091566 1.19637833768494 1.76648168687959 -1.0547421436747 -1.07161874704031 1.76648168687959 -1.0547421436747 -1.07161874704031 1.769396833126586150 3.66948424000055 4.83313265885150 3.66948424000055 4.83313265885150 3.66948424000055 4.8331326588150 3.66948424000055 4.83313265882764 1.79999683832468 5.18729739898977 5.53697483304088 6.14895078414520	c sing [1] ²⁺ 2.9202972859950 2.9202972859950 2.029272859950 2.029272859950 2.0292785846520 2.0298865799167 2.63628272149615 2.636286273149615 3.74882930213350 1.46608667350958 3.24829189623914 1.84479292423000 2.959584608503107 2.7354220189633 5.168962583161046 0.0743071816077 2.925647860828745 0.9113743526203 2.92564786092273 2.40700973243585 2.08965253718889 2.08965253718889 2.08965253718889 2.04070973243585 2.08965253718889 2.0400817506740 2.63647714094177 3.96277981679329 2.135799162444622	0.52084122656546 1.296732.40746397 0.75419368039073 -2.69992582522569 -2.46983366371063 -2.14575757648773 -1.86401549550671 -1.61668989249457 2.35996188697230 0.30622255176950 -3.47023851715834 -2.81626636277268 -2.18214431496753 -1.58261367385847 -1.02673822128828 3.7094353934579 3.12224522490416 0.75681657603833 4.69629285053729 0.4902976113438303 4.69629285053729 0.45275317639583 -1.18067451991068177 0.45275317639583 -1.8067451991068177
	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.83368850960539 0.9355708228671 1.25155943428491 -0.28096142664570 0.0381028093284 1.3442202096690 2.7625961142395 4.37389129862140 3.12577478091566 1.1054783768494 1.76648168687959 -1.05474743091566 1.105478415867947 -1.07161874704031 0.8394055686150 0.83940456586150 1.536748313265882764 5.2324003403841 1.79989683832496 3.18729739898977 -0.304270941004978	C Sing [1] ²⁺ 2.9202972859950 3.30440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829198623914 1.8447929423000 2.95595884009903 2.89163356801307 2.7554284139 2.89163356801307 2.7554284139 2.89163356801307 2.7554786992273 2.92564786992273 2.92564786992273 2.92564786992273 2.92564786992273 2.92564786992273 2.92564786992273 2.9256478697273 2.9257812835 2.08965253718889 3.8415636757566 2.64100817506740 2.36847714904177 3.96277981673329 2.19579242444622 3.1338879916245 3.58778803179864	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 -2.14575757648773 -1.86401549550671 -1.6166889249457 2.35996188697230 0.30622255176950 3.47023587115834 -2.81626636277268 -2.8162663677268 -2.8162663677268 -3.826167385247 -1.02673822128828 3.70943539344579 -1.58261876385847 -0.2673822128828 3.70943539344579 -1.82626167385247 -0.267382212840416 0.75881657603833 0.90976113438303 4.66629285053729 4.40046011698177 0.45275317635833 -1.8067451991049 0.5792737461034 1.473067383589544
	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758188251197 1.83368850960532 0.93557082828671 1.25155943428491 0.2809614264570 0.2809614242020866973 1.3442202086979 1.3442202086142 3.76259611423955 4.37389129862140 1.25047241369747 1.07161874704031 1.76648168687959 1.50547241369747 1.07161874704031 1.769481688675615 3.66948424000858150 3.66948424003430841 1.79989683832496 5.23240034303841 1.79989683832496 5.4189507483304088 6.14895074413520 7.00304078832444 0.34270941004978 2.88985589219787	2.92029772859950 3.0440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829188623914 1.84479292423000 2.9659584009903 2.9659584009903 2.9659584009903 2.9659584009903 2.9659584019903 2.65916528484193 2.858470180675 4.04625860850845 0.91137435326203 2.92564786992273 2.40700973243585 2.92564786992273 2.40700973243585 3.84156367577506 2.64100817505705 2.64100817505705 2.6540714904177 3.96277981673329 2.1957924244422 3.1338877916245 3.58778803179864	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 -1.61668989249457 2.35996188697230 2.05640688505471 0.30622255176950 3.47023587115834 -2.8126636277268 2.18214431496753 -1.826613673822128828 2.18214431496753 -1.826613673822128828 3.7094539344579 3.12224522490416 0.75581657603833 0.90976113438303 4.6662928053727 0.45275317639583 1.18067451991049 -0.57927397461034 4.454224684774186
	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.83368850960539 0.9355708282671 1.25155943428491 1.25155943428491 1.26259611423955 4.37389129862140 3.12577478091566 1.19637833768494 1.76648168687959 1.50547241369747 -1.07161874704031 0.89340556586150 3.66948424000055 4.83313265882764 3.1872973989877 6.53677443304088 6.14895078414520 6.548974833444 -0.342793498977 6.54587443304088 6.14895078414520 7.0030407832444 -0.34270941004978 2.8895589219787 3.75818191528375	C Sing [1] ²⁺ 2.9202972859950 2.9202972859950 2.029272859950 2.63628272149615 2.63628272149615 2.63628272149615 3.74889393123350 1.46608667350958 3.74862930423350 1.46408667350958 3.482918623914 1.84479292423000 2.959584009903 2.895988409903 2.89163356801307 2.7354220819863 5.16896258161046 0.07430718160776 4.046258608764 0.0137435326203 2.9256478692273 2.04070973243585 2.0856253718889 2.0856253718889 2.0856253718889 2.0856253718889 2.0577961679329 2.15779162444622 3.1338879916245 3.1338879916245 3.13887916243 3.857780017924246 2.8203395542036	0.52084122656546 1.296732.40746397 0.75419368039073 -2.69992582522569 -2.46983366371063 -2.14575757648773 -1.86401549550671 -1.61669892349457 2.35996188657230 -3.0524068805471 0.30622255176950 -3.4702358717834 -2.8162666277268 -2.18214431496753 3.152261367385347 -1.02673822128828 3.7094353934579 3.12224522490416 -0.75681657603833 4.69629285053729 4.40046011698177 0.45275317639583 -1.18067451991049 0.57927397461034 1.47306383589534 -3.34114018396332
IF IN N C C C C C C C C C C C C C C C C C	CNPhH 20x 1.41088720406001 0.6243248060008 0.30578138251197 1.83368850960539 0.9355708228671 1.25155943428491 -0.28096142664570 0.0381023093284 1.3442202096693 4.3745912862140 3.12577478091566 1.1053783768494 1.76648168687959 -1.07161874704031 0.83940556586150 0.8394056586150 0.8394056586150 0.8394056586150 0.8394056586150 0.8394056586150 0.8394056586150 0.8394056586150 0.8394056832496 5.326748340086 6.14895078414520 7.00304078832444 6.34270941004978 2.888558219787 3.7581811528375 3.7581811528375 3.7024008262280	C Sing [1] ²⁺ 2.9202972859950 3.0440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829198623914 1.8447929423000 2.95559884009903 2.89163356801307 2.7554220819863 5.168962583161046 0.07430718160776 4.04625860850845 0.91137435326203 2.92564786992273 2.92564786992273 2.92564786992273 2.92564786992273 2.92564786992273 2.92564786992273 2.9256478697273 2.9256478697273 2.9579242444622 3.1338897916245 3.5877803179864 2.82033955942036 3.62089515842087	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 -2.14575757648773 -1.86401549550671 -1.61668898249457 2.35996188697230 0.30622255176950 3.47023587115834 -2.81626636277268 -2.8162663677268 -2.8162663677268 -2.816267435834 -1.02673822128828 3.70943539344579 -1.58261876385847 -1.02673822128828 3.70943539344579 3.12224522409416 0.75681657603833 0.9097611343830 4.69622925053729 4.40046011698177 0.4527531763583 -1.1867451991049 0.5792737461034 -1.47306383589634 4.54224684774186 3.34114018896332 -3.81788538051502 -3.81788538051502
	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758188251197 1.83368850960532 0.93557082828671 1.25155943428491 0.2809614264570 -0.2809614242020866973 1.3442202086973 1.3442202086973 1.34242020864570 -0.8310238093284 1.34422020864570 1.34372739858150 3.1557478091566 1.19637833768494 1.76648168687959 1.50547241369747 1.07161874704031 1.76948168682764 5.23240034303841 1.7998968382764 5.23240034303841 1.7998968382496 5.48891578414520 7.0304078832444 0.34270941004978 2.8898558219787 3.70724008262280 2.2597928992060 2.2597928992060	2.9202972859950 3.0440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829188623914 1.84479292423000 2.9659588409903 2.65916592484193 2.8916328601307 2.73543220819863 5.16896258161046 0.07430718160776 4.04625860850845 0.91137435326203 2.92564786992273 2.40700973243585 2.86847714904177 3.96277981679329 2.85847714904177 3.96277981679329 2.1575924244622 3.1388979916245 3.58778803179864 2.8203395542036 1.85331671323246 2.8203395542036	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 -1.61668989249457 2.35996188697230 2.05640688505471 0.30622255176950 3.47023587115834 -2.8126636277268 2.1821443146753 -1.826613673822128828 2.1821443146753 -1.82673822128828 2.1821443146753 3.1224522490416 0.75681657603833 0.90976113438303 4.66629285053729 1.122652490416 0.7558157630333 0.90976113438303 4.66629285053729 1.18067451991049 0.57927397461034 4.54224684774186 -3.34114018396332 -3.18788538051502 -2.99465482241908
	CNPhH 20x 1.41088720406001 0.6243248060080 3.05758138251197 1.83368850960539 0.9355708228671 1.25155943428491 1.25155943428491 1.26259611423955 4.37389129862140 3.12577478091566 1.19637833768494 1.76648168687959 -1.0547241369747 -1.07161874704031 0.89340556586150 3.66948424000055 4.83313265882764 3.36948424000055 4.83313265882764 3.36948424000055 4.83313265882764 3.36948424000055 4.83313265882764 3.36948424000055 4.83313265882764 3.659474330481 1.7999863832446 -0.34270941004978 2.88985589219787 3.75818191528375 3.70724008262280 0.833875002330 0.8416255529097	C Sing [1] ²⁺ 2.9202972859950 2.9202972859950 2.029272859950 2.029272859950 2.029272859550 2.029272859550 2.029272859550 2.02927285846520 2.0298865799167 2.02628623141 2.02959884009903 2.03959884009903 2.03959884009903 2.03959884009903 2.03959884009903 2.03959884009903 2.03959884009903 2.03959884009903 2.0359884009903 2.0359884009903 2.0359884009903 2.0359884009903 2.0359884009903 2.035988409903 2.0359884099273 2.04070973243585 2.08965233718889 2.03696523718889 2.0359786027796 2.04070973243585 2.0369757506 2.64100817506740 2.1358979916245 3.53678803179864 8.2803957102256 3.5565843316917 5.84305967101256 4.30209505410917 5.84305967101256	0.52084122656546 1.296732.40746397 0.75419368039073 -2.69992582522569 -2.46983366371063 -2.14575757648773 -1.86401549550671 -1.864054989249457 2.35996188697230 0.30622255176950 -3.0524068805471 0.30622255176950 -1.8261367385847 -1.02673822128828 -2.18214431496753 -1.5261367385847 -1.02673822128828 3.7094533934579 3.12224522490416 -0.75681657603833 4.69629285053729 0.90976113438303 4.69629285053729 0.45275317639583 -1.180674519910698177 0.45275317639583 -1.38067451991063817 -4.55224684774186 -3.34114018396332 -3.8788538051502 -2.99465482241908 -2.02378341273919
I INN 000000000000000000000000000000000	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.85368850960539 0.9355708228671 1.25155943428491 0.28096142664570 0.0381028093284 1.34422020966903284 1.3442202096693284 1.3442202096142 2.76259611423955 4.37389129862140 3.12577478091566 1.1963783758494 1.76648168687959 1.0567421430747 1.07161874704031 0.8394056586150 0.85397481326584152 3.18729739898977 1.0716187470400055 4.833132658832446 5.336748340488 6.14895078414520 0.03407832444 -0.34270941004978 2.88985589219787 3.7074008262280 0.2597992892060 0.643167565520087 -1.9119167871878	C Sing [1] ²⁺ 2.920297285950 3.0440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829198623914 1.84479292423000 2.95595884009903 2.95595884009903 2.89163356801307 2.73543220819863 3.6896258161046 0.07430718160776 4.04625860850845 0.91137435326203 2.92564786992273 2.40700973243585 2.08965253718889 2.92564786992273 2.40700973243585 2.08965253718889 2.925647789016245 3.58778803179664 2.82033955942036 3.58778803179664 2.82033955942036 3.58778803179664 2.82033955942036 3.58778803179664 2.82033955942036 3.58778803179664 3.58778803179664 3.58778803179664 3.58758051123246 3.58658453416917 5.34521291206967 3.3980598220213	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 -2.14575757648773 1.86401549550671 -1.61668898249457 2.35996188697230 0.3622255176950 3.47023587115834 -2.81626636277268 2.18214431496753 -1.8261367438547 -1.02673822128828 3.709435334457 -1.8261367438547 -1.02673822128828 3.709435334457 -1.8261367438547 -0.7558165703833 0.90976113438303 4.69629285053729 4.40046011698177 -0.4527531763583 -1.1867451991049 0.5792739741034 1.47306383589634 4.52424684774186 3.3411401836332 -3.81788538051502 2.99465482241988 -2.02378341273919 -3.73379660195521
IFNNCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758188251197 1.83368859060532 0.93557082828671 1.25155943428491 0.2809614264570 0.08310238093284 1.344202006697 1.34212020866975 1.34242020864570 0.280961423955 4.37389129862140 1.76648168687959 1.50547241369747 1.07161874704031 1.76648168687959 1.50547241369747 1.07161874704031 1.76948424000065 4.83313265882764 5.23240034303841 1.79998683832495 0.489507483304088 6.148950748134000 5.14892074414520 7.00304078832444 0.34270941004978 2.48948589219787 3.7584191528375 3.70724008262280 2.2597928992060 0.843875002330 0.646167565520087 2.19714843781878	C Sing [1] ²⁺ 2.9202972859950 2.9202972859650 2.9202972859650 2.9202972859650 2.92989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.74889930123350 1.46608667350958 2.96595884009903 2.669116592484193 2.89163356801307 2.7354322018963 5.168326801307 2.7354322018963 5.1689258161046 0.7430748160776 4.04625860850845 0.91137435326203 3.84156367577506 2.64100817506741889 3.84156367577506 2.6410081750674178 3.86847714904177 3.9627798167329 1.35877803179864 3.85877803179864 3.858758031673224 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.3658453416917 5.368453416917 5.368453416917	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.4698336637163 2.14575757648773 1.86401549550671 1.6166898249457 2.35996188697230 2.05640688505471 0.30622255176950 2.35961868505471 0.30622255176950 2.18214431496753 -1.82661367385218824 2.18214431496753 -1.82661367385247 -1.02673822128828 2.18214431496753 -1.52661367385487 -1.02673822128828 2.1821443149753 -1.52661367385487 -0.57927397461034 1.457263851501502 -2.99465482241908 2.0237834127391 -3.73376660155021 -3.7387660155021 -3.7387660155021 -3.4387678266615
Ігххоосососососососососостнининии	CNPhH 20x 1.41088720406001 0.6243248060080 3.05758138251197 1.83368850960539 0.9355708228671 1.25155943428491 0.28096142664570 0.08310238093284 1.344220206697 1.3424202096697 1.3424202096697 1.3424202096697 1.3547478091566 1.19637833768494 1.75648168687959 1.05647241369747 -1.07161874704031 0.89340556586150 3.66948424000055 4.83313265882764 3.18729798986332444 -0.34279490498977 6.56367443304088 6.14895078414520 0.636974332444 -0.3427941004978 2.88985589219787 3.75818191528375 3.70724008262280 0.8438755052307 -2.19718483781878 -1.28343869037181 -2.06372051243299	C Sing [1] ²⁺ 2.9202972859950 2.9202972859950 2.63628272149615 2.63628272149615 2.63628272149615 3.7488930213350 1.46608667350958 3.74882930213350 1.46608667350958 3.2482198623914 3.2482198623914 3.2482198623914 3.2482198623914 3.24821986038045 0.013743526203 2.1557860377506 2.64100817506740 2.1557780173624 3.5362877180479329 2.1557780179816479329 2.1557780179824469177 3.96277981679329 2.15577801798624 3.536584734094177 5.84531671323246 3.536584734094177 5.84531671323246 3.53658453416917 5.845331671323246 5.3558843416917 5.84305967101256 5.343209206997 3.8095987202139 5.0393078012545 3.8039307802168 3.80395987202139 5.0393078012545	0.52084122656546 1.296732.40746397 0.75419368039073 -2.69992582522569 -2.46983366371063 -2.14575757648773 -1.86401549550671 -1.86401549550671 -1.86401549550671 -0.30622255176950 -2.18214431496753 -2.18214431496753 -1.52661367385247 -1.02673822128828 -2.18214431496753 3.12224522490416 -0.75681657603833 3.12224522490416 -0.75681657603833 4.69629285053729 0.90976113438303 4.69629285053729 0.90976113438303 4.69629285053729 0.57927397461034 1.47306383589634 1.47036383589634 1.47036383589634 1.47306383589634 1.47306383589634 1.47306383589634 1.47306383589634 1.37307660159521 -2.937634221908 -2.02378341273919 -2.037874221908 -2.037874221908 -2.0378341273919 -2.037874221908 -2.03783427394 -2.037874221908 -2.03783427394 -2.037874221908 -2.037874221908 -2.037874221908 -2.037874221908 -2.037874221908 -2.037874221908 -2.037874221908 -2.037874221908 -2.037874221908 -2.037874221908 -2.037874221908 -2.037874221908 -2.037874221988 -2.037841273919 -2.037841273919 -2.0378421279419 -2.0378421279419 -2.0378421279419 -2.0378421279419 -2.0378421279419 -2.0378421279419 -2.0378421279419 -2.0378421279419 -2.0378421279419 -2.0378421279419 -2.0378421279419 -2.0378421279419 -2.0378421279419 -2.03784421279419 -2.03784421279419 -2.03784421279419 -2.03784421279419 -2.03784421279419 -2.03784421279419 -2.03784421279419 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.037844212794 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -2.03784421908 -
I INNOUCOUCOUCOUCOUCOUCT Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.85368850960539 0.9355708228671 1.25155943428491 0.28096142664570 0.0381028093284 1.344220209669039284 1.344220209669039284 1.3442202096693284 1.3424202096693284 1.356747478091566 1.1963783768494 1.76648168687959 1.05674241369747 1.07161874704031 0.8394056586150 0.839405688332496 3.18729739898977 1.0716187470400055 4.83313265882764 4.53297480400055 4.83313265882764 0.34270941004978 3.28895078414520 0.0304078832444 0.34270941004978 2.88985589219787 3.7074008262280 0.2597992892060 0.8438750002330 0.64167565520087 -2.1971848718787 8-128343869037181 2.0637205124329	<b>Sing [1]</b> ²⁺ 2.920297285950 2.920297285950 2.72989865799167 2.63628272149615 3.7488930123350 1.46608667350958 3.24829188623914 1.84479292423000 2.9559584009903 2.69116592484193 2.8951682018963 3.24829186238161046 0.9113748536601307 4.04625860850845 0.91137435326203 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786992273 3.841556740 2.36847714904177 3.96277981679329 2.1957924244622 3.13388979916245 3.587780179864 2.82033955942036 1.85331671323246 3.56288453416917 5.3626845316716256 5.4321291206967 5.4320379587202139 5.10932078012156 5.4321291206957	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 1.61668898249457 2.35996188697230 0.3622255176950 3.47023587115834 2.81626636277268 2.18214431496753 3.709435334457 1.58261367438547 1.02673822128828 3.709435334457 1.582613674538547 1.02673822128828 3.709435334457 1.02673822128828 3.709435334457 1.582613674538547 1.02673822128828 3.709435334457 1.52613674538547 1.02673822189834 4.69629285053729 4.40046011698177 1.47306383589634 4.52424684774186 0.57927397461034 1.47306383589634 4.54224684774186 2.99465482241988 2.02378341273919 3.73379660159521 3.41410325146135 0.7087878815779 2.90636119776324
IFNNOCCOCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758188251197 1.83368859060532 0.93557082828671 1.25155943428491 0.28096142664570 0.08310238093284 1.344202006697 1.3424202096697 1.3424202096697 1.3438129862140 1.3424202096697 1.3438129862140 1.2504742041049747 1.07161874704031 1.7664816887959 1.250474214369747 1.07161874704031 1.769484126082764 5.23240014303841 1.79989683832496 1.489507483304088 6.148950748134048 0.3427941004978 2.3597483304088 6.14895074813420 7.00304078832444 0.3427941004978 2.3597483304088 0.4895074832444 0.3427941004978 2.5597928992080 0.843875002330 0.64167555520087 2.19718483781878 2.12834850837181 2.06372051243299 4.71139354118920	<b>c sing [1]</b> ²⁺ 2.920297285950 2.920927285950 2.63628272149615 3.7488930123350 1.46608667350958 3.7488930123350 2.9659588400900 2.9659588400900 2.9659588400900 2.9659588400900 2.9659588400900 2.9659588400900 2.965958840190 2.7354322019863 5.16896258161046 0.0743071816076 4.0462586085045 0.0743071816076 4.0462586085045 0.0743071816076 3.92564786092273 2.40700973243585 3.84156367577566 2.6410081750574 3.8684771408745073 2.1957924244622 3.13388979916245 3.35778031798154203 5.3658453416917 5.8430595942036 1.8533167132246 3.62089515842087 5.36568453416917 5.8430595942036 1.8533167132246 5.3658453416917 5.8430595942036 1.8533167132246 5.3658453416917 5.8430595942036 1.8533167132246 5.3658453416917 5.8430595942036 1.8533167132246 5.363953120265 5.1032070812168 3.6369133102545 2.17444087145073 2.00565520571418	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 -1.61668989249457 2.35996188697230 2.05640688505471 0.30622255176950 2.16216638505471 0.30622255176950 2.18214431496753 -1.82661367385247 -1.02673822128828 2.18214431496753 -1.58261367385547 -1.02673822128828 2.18214431496753 -1.582613673854477 -1.02673822128828 2.18214431496753 -1.5826136738547 -1.02673822128828 -0.7568155763833 0.90976113438303 4.6562285053729 0.90976113438303 4.6562285053729 0.90976113438303 4.654224684774186 -3.34114018396332 -2.934654822419018 2.02378341273919 -3.73379660195921 -2.38767826601552 -2.94654822146135 -0.70878798815779 2.90636119776324 5.21045098024899
	CNPhH 20x 1.41088720406001 0.6243248060080 3.05758138251197 1.83368850960539 0.9355708228671 1.25155943428491 0.28096142664570 0.08310238093284 1.344220206697 1.3424202096697 1.3424202096697 1.3424202096697 1.3547478091566 1.19637833768494 1.75648168687959 1.05647241369747 -1.07161874704031 0.89340556586150 3.66948424000055 4.83313265882764 3.1872973989877 6.53677443304088 6.14895078414520 1.7030407832444 -0.3427934089877 6.53697443304088 6.14895078414520 1.7030407832444 -0.34270941004978 2.889558591219787 3.7581811528375 3.70724008262280 0.8433875002330 0.6416755002330 -2.1971848378188 -1.2834386037181 -2.06372051243299 4.7113354118920 4.7113354118920	<b>Sing [1]</b> ²⁺ 2.9202972859950 3.0440555846520 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.74889930123350 1.46608667350958 3.2482918623914 3.2482918623914 3.2482918623914 2.89163356801307 2.7354322018963 5.168962583169164 0.0743071816077 2.7354322018963 5.1689625831689 2.92564786092273 2.40700973243585 2.92564786092273 2.40700973243585 2.08965253718889 2.92564786092273 2.40700973243585 2.08965253718889 3.8415536757506 2.64100817506740 2.63647714904177 3.96277981679329 2.135789916245 3.53658453416917 5.84305967101256 5.3558454316917 5.84305967101256 5.3558454316917 5.84305967101256 5.3558453102545 3.38095987202139 5.10932078012545 3.8639513102545 2.17444087145073 3.8095987202139 5.10932078012545	0.52084122656546 1.296732.40746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 1.61668989249457 2.35996188697230 0.30622255176950 2.35996188657230 2.32617453715834 2.81626636277268 2.18214431496753 1.5261367385247 1.02673822128828 3.12224522490416 0.75681657603833 3.1224522490416 0.75681657603833 3.1224522490416 0.75681657603833 4.69629285053729 4.40046011698177 0.45275317639583 1.18067451991049 0.57927397461034 1.47306383589534 1.430673451991049 0.57927397461034 1.47306383589534 1.43027451991049 2.332786105921 2.332784127319 2.99465482241908 2.02378341273919 2.3337660159521 2.43876782666715 1.44110325146135 2.0178782421908 2.02378341273919 2.0337842139851577 2.90636119776324 2.0178782426905499 5.73797149967400
I I Z Z U U U U U U U U U U U U U U U U	CNPhH 20x 1.41088720406001 0.62432480600080 3.05758138251197 1.85368850960539 0.9355708228671 1.25155943428491 0.28096142664570 0.0381028093284 1.344220209669039284 1.344220209669039284 1.3442202096693284 1.342202096693284 1.356747478091566 1.1963783768494 1.76648168687959 1.05674241369747 1.07161874704031 0.89340556586150 0.85367481304085 4.83313265882764 4.53297480400055 4.83313265882764 4.53297480400055 4.83313265882764 0.34270941004978 2.8898558219787 3.7074008262280 0.2597992892060 0.8438750002330 0.64167565520087 2.1971848718787 8-128343869037181 2.266772051243299 4.71133354118200 3.85284953451820	<b>Sing [1]</b> ²⁺ 2.920297285950 2.920297285950 2.72989865799167 2.63628272149615 3.7488930123350 1.46608667350958 3.24829188623914 1.84479292423000 2.9559584009903 2.69116592484193 2.8916336601307 2.9559284009903 2.69116592484193 2.8916336601307 2.9559284009903 2.69116592484193 2.8916335601307 4.04625860850845 0.091137435326203 2.925647866992273 2.925647866992273 2.40700973243585 2.08956253118889 3.8415636757506 2.36847714904177 3.96277981679329 2.1957924244622 3.13388979916245 3.587780179864 2.8351584234169127 3.535584534169127 3.5420395520571256 5.4321291206987 2.17444087121567 3.9809587202139 5.10332078012168 3.8639133102545 2.17444087145073 2.09565520571418	0.52084122656546 1.29673240746397 0.75419368039073 2.6999258222569 2.46983366371063 2.14575757648773 1.86401549550671 1.61666989249457 2.35996188697230 2.05640688505471 0.30622255176950 1.3202618715834 2.8126636277268 2.182143149673 1.1826636277268 2.182143149673 2.182143149673 2.182143149673 3.1224522490416 0.75581657603833 0.90976113438305 4.6962928053729 4.40046011698177 0.45275317639583 1.18067451991049 0.575927397461034 4.54224684774186 3.34114018396332 3.1878538051502 2.99465482241908 3.31878538051502 2.99465482241908 3.31878538051502 2.99465482241908 3.187878548051502 2.99465482241908 3.187878548051502 2.99465482241908 3.187878548051502 2.99465482241908 3.187878548051502 2.99465482241908 3.1878785480532 3.187895480532 3.187895480532 3.187895480532 3.187895480532 3.1878954805459 3.9078794854578 3.9078794854578 3.9078794854578 3.9078794854578 3.9078794854578 3.9078794854578 3.9078794854578 3.9078794854578 3.9078794854578 3.90767624 3.92874845978844 3.4078776777777777777777777777777777777777
II I I N N C C C C C C C C C C C C C C C	CNPhH 20x 1.4108720406001 0.62432480600080 3.05758138251197 1.8336885906052 0.93557082828671 1.25155943428491 0.28096142664570 0.08310238093284 1.344202096697 1.3421202096697 1.3421202096697 1.34321202086978 1.34321202086979 1.35424091566 1.19637833768494 1.7664816887959 1.250474214309747 1.07161874704031 1.769484160802586150 3.65948424000055 4.83313265882764 5.23240014303841 1.79989683832496 5.4389459854159 3.6597481340483 5.4389459854159 3.7072400282280 2.25979928992060 0.843387500230 2.459718483781878 3.78818191528375 3.7072400262280 2.25979928992060 0.84387505520087 2.19718483781878 3.7881891528375 2.19718483781878 2.12834850937181 2.06372051243299 4.7113954118920 3.8529484595346 1.47861455281002 -0.1553895704973 4.8529484595346 1.47861455281002 -0.1553895704973 4.8529484595346 1.47861455281002 -0.1553895704973 4.8529484595346 1.47861455281002 -0.1553895704973 4.8529484595346 1.47861455281002 -0.1553895704973 4.8529484595546 1.47861455281002 -0.1553895704973 4.8529484595546 1.47861455281002 -0.1553895704973 4.8529484595546 1.47861455281002 -0.1553895704973 4.8529484595546 1.47861455281002 -0.1553895704973 4.8529484595546 1.47861455281002 -0.1553895704973 4.8529484595546 1.47861455281002 -0.1553895704973 4.8529484595546 -0.1553895744524020 -0.1553895744524020 -0.1553895744520574424 -0.1553895744528002 -0.1553895744528002 -0.1553895744528002 -0.155895744528002 -0.155895744528002 -0.155895744528002 -0.1558957445528002 -0.15885495744528002 -0.1558957445528002 -0.1558957445528002 -0.15589574455528002 -0.15588549574455528002 -0.15588549574492 -0.15588549574492 -0.15588549574492 -0.15588549574492 -0.1558854957497 -0.15588549574492 -0.15588549574492 -0.15588549574492 -0.1558854957497 -0.1558854957497 -0.1558854957497 -0.1558854957497 -0.1558854957497 -0.1558854957497 -0.1558854957497 -0.1558854957497 -0.1558854957497 -0.1558854957497 -0.1558854957497 -0.1558854957497 -0.1558854957497 -0.1558854957497 -0.1	<b>c</b> Sing [1] ²⁺ 2.920297285950 2.920297285950 2.636846520 2.73698865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.24829188623914 1.84479292423000 2.96595884009903 2.69116592484193 2.89163356801307 2.7354322018963 5.16896258161046 0.07430718160776 4.04625860850845 0.07430718160776 4.04625860850845 0.07430718160776 4.04625860850845 0.92564786092273 2.40700973243585 2.858475404177 3.96277981679329 2.1957924244622 3.13388979916245 3.36877718041797 3.96277981679329 2.1957924244622 3.13388979916245 3.3684751404177 5.8430597916245 3.5658453416917 5.8430597916245 3.5658453416917 5.843059712165 5.43212912069659 5.303207812165 5.17444087145073 2.09565520571418 2.6030101432841 3.1228140628095	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 -1.61668989249457 2.3599618869723 2.05540688505471 0.30622255176950 2.18214431496753 -1.82661367385247 -1.02673822128828 2.18214431496753 -1.58261367385344579 3.12224522490416 0.75681657603833 0.90976113438303 4.69629285053729 0.90976113438303 4.69529285053729 0.455275317639583 -1.8067451991049 0.57927397461034 1.47306383596015921 2.31878858051502 2.99465482241908 2.0237834127391 2.33876782660155921 2.343876782660155921 2.343876782660155921 2.343876782660155921 2.343876782660155921 2.343876782660155921 2.343876782660155921 2.343876782660155921 2.343876782660155921 2.343876782660155921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601595921 2.3438767826601597620 2.343876782660159776324 3.3287484577884 2.3447767876787678767876 3.328748477786778767876 3.34876787678767876 3.34876787678767876 3.34876787678767876 3.3487678767876 3.3487678767876 3.3487678767876 3.348767877876 3.3487678767876 3.34877777776 3.348777777777777777777777777
I I I N N C C C C C C C C C C C C C C C	CNPhH 20x 1.41088720406001 0.6243248060080 3.05758138251197 1.83368850960539 0.9355708228671 1.25155943428491 0.28096142664570 0.08310238093284 1.344220206697 1.3424202096697 2.7625961142975 2.7625961142975 2.7625961142975 1.3054724130747 1.0761874704031 0.89340556586150 3.66948424000055 4.83313265882764 3.1872973989877 6.53679443304088 6.14895078414520 1.03640474332444 0.34270941004978 2.88958589219787 3.7581811528375 3.70724008262280 0.84384750052030 -2.19718483761878 1.26367443781878 1.2636724132992060 0.84387550502300 -2.19718483781878 1.26367261243299 4.71139354118920 0.8352485455346 1.47861455281002 -0.15538996704973 1.8552845521092	C Sing [1] ²⁺ 2.9202972859950 2.9202972859950 2.63628272149615 2.63628272149615 2.63628272149615 3.74889930123350 1.46608667350958 3.74889930123350 1.46608667350958 3.2482198623914 3.2482198623914 3.2482198623914 3.2482198623914 3.2495198260850845 0.013743526203 2.9563786092273 2.40700973243585 2.0865253718889 3.92563786092273 2.40700973243585 2.08695253718889 3.92563786092273 2.40700973243585 2.08695253718889 3.1338897916245 3.53658453196244 2.35658453416917 5.84305967101256 5.35658453416917 5.84305967101256 5.3658473409477 3.8095987202139 5.039207801256 5.1039207801256 3.8095987202139 5.0392078012543 3.82728013102545 2.12444027445027 3.98095987202139 5.039207801256 5.1393078012565 5.1393078012565 5.127444087145073 2.1352571418 2.0956552071418 2.0956552071488 2.03501525366415 3.135087963752 1.35051523636415	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 1.86401549550671 1.61669892349457 2.359961886597230 0.30622255176950 2.18214431496753 1.52616374515834 2.281626636277268 2.18214431496753 1.526163745584 7.102673822128828 3.70243539344579 3.1224522490416 0.75681657603833 4.69629285053729 4.0040611698177 0.45275317639583 1.18067451991049 0.57927397461034 1.47306383589534 1.4807451991049 0.57927397461034 1.47306383589534 1.4807451991049 3.332766105921 2.43876782666715 1.44110325146135 2.02378341273919 3.7337666195921 2.43876782666715 1.44110325146135 2.02378341273919 3.73379660159521 2.43876782666715 1.44110325146135 2.02378341273919 3.7337966025921 3.52874845978894 5.73797149967406 3.92874845978894 1.1813740525710
<b>Г</b> I I N N C C C C C C C C C C C C C C C C	CNDPhH 20x 1.41088720406001 0.62432480600080 3.05758188251197 1.83368850960532 0.93557082828671 1.25155943428491 0.03357082828671 1.25155943428491 1.3442020366979 1.34242020366979 1.342420203697979 1.342420203697979 1.37614874704031 1.25047840741369747 1.0761874704031 1.76648168687959 1.50547241369747 1.0761874704031 1.76948168687595 1.50547241369747 1.0761874704031 1.79989683832496 5.23240034303841 1.79989683832496 5.23240034303841 1.79989683832496 5.48891578414520 7.00304078832444 0.34270741004978 2.8597928992060 0.5416756552087 2.1971848378187 2.2597928992060 0.6416756552087 2.1971848378187 2.2597928992060 0.5416756552087 2.1971848378187 2.2594854595346 1.718345118202 3.85294854595346 1.4786145528102 -0.1553896704973 4.85268549621590 3.85007736402556	C Sing [1] ²⁺ 2.9202972859950 2.92029728596520 2.92029728596520 2.9298865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.74889930123350 1.46608667350958 2.69116592484193 2.8916336601307 2.69116592484193 2.8916336601307 2.7354322018963 5.16896258161046 0.07430718160776 4.0462860850845 0.07430718160776 4.0462860850845 0.07430718160776 4.0462860850845 0.07430718160776 4.0462860850845 0.07430718160776 4.0462860850845 2.92564786992273 2.40700973243585 2.64100817506740 2.36847714904177 3.96277981679329 3.8138879916245 5.35578584531679266 5.432039710256 5.43203970122168 3.8809138102545 5.1032076012168 3.8809138102545 5.17440871745073 2.09565520571418 2.003010042841 3.12298194628095 4.50379997643752 1.09520778145073 2.0956520571418 3.12298194628095 4.50379997643752 1.0952077815636415 0.0512767882298132 0.05277882298132 0.0527788298132 0.0527788298132	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 1.61666989249457 2.35996188697230 2.056440688505471 0.30622255176950 3.47023827115834 2.81626636277268 2.1821443149673 3.1224522490416 3.7094353944579 3.1224522490416 0.7558165760383 0.90976113438303 4.6962928053729 4.40046011698177 0.45275317639583 0.90976113438305 1.18067451991049 0.57582165763833 0.90976113438305 1.18067451991049 0.575821657038359634 4.54224684774186 3.341140183965312 2.93965482241908 3.33379660195921 2.43876782666715 1.44110325146135 0.70878798815779 3.73379960195921 2.43876782666715 1.44110325146135 0.70878798815779 3.73379960195921 2.43876782666715 1.44110325146135 0.70878798815779 3.73379960195921 2.4387678266715 1.44110325146135 0.70878798815779 3.732714997406 3.9287484597894 1.58288711286888 3.9287484597894
II II N N C C C C C C C C C C C C C C C	CNPhH 20x 1.41088720406001 0.6243248060080 3.05758138251197 1.83368850960539 0.28096142664570 0.08310238093284 1.344202096697 1.25155943428491 1.26155943428491 1.344202096679 1.3424202096679 1.35424202096679 1.3542420296679 1.3542420296679 1.353476415882764 1.35424094055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.65948424000055 3.707240025280 2.259792892000 0.84338750002330 0.84325850073181 2.263720512432989 4.7113334118920 0.1553895704973 4.85268549621899 4.1570254574832 4.85268549621899 4.15702545748324055 1.4347369627044 3.95711448745055 1.4347369627044 3.95711448740655 1.4347369627044 3.95711448740655 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555 3.45607736402555	<b>c</b> Sing [1] ²⁺ 2.9202972859950 2.9202972859950 2.6362884520 2.63628272149617 2.63628272149617 2.63628272149617 2.63628272149617 2.63628272149617 2.63628272149617 2.63916529484193 2.89163356801307 2.95595884009903 2.85952844193 2.89163356801307 2.7354322018963 5.16896258161046 0.07430718160776 4.04625860850845 0.07430718160776 4.04625860850845 0.07430718160776 4.04625860850845 0.07430718160776 4.04625860850845 0.07430718160776 4.04625860850845 0.07430718160776 4.04625860850845 0.07430718160776 4.04625860850845 0.07430718160776 4.04625860850845 0.07430718160776 4.04625860850845 0.07430718160775 6.3640714907 2.9556784544622 3.13388979916245 3.35778803179864 4.8203957101256 5.432129102565 3.09305987202139 5.0932078012168 3.68369133102545 2.17444087145073 3.12298149628095 4.5037997643752 1.3507688192891 0.02672882598132 0.034382659477	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 1.86401549550671 1.36201549550671 0.30622255176950 0.30622255176950 2.18214431496753 1.1826636277268 2.18214431496753 1.1826636277268 2.18214431496753 1.182673822128828 2.18214431496753 1.182673822128828 3.7094539344579 3.1224522490416 0.75681657603833 0.90976113438303 4.69629285053729 3.1224522490416 0.75681657603833 0.90976113438303 4.69629285053729 3.1224522490416 0.75681657603833 0.90976113438303 4.69629285053729 3.123673737461034 1.47306383589634 4.54224684774186 3.3337660159521 2.934876782666715 9.73874123146135 -0.70878798815779 2.90651977632146135 -0.70878798815779 2.906511977632146135 -0.70878798815779 2.906511977632146135 -0.70878798815779 2.906511977632146135 -0.70878798815779 2.906511977632146135 -0.70878798815779 2.9065611977632146135 -0.70878798815779 2.906541274688871128688 -1.18113740525710 -2.22678730882504 -1.31856547622384
<b>Г</b> I I N N C C C C C C C C C C C C C C C C	CNPhH 20x 1.41088720406001 0.6243248060080 3.05758138251197 1.83368850960539 0.9355708228671 1.25155943428491 1.25155943428491 1.26155943428491 1.26155943428491 1.2615943428491 1.3442202066979 4.37389129862140 3.12577478091566 1.19637833768494 1.76648168687959 1.0564741430747 -1.07161874704031 1.07648168687959 1.50547241369747 -1.07161874704031 0.83340556586150 3.66948424000055 4.83313265882764 3.1872973989877 6.5367443304088 6.14895078414520 1.03644455281002 -0.54594837418528 3.75818191528375 3.70724008262280 0.6416756550087 -2.19718483761878 1.28434860937181 -2.663702143299 4.711393411820 3.852845455346 1.4786145281002 -0.15538996704973 4.8552854621590 4.15702545744839 2.86007736402656 1.53726523052790	C Sing [1] ²⁺ 2.9202972859950 2.9202972859950 2.63628272149615 2.63628272149615 2.63628272149615 3.74889393123350 1.46608667350958 3.74882930123350 1.46608667350958 3.2482198623914 1.84479292423000 2.959584609203 2.951958460370 2.7354220819863 5.16896258161046 0.0743071816077 2.7354220819863 5.16896258310808 2.9256478609273 2.40700973243585 2.0865253718889 2.9256478609273 2.40700973243585 2.0865253718889 3.925674809273 2.40700973243585 2.0865253718889 3.8415636757506 2.64100817506740 2.15577842444622 3.35658433102545 3.35658433102545 3.35658433102545 3.38095987202139 5.0392076012168 3.8095987202139 5.0392076012168 3.8095987202139 5.0392076012168 3.8095987202139 5.0392076012168 3.8095987202139 5.0392076012168 3.8095987202139 5.0392076012168 3.8095987202139 5.0392076012168 3.320955527141 3.60301010432841 3.12281946280955 1.35051523636415 0.0267288258132 0.0267288258132 0.0360768912969	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 1.5166898249457 2.35996188657230 0.30622255176950 3.4702358711834 2.81626636277268 2.18214431496753 1.52616373852178354 1.526163738547 1.02673822128828 3.7094535934579 3.1224522490416 0.75581657603833 4.69629285053729 4.40046011698177 0.45275317639583 1.18067451991049 0.57927397461034 1.47306383589534 4.54224684774186 3.34114018396332 3.1878538051502 2.0378742129624 3.341401839632 3.31878538051502 2.0378742266715 1.44110325146135 2.0378742666715 1.44110325146135 2.0378748266715 1.44110325146135 2.0378748266715 1.44110325146135 2.0378748266715 1.44110325146135 2.0378748266715 1.44110325146135 2.0378748266715 1.4411032541408 3.32874845978894 5.1318740525710 2.22678730882504 -1.3186547622384 -3.850891269902
II IN N C C C C C C C C C C C C C C C C	CNDPhH 20x 1.41088720406001 0.62432480600080 3.05758188251197 1.83368859060532 0.93557082828671 1.25155943428491 0.2809614264570 0.08310238093284 1.3442202086979 1.3421202086979 1.34242020864570 0.2809614220956 1.3637833768494 1.76648168687959 1.50547241369747 1.07161874704031 1.76648168687959 1.50547241369747 1.07161874704031 1.76948168685150 3.65948240003841 1.7999868382764 5.22240034303841 1.7999868382764 5.22240034303841 1.7999868382496 0.8433152688575 4.83313265885150 3.659483304088 6.14895078414520 7.0034078832444 0.34270941004978 2.8898558219787 3.758418522807 2.59792899260 0.843387500230 0.6416755520087 2.19718483781878 2.859485455360 1.4385458514820 3.8529485455366 1.4476455281002 3.85294854595366 1.47861455281002 3.85294854595366 1.47861455281002 3.85294854595366 1.47861455281002 3.85294854595366 1.47861455281002 3.85294854595366 1.434736969270447 3.85286549621690 3.4536748339 2.8600736402656 1.43473696927044 1.3917118471405 1.57286233052790	Sing [1] ²⁺ 2.9202972859950 2.9202972859950 2.92029728596520 2.92089865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.74889930123350 1.46608667350958 2.69116592484193 2.8916336601307 2.69116592484193 2.8916336601307 2.7354322018963 5.16896258161046 0.07430718160776 4.04625860850845 0.91174353260740 2.36847714904177 3.9627781679329 2.8045025718889 3.8415636757506 2.64100817506740 2.36847714904177 3.96277981679329 2.1357824244622 3.138879916245 5.36578453416917 3.9609558720319 5.36574714904177 3.96277981679329 5.3658453416917 3.9609558720319 5.3093207811256 5.43212912069697 3.98095587202139 2.0363013102545 5.10932078145073 2.0956520571418 2.17444087145073 2.0956520571418 2.132444529 4.53079997643752 2.051076581266415 0.02672882598132 0.51507658126417 0.3404696552251470 0.3404696552251470 0.340452547170 0.3404696552251470 0.3404696552251470 0.3404696552251470 0.34046965522547170 0.34046965522547170 0.34046965522547170 0.34046965522547170 0.34046965522547170 0.34046965522547170 0.34046965522547170 0.34046965522547170 0.34046965522547170 0.34046965522547170 0.340469655225471920	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 1.61668989249457 2.35996188697230 2.05640688505471 0.30622255176950 3.47023587115834 2.8126636277268 2.18214431496753 1.582613673822128828 2.18214431496753 1.582613673822128828 2.18214431446753 1.582613673822128828 3.7094539244597 3.12224522490416 0.75681657630833 0.90976113438303 4.696292505372 3.1224522490416 0.75681657630833 0.90976113438303 4.696292505372 3.1224522490416 0.7568165763833 0.90976113438303 4.696292505372 3.1287451891049 0.57927397461034 4.4004601597897 4.4004601597897 4.5224684774186 3.34114018396334 4.54224684774186 3.3417405835051502 2.9965461277391 2.238767226651 2.9063611976524 5.73797149967406 3.9287445978894 1.68888711268883 1.81813740525710 2.22678730882504 1.3186474525710 2.22678730882504 1.3186476225731 3.9287445978894 1.6888871268980 3.938912699906 3.9287445978894 3.0380812699906 3.92874445978894 3.0380812699906 3.4527029488456 3.4527029488456 3.4527029488456 3.4527029488456 3.4527029488456 3.4527029488456 3.4527029488456 3.4527029488456 3.4520292488456 3.4520292488456 3.45202924984556 3.4520292498456 3.45202924984556 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.4520292498456 3.452029248456 3.452029248456 3.452029248456
II INN СССССССССССССССССССНННННННННННННН	CNPhH 20x 1.41088720406001 0.6243248060080 3.05758138251197 1.83368850960539 0.935570828671 1.25155943428491 0.28096142664570 0.08310238093284 1.344202096697 2.76259611423955 4.37389129862140 1.1637833768494 1.76648168687959 1.05647241369747 1.07161874704031 1.76648168687959 1.05647241369747 1.07161874704035 3.66948424000055 4.8331326586150 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.66948424000055 3.67074832444 0.342709410049282 2.889558501978 3.70724008252800 2.25979928992060 0.8433875002330 0.01538395744339 3.8520485495346 1.4786455281002 0.0155389574973 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85268549621690 4.1570254574833 4.85564962	<b>c</b> Sing [1] ²⁺ 2.9202972859950 2.9202972859950 2.63628272149615 2.63628272149615 2.63628272149615 2.63628272149615 2.63628272149615 2.63628272149615 2.63916529384109 2.95595884009003 2.96595884009003 2.96595884009003 2.96595884009003 2.96595884009003 2.96595884009003 2.9659786019863 5.16896258161046 0.07430718160776 4.04625860850845 0.07430718160776 4.04625860850845 0.07430718160776 4.04625860850845 2.08965253718889 3.8815636757506 2.6410081750760 2.6400081750760 2.6407097324385 2.0896525371889 3.1338979916245 3.53778803179864 3.6208515842087 5.35658453416917 5.84305967101256 3.6208515840287 5.3658453416917 5.84305967101256 3.6208515840287 5.3658453416917 5.84305967101256 3.6208515840287 5.3658453416917 5.84305967101256 3.6208515840287 5.3658453416917 5.84305967101256 3.6208515840287 3.30905987202139 5.10932078412525 3.131022353412 2.0515075812809 4.53379997643752 1.3501523634529477 0.3406496552623 0.18571254719029 1.4471118333800	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 1.86401549550671 1.36201549550671 0.30622255176950 0.30622255176950 1.52261367385217834 2.81626636277268 2.18214431496753 1.52261367385217834 2.81626636277268 2.18214431496753 1.52261367385247 1.52261367385247 1.52261367385247 1.52261367385247 1.52261367385247 1.52261367385247 1.52261367385247 1.52261367385247 1.52261367385247 1.52261367385247 1.52261367385247 1.5226136738547 1.52731763583 1.57921397461034 1.47306385589534 1.4524548774186 3.341740638558953 1.373786015921 2.43876782666715 1.44110325146135 1.4410325146135 1.4410325146135 1.4410325146135 1.44110325146135 1.44110325146135 1.44110325146135 1.21245978344173819 2.5278730882504 1.318547622384 1.885871286883 1.1811374055772384 1.885877834857834 1.8858778348857834 1.885476223844 1.8858778348857834 1.885476223844 1.885476223844 1.385547622384 1.385547622384 1.385547622384 1.385547622384 1.385547622384 1.38547622384 1.385547622384 1.3854434880163 0.3452072498456 0.47238813764077
II INN CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	CNPhH 20x 1.4108720406001 0.6243248060080 3.05758138251197 1.83368850960539 0.9355708228671 1.25155943428491 0.2809614266457 0.08310238093284 1.34422020966979 2.7625961143975 4.37389129862140 3.12577478091566 1.19637833768494 1.76648168687959 4.37389129862140 1.76648168687959 4.37389129862140 1.76648168687959 4.3331265882764 1.07161874704031 0.8394056586150 3.66948424000055 4.83313265882764 5.2340043418527 1.07161874704031 0.8395078413520 3.1872973898977 6.53697483304088 6.14895078414520 1.036407832444 0.34270541004978 2.85958928977 3.75718191528375 3.70724008262280 0.64167565520087 2.19718483781878 1.28343869037181 1.26362705143299 4.7113354118920 3.8526454621590 4.1570254574839 2.86007736402656 1.5726632302790 0.6062989284189 2.8007736402656 1.5726632052790 0.6062989284189 2.800573640255	<b>Sing [1]</b> ²⁺ 2.9202972859950 2.9202972859950 2.72989865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.74889930123350 2.8591860283161 1.46608667350958 2.85918602931 2.85918601907 4.04625860850845 5.16896258161046 0.9113743532603 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.92564786692273 2.935778167932 3.8431563777506 2.36847714904177 3.9627798167932 3.15979242444622 3.13388979316245 3.5877803179864 2.82533167132346 3.8389719316255 5.4321291206957 5.43212912069743752 3.9809587202139 5.103407487145073 2.055505571418 3.88369133102545 5.17244087145073 2.0555055125148 3.83809133102545 5.17244087145073 2.055507634125 4.50379997643752 1.35015253636415 0.02677882598132 0.035074832598132 0.0350748552631 0.035074852598132 0.035074852598132 0.035074852598132 0.035074852598132 0.035074852598132 0.035074832598132 0.035074832598133 0.03507495552633 0.18571554719029 1.44711918333800	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 1.6166888249457 2.35996188697230 0.30622255176950 3.4702358715834 2.81626636277268 2.18214431496753 1.5261637435847 1.02673822128828 3.70943539344579 3.1224522490416 0.75581657603833 4.69629285053729 4.40046011698177 0.45275317639583 1.18067451991049 0.57927397461034 1.47306383589534 4.54224684774186 3.34114018396332 3.1378538051502 2.02378341279319 3.73379660159511 2.43876782666715 1.44110325146135 2.07087898815779 2.90636119776324 5.2194598815779 2.90636119776324 5.2194598815779 2.90636119776324 5.2194598815779 2.90787308815779 2.90636119776324 5.2194598245978894 5.118137405257100 2.22678730882504 1.13185476223884 3.05808912699906 1.8264434801163 0.34520729498455 0.47238813764077
I IN N C C C C C C C C C C C C C C C C C	CNPhH 20x 1.4108720406001 0.62432480600080 3.05758188251197 1.83368850960532 0.93557082828671 1.25155943428491 0.2809614264570 0.08310238093284 1.344202006697 1.34212020866973 1.34242020864570 0.280961423955 4.37389129862140 1.76648168687959 1.50547241369747 1.07161874704031 1.76648168687959 1.50547241369747 1.07161874704031 1.76948424000055 4.83313265885150 3.65948424000055 4.83313265885150 3.659482300433841 1.79998683832495 0.489507483304088 0.489507483304088 0.4895074832444 0.3427094100497 2.5397928992080 0.8433875002330 0.6416755520087 2.59792899260 0.8433875002330 0.6416755520087 2.19714843781878 2.859458549118920 3.8529485459536 1.47861455281002 3.8529485459536 1.4786145281002 3.8529485459536 1.47861455281002 3.8529485459536 1.434736969270447 3.8528549621690 0.45339704973 4.85268549621690 0.45339704973 4.8526854921944 1.57254744399 2.8007736402656 1.43473696927044 1.39371118471405 1.57286233052790 0.6062628824819 3.80356064374839 2.80356043748439 2.803560436437868 7.1955865319748 3.03560436437868 7.19558653052790 3.803560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.03560436437868 3.0356043437868 3.035604343788 3.035604343788 3.0356043643788 3.0356043643788 3.035604343788 3.035604343788 3.035604343788 3.035604343788 3.035604343788 3.035604343788 3.035604343788 3.035604343788 3.0356043438 3.035604343788 3.0356043434788 3.0356043434788 3.035604343788 3.035604343788 3.035604343788 3.035604343788 3.035604343788 3.035604343788 3.0356043438 3.035604343788 3.035604343788 3.035604343788 3.035604343788 3.035604343788 3.035604343788 3.0356043434788 3.0356043434788 3.035604343788 3.035604343788 3.03	<b>c</b> Sing [1] ²⁺ 2.920297285950 2.92089865799167 2.63628272149615 3.74889930123350 1.46608667350958 3.74889930123350 1.46608667350958 2.69116592484193 2.8916328623914 1.84479292423000 2.9659584009903 2.69116592484193 2.8916336601307 2.7354322018963 5.16896258161046 0.07430718160776 4.04625860850845 0.91137435362073 2.40700973243585 2.64100817506740 2.36847714904177 3.96277981679329 2.1957924244622 3.1388979916245 3.58778803179864 2.8203395542036 1.8533167132246 2.843059542036 1.8533167132246 3.58778803179864 3.58778803179864 3.58778803179864 2.84305954701256 5.43212912069697 3.3809558720318 2.0390558720318 2.039055872012168 3.63639133102545 2.17444087145073 2.09565520571418 2.60301010432841 3.1228194628095 4.50379997643752 2.051507658912969 4.50379997643752 2.051507658912969 0.0438204552477 0.3406496555267 0.183715929 1.44711918393800 2.207603480707 4.7006733002218	0.52084122656546 1.29673240746397 0.75419368039073 2.69992582522569 2.46983366371063 2.14575757648773 1.86401549550671 1.61668989249457 2.35996188697230 2.05640688505471 0.30622255176950 3.47023587115834 2.8126636277268 2.1821443146753 1.58261367382514637 1.58261367382514637 1.58261367382514637 1.58261367382514637 1.58261367382514637 1.582613673854457 1.58261367382514637 1.58261367385457 1.58261367385457 1.58261367385457 1.58261367385214838 0.90976113438303 4.69629285053729 1.122652490416 0.7588156763833 0.90976113438303 4.69629285053729 1.1807451991049 0.57927397461034 4.69424459784053 2.394764264774186 3.3414018396334 4.5422464774186 3.3414018396334 2.9093641273919 2.33737660195921 2.43876782666715 0.70878798815779 2.9063611976524 5.2194508024899 5.73797149957406 3.92874445978894 1.68888711286883 3.92874445978894 1.688474525710 2.22678730882504 1.3136547622384 3.0380812699906 1.8264434880163 0.931544551467 0.45272948456 0.472288137607 0.9159485028431 0.915948508413 0.931544551467 1.505467 0.45272948455 0.45227948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.4522948455 0.452571 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5567 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.55777 0.5577

#### IrNPhH 1ox dub [1]⁺

Ir	1.27250370216992	2.66065225100001	-0.40566844950282
N	0.49525076430211	2.56640645025630	1.43463497168755
N	2.9253/25193126/	2./3850/2/510534	0.76841702729670
c	1.95610854325086	2.70870688500798	-2.507/3442884457
c	1.10910011373429	3.83601676495339	-2.21045907366082
c	1.193446/1552481	1.51545/30/03/31	-2.23182295792826
c	-0.21695981632337	3.33704049522214	-1.82957052926271
c	-0.166263/3052119	1.90831600377806	-1.84485588810112
c	1.32944789020000	2.62233084000392	2.4815131/4/245/
c	2./34262/63599/6	2.72870831992991	2.09889205212271
C	4.23940107961831	2.84409849901616	0.22493981954/1/
C	3.33801/9122/632	2.76988932445793	-3.0554/9803/46/5
C	1.510/430454/803	5.26697508844582	-2.29502534922377
C	1.68499770519096	0.11554443450638	-2.34/31802885851
C	-1.41614668437326	4.1/321/6699132/	-1.54991233922865
c	-1.3066/0584/0230	0.99167404802521	-1.56614895/99560
c	0.97544097369509	2.56552/060/2240	3.65311457462209
c	3./351616/39/036	2.803/3626869/08	3.10515898737266
c	4.90447878368676	1.68483906028306	-0.18304747537225
C	4.82958652172600	4.10240128128892	0.06309708054082
C	1.9/106/90822694	2.6/1238/0142235	4.79920494692470
C	3.34955678013804	2.78049646678437	4.42392775332086
Ċ	6.09614886731461	4.19343693937745	-0.51/90825698640
C	6.17505156033493	1.78492339695638	-0.75344620720380
	6.76912458281245	3.03868326884718	-0.92544904571773
н	-0.49816508424490	2.49192329772376	1.64574503468582
н	3.29748500966583	2.75676650013355	-4.15491963981809
н	3.94844445304487	1.91965257420452	-2.73320206444456
н	3.8629654128/182	3.68549043065280	-2.75261769939311
н	2.60233716640027	5.350/5168205110	-2.2/1/0465405/02
н	1.103/0548585321	5.85683857493535	-1.461/83/50/2009
н 	1.15/300402///62	J./2//JI28826//5	-3.23249122037759
п	-2.09393388208035	4.1/034493346362	-2.41995505/94618
н	-1.152914/23/58/9	5.21950746249366	-1.356/3564246934
н	-1.999083/536/335	3.80029184877866	-0.69599212478346
н г	4.78035004203424	2.6/0/3084682965	2.6308492644/985
н	4.104/214/292493	2.8390//209526//	5.20591657869100
н	1./256838425/163	2.64666092605235	5.86039807522205
н	-0.0/424090/06/68	2.48914185288853	4.1316528321/918
н	4.29568788355507	4.98979046246618	0.40514189318140
н	4.41636373855636	0.71770961382831	-0.05859184868982
н	2.78012564055149	0.07573645240890	-2.31086452113497
н	1.29516137493370	-0.51666447064837	-1.53777972988039
н	1.37126545013383	-0.34135827854458	-3.30134397304620
н	-1.99456111446452	0.96681065471545	-2.42/46/052/0531
н	-0.97809319492176	-0.03882556054695	-1.386/943498/982
н	-1.89484246227659	1.32766126996122	-0./018041611/53/
н	7.76453046209501	3.11660256601713	-1.3651/883191952
н	6.56862057927220	5.1/015625864945	-0.63221596/135/2
н	6.70860051380217	0.8844/1482652/9	-1.06061498558939
١r	Me native	· [2]+	
		. [-]	
Ir	0.69345166687752	-0.15616795923605	0.02697364549431
lr N	0.69345166687752 0.41083395806592	-0.15616795923605 -2.10719802049580	0.02697364549431 -0.28625359487150
lr N N	0.69345166687752 0.41083395806592 -1.28797237588811	-0.15616795923605 -2.10719802049580 -0.35378824597376	0.02697364549431 -0.28625359487150 0.20543984317884
Ir N N C	0.69345166687752 0.41083395806592 -1.28797237588811 2.65516485399466	-0.15616795923605 -2.10719802049580 -0.35378824597376 0.28561958723051	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282
Ir N C C	0.69345166687752 0.41083395806592 -1.28797237588811 2.65516485399466 2.66628632136956	-0.15616795923605 -2.10719802049580 -0.35378824597376 0.28561958723051 0.85560664803273	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 0.31965476307846
	0.69345166687752 0.41083395806592 -1.28797237588811 2.65516485399466 2.66628632136956 1.58626644745223	-0.15616795923605 -2.10719802049580 -0.35378824597376 0.28561958723051 0.85560664803273 0.90979617694091	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 0.31965476307846 -1.74734913649692
	0.69345166687752 0.41083395806592 -1.28797237588811 2.65516485399466 2.66628632136956 1.58626644745223 1.57795397093653	-0.15616795923605 -2.10719802049580 -0.35378824597376 0.28561958723051 0.85560664803273 0.90979617694091 1.82566487688883	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 0.31965476307846 -1.74734913649692 0.40534301111973
	0.69345166687752 0.41083395806592 -1.28797237588811 2.65516485399466 2.66628632136956 1.58626644745223 1.57795397093653 0.92827361409556	-0.15616795923605 -2.10719802049580 -0.35378824597376 0.28561958723051 0.8556064803273 0.90979617694091 1.82566487686883 1.86127803729631	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 0.31965476307846 -1.74734913649692 0.40534301111973 -0.88133294718497
	0.69345166687752 0.41083395806592 -1.28797237588811 2.65516485399466 2.66628632136956 1.58626644745223 1.57795397093653 0.92827361409556 -3.11405176009872	-0.15616795923605 -2.10719802049580 -0.35378824597376 0.28561958723051 0.85560664803273 0.90979617694091 1.82566487686883 1.86127803729631 1.03250522520081 0.7302467264504	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 0.31965476307846 -1.74734913649692 0.40534301111973 -0.68133294718497 -0.62924975252470
	0.69345166687752 0.41083395806592 -1.28797237588811 2.65516485399466 2.66628632136956 1.58626644745223 1.5779539709367 -3.11405176009872 -2.15038463045955	-0.15616795923605 -2.10719802049580 -0.35378824597376 0.2856198723051 0.85560664803273 0.90979617694091 1.82566487686883 1.86127803729631 1.03250522520081 0.77022467845021 2.1632607290076	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 0.31965476307846 -1.74734913649692 0.40534301111973 -0.88133294718497 -0.62924975252470 0.35338084105093
	0.69345166687752 0.41083395806592 -1.2879723758811 2.65516485399466 2.66628632136956 1.58626644745223 1.57795397093653 0.92827361409556 -3.11405176009872 -2.15038463045965 -3.92226634354573	-0.15616795923605 -2.10719802049580 -0.35378824597376 0.85560664803273 0.90979617694091 1.82566487686883 1.86127803729631 1.0325052520081 0.77022467845021 2.16316967089956	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 0.31965476307846 -1.74734913649692 0.40534301111973 -0.88133294718497 -0.6292497525470 0.35338084105093 -0.51541104415686 0.3292052104716
	0.69345166687752 0.41083395806592 1.2879723758811 2.65516485399466 2.66628632136956 1.58626644745223 1.57795397093653 -3.11405176009872 -2.15038463045965 -3.92226634354573 -1.79443937968677	-0.15616795923605 -2.10719802049580 0.28561958723051 0.855605861958723051 0.8556664803273 0.90979517694091 1.82566487686883 1.86127803729631 1.03250522520081 0.77022467845021 2.16316967089956 -1.60837386682183 0.685168475410	0.02697364549431 -0.28625359487150 0.02543984317884 -0.99529158066282 0.4053470846 -1.74734913649692 0.40534301111973 -0.62924975252470 0.35338084105093 -0.51541104415886 0.23382035194716
	0.69345166687752 0.41083395806592 1.2879723758811 2.65516485399466 2.66628632136956 1.5826644745223 1.57795397093653 0.92827361409556 -3.1202165009872 -3.15038463045965 -3.92226634354573 -1.79443937968677 3.64134247856537 0.92314624142842	-0.15616795923605 -2.10719802049580 0.3537824597376 0.28561958723051 0.85560664803273 1.86127803729631 1.8256487686883 1.86127803729631 0.37022467845021 2.1631696708956 -1.60837386682183 -0.68616884475410	0.02697364549431 -0.28625359487150 0.2054398431784 -0.99529158086282 0.31965476307846 -1.74734915469692 0.40534301111973 -0.682347252470 0.53338084105093 -0.51541104415686 0.23382035194716 -1.54912055719563
	0.69345166687752 0.41083355806592 1.2879223758811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 -3.11405176009872 -2.15038463045965 -3.1226634354573 -1.79443937968677 -0.80314681416843 0.4270652740140	-0.15616795923605 -2.10719802049580 0.33378824597376 0.28561958723051 0.8556064803273 0.90979617694091 1.82556487686883 1.68127803729631 0.77022467845021 2.16316667089956 -1.60837386682183 -0.686168475410 -2.61839484210031	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -0.31366476307846 -1.74734913649692 0.40534301111973 -0.633430111973 -0.632924975252470 -0.535348084105093 -0.51541104415686 0.23382035194716 -1.54912055719563 -0.04510719905666 -0.34510719905666
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 2.66628632136956 1.5822664475223 1.57795397093653 -3.11405176009872 -2.15038463045965 -3.92226634354573 1.79443937968677 3.64134247856537 -0.80314681415843 3.67965539440140	-0.15616795923605 -2.10719802049580 0.35378824597376 0.285661958723051 0.85560664803273 0.90979517694091 1.82566487686883 1.86127803729631 1.03250522520081 0.77022467845021 2.16316967089956 -1.60837386682183 -0.68616884475410 0.59757727809359 1.98848210031	0.02697364549431 -0.28625359487150 0.02543984317884 -0.99529158066282 0.4053470846 -1.74734913649692 0.40534301111973 -0.88133294718497 -0.62924975252470 0.35338084105093 -0.51541104415886 0.23382035194716 -1.54912055719563 -0.04510719905666 1.38156009702597
	0.69345166687752 0.41083355806592 1.287927358811 2.65516485399466 1.58626644745223 1.57795397093653 0.92827361409556 -3.11405176009872 2.15038463045965 -3.92226634354573 -0.80314681416843 0.64134247856537 -0.80314681416843 3.67965539440140 -3.3658664413353	-0.15616795923605 -2.10719802049580 -0.35378824597376 0.28561958723051 0.855606486803273 0.9875606486883 1.86127803729631 1.03250522520081 2.16316967089956 -1.60837386682183 -0.68616884475410 -2.61839484210031 0.59757727803359 -1.98953730162681	0.02697364549431 -0.28625359487150 0.02543984317884 -0.99529158086282 -0.31965476307846 -1.74734913649692 -0.40534301111973 -0.8813329473252470 -0.53338084105093 -0.51541104415868 -0.23382035194716 -1.54912055719563 -0.04510719905666 -1.38156009702597 0.49444719345709 0.15667689702597
Ir N N O O O O O O O O O O O O O O O O O	0.69345166687752 0.41083355806592 1.2879223758811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 -3.11405176009872 -2.15038463045965 -3.1226634354573 -1.79443937968677 -0.80314681416843 3.6796553944012 -3.13658664413353 -2.48902157526632 -1.1755078214424	-0.15616795923605 -2.10719802049580 0.28561958723051 0.285661958723051 0.8556064803273 0.90979617694091 1.82566487686883 1.66127803729631 1.02250522520081 0.77022467845021 2.16316967089956 -1.60837386682183 0.6861684475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.618494475410 -2.61849447540 -2.61849447540 -2.61849447400 -2.61849447400 -2.61849447400 -2.61849447400 -2.61849447400 -2.61849447400 -2.61849447400 -2.61849447400 -2.61849447400 -2.618494400 -2.618494400 -2.618494400 -2.618494400 -2.618494400 -2.618494400 -2.618494400 -2.618494400 -2.618494400 -2.618494400 -2.618494400 -2.618494400 -2.618494400 -2.618494400 -2.618494400 -2.61849400 -2.618494000 -2.6184940000000000000000000	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -1.74734913649692 0.40534301111973 -0.62924975252470 0.3533808410593 -0.51541104415686 0.23382035194716 -1.54912055719563 -0.04510719905666 1.3815609702579
	0.69345166687752 0.41083395806592 1.2879723758811 2.65516485399466 2.66628632136956 0.92827361409556 3.11405176009872 -2.15038463045965 3.92226634354573 -1.79443937968677 3.64134247856537 -0.80314681415843 3.67965539440140 -3.13658664413353 -2.48902157526632 -1.7552087914434	-0.15616795923605 -2.10719802049580 0.35378824597376 0.28561958723051 0.8556064803273 0.90979617694091 1.82566487686883 1.86127803729631 1.03250522520081 0.77022467845021 2.1631697089956 -1.60837386682183 -0.68616884475410 0.5957727809359 -1.98953730162681 -3.98692247435299 -3.98692247435299	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 0.31665476307846 -1.74734916349692 0.40534301111973 -0.88133294718497 -0.62924975252470 0.53538084105093 -0.51541104415886 0.23382035194716 -1.549120557195656 1.38156009702597 0.4944719345709 0.15606508296251 -0.0767669338490 0.4496638184570
	0.69345166687752 0.41083395806592 1.2879223758811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 -3.11405176009872 -3.1240547609872 -3.1240547609872 -3.1240547856337 -0.80314681416843 3.6796553940140 -3.13658664413353 -2.48902157526632 -1.17552087914434 -3.46535957667757	-0.15616795923605 -2.10719802049580 0.28561958723051 0.285664864803273 0.90979617694091 1.82566487686883 1.632250522520081 1.03250522520081 0.77022467845021 2.16316967089956 -1.60837386682183 0.68616884475410 -2.61839484210031 -0.6871684475410 -3.98852724735299 -3.39252346864384	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -0.4053430111973 -0.8133294718497 -0.62924975252470 -0.5333804105093 -0.51541104415686 0.23382035194716 -1.5491205719563 -0.04510719905666 1.3815600702597 0.49444719345709 0.15606508296251 -0.00776766338490 0.49466868189579 -1.4788457496403
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 2.66628632136956 1.58626644745223 1.57795397093653 -3.11405176009872 -2.15038463045965 -3.2126634354573 1.79443937968677 -0.80314681416843 3.67965539440140 3.31365864413353 -2.48902157526632 -1.1755208791434 -3.46635957667757 -0.15430853379651	-0.15616795923605 -2.10719802049580 0.23578824597376 0.28561958723051 0.85560664803273 0.90979617694091 1.8256648786883 1.86127803729631 1.03250522520081 0.77022467845021 2.16316967089956 -1.60837386682183 0.6861688475410 0.5861688475410 0.5861688475410 0.5861688475410 -2.61839484210031 0.59757727809359 -3.32523648644384 2.89924469673019 2.7676442469234	0.02697364549431 -0.28625359487150 0.02543984317884 -0.99529158066282 0.4053470846 -1.74734913649692 0.40534301111973 -0.62924975252470 0.5338084105093 -0.51541104415886 0.23382035194716 -1.5491205719563 -0.04510719905666 1.38156009702597 0.04504719345709 0.15606508296251 -0.0776769338490 0.44966686189579 -1.27836517549603 1.533807672479
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 1.58622644745223 1.57793397093653 2.66628621409556 -3.11405176009872 -3.1503463045965 3.92226634354573 -0.80314681416843 3.6796553940140 -3.13658664413353 -0.80314681416843 -3.48902157256632 -1.17552087914434 -3.4655595766772 -0.15430853379651 1.34263615462090	-0.15616795923605 -2.10719802049580 -0.35378824597376 0.285561958723051 0.855666486803273 0.9875606486803273 0.90979617694091 1.82256487686821 1.63250522520081 0.7702246784521 2.16316967089956 -1.60837386682183 -0.68616884475410 -2.61839484210031 -0.59757727803539 -1.98953730162681 -3.98692247435299 -3.32523648644384 -3.8892446573019 2.76764342692374	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -0.31965476307846 -1.74734913649692 -0.4053430111973 -0.88133294718497 -0.62924975252470 -0.35338084105093 -0.51541104415866 -1.54912055719563 -0.04510719905666 -1.38156009702597 0.49444719345709 0.15606508296251 -0.07767669338490 0.4496686189579 -1.27836517549603 1.53938005674799
	0.69345166687752 0.41083395806592 1.2879223758811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 -3.11405176009872 -3.13446349556 -3.11405176009872 -3.126634354573 -3.9226634354573 -3.92443937968677 -3.9344585337 -0.83146841416843 -3.1355866441333 -2.48902157526632 -1.17552087914434 -3.4653957667757 1.34263615462090 1.22774711105381	-0.15616795923605 -2.10719802049580 0.28561958723051 0.8556064803273 0.90979617694091 1.82566487686883 1.68127803729631 1.03250522520081 0.77022467845021 2.16316967089956 -1.60837386682183 0.68616884475410 -2.61839484210031 0.5975772789359 -1.98933730162681 -3.398692247435299 -3.392523648644384 2.80924469673019 2.767643424592374 0.65168224713682 2.767643424592374	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -1.74734913649692 0.40534301111973 -0.8813329473252470 -0.83133294105093 -0.51541104415686 0.23382035194716 -0.3533884015093 -0.51541104415686 1.3491205719563 -0.04544719345709 0.15606508296251 0.49444719345709 0.15606508296251 -0.0776766338490 0.4966868189579 -1.27836517549603 1.53338005674799 -3.37499290588863
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 2.6662863218056 1.58226644745223 1.57795397093653 0.92827361409556 -3.11405176009872 -2.15038463045965 3.02226634354573 -1.79443937968677 3.64134247856537 -0.80314681416843 3.67965533440140 3.313658664413353 -2.48902157526632 -1.17552087914434 -3.46633597567757 0.15430853379661 1.34263615462090 1.22774711105381 -3.77646482444485	-0.15616795923605 -2.10719802049580 0.28561958723051 0.28561958723051 0.85560664803273 0.90979517634091 1.8256648786883 1.86127803729631 1.03250522520081 0.77022467845021 2.16316967089956 -1.60837386682183 -0.68616884475410 -2.61839484210031 0.59757727809359 -3.32523648644384 2.8092446973019 2.376764346292374 0.65168224713682 3.02139614208224	0.02697364549431 -0.28625359487150 0.02543984317884 -0.99529158066282 0.4053470846 -1.74734913649692 0.40534301111973 -0.62924975252470 0.53338084105093 -0.51541104415886 0.23382035194716 -1.54912055719563 -0.04510719905666 1.38156009702597 0.1566508296251 -0.07576769338490 0.44966668189579 -1.27836517549603 1.5393800574799 -3.17499290588863 0.57779447330058
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485395466 1.58626644745223 1.57795397093653 3.11405176009872 -3.12405176009872 -3.92226634354573 -1.794439379686457 -3.92226634354573 -1.79443937968477 -0.803146841416843 -3.43658664413533 -2.489021575268740140 -3.13658664413533 -2.4890215752687914324 -3.46635957667757 1.34263615462090 1.22774711105381 -3.77646482444485 -2.81789680605112	-0.15616795923605 -2.10719802049580 0.28561958723051 0.285661958723051 0.8556064803273 0.90979617694091 1.82566487686883 1.68127803729631 1.03250522520081 0.77022467845021 2.16316967089956 -1.60837386682183 0.6861684475410 -2.61839484210031 -0.6871684475410 -3.9865274735299 -3.32523648644384 2.80924466473019 2.7676434269234 0.65168224713622 3.02139614208224 2.74701150469074	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -0.31965476307846 -1.74734913649692 0.40534301111973 -0.62924975252470 -0.533804105093 -0.51541104415686 0.2338203519571 -0.04510719905666 -1.54912055719563 -0.045410719905666 -1.3815600702597 0.49444719345709 0.1566508296205 -0.0776769338490 0.4966686189579 -1.27836517549603 1.53938005674799 -3.1749290588863 0.57779447330058 1.55797355661867
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 -3.1140517600872 -3.15038463045965 -3.92226634354573 -1.79443937968677 -0.80314681416843 3.67965533440140 3.1365864413353 -2.48902157526632 -1.1755208791444 -3.46635957667757 -0.15430853379651 -3.47648244435 -3.7764648244485 -3.179680605112 -3.978430195286	-0.15616795923605 -2.10719802049580 0.28561958723051 0.285661958723051 0.85560664803273 0.90979617694091 1.82566487686883 1.602255220081 0.77022467845021 2.16316967089956 -1.60837386682183 0.6861688475410 -2.61839484210031 0.59757727803162681 -4.32277961372662 -3.32523648644384 2.80924469573019 -3.32523648644384 2.80924469573019 -3.32523648644384 2.80924469573119 -3.32523648644384 2.80924469573119 -3.32523648644384 2.80924469573119 -3.32523648644384 2.80924469573119 -3.32523648644384 2.80924469573119 -3.32523648644384 2.80924469573119 -3.32523648644384 2.80924469573119 -3.32523648644384 2.80924469573119 -3.32523648644384 2.80924469573119 -3.32523648644384 2.80924469573119 -3.325364877369 -3.3253777789 -3.3253777787 -3.32537777777 -3.325377777777 -3.3253777777777 -3.32537777777777777777777777777777777777	0.02697364549431 -0.28625359487150 0.02543984317884 -0.99529158086282 0.4053476307846 -1.74734913649692 0.40334301111973 -0.63224975252470 0.53538084105093 -0.51541104415686 0.23382035194716 -1.54921055719563 -0.04510719905666 1.3815609702597 0.15606508296251 -0.0776766938490 0.44966868189579 -1.27836517549603 0.537305674799 -3.17499290588863 0.5779447330058 1.5579355661867 1.4471935124308
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 1.58626644745223 1.57793397093653 0.57793397093653 3.21405176009872 -3.11405176009872 -3.12405176009872 -3.215038463459556 -3.22226634354573 -0.80314681416843 -0.80314681416843 -3.3658664413353 -0.530346853976677526632 -1.17552087914434 -3.4636359576677526632 -1.17552087914434 -3.46363597667730 -0.15430853379651 -1.2277471105381 -3.277646482444855 -2.81789680605112 -1.99783311952586 -3.1984044051851	-0.15616795923605 -2.10719802049580 -0.35378824597376 0.285561958723051 0.8556064876803273 0.90079617694091 1.82266487686833 1.63227803729631 1.03250522520081 2.16316967089956 -1.6083736682183 -0.68616884475410 -2.61839484210031 -0.5975772780359 -1.98953730162681 -3.3252364864384 2.80924469673019 2.76764342692374 -3.225264864384 2.80924469673019 2.76764342692374 0.65168224713582 3.02139614208224 1.62361217543718 0.34848157747490	0.02697364549431 -0.28623359487150 0.20543984317884 -0.99529158086282 -0.31965476307846 -1.74734913649692 -0.4053430111973 -0.88133294718497 -0.62924975252470 -0.53338084105093 -0.51541104415686 -1.54912055719563 -0.04510719905666 -1.3815600702597 0.4946808189579 -0.15606508296251 -0.07767669338400 0.449668619579 -1.27836517549603 1.53938005674799 1.5379355661867 1.44930234677041 -1.47193815243808 0.37771546560243
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 -3.11405176009872 -3.13405176009872 -3.1340547609872 -3.9226634354573 -3.9226634354573 -3.92443937968677 -3.93443937968677 -3.93443937968677 -3.9344585337 -0.83414585537 -0.83414585537 -0.83414585537 -0.3346841416843 -3.48653957667757 -0.15430853379514 -3.475526642 -3.17952486441353 -3.47564515462090 1.22774711105347 -3.3776648515462090 1.22774711105286 -3.19984044051851 -2.8283094160066 -3.19984044051851 -2.8283094160066	-0.15616795923605 -2.10719802049580 0.28561958723051 0.28566486803273 0.90979617694091 1.82566487686883 1.86127803729631 1.03250522520081 0.77022467845021 2.16316967089956 -1.60837386682183 0.77022467845021 2.68816884475410 -2.61839484210031 -0.68816884475410 -3.98692247435299 -3.32523648644384 2.80924469673019 2.76764342692374 0.65168224713682 2.30213942469673019 2.76764342692374 0.65168224713682 3.0213961248243718 0.63816824713682 3.02139612482443718 0.63816824713682 3.02139612482443718 0.33848157747490 -5.37214481558543	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -1.74734913649692 0.40534301111973 -0.62924975252470 -0.6333804105093 -0.51541104415686 0.23382035194716 -0.4510719905666 1.3815600702597 0.49444719345709 0.15606508296251 -0.0776760338490 0.49466868189579 -1.2783615749603 1.53938005674799 -3.17499290588863 0.57779447330058 1.55797355661867 1.44992034677041 -1.47193315243808 0.13775169660243 0.2881546119306
IL N N O O O O O O O O O O O O O O O O O	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 2.66628632136956 1.58626644745223 1.57795397093653 -3.11405176009872 -2.15038463045965 -3.2126634354573 -0.80314681416843 3.67965539440140 3.13658664413353 -2.48902157526632 -1.1755208791434 -3.466352957667757 -0.15430853379651 -1.34266315462090 1.22774711105381 -3.77646482444485 -3.77646482444451 -3.7984341952586005112 -1.9783311952586 0.42033526620076 0.42033526620076	-0.15616795923605 -2.10719802049580 0.33378824597376 0.28561958723051 0.85560664803273 0.90979617694091 1.82566487686883 1.6022552250081 0.77022467845021 2.16316967089956 -1.60837386682183 0.6861688475410 -2.61839484210031 0.58757727809359 -3.32523648644384 2.80924469673019 -3.32523648644384 2.80924469673019 2.76764342692374 0.56168224713682 3.02139614208224 2.74701150469074 1.62361217543718 0.34848157747490 -5.37214481252114 -4.74433185588353	0.02697364549431 -0.28625359487150 0.02543984317884 -0.99529158066282 0.405347804 -1.74734913649692 0.40534301111973 -0.632924975252470 0.35338084105093 -0.51541104415686 0.23382035194716 -1.54921055719563 -0.04510719905666 1.3815609702597 0.15606508296251 -0.07767669338490 0.44966686189579 -1.27836517549603 1.539380574799 -3.17499290588863 0.5777944730058 1.55797355661867 1.4479325467409 -1.471931524308 0.13775169660243 -0.2881540119306 -1.558815541019306
IL N N O O O O O O O O O O O O O O O O O	0.69345166687752 0.41083355806592 1.287927358811 2.65516485399466 1.58626644745223 1.57795397093653 2.6622632146956 -3.11405176009872 -3.11405176009872 -3.1244393796864 -3.1362447856537 -0.80314681416843 -2.48902157526532 -0.80314681416843 -2.48902157526532 -1.7552087914434 -3.46355957667757 -0.554085379651 1.34263615462090 -0.1543085379651 1.34263615462090 -1.257274711105381 -3.77646482444485 -2.81789680605112 -2.78283094160066 -0.42033526620076 0.29158366096974	-0.15616795923605 -2.10719802049580 0.28561958723051 0.28566486803273 0.90979617694091 1.8256648768683 1.686127803729631 1.03250522520081 2.16316967089956 -1.60837386682183 -0.68816884475410 -2.61839484210031 0.59757727809359 -1.99853730162681 -3.98652247435299 -3.32523648644384 -3.9263247435299 -3.32523648644384 -3.92634247435299 -3.32523648644384 -3.92634247435299 -3.32523648644384 -3.921796137642 -3.96632247435299 -3.325364247382 -3.96632247435299 -3.325364247382 -3.96632247435293 -3.96632247435293 -3.96632247435293 -3.92164208224 -3.74701150469074 1.62361217543718 0.3484815774740 0.537214471254174 -4.74433158558535 3.77622790712216	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -1.74734913649692 0.40534301111973 -0.62924975252470 -0.6333804105093 -0.51541104415686 0.23382035194716 -1.54912055719563 -0.04510719905666 1.3815600702597 0.9444719345709 0.15406508296251 -0.07767669338490 0.4966668189579 -1.2783615749603 1.53938005674799 -3.1749929058863 0.57779447330058 1.557973556618677 -1.44930234677041 -1.47193815243805 0.1377516660243 -0.28815460119306 -1.5583655197450
IL N N O O O O O O O O O O O O O O O O O	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 3.11405176009872 -2.15038463045965 -3.11405176009872 -2.15038463045965 -3.1226634354573 -0.80314681416843 3.67965539440140 -3.13658664413353 -2.48902157526632 -1.795208791434 -3.4653957667757 -0.15430853379514 -1.34263615462090 1.22774711105381 -3.3776464515462090 1.22774711105381 -3.3776464244855 -2.81789680605112 -1.9783311952586 -3.19984044051851 -2.78283094160056 0.4203354260076 0.4203354260076 0.2315464267256		0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -1.74734913649692 0.40534301111973 -0.6323430111973 -0.632343013194716 0.35338084105093 -0.51541104415686 0.23382035194716 -1.5491205719563 -0.04544719345709 0.15606508296251 -0.0776760338490 0.49466868189579 -1.2783651759613867 -1.2783651759613867 -1.47493055618677 -1.47493055618677 -1.4749315243808 0.37775169660243 0.2881546119306 -1.55836555197450 -0.283126119306
IN N O O O O O O O O O O O O O O O O O O	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 1.58626644745223 1.57793397093653 1.57793397093653 3.124409556 -3.11405176009872 -3.1503863045965 3.92226634354573 1.79443937968677 3.64134247856537 -0.803146841416843 3.46559576677526632 -1.17552087914434 -3.46559576677526632 -1.17552087914434 -3.46559576677526632 -1.17552087914434 -3.465595766712 -1.1758685379651 1.34263615462090 -1.5378648244485 -2.8178968065112 -1.9783311952586 -3.19984044051851 -2.778240140505512 -2.78283094160066 0.4203526620076 0.2915836606974 -0.53387685470821 -0.73186448267256	-0.15616795923605 -2.10719802049580 -0.35378824597376 0.285561958723051 0.855666486803273 0.9855606486803273 0.9855606486803273 0.9825602648668213 1.63225220081 2.16316967089956 -1.6083736682183 -0.68616884475410 -2.61839484210031 -1.6083736682183 -0.68616884475410 -2.61839484210031 -3.98569234745299 -3.32523648644384 -3.98692247435299 -3.32523648644384 2.3279761372662 -3.98692247435299 -3.3252346444384 2.3279761372662 -3.98692247435299 -3.325234644384 2.3271912464573119 2.76764342692374 1.62361217543718 0.34848157747490 0.53.72214481252114 -4.74433158558533 3.77622790712216 2.97727315359423 2.43832007301112	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -0.31965476307846 -1.74734913649692 -0.4053430111973 -0.68213294718497 -0.62924975252470 -0.53338084105093 -0.51541104415866 -1.54912055719563 -0.04310719905666 -1.5491205719563 -0.04310719905666 -1.5491205719563 -0.045608296251 -0.07767669338490 0.44966868189579 0.945668296251 -1.27836515749603 -1.538360574799 -1.5479355661867 -1.44930234677041 -1.47193815243808 0.1377515660243 -0.2581540119306 -1.5588365197450 -0.45328704641903 -2.1474332915732
Ir N N C C C C C C C C C C C C C C C C C	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.66628632186956 1.58626644745223 1.57795397093653 3.12405176009872 -3.13405176009872 -3.13405176009872 -3.1340547856337 -0.80314681416843 -3.13658664413353 -2.48902157526632 -1.1755208731434 -3.46635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.3426635957667757 1.342663595767757 1.342663595767757 1.342663595767757 1.342663595767757 1.342663595767757 1.342663595767757 1.375656006974 1.39765718798164	-0.15616795923605 -2.10719802049580 0.35378824597376 0.38561958723051 0.8556064803273 0.90979617694091 1.822566487686883 1.632255220081 1.03250522520081 1.03250522520081 0.707224767845021 2.16316967089956 -1.60837386682183 0.68516884475410 -2.61839484210031 -0.68516884475410 -2.61839484210031 -3.98652247435299 -3.32523648644384 2.802446947319 2.76764342692374 0.65168224713682 2.30213964673019 2.76764342692374 0.635168224713682 3.02139614208224 2.74701150469074 1.6336127543718 0.34848157747490 -5.37214481255114 0.34848157747490 -5.37214481255114 2.9772731559423 2.772731559423 2.43832007301112 -3.28869910560274 -3.27824854805779	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -1.74734913649692 0.40534301111973 -0.62924975252470 -0.6333404105093 -0.51541104415686 0.23382035194716 -0.4531074905666 -1.5491205719563 -0.045410719905666 -1.5491205719563 -0.04757696338490 0.4966868189579 -1.27836517549603 1.53938005674799 -3.17499290588863 1.55797355661867 -1.4793920588863 0.5777944730058 1.55797355661867 -1.479326477041 -1.471938152430880 0.1377516966027 -0.2838555197450 0.28315460119306 -1.55836555197450 0.28315460119306 -1.55836555197450 0.28315460119306 -1.55836555197450 0.28315460119306 -1.55836555197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.28315460119306 -1.5583655197450 0.2831546019306 -1.5583655197450 0.2831546019306 -1.5583655197450 0.2831546019306 -1.5583655197450 0.2831546019306 -1.5583655197450 0.2831546019306 -1.5583655197450 0.2831546019306 -1.5583655197450 0.2831546019306 -1.5583655197450 0.2831546019306 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.5583655197450 -1.55836
Ir N N С С С С С С С С С С С С С С С С С	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 -0.92827361409556 -3.11405176009872 -2.15038463045965 -3.92226634354573 -0.80314681416843 3.6796553944014856537 -0.80314681416843 3.679655394401485 -3.13658664413353 -2.48902157526632 -1.1755208791434 -3.16358664413353 -2.48902157526632 -1.34263615462090 1.22774711105381 -3.776648244485 -3.1988044051851 -2.78283094160066 -0.4203356600974 -0.5313646267256 -4.9296325625791 1.15165718798164 -3.8736802544139	-0.15616795923605 -2.10719802049580 0.28561958723051 0.285661958723051 0.8556064803773 0.90979617694091 1.82566487686883 1.6812780329631 1.02250522520081 1.02250522520081 0.77022467845021 2.16316967089956 -1.60837386682183 0.6861684475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -2.6183948475410 -3.98692244692314 0.5975772789339 -3.92523648644384 2.80924469673019 -3.32523648644384 2.8092446973019 -3.325214841252114 0.531612747359 -3.325214841252114 0.53481257747490 -5.37214841252114 -2.438318858535 3.77622790712216 2.97727315359423 2.43832007301112 -3.62869910560274 -1.2372109300097	0.02697364549431 -0.28625359487150 0.02543984317884 -0.99529158086282 -1.74734913649692 0.40534301111973 -0.62924975252470 0.5338084105093 -0.05134104415886 0.23382035194716 -1.54912055719563 -0.04544719345709 0.15606508296251 -1.38156009702597 0.49444719345709 0.15606508296251 -1.3832805674799 -3.749920588863 0.57779447330058 1.5597355661867 1.44793815448019306 -1.55836555197450 -0.48328704641903 -1.5583815540119306 -1.558328704641930 -0.48368609398282 0.72512921800964
Ir N N С С С С С С С С С С С С С С С С С	0.69345166687752 0.41083355806592 1.287927358811 2.65516485399466 2.66626832186956 1.5795397093653 1.57795397093653 3.12405176009872 2.15038463045965 3.92226634354573 1.79443937968677 3.64134247856537 -0.80314681416843 2.48902157526632 -1.17552087914434 3.46635957667757 1.342636154620926 -1.4525087914434 -3.46635957667757 1.342636154620926 -1.47592087914434 -3.46635957667757 1.342636154620926 -0.1534085379651 -2.47896800612 -2.778210105381 -2.77824104451851 -3.376448244485 -2.81789680065174 -0.85387685470821 -0.73136446267256 -0.42033526527911 1.5165718798164 -3.87376802544139	-0.15616795923605 -2.10719802049580 -2.10719802049580 -0.35378824597376 0.285561958723051 1.82566486803273 0.9855606486803273 0.9855606486803273 0.982560264862183 -0.68516884475410 -2.61839484210031 -0.58516884475410 -2.61839484210031 -0.59757727803359 -1.98953730162681 -3.98692247435299 -3.32523648644384 -3.2802446973019 2.76764342692374 0.55168224713582 3.02139614208224 2.74701150469074 0.55168224713582 3.02139614208224 2.74701150469074 0.5518224713582 3.77622790712543718 0.34848157747490 5.3721441252114 -4.7443318858853 3.77622790712216 2.97727315359423 2.43832007301112 2.36286910560274 -2.8284758405779 -1.22372109300097	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -0.31965476307846 -1.74734913649692 -0.40534301111973 -0.62924975252470 0.333804105093 -0.51541104415868 -0.3338041055719563 -0.04510719905666 -1.54912055719563 -0.04510719905666 -1.54912055719563 -0.04510719905666 -1.54912055719563 -0.04767669338490 0.4496686189579 0.94464719345709 -1.2783615749603 1.53938005674799 -3.1749292088863 0.5777944730058 1.557973566186 0.5777944730058 1.557973566184 -1.55836555197450 -0.45328704641903 -1.55836555197450 -0.45328704641903 -1.5436680936982 -0.72513291800964 -2.1193186669089
Ir N N СССССССССССССССССССССССССНННННННННН	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 3.12405176009872 -2.15038463445955 -3.11405176009872 -2.15038463445955 -3.1246534354573 -0.80314681416843 -3.4586541416843 -3.4586541416843 -3.4586541416843 -3.4580505765755 -0.1543085337651 -1.7552087914434 -3.4653957667757 -0.15430853379514 -3.47564515462090 1.22774711105381 -3.776646354542090 1.22774711052586 -3.19984044051851 -2.78283094160065 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.4203352682791 1.516571878164 -3.837680254139 4.40975052278319 3.18435072810977	- -0.15616795923605 -2.10719802049580 0.35378824597376 0.28561958723051 0.8556064803273 0.90979617694091 1.82556487686883 1.03250522520081 1.03250522520081 0.77022467845021 2.16316967089956 -1.60837386682183 0.68616884475410 -2.61839484210031 -0.68616884475410 -2.61839484210031 -3.98692247435299 -3.32523648644384 2.8092469673019 2.8072446973019 2.3021842459214 2.8072446947319 2.0536124743529 -3.325214481557144 0.54681274713682 3.07136124734718 0.3484157747490 -5.3721448155714 0.3484157747490 -5.3721448155734 2.43832007301112 -3.2886910560274 -2.7824878405779 -1.23272109300097 -0.14033829528636 -1.33599733439579	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -1.74734913649692 0.40534301111973 -0.62924975252470 -0.6333404105093 -0.51541104415686 0.23382035194716 -0.453210905666 1.3815600702597 0.49444719345709 0.15606508296251 -0.0776760338490 0.4966868189579 -1.278365175403 0.4944471330056 1.5393005674799 -3.17499290588863 0.57779447330058 1.5797355661867 1.44930236677041 -1.47193315243808 0.3775169560243 0.2881546119306 -1.5883655197450 0.4532870461933 -0.2881546119306 -1.5583655197450 -0.4836680935082 0.72513291800964 -2.11931868690689 -2.25405663360932
Ir N N С С С С С С С С С С С С С С С С С	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 1.58626644745223 1.57793397093653 1.57793397093653 1.57793397093653 3.0222663454755 3.9222663454673 3.64134247856537 -0.80314681416843 3.6796553940140 -3.1365866441335 -2.48902157256632 -1.17552087914434 -3.4653595766772 -0.15430853379651 1.34263615462090 -0.15430853379651 1.34263615462090 -0.15430853379651 -2.8789680605112 -1.9783311952586 -3.19984044051851 -2.77824014051851 -2.77824014051851 -2.77824014051851 -2.77824094160066 -0.42033526525791 1.15165718798164 -0.429265252781 1.5165718798164 -4.492652525791 1.5165718798164 -4.49265252781 1.5165718798164 -4.492632525781 -3.578789841439 -0.7315644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644267256 -0.7431644448 -0.74444854578 -	-0.15616795923605 -2.10719802049580 -2.10719802049580 -0.35378824597376 0.285561458723051 0.8556054846803273 0.90079617694091 1.8225648768483273 0.90079617694091 1.8225648768682183 -0.688616884475410 -2.61839484210031 -1.6083736862183 -0.688616884475410 -2.61839484210031 -1.6083736862183 -0.688616884475410 -2.61839484210031 -3.95957727309359 -1.98953730162681 -3.92564342692374 -3.225264864384 2.80924469573019 2.76764342692374 -3.225264864384 2.80924465973019 2.76764342692374 -3.225264864384 2.80924465973019 2.76764342692374 -3.225264864384 2.80924465973019 2.76764342692374 -3.225264864384 2.80924465973019 2.76764342692374 -3.32548455541352 -3.377622790712216 2.9777315359423 2.4382007301122 -3.62869910560274 -2.72248758405779 -1.2337210300097 -1.233720300097 -1.26516507642564	0.02697364549431 -0.28623359487150 0.02543984371884 -0.99529158086282 -0.31965476307846 -1.74734913649692 -0.4053430111973 -0.88133294718497 -0.62924975252470 -0.53338084105093 -0.51541104415686 -1.54912055719563 -0.04380107907576 -0.438010702597 0.43444719345709 0.15606508296251 -0.07767669338400 0.4496686189579 -1.27836517549603 1.53938005674799 1.53938005674799 1.53938005674799 1.53938023677741 -1.47193815243808 0.37775482917535 -0.4536819740 -1.5588655197450 -0.453287046119305 -0.453287046119305 -0.45328704611933 -0.654565817451 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.453287046119305 -0.4532870461932 -0.4532870461932 -0.45328704725 -0.45328704725 -0.45328704725 -0.453287047
$[ \ \square \ $	0.69345166687752 0.41083355806592 1.287927358811 2.65516485395466 2.6662464745223 1.57795397093653 3.11405176009872 -3.11405176009872 -3.12405176009872 -3.124043937968677 1.79443937968677 -3.03146841416843 -3.4635957667757 -0.543042745533 -0.4890157526537 -0.5430425379651 1.34263615462090 1.22774711105381 -3.77646482444485 -2.81789680605112 -2.78283094160066 -0.42033526620076 0.29138366096974 -0.85387685470821 -0.73136446267256 -4.4929632562791 1.15165718798164 -3.8376802543199 1.8435718798164 -3.8376802543199 -1.640436403483 4.19202382682490	-0.15616795923605 -2.10719802049580 0.3537824597376 0.38561958723051 0.8556064803273 0.90979617694091 1.82266487686883 1.86127803729631 1.03250522520081 2.16316967089956 -1.60837386682183 -0.68616884475410 -2.61839484210031 -0.68716884475410 -2.61839484210031 -0.68716884475410 -3.08953730162681 -4.32277961372662 -3.9869224743529 -3.382523648644384 -4.322779613746673019 2.76764342692374 -3.0213964208224 2.37071354218 0.36484515743788 0.36484515743788 0.36484515744788 0.36484515747490 0.5517543718 0.34848157747490 0.537822790712216 -3.2782487559423 2.47823559423 2.43832007301112 -2.782487554405779 -1.22372109300097 -0.1403382528636 -1.35959793439579 -1.265165074254	0.02697364549431 0.0263984317884 0.09529158086282 0.405384308417884 0.99529158086282 0.40534301111973 0.62924975252470 0.533804105093 0.51541104415686 0.23382035194716 0.53380410593 0.051541104415686 0.23382035194716 0.4350702597 0.49444719345709 0.1560508296251 0.00776769338490 0.4966868189579 0.12783651594503 0.53779447330058 1.5597355661867 1.44930234677041 1.447193815243808 0.13775169660243 0.28815460119306 1.55836555197450 0.4383650547193 2.13473423915732 2.13473423915732 2.13473323915732 2.13473323915732 2.13473323915732 2.13473323915732 2.13473323915732 2.13473323915732 2.13473323915732 2.13473323915732 2.13473323915732 2.13473323915732 2.13473323915732 0.45365042715136 0.45365045715136 0.45365045715136 0.4536506847215 1.22849458965818
$[ \ \square \ $	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 3.12405176009872 -2.15038463045965 -3.11405176009872 -2.15038463045965 -3.1226634354573 -0.80314681416843 3.67965539440140 -3.13658664413353 -2.48902157526632 -1.795208791434 -3.46635957667757 -0.1543085337651 -1.375266315462090 1.22774711105381 -3.7766426305766775 -0.5138768540825 -2.81789680605112 -1.7952087444485 -2.81789680605112 -1.928337685470821 -0.7313644267256 -4.4296325627810 1.515671878164 -3.87376802544139 4.40975052278319 -1.81435072810977 4.16040366403483 -1.920328219977 4.16040366403483 -1.92032822997		0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -1.74734913649692 0.4053430111973 -0.632924975252470 0.533430111973 -0.51541104415686 0.23382035194716 -1.5491205719563 -0.04510719905666 1.38156009702597 0.49444719345709 0.15606508296251 -0.0776760338490 0.49466868189579 -1.27836517549603 1.5393005674799 -3.1749220588863 0.57794347330058 1.55797355661867 1.44930234677041 -1.47193315243808 0.37775169660243 0.2881546119306 -1.5588655197450 0.453287046119306 -1.5588655197450 0.453287046119306 -1.5583655197450 0.453287046119306 -1.5583655197450 0.453287046119306 -1.5583655197450 0.453287046119306 -1.5583655197450 0.453287046119306 -1.5583655197450 0.453287046119306 -1.5583655197450 0.453287046119306 -1.5583655197450 0.453287046119306 -1.5583655197450 0.45368047215 0.57533291800964 -2.119318686906889 2.254056530932 0.77543880647215 -1.2284498965818 2.38459048593886
	0.69345166687752 0.41083355806592 1.287927358811 2.65516485399466 2.66626832186956 3.11405176009872 3.15795397093653 3.9222663454955 3.9222663454573 1.79443937968577 3.64134247856537 -0.80314681416843 3.67965532440140 3.13658664413353 2.48902157526632 -1.17552087914434 3.46635957667757 1.342636154620926 -0.1534085379651 1.342636154620926 -0.1534085379651 1.342636154620926 -0.2913834600567 -0.2913834600567 -0.291316448244485 2.8179984044051851 -2.7782804160066 -0.42033526620076 0.2913834650696974 -0.35337685470821 -0.73136446267256 -0.4203352625791 1.51565718798164 -3.87376802544139 3.443957281097 -1.1604036403483 4.19202382682400 3.23845560726678	-0.15616795923605 -2.10719802049580 -2.10719802049580 -2.80719802049580 -2.80719802049580 -2.85560548273051 -2.85560548459376 -0.85560548403273 -0.85560548403273 -0.855605467845021 -2.6136967089956 -1.60837386682183 -0.68616884475410 -2.61839484210031 -2.61839484210031 -0.59757727803359 -1.98953730162681 -3.98692247435299 -3.32523648644384 -3.2277961372662 -3.98692247435299 -3.32523648644384 -3.2279761372662 -3.98692247435299 -3.32523648644384 -2.65185224713582 -3.926324713582 -3.926324713582 -3.926324713582 -3.9217315359423 -3.6286910560274 -2.8284758405779 -1.22372109300097 -0.14033829528636 -1.39599793439579 -1.255155074254	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -0.31365476307846 -1.74734913649692 0.40334301111973 -0.62924975252470 0.3333804105093 -0.51541104415866 -1.54912055719563 -0.04510719905666 -1.54912055719563 -0.04510719905666 -1.3815600702597 0.94444719345709 0.4596289251 -0.07767669338490 0.4496686189579 0.9496686189579 0.9496686189579 0.9496686189579 -1.2783615749603 1.53938005674799 -3.1749292088863 0.5777944730058 1.557973566186 -1.55836555197450 -0.45328704641903 -1.5438650936882 -1.558365517450 -0.45328704641903 -1.5438660936882 -1.5531291800964 -2.1193166690689 -2.25405663360392 -2.38459647151 -2.384596864715 -2.3849588664715 -2.384598664715 -2.384598664715
к N N C C C C C C C C C C C C C C C C C	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 3.12405176009872 -2.15038463045965 -3.11405176009872 -2.15038463045965 -3.124653454573 -1.79443937968677 -0.631468474856537 -0.80314681416843 -3.4653957667757 -0.1543085337661 -1.75520871434 -3.4653957667757 -0.1543085337651 -1.7952085470821 -0.793311952586 -3.1998444051851 -2.78283094160066 0.420335662076 0.4203356260076 0.4203356260076 0.4203356260076 0.4203356260076 0.4203356260076 0.4203356260076 0.4203356260076 0.4203356260076 0.4203356260076 0.4203356260076 0.4203356262077 4.154043644267256 -4.4296525278319 3.1843507281097 4.16040366403843 -1.92082282190 -2.8321290822570 -4.33851290822570 -4.33851290822570 -4.33851290822576	-     -     -     0.15616795923605     -2.10719802049580     -2.00719802049580     -2.80719802049580     -2.80719802049580     -0.35378824397376     -0.36561958723051     1.825266487686883     1.60837386682183     1.60387386682183     -1.60837386682183     -2.6381684475410     -2.61839484210031     -2.61839484210031     -2.6381684475410     -2.61839484210031     -3.98692247435299     -3.32523648644384     -3.2277961372662     -3.98692247435299     -3.3253648644384     -2.66454844210231     -2.66454844210231     -2.6764342692374     0.65168224713682     -3.926924735299     -3.32214481257144     0.548645844     -2.474315585353     -3.7622790712216     -2.782487858935     -3.762279071221     -3.22865910560274     -2.3724848155714790     -3.372843805779     -1.2337210930097     -0.1403382528636     -3.9599793439579     -1.2516507642544     -3.35768451802480     0.604284558418     1.3960825704327     -3.89937039237136	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -1.74734913649692 0.4053430111973 -0.62924975252470 -0.6333404105093 -0.51541104415686 0.23382035194716 -0.4532719563 -0.045410719905666 -1.5491205719563 -0.04541719905666 -1.3815600702597 0.49444719345709 0.15606508296251 -1.27836517549603 -1.27836517549603 -1.27836517549603 -1.27836517549603 -1.27836517549603 -1.47193815243808 0.1377516966044 -0.281346477041 -1.47193815243808 0.1377516966044 -0.281346411930 -2.1347323915732 0.64565842715136 -0.4835680938982 0.72513291800964 -1.21394680689 -2.25405663360932 -0.72513291800964 -1.2284958690689 -2.25405663360932 -0.75148380647503 -1.2284945895188 -3.8459048593866 1.3620657431076 0.66367675802304
Ir N N С С С С С С С С С С С С С С С С С	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 1.58626644745223 1.57793397093653 1.57793397093653 3.124409556 -3.11405176009872 -3.1503863045965 3.92226634354573 -0.80314681416843 3.6796553940140 -3.13658664413853 -1.7552087914434 -3.465659576677526632 -1.17552087914434 -3.4656595766772 -0.15430853379651 1.34263615462090 0.15430853379651 1.34263615462090 0.291583606974 -0.831876854708214 0.73186448264256 -3.19984044051851 -3.7786468244485 -3.1789680605112 -1.9783311952586 -3.19984044051851 -3.7786468244485 -3.1876685257591 1.15165718798164 -0.4292632525791 1.15165718798164 -4.4292632525791 1.15165718798164 -4.429632527819 -3.433072810977 -4.16040366403483 4.19203822570 -3.2884550756678 -4.4146585418910 -2.708437838164	-0.15616795923605 -2.10719802049580 -2.10719802049580 -0.35378824597376 0.285561458723051 1.825664876863273 0.9875607648603273 0.9875607648603273 0.9875607845521 2.16316967089956 -1.60837368628183 -0.68616884475410 -2.61839484210031 -1.60837368628183 -0.68616884475410 -2.61839484210031 -3.98569247435299 -3.32523648644384 -3.98692247435299 -3.32523648644384 2.802944697301 2.76764342692374 -0.85168224713529 -3.232348644384 2.74701150469741 1.62361217543718 0.34848157747490 0.53.7214481252114 -4.74433158558533 3.77622790712216 2.977727315359423 2.43832007301112 -3.62869190560274 -2.78248758405779 -1.235710900097 -1.235710900097 -1.23571690560274 -2.78248758405779 -1.2357568451802480 0.50024246558418 1.3960825704327 3.8993703923136 3.341699526683015	0.02697364549431 -0.28625359487150 0.02543984317884 -0.99529158086282 -0.31366476307846 -1.74734913649692 -0.4053430111973 -0.68133294718497 -0.62924975252470 -0.53338084105093 -0.51541104415686 -1.54912055719563 -0.04510719905666 -1.5491205719563 -0.04510719905666 -1.5491205719563 -0.04510719905666 -1.5491075796473 -0.4592682651 -0.07767669338490 0.44966868189579 0.5496682754709 -1.27836517549603 1.53938005674799 -1.27836517549603 1.5597355661867 1.44930234677041 -1.47193815243808 0.377516560243 -0.45328704641903 -2.15486609326992 -2.54056332715136 -0.453628715136 -0.4536280936982 -2.2540563360932 -0.77548380647215 -2.2849558858 -2.38495895866 -3.28495895866 -3.28495895866 -3.28495895866 -3.2849549234255
Г 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.6662864745223 1.57795397093653 3.12405176009872 -3.11405176009872 -3.12405176009872 -3.12405176009872 -3.13405176009872 -3.134586537 -0.80314681416843 -3.4365866441353 -3.48902157526632 -1.7552083791434 -3.46635957667757 1.34263615462090 1.227747111053879663 -3.19984044051851 -3.7764648244485 -3.1798400605112 -2.78283094160066 -0.42033526620076 0.29153366096974 -0.85387685470821 -0.73136446267256 -4.4929632565791 1.15165718798164 -3.83776802543199 -1.843507281097 4.1604036403433 4.19203282682490 3.238512908225570 -3.7864643434 -1.927831260576678 -4.4445855418910 -2.708437836164 -3.83090301478	- -0.15616795923605 -2.10719802049580 0.35378824597376 0.28561958723051 0.8556064803273 0.90979617694091 1.822566487686883 1.63225522081 1.0325052252081 1.0325052252081 2.1631696708956 -1.608373866847510 -2.61839484210031 -0.68516884475410 -2.61839484210031 -0.68516884475410 -2.61839484210031 -3.986953730162681 -3.9869527435299 -3.32523648644384 -3.32523648644384 -3.325364864384 -3.302139614208224 2.74701150469074 1.6236127543718 0.3484815774740 0.6516822471352914 -3.7262290712216 -3.3269910560274 -3.728248758405779 -1.2837210930097 -1.2837545405779 -1.2537210930097 -1.253754542 -3.378558052 -1.395997343857 -1.2651650764258 -1.39599734387 -1.2651650764258 -1.39599734387 -1.2651650764258 -1.39599734397 -1.2651650764258 -1.39599734397 -1.2651650764326 -1.39599734397 -1.2551650764327 -3.39897039237136 -3.3468952663605 -2.4787715216711	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -1.74734913649692 0.40534301111973 -0.62924975252470 -0.8313329418497 -0.62924975252470 -0.51541104415686 0.2338203519513 -0.04510719905666 -1.5491025719563 -0.04540719905666 -1.5491025719563 -0.04944719345709 0.15606508296251 -0.0776769338490 0.44966868189579 -3.17499290588863 0.57779447330058 1.55797355661867 -1.4793024677041 -1.4793815243806 0.13775169660243 -0.28815460119306 -1.55836555197450 0.4583655197450 0.4583655197450 0.4583655197450 -0.45328704641903 -2.113918680689 -2.2540566336932 0.775488606389 -2.2540566336932 0.7754880647255 -1.2284458958861 2.38459048593866 2.38459048593866 2.364578427167
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 3.12405176009872 -2.15038463045965 -3.11405176009872 -2.15038463045965 -3.1226634354573 -0.80314681416843 3.67965539440140 -3.13658664413353 -2.48902157526632 -1.795208791434 -3.46635957667757 -0.1543085337651 -1.375266315462090 1.22774711105381 -3.77664261545620976 0.29158366096974 -0.7313644267256 -4.492963256278319 1.515677878164 -3.8776802544139 4.4097552278319 2.1843550756678 -4.9296325278319 1.516571878164 -3.87376802544139 4.4097552278319 2.18435507286139 -1.23284299325278 -1.1940366403483 -1.232804940515278164 -3.87376802544139 -1.03284258027667 -2.23845560756678 -1.2328425907557 -1.640366403483 -1.232803901478 -2.23845507566788 -2.23851290822570 -2.3384556075678	-0.15616795923605 -2.10719802049580 -2.10719802049580 -0.35378824597376 0.285560548297376 0.285560548297376 0.28556054803273 0.90079617694091 1.8256648768403273 0.93250522520081 1.03250522520081 -1.6083736682183 -0.68616884475410 -2.61839484210031 -2.61839484210031 -0.59757727809359 -1.98953730162681 -0.59757727809359 -1.98953730162681 -3.325264864384 2.80924463673019 2.76764342692374 -3.325264864384 3.20139614208224 0.055168224713582 3.37762279071216 2.97727315359423 2.438207071112 -3.62869910560274 -2.322484758405779 -1.26516507642564 -1.395997343579 -1.26516507642564 -1.395997343579 -1.26516507642564 -1.395997343579 -1.26516507642564 -1.395997343579 -1.26516507642564 -1.395997343579 -1.26516507642564 -1.3959973237136 3.41689526683015 2.4778715216711	0.02697364549431 -0.28623354871784 0.0254398431784 0.0254398431784 -0.99529158086282 -0.31365476307846 -1.74734913649692 -0.483324718497 -0.62924975252470 0.5333808410593 -0.51541104415866 -1.54912055719563 -0.045107190563 -0.045071905297 0.49444719345709 0.15606508296251 -0.07767669338490 0.4496686189579 -1.27836517549603 1.539338005674799 0.4496686189579 -1.47836317549603 1.539338056517450 0.43966864175150 -0.5565055197450 -0.5582704641903 -0.55828704641933 -0.5582197450 -0.5582197450 -0.55828704641933 -0.558365197450 -0.55328704641933 -0.558365197450 -0.55328704651935 -0.24845809389380 -2.1347323915722 -0.755438064721536 -0.43666093280946 -2.13913866609389 -2.254065630932 -0.7754838064721536 -0.435680938866 -3.226495782034 -2.254056578234 -2.254056578234 -2.384594285818 -3.384594275862 -3.581274247586 -3.581274242587 -3.581274242587 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.591724247586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586 -3.59172447586
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 2.66626832186956 3.11405176009872 3.15795397093653 3.12405176009872 3.12405176009872 3.124043937968677 3.64134247856537 -0.80314681416843 3.67965532404140 3.13658664413353 2.489021575667757 -0.15340853796617 1.342636154620926 -0.1534085379651 1.342636154620926 -0.29318366096974 4.3476565278319 1.5165718798164 -3.8776802544139 3.1843507281097 1.15165718798164 -3.8776802544139 3.1843507281097 1.15165718798164 -3.87376802544139 3.1843507281097 1.15165718798164 -3.87376802544139 3.1843507281097 1.15165718798164 -3.87376802544139 3.1843507281097 -1.16040366403483 4.19202382682490 3.23851290822570 -4.4344556075678 -4.4344556075678 -4.434455075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.43445855075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585075678 -4.4344585	-0.15616795923605 -2.10719802049580 -2.10719802049580 -2.80719802049580 -2.80719802049580 -2.80719802049580 -2.80719802049580 -2.80540564803273 -0.8556654803273 -0.8556654803273 -0.8556654868313 -0.86516884475410 -2.61839484210031 -2.61839484210031 -2.61839484210031 -0.5975772780339 -1.98953730162681 -3.98692247435299 -3.32523648644384 -3.3267961372662 -3.98692247435299 -3.32523648644384 -3.3273761372662 -3.98692247435299 -3.32523648644384 -3.2277961372662 -3.3964324203374 -0.551862247435293 -3.5214441352114 -4.7443318558535 -3.77244713559423 2.43832007301112 -3.62869190560274 -2.7227413559423 2.43832007301112 -1.25515507642564 -1.35599793439579 -1.2251507642564 -1.35599793439579 -1.25515507642564 -1.35959793439579 -1.25515507642564 -3.35768451802480 0.60042846558418 -1.3960825704327 -3.848751802480 0.60042846558418 -3.47689527034327 -3.8939739237136	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 0.40534300111973 -0.632924975252470 0.4333400111973 -0.632924975252470 0.5333804105093 -0.51541104415686 0.23382035194716 -1.54912055719563 -0.04510719905666 1.3815600702597 0.9444719345709 0.15606508296251 -0.07767669338490 0.4496686189579 0.9496686189579 0.9496686189579 0.9496686189579 -1.2783615749603 1.53938005674799 -3.1749290288863 0.5777944730058 1.557973561618 0.4396660243 -0.28815460119306 0.4532670461 -1.47193815243805 0.28815460119306 0.45326704611933 -2.15436660243 -0.28815460119306 0.45326704611933 -2.1543166660689 -2.25405663360932 -2.25405663360932 -2.25405663360932 -2.25405663360932 -2.25405663360932 -2.254056637431076 0.66367675802304 .40978092185256 2.50517294247586 2.36517294247586 2.36517294247586 -3.650657431076 0.66367675802304 .40978092185256 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586 -3.0517294247586
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 3.12405176009872 -2.1503843045955 -3.12405176009872 -2.1503843045955 -3.12458537 -0.80314681416843 -3.13658664413353 -2.48902157526632 -1.7552087914434 -3.4653557667757 -0.15430853379651 -1.34263615462090 1.2277471110537 -3.37766425444855 -3.178968006517 -0.453307565470821 -0.453307585470821 -0.73136446267256 -4.4296325625791 4.155456470821 -0.73136446267256 -4.4296325627819 3.18435072810977 4.160403664038576678 -4.4384550756678 -4.4384550756678 -4.4384556418910 -2.70984373336164 -3.83376802541399 -2.3326489301478 -3.2354112314333 -2.332648935448190 -2.33456418910 -2.70984373336164 -2.33456418910 -2.70984373336164 -2.33456418910 -2.70984373336164 -2.33456418910 -2.70984373336164 -2.33456418910 -2.70984373336164 -2.33456418910 -2.70984373336164 -2.33456418910 -2.70984373336164 -2.33456418910 -2.70984373336164 -2.33456321025755 -1.23551112314133	-0.15616795923605 -2.10719802049580 0.35378824597376 0.385661958723051 0.8556064803273 0.90979617694091 1.822566487686883 1.0325052252081 1.0325052252081 1.0325052252081 2.16316967089956 -1.60837386682183 0.70224784521 2.16316967089956 -1.60837386682183 0.85816884475410 -2.61839484210031 -3.98652247435299 -3.32523648644384 2.802446947319 2.76764342692374 0.65168224713682 2.3021964673019 2.76764342692374 0.635168274713682 3.0213961428528535 3.77622790712216 0.34848157747490 -5.37214481252114 2.782478585535 3.77622790712216 -3.2868910560274 -3.2724713559423 2.43832007301112 -3.2868910560274 -3.2724748528636 1.39599793439579 -1.2516507642528636 0.5004284558418 1.39508728636 0.5004284558418 1.39508728436 2.24787715216711 3.2750650158188 3.5147986621225 1.40813715887020 1.256812824015 3.5147986621225 1.40813715887020 1.600428451287 1.40813715887020 -1.6004124558418 3.5147986621225 1.40813715887020 -2.0004784558758 -2.4787715287070 -1.6750500158188 -2.4787715287070 -2.4787715216711 3.7506500158188 -2.4787715216711 3.7506500158188 -2.4787715216711 3.7506500158188 -2.4787715216711 3.7506500158188 -2.4787715216711 3.7506500158188 -2.4787715216711 3.7506500158188 -2.4787715216711 3.7506500158188 -2.4787715216711 3.7506500158188 -2.4787715216711 3.7506500158188 -2.4787715216711 3.7506500158188 -2.4787715216711 3.7506500158188 -2.4787715216711 -2.74848157877020 -2.4787715216711 -2.74848157887020 -2.4787715216711 -2.74848157887020 -2.4787715216711 -2.74878715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216711 -2.7478715216	0.02697364549431 0.02639784517884 0.09529158086282 0.40534301111973 0.43196476307846 -1.74734913649692 0.4053430111973 -0.632924975252470 0.5333084105093 -0.51541104415686 0.23382035194716 -0.4532719563 -0.04510719905666 1.3815600702597 0.49444719345709 0.15606508296251 -0.0776769338490 0.49966868189579 -1.27836517549603 1.53938005674799 -3.17499290588863 0.57779447330058 1.55797355661867 -1.27836477041 -1.47193815243088 0.1377516966037 -0.4836680793 -2.1347323915732 0.645684471033 -2.1347323915732 0.6456844715136 -0.4835680936982 -0.7513291800964 -1.2583655197450 0.48366809389582 0.72513291800964 -1.2583655197450 0.4835680936982 -0.75458454715136 -1.324945925818 2.34459048593866 1.3220497541076 0.66367675802304 2.40978092185256 1.33781142427871 1.5514313738557 2.15607483364377 2.15607483364377 2.1560748336437
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 1.58626644745223 1.57793397093653 1.57793397093653 3.12441405176009872 2.15038463045965 3.22226634354573 1.79443937968677 3.64134247856537 -0.80314681416843 3.6796553940140 3.365866441335 2.48902157256632 -1.17552087914434 -3.4656595766772 -0.15430853379651 1.34263615462090 0.15430853379651 1.34263615462090 0.291583606974 -0.291583606974 -0.291583606974 0.291583606974 0.291583606974 0.2915836262076 0.291583606974 0.3136448267256 -0.4292052525791 1.15165718798164 4.429265255791 1.15165718798164 4.429265255791 1.15165718798164 4.383768241097 4.16040366403483 4.192038226570 2.3845560756678 -4.4146555618910 -2.7084378336164 1.3280390301478 -1.2355112313133 0.1412241786920	-0.15616795923605 -2.10719802049580 -2.10719802049580 -0.35378824597376 0.285561458723051 1.825664876803273 0.90979617694091 1.825664876868213 1.03250522520081 2.16316967089956 -1.6083736682183 -0.68616884475410 -2.61839484210031 -1.6083736682183 -0.68616884475410 -2.61839484210031 -3.95957727309359 -1.99953730162681 -3.98692247435299 -3.325236466473019 2.76764342692374 -3.2279614278224 -3.9869224713529 -3.325344645973019 2.76764342692374 -3.2279413528 3.02139614208224 2.74701150469074 1.62361217543718 0.34848157747490 0.53.7214481252114 -4.74433158558533 3.7762279012216 2.97727315359423 2.43832007301112 -3.62869190500274 -2.78248758405779 -1.235710300097 -0.14033829528636 -1.3959793439579 -1.26516507642564 -0.357684518024800 .50202486558418 1.3960825704327 -3.8993703237136 3.41689526683015 2.24787715216711 .27506500183188 3.33147986621225 -2.4787715216711 .27506500183188 -3.3214986621225 -2.4787715216711 .27506301518188 -3.3147986621225 -2.4787715216711 .2750630158188 -3.3147986621255 -2.4787715216711 .2750630158188 -3.3214986621255 -2.4787715216711 .2750630158188 -3.321498662125 -2.4787715216711 .2750630158188 -3.3214798662125 -2.4787715216711 .2750630158188 -3.321479862125 -2.4787715216711 -2.5750645500227 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500216 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.275063500210 -3.27506350021	0.02697364549431 -0.28625359487150 0.20543984717884 -0.99529158086282 -0.31366476307846 -1.74734913649692 -0.4053430111973 -0.68133294718497 -0.62924975252470 -0.35338084105093 -0.51541104415686 -1.54912055719563 -0.04510719905666 -1.5491205719563 -0.0430702597 0.49444719345709 0.456668189579 -1.2783615749603 1.53938005674799 0.456668189579 -1.2783615749603 1.53938005674799 -1.2783615749603 1.55930561877 1.44930234677041 -1.47193815243808 0.377516560243 -0.45328704641903 -2.154866005936982 -2.5506633609326 -2.5545632715136 -0.4536680936982 -2.2540566360932 -0.7548380647215 -2.2849589566 -3.284959866 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.28495898586 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589856 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.2849589836 -3.284958985 -3.284958985 -3.284958985 -3.284958985 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284958985 -3.284958985 -3.284958985 -3.284958985 -3.284958985 -3.284958985 -3.284958985 -3.284958985 -3.284958985 -3.284958985 -3.284958985 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.284959885 -3.
	0.69345166687752 0.41083355806592 1.287927358811 2.65516485399466 1.58626644745223 1.57795397093653 2.66226821469556 3.11405176009872 -3.1405176009872 -3.12405176009872 -3.13405176009872 -3.13405176009872 -3.13405176009872 -3.13658664413835 -3.4800157526632 -1.7552087914434 -3.465615462090 1.2277471105381 -3.77646482444485 -3.8789680605112 -2.78283094160066 -0.42033526620076 0.29158366096974 -0.85387685470821 -0.73136446267256 -4.4929632562791 -1.5165718798164 -3.87376802543189 -1.85478128094 -3.87376802543189 -1.85478128094 -3.87376802543189 -1.85481280278319 -3.834264934854 -3.8376802543189 -3.834264934854 -3.8376802543189 -3.834264934854 -3.2376802543189 -3.83426493483 4.19202382682490 -3.238511290228570 -2.2708437383164 -3.35800390301478 0.37265189334640 0.3726518934649 0.3726518934649 0.3728518132418939 -1.8458554189310 -3.72654183301 -3.72654833464 0.372851812341133 -3.72854183246892 -3.2708437383164 -3.3580039031478 0.372851812341133 0.372851812341133 0.372851812341133 -3.760027557 -1.23551112314133 -1.345800297557 -1.23551112314133 -1.345800297557 -1.23551112314133 -1.345800297557 -1.2355111234133 -1.345800297557 -1.2355111234133 -1.345800297557 -1.2355111234133 -1.345800297557 -1.23551112344133 -1.345800297557 -1.23551112344133 -1.345800297557 -1.23551112344133 -1.345800297557 -1.25551112344133 -1.3580039031478 -1.3580039030478 -1.3580039030478 -1.3580039030478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.358003903478 -1.3580039	-0.15616795923605 -2.10719802049580 0.28561958723051 0.28561958723051 0.85566486803273 0.90979617694091 1.8226648768683 1.86127803729631 1.03250522520081 2.160837386682183 0.68616884475410 -2.61839484210031 0.5975772789359 -1.98953730162681 -3.9869224743529 -3.39253264644384 -3.3227361372662 -3.9869224743529 -3.32523648644384 -3.322364864384 -3.302139614208224 2.74701150469074 1.6236117543718 0.36484515744740 0.65168224713522 3.02139614208224 2.74701150469074 1.6236117543718 0.3484815774740 0.5537214481255144 -2.78248758405779 -1.22372109300097 -1.237213559423 2.6286910560274 -2.78248758405779 -1.22372109300097 -1.2357645458418 2.3547986451802480 0.60042846558418 2.354798663015 2.24787715261711 3.2750650158188 3.5314798661225 1.40813715887020	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -1.74734913649692 0.40534301111973 -0.62924975252470 0.6333804105093 -0.51541104415686 0.23382035194716 -1.54912055719563 -0.04510719905666 0.23382005719905 -0.045407092597 0.49444719345709 1.5491205719561867 -0.04767669338490 0.4966868189579 -1.27836517549603 1.53938005674799 -3.174992058863 0.57779447330058 1.557973556618677 -1.44930234677041 -1.47193815243806 0.13775169660243 -0.28815460119306 -1.55836555197450 0.45328704715136 -0.48366809936828 0.72513291800964 -1.538459048593866 -0.47548459048593866 -0.775438459048593866 1.3260457431076 0.6363675802304 .2409740218526 2.50517294247586 1.36214957431076 0.63637675802304 .2409748137338657 2.19007483361347 .56143137338657 2.19007483361347 .56143137338657 2.19007483361347 .29674825700556 -3.5412742628233
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.66628632136956 1.58626644745223 1.57795397093653 3.12405176009872 2.15038463445955 3.1246543454573 3.92226634354573 3.92226634354573 3.07965539440140 3.13658664413333 3.67965539440140 3.13658664413333 3.47965539440140 3.13658664413333 3.48902157526632 1.1755208791434 3.46635957667757 0.15430853379511 1.34263615462090 1.22774711105381 3.37766426505767757 4.34789680069112 2.7983311952586 3.19948440451581 2.78283094160066 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.42033526620076 0.420335268207810 3.15165718788164 3.8737680254139 4.4097552278319 3.18435077810977 4.1604366403483 4.409755278319 3.18435077810977 4.1604366403483 4.43955675678 4.41465856418910 2.70984378336164 3.128351290825570 4.438455675678 4.41465856418910 2.70984378336164 3.12835112314133 0.14122941786992 1.23551112314133 0.14122941786992 1.23551112314133 0.14122941786992 1.23551112314133 0.14122941786992 1.23551112314133 0.14122941786992 1.23551112314133 0.14122941786992 1.23551112314133 0.14122941786992 1.23551112314133 0.1422941786992 1.23551112314133 0.1422941786992 1.23551112314133 0.1422941786992 1.23551112314133 0.1422941786992 1.23551112314133 0.1422941786992 1.2355112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314133 0.1422941786992 1.2359112314134 1.3450179555 1.2359112314134 1.3450179555 1.2359112314134 1.3450179555 1.2359112314134 1.34692012575 1.2359112314134 1.345017955 1.2359112	-     -     -     0.15616795923605     -2.10719802049580     -2.10719802049580     -2.10719802049580     -2.856054824957376     0.28556654824957376     0.285561588723051     1.8252648768403273     0.98561684843273     1.03250522520081     1.03250522520081     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.61839484210031     -2.632642463673019     2.7672143526     3.25236484384     3.26024463673019     2.7621435258535     3.27621790420524     -3.32648758405779     -1.2357210300097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.237210390097     -1.23721359423     0.60042446558418     -356451802480     0.6004244558418     -356685118     -376650158188     -3147986621225     -2747871587020     0.522603360210     -27200312847     -43235824827653	0.02697364549431 -0.28623354871784 0.02513984317884 -0.99529158086282 -0.31965476307846 -1.74734913649692 -0.48332494718497 -0.62924975252470 0.4353480410593 -0.51541104415686 -0.4352035194716 -1.54912055719563 -0.04509702597 0.49444719345709 0.1560560296251 -0.0776769338490 0.1560560296251 -0.0776769338490 0.1560560296251 -0.0776769338490 0.1560560288863 0.57779447330058 0.4396848189579 -1.27836517549603 1.53933605674799 0.439648189579 -1.27836517549603 1.5393350561867 1.4993234677041 -1.47193815243988 0.3775169660243 0.23827046419030 -0.5583655197450 -0.653676519230 -0.75513915072 0.65456842715136 -0.84366093936932 -0.755439310572 0.7554380647215 1.228445896360393 -2.254056530230 2.384590445938866 -3.2605957431076 -0.6633675802304 2.40978092185256 -3.3841242478586 -3.3841242478586 -3.4313433861347 -3.29674585700556 -3.5412244258321 -3.5412244258321 -3.5412244258233 -3.81080204202836
	0.69345166687752 0.41083355806592 1.287927358811 2.65516485399466 2.66626832186956 3.11405176009872 3.15795397093653 3.9222663454955 3.9222663454573 1.79443937968577 3.64134247856537 -0.80314681416843 3.67965532440140 3.13658664413353 2.48902157526632 -1.17552087914434 3.46635957667757 1.34263615462092 0.1543085379651 1.34263615462092 0.25317682540140 0.25387685470821 0.25318366096974 4.3276412105381 -2.7782104450525781 1.51565718798164 -3.87376802544139 3.1843507281097 1.514552278319 3.1843507281097 4.429645225791 1.5165718798164 -3.87376802544139 3.483507281097 -2.70843738316164 -3.87376802544139 3.445556787831 -1.270843738316164 -3.27376802544139 3.44556578336164 -3.2738361643433 4.19202382682490 3.23851102312935480 3.238511023124133 4.19453554112314133 3.192354123446992 1.5740923393000 -4.66120778898629 -1.5740923339300 -4.66120778898629 -1.5740923339300 -4.66120778898629 -1.5740923339300 -4.56120778898629 -1.5740923339300 -4.56120778898629 -1.5740923339300 -4.56120778896629 -1.5740923339300 -4.56120778896629 -1.5740923339300 -4.56120778896629 -1.5740923339300 -4.56120778896629 -1.5740923339300 -4.56120778896629 -1.5740923339300 -4.56120778896629 -1.5740923339300 -4.56120778896629 -1.5740923339300 -4.56120778896629 -1.5740923339300 -4.5612077889629 -1.5740923339300 -4.5612077889629 -1.5740923339300 -4.5612077889629 -1.5740923339300 -4.5612077889629 -1.574092325779 -1.5740923239300 -1.57409232570 -1.5740923239300 -1.5740923239300 -1.57409232570 -1.5740923239300 -1.57409232570 -1.5740923239300 -1.57409232570 -1.57409232570 -1.57409232570 -1.57409232574 -1.57409232574 -1.57409232574 -1.57409232574 -1.57409232574 -1.57409232574 -1.574092455 -1.2555112344133 -1.574092455 -1.2555112344133 -1.574092455 -1.2555112344133 -1.574092455 -1.2555112344133 -1.574092455 -1.2555112344133 -1.574092455 -1.2555112344133 -1.574092455 -1.2555112344133 -1.574092455 -1.2555112344133 -1.574092455 -1.2555112344133 -1.5	-0.15616795923605 -2.10719802049580 -2.10719802049580 -2.80719802049580 -2.80795861958723051 -2.8561958723051 -0.855606486803273 -0.855606486803273 -0.855606486803273 -0.85560546784521 -2.16136967089956 -1.60837386682183 -0.68616884475410 -2.61839484210031 -2.61839484210031 -0.5975772780339 -1.98953730162681 -3.98692247435299 -3.32523648644384 -4.32277961372662 -3.98692247435299 -3.32523648644384 -2.65186224713582 -3.98692247435299 -3.32523648644384 -2.65186224713582 -3.92642473529 -3.3223484515744740 -5.518224471354218 -3.6286910560274 -2.72248758405779 -1.2237210930097 -0.14033829528636 -1.39599793439579 -1.225155704322 -3.3568451802480 -0.60042846558418 -1.39608257043427 -3.84937039237136 -3.441592663915 -2.4787715216711 -3.27506500158188 -3.416895663015 -2.4787715216711 -1.8235800210 -0.272000318284750 -0.582643560210	0.02697364549431 -0.28625359487150 0.20543984317884 -0.99529158086282 -0.31365476307846 -1.74734913649692 -0.40534301111973 -0.62924975252470 -0.4053430111973 -0.5333084105093 -0.51541104415866 0.23382035194716 -1.54912055719563 -0.04510719905666 -1.54912055719563 -0.04510719905666 -1.54912055719563 -0.04510719905666 -1.5491205719563 -0.07767669338490 0.4496686189579 0.94506296251 -0.07767669338490 0.4496686189579 -0.1560560243 1.53938005674799 -3.1749292088863 0.57779447330058 1.557973546180 -1.5836555197450 -0.45328704641903 -1.55836555197450 -0.45328704641903 -1.55836555197450 -0.45328704641903 -1.55836555197450 -0.45328704641903 -1.55836555197450 -0.45328704641903 -1.55836555197450 -0.45328704641903 -1.55836555197450 -0.45328704641903 -1.55836555197450 -0.45328704641903 -1.5584595866 -1.528495856 -3.5413274263233 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.5413274263231 -3.8108020242836 -3.541327426323 -3.8108020242836 -3.541327426323 -3.8108020242836 -3.541327426323 -3.8108020242836 -3.541327426323 -3.8108020242836 -3.541327426323 -3.8108020242836 -3.541327426323 -3.8108020242836 -3.541327426323 -3.8108020242836 -3.541327425327 -3.55614327452524 -3.556
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485393466 2.6662863218056 2.6662864745223 1.57795397093653 3.12405176009872 2.1503463045955 3.32226634354573 3.79443937968677 3.6413424785537 -0.80314681416843 3.6796553940140 -3.13658664413353 2.48902157526632 -1.7552087374343 3.46635957667757 1.354642544485 -3.17896800617 1.3426615462090 1.227747111053379651 1.3426635957667757 0.1543085379651 1.3426635957667757 1.3752685470821 -0.73136446264256 -3.19984044051851 -2.78283094160066 0.42033526620076 0.29158366096974 4.085387685470821 -0.73136446267255 4.49296325625791 1.5165718798164 -3.8377680254139 3.184507281097 4.1604036403433 4.19201382682490 3.23851290822570 2.70984378336164 1.3580390301478 0.3726189354618910 -2.70984378336164 1.3580390301478 0.37261893544137 1.5365112341437 1.53601205755 -1.23551112314133 0.141229417869820 0.85407589529 0.85407581989529 0.85407589529 0.85407589529 0.85407589529 0.8540758789529 0.85407589529 0.8540758789529 0.85407589529 0.85407589529 0.85407589529 0.85407589529 0.85407589529 0.85407587889529 0.854075472411437 1.57409923393900 0.451229417889529 0.8540758788529 0.8540758788529 0.85407588529 0.85407547829 0.85407588529 0.85407547241437 1.57409923393900 0.5755 1.23551112314133 0.1412294178898529 0.8540758788529 0.85407588529 0.8540758788529 0.854075878 0.454274741137 0.5740922339390 0.5755 0.25551 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0.2575 0	-0.15616795923605 -2.10719802049580 0.28561958723051 0.28566486803273 0.90979617694091 1.8256648768683 1.6325052252081 1.0325052252081 1.0325052252081 2.16316967089956 -1.60837386682183 0.70224784521 2.16316967089956 -1.60837386682183 0.6851684475410 -2.61839484210031 -3.98652247435299 -3.32523648644384 -4.32277961372662 -3.98652247435299 -3.32523648644384 2.80924469234 0.655168224713589 -3.9865224713529 -3.32523648644384 0.63516822471362 3.02139614208224 2.747701150469074 -5.37214481252114 4.7443315858535 3.77622790712216 -3.32689910560274 -2.78248758405779 -1.2237210930097 -1.2537504327 3.89937033227135 3.4168952663315 3.24787715216711 3.27506500158188 3.4168952663305 3.24787715216711 3.27506500158188 3.4168952663305 3.2478771521771 3.27506500158188 3.4168952663305 3.24787715216711 3.27506500158188 3.4168952663305 3.24787715216711 3.27506500158188 3.4168952663305 3.24787715216711 3.27506500158188 3.4168952663305 3.24787715216711 3.27506500158188 3.4168952663305 3.24787715216711 3.27506500158188 3.4168952663305 3.24787715216711 3.27506500158188 3.4168952663305 3.24787715216711 3.27506500158188 3.4168952663305 3.24787715216711 3.27506500158188 3.4168952663305 3.24787715216711 3.27248918661356 3.24787715216711 3.27248918661356 3.24787715216711 3.27248918661356 3.24787715216711 3.27248918661356 3.24787715216711 3.2724821282427503 3.31478861255 3.3414812582427503 3.3414812582427503 3.34148125842427503 3.341484544124228 3.341478454412428 3.341478454412428 3.341478454412428 3.341478454412428 3.341478454412428 3.341478454412428 3.341478454412428 3.3414784544124428 3.3414784544124428 3.3414784544124428 3.341478454412428 3.341478454412428 3.341478454412428 3.341478454412428 3.341478454421254428 3.341478454412428 3.3414784544124428 3.3414784544124428 3.341478454412428 3.341478454412428 3.341478454412428 3.341478454412428 3.341478454412428 3.341478454412428 3.341478454412428 3.341478454412428 3.341478454412428	0.02697364549431 0.0265398471580 0.0254398471884 0.09529158086282 0.40534301111973 0.62924975252470 0.633340111973 0.0533804105093 -0.51541104415686 0.23382035194716 1.5491205719563 -0.04510719905666 1.3815600702597 0.49447193457091 0.070767669338490 0.4966868189579 0.156650292647 1.2783615749603 1.53938005674799 -3.17499200588863 0.57779447330058 1.5579735561867 -1.479024747330058 1.5579735561867 0.48466093660243 0.28815460119306 -1.5583655197450 0.4582674715136 0.48366809366932 0.75754880641933 -2.134736295818 2.3240566366936932 0.75749458958618 2.3240566366936932 0.75749458958618 2.32405673417515 0.48366809356389 2.254056336932 0.757494380647215 1.32206957431076 0.6367675802304 2.4097802185256 1.327452741076 0.6367675802304 2.4097802182556 1.3274459545818 1.382064724587 1.5644313738657 2.1960748336147215 1.5644313738657 2.196074833614725 1.3607458730656 1.352144229871 1.5644313738657 2.196074833614429871 1.5644313738657 2.196074833614429871 1.320695745870056 1.354144229871 1.5644313746263233 -3.18080202422836 -3.4182744262323 -3.18080202422836 -3.4182744262323 -3.18080202422836 -3.4182744262323 -3.18080202422836 -3.4182744262323 -3.418080202422836 -3.4182744262323 -3.418080202422836 -3.4182744262323 -3.418080207277548 -3.418414429871 -3.2960748351414429871 -3.29607483514472556 -3.541417327657 -3.541417327657 -3.541417327657 -3.541417327657 -3.541417327657 -3.541417327757 -3.541417327657 -3.541417327657 -3.541417327657 -3.541417327657 -3.541417327657 -3.541417327657 -3.541417327657 -3.541417327657 -3.541417327657 -3.5414417327657 -3.541417327657 -3.54144174597 -3.541441429871 -3.541441429871 -3.541441429871 -3.541441429871 -3.5414414429871 -3.5414414429871 -3.54144429871 -3.541444429871 -3.541444429871 -3.541444429871 -3.541444429871 -3.541444429871 -3.541444429871 -3.541444429871 -3.54144444987 -3.54144444987 -3.54144444987 -3.54144444987 -3.54144444987 -3.54144444987 -3.54144444987 -3.541444449
	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 1.58626644745223 1.57793397093653 1.57793397093653 1.57793397093653 3.179443937968677 3.64134247856537 -0.80314681416843 3.6796553940140 3.1365866441335 -2.4890215725632 -1.17552087914434 -3.4653595767732 -0.15430853379651 1.34263615462090 -0.15430853379651 1.34263615462090 -0.15430853379651 1.34263615462090 -0.15430853379651 1.34263615462090 -0.15430853379651 1.34263615462090 -0.15430853379651 1.34263615462091 -2.77828044051851 -2.7782804160066 -0.42033526525791 1.15165718798164 -0.4292632525791 1.15165718798164 -0.37316446267256 -0.3136446267256 -0.329387685470821 -0.73136446267256 -0.329387685470821 -0.73136446267256 -0.4292632525791 1.15165718798164 -0.3285418907 -2.7084378336164 1.358003903142 -2.70984378336164 1.358003903142 -1.2355112314133 0.1412241786992 1.68700472411377 1.55740923393000 -4.66120778988629 1.657047241537 -2.758424725535 -0.758424725535 -0.758424725535 -0.758424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424725535 -0.75928424	-0.15616795923605 -2.10719802049580 -2.10719802049580 -2.80795861958723051 0.2855605484597376 0.2855605484597376 0.2855605484597376 0.285560548459273 0.855605468483273 0.98567245921 2.16316967089956 -1.60837368628183 -0.68616884475410 -2.61839484210031 -2.61839484210031 -2.61839484210031 -0.59757727809359 -1.98953730162681 -3.3252364864384 2.80924469673019 2.76764342692374 -3.3252364864384 2.80924469673019 2.76764342692374 -3.3252364864384 2.80924469673019 2.76764342692374 -3.3252364864384 2.80924469673019 2.76764342692374 -3.325264864384 2.80924469673019 2.76764342692374 -3.325484518558433 2.377624790712216 2.9777315359433 2.43832007301112 -3.62869910560274 -2.78248758405779 -1.235710930097 -0.14033829528636 -1.3959793439579 -1.26516507642564 -0.35768451802480 0.560625704327 -1.23750455074226 -3.37568451802480 0.560625704327 -3.2758451802480 0.560625704327 -3.2758451802480 0.560625704327 -1.48235584627503 3.3715641921651818 3.3314798662125 2.4787715216711 -0.27200032182847 -1.4823524827503 2.3715641294122847 -0.7243818661356	0.02697364549431 -0.28623359487150 0.2054398471584 -0.99529158086282 -0.31365476307846 -1.74734913649692 -0.4053430111973 -0.68133294718497 -0.62924975252470 -0.53338084105093 -0.51541104415686 -1.54912055719563 -0.04510719905666 -1.54912055719563 -0.04510719905666 -1.5491205719563 -0.045686189579 -0.4466868189579 -1.27886517549603 1.53938005674799 0.44966868189579 -1.27886517549603 1.53938005674799 -1.27886517549603 1.5393805561867 -1.47930234677041 -1.47193815243808 0.377516560243 -0.2881540119306 -0.45328704641903 -0.45328704641903 -0.45328704641903 -0.45328704641903 -0.45328704641903 -0.45328704641903 -0.45328704641903 -0.45328704641903 -0.45328704641903 -0.45328704641903 -0.4532870441903 -2.34459489581742 -0.7543830647215 -3.284594295856 -3.284594295856 -3.284594295856 -3.284594295856 -3.284594295856 -3.284594295856 -3.240978092185256 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.5413427458 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.541327426283 -3.54132746283 -3.541327
$ \begin{array}{c} \mathbf{x} \mathbf{x} \mathbf{x} \mathbf{x} \mathbf{y} \mathbf{y} \mathbf{y} \mathbf{y} \mathbf{y} \mathbf{y} \mathbf{y} y$	0.69345166687752 0.41083395806592 1.287927358811 2.65516485399466 2.66626823186956 2.662268231469556 3.11405176009872 2.1503843045955 3.92226634354573 1.79443337968473 3.64134247856537 -0.80314681416843 2.48902157526632 -1.7552087914434 -3.46535957667757 -0.543085379651 1.34263615462090 0.25126632 -1.7552087914434 -3.46535957667757 -0.543085379651 1.34263615462090 0.251378968005511 2.27828094160066 -0.42033526620076 0.29158366096974 -0.85387685470821 0.73136446252556 -1.9783416005 -0.42033526620076 0.29158366096974 -0.4203352652071 1.5165718798164 -3.87376802544139 3.1843507281097 1.15165718798164 -3.87376802544139 3.1843507281097 -1.27084373831614 1.3500390301478 4.4345556489310 0.3726518354800 2.1346901205755 -1.25551112314133 0.1422941786992 1.6570472411437 1.5740923339300 -4.66120778989629 0.85409550868798 1.6528442725533 1.07816295152565	-0.15616795923605 -2.10719802049580 -2.10719802049580 -2.80719802049580 -2.80719802049580 -2.80719802049580 -2.805405648459376 -0.855665484957376 -0.85566546803273 -0.855665468831 -0.85566546842183 -0.68516884475410 -2.61839484210031 -2.61839484210031 -0.5975772780339 -1.98953730162681 -3.9869224743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.3926424743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.392524743529 -3.39254743529 -3.39254743529 -3.3925454548484 -3.75645450560274 -2.7224731559423 -1.2551557642544 -0.35768451802480 -0.60042845554818 -1.3950825704327 -3.89397039237136 -1.255155704254 -1.39568451802480 -0.6004284558418 -1.395684551084327 -3.3756845500210 -0.27200032182847 -1.4823582427503 -1.4825580210 -0.2720032182847 -1.4823582427503 -1.48255604515818 -1.48555604515818 -1.345155014098	0.02697364549431 0.0265398471584 0.0255398471584 0.0255398471884 0.99529158086282 0.40534301111973 0.62924975252470 0.6831329214786 0.5831329475252470 0.5333804105093 0.51541104415686 0.23382035194716 1.54912055719563 0.04510719905666 1.3815600702597 0.9444719345709 0.15606508296251 0.07767669338490 0.44966565189579 0.944671934579403 1.53938005674799 -1.27836157549603 1.5393800564799 -1.2783615749603 1.5393800564799 -1.4793025647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647877 1.4493023647151 1.449302386593883 2.38459048593866 1.3520657431076 0.6636767802304 2.3849048593866 1.3520657431076 0.6636767802304 2.409780278570656 3.3413274262333 3.31080020422366 -1.2888411046909 2.06940722276368 3.511227427586 -3.511227427586 -3.511227427586 -3.511274267233 -3.510802022737115 -2.1258864230569 -2.36474788504

#### IrMe 1red [2] 0.74723951249808 0.46551523097126 99379595432 0.08683820905166 N N C -2.12523558904867 -0.28308757243802 -1.29093264111277 2.60752850992090 -0.36478947995004 0.22290382408901 0.21025689756575 -1.04368774622934 2.67911049138586 0.85000692781144 0.25143447388366 CCCC 1.54156397161116 1.61262206056446 0.84697232989112 1.83901512817993 -1.80729260654532 0.32367498022532 0.92431141279827 1.81992164725336 -0.94867705213277 -3.14303627689743 -2.14428625479798 1.00149900032426 0.74357788750864 -0.60370448043728 0.35166295581987 2.14252250727606 -1.63796045887244 -0.80936782799780 -0.50369513650777 0.14323147031422 -1.58007280593461 -3.93693137378892 -1 78195434204010 -1.78193434204010 3.54360749064813 -0.77705947355704 3.70442681427669 -3.11871902260324 -0.80936782799780 -0.80936782799780 -0.6385295885385 -2.04305024987679 -4.35951345400916 -3.99002928703979 -3.38810802356851 2.78876076434282 2.83362155770017 0.554657787388 1.64371034017022 -2.78415388212843 1.64371034017022 -0.29539603(512591 -1.58007280593461 -0.13010497648473 1.31065939685897 0.34550351759062 -0.04105178141527 0.22427364014807 0.25178923794313 -1.33218976331370 -3.22253866361855 0.54983934226414 1.50532925038222 -3.11871902260324 -2.47634991843886 -1.15057297899926 -3.45693093062469 -0.17301233687796 1.40768491872711 1.15201890935894 -3.74825539011198 2.76996(1722)278 -2.75989617222788 -1.96227110906172 1.50539295038222 1.41253750789290 0.29539630512591 -5.41419566893113 -4.73597218827842 Н -3.26094326525402 -1.42370074218248 H H -2.74638536060341 -0.38157125250883 -0.09863711269223 -0.43305232581998 Н 0.25772317383473 3.72841066828302 -1.62906685606064 H H -0.85664694421216 -0.76734426807383 2.92959599966896 2.37548060794697 -0.49320516109881 -2.17194748584529 -2.17194748584529 0.41531456615563 -0.43058470513938 0.58034497603505 -2.20399703716275 -2.23045920835049 -0.79235387937868 1.18745860776268 2.30759865194804 1.28061693189875 0.62301995027584 H H H -3.68819986733138 -2.80288521537006 -1.29012237621939 -4 49244113419996 1.21149780342596 -3.86879508167613 4.31865247926130 3.0282189927469 4.05549057639208 4.20796935064140 3.24742505856747 4.47077209674617 -4.37273479342119 2.60854114086204 1.44312921731169 0.43735770810223 2.19435139473365 -1.29012237621939 -0.33390405982285 -1.53187951578699 -1.37701308709178 -0.34130153697850 0.65133436096453 1.41611747965424 3.93221920730841 3.48286204507233 2.35778008004888 H H H H H H 0.62401995022584 2.32791189328386 2.35278908994888 3.33195302157029 H H 2.40407444906940 1.31308544538892 1.40111789389253 2.19435139473365 Н 3.60640160479617 H H -1.17851403310399 1.44800166709825 2.14286437011186 -3.31639449353825 0.06230786008782 0.47546475830473 Н 1.59694506820371 -0.38588548534499 -3.56656918841871 H H 1 48288275360182 1.35805823455103 2.33482679456107 -3 90141583297964 -4.69262543451276 -1.26555268892653 0 74574136380053 -0 75333383013305 2 11105193919431 H H H 1.66126449279827 0.69225332818430 -1.32198463610609 0.08886106254213 2 33844845587490 2.550440455007450 -0.11470201816050 -1.40730700007890 2.30652789827721 IrCl Ir 3.24416348533836 Cl 2.50690137004877 2.04635464456639 17.51927099940094 3.24416348533836 2.50690137004877 4.78182430070674 1.87634105734610 5.32923140982803 1.59360715719865 5.12115494245642 5.13307112067144 4.73982149636683 1.54141262177729 4.524030272552 2.04635464456639 4.30905911949233 1.27084718495563 1.74208866912136 2.63929148375957 1.49269452975693 1.31339173691271 2.60674723714185 0.46356034508043 1.40973569173247 0.77277254794519 17.59927830301823 18.89707910344297 18.89707910344297 16.04106462730468 17.06862548355086 18.51883594667846 16.56968843848080 18.52507987576022 17.68572614335662 19.53666583659171 20.27769012896299 4.52440320272532 0.61044281249386 0.77277254794519 1.52572988554414 20.27769012896299 16.41371982464571 2.22770028011269 1.85640414694076 14.66929710905345 5.78153122062608 3.82670348355280 1.37579058914044 16.29143478334355 17.85451401737456 0.45495687293880 5.31963669385618 0.85159527267021 15.16945843790352 5.34718262238101 4.48708641685280 3 75952129425597 19.44152587092071 17.61689799394672 -1.00429414321327 1.45101605446576 3.04080367725721 0.76850110855404 -0.53799376341631 15 57266611801790 2.81714881422282 14.20848381923842 13.80681735300224 2.03668104340816 2.03668104340816 -0.83112934910173 -1.75750187394613 3.20325087814220 2.44543810502105 -1.90406378261180 3.02579614853518 2.95008028668716 3.78383114513551 4.17444072263997 5.45685614117135 5.59892866995392 0.76850110855404 1.11278481162208 1.20160653378018 3.13627049080533 0.87047250217585 1.02109154905731 2.05180923931807 3.87196603687276 -0.037160668094206 1.57548883572384 0.37021469589095 3.69565969325572 13 80681735300224 18.41119570233812 16.14798445593499 12.87256656458729 12.47642121420274 17.56458470950967 12.00571445505140 14.9011045825325 20.70241069780821 15.21852862423314 16.43702337175003 H H Н H H $\begin{array}{c} 5.59892866995392 \\ 6.86208321084704 \end{array}$ 3.69565969325572 3.97923122344945 5.26230165401036 5.17996736032035 4.63603280702232 Н 4.73483451044481 16.62389406937705 H H 1.66406624687338 0.03511410765964 14.44821365631871 14.90902580681944 Н 6.34882211252493 0.47426341292025 15.06430558753267 H H 6.42549183108316 4.84378543653847 3.87530647555767 3.61001456617133 19.63336708261648 20.40388086205428 4.69175451546507 -1.33646535999964 -1.54651319365824 20.4038080203428 18.99764021505261 18.42002311170512 17.72412915282936 16.65502271052546 4,97715931725028 н н 3.81878977358347 5.44015617341075 ц 5.44015617341075 4.04529259573220 -0.43843171255670 1.60024379900272 -0.93627074480502 -2.64716482311956 3.64941819219223 2.31458949256838 -2.89765646840763 3.34315772321749 -1.54651319365824 -1.29107537417922 1.60299750472613 -0.15459861746560 0.99727066558905 1.15169176999336 4.06202964977836 0.01871615166277 0.82557727091575 2.12692638690272 14.49963742766945 14.18915499456737 14.18913499456737 19.49018836428845 15.51999774314230 12.50764478890301 11.80822208262711

H H

Ľ	2] ²⁻ . IrMe	3red	
Ir	0.74971602017080	-0.06225315437802	0.39384784518328
Ν	0.48721500373394	-2.11528913810663	0.01792445230411
Ν	-1.42714789162027	-0.36746827168270	0.33528462827663
С	2.82952545027859	0.46083146588825	-1.21609691287654
С	2.77877152254180	0.70691546346824	0.23111794352206
Ċ	1.62653648203027	1.04220630005954	-1.73737053824159
Ċ	1.77679889056089	1.76101676612894	0.49849626187611
С	1.01500102309501	1.87733411793093	-0.73100590333810
Ċ	-3.34028645774894	0.87598441961181	-0.61850729777762
С	-2.29465632138624	0.69017279153503	0.34210532953344
С	-4.12686472455742	2.02341898036880	-0.62434334940201
Ċ	-1.84132808978693	-1.67149048555276	0.16531581500567
С	3.52245296469361	-0.70834674354880	-1.84591129413289
С	-0.76321263123786	-2.63796155352595	0.07189679498712
С	3.92393315552850	0.45031045061317	1.16416458287308
С	-3.16590794405109	-2.14473890609326	0.21355415904489
С	-2.43121387411500	-4.45567139809143	0.07807226230471
С	-1.09759458525247	-4.01230576766901	0.05309282382754
С	-3.46766940094473	-3.52220952809124	0.18405984583740
С	-0.04690571745796	2.89564115959331	-1.01831961839956
С	1.78941128870811	2.69249608718794	1.66756315213072
С	1.11242386257459	0.89650486350538	-3.13286125195772
С	-3.94722813736851	3.04237030108732	0.32943475705693
С	-2.94606856079979	2.85810283228120	1.30693316736224
С	-2.13332003867480	1.73228280238553	1.30330021311220
Н	-3.46694740759827	0.10188656562225	-1.37514442727748
Н	-2.63140999648647	-5.53094905852196	0.07316021554660
Н	-0.28156989950996	-4.74093895850269	-0.00230471664978
Н	0.39563257888318	3.88783485327192	-1.24567663394314
Н	-0.74587201787463	3.00725412616153	-0.18165571867813
Н	-0.65074382555237	2.59122571421748	-1.88504424258705
Н	-4.51471518304355	-3.83842759526319	0.21307402680687
Н	1.22083145089152	-2.80329636132470	0.18474265171756
Н	-3.97320189517640	-1.42150540565892	0.33071784108781
Н	4.28022059482215	-0.42512008742967	-2.60024744638099
Н	2.79917229100295	-1.37162714950846	-2.36231005898176
Н	4.04128078705142	-1.32234335235935	-1.09030091311983
Н	4.42896647525735	-0.50725669117204	0.95115636968074
Н	3.60040741147852	0.42781673894801	2.21661625950428
Н	4.69807838478652	1.24675179283962	1.09439477450925
Н	-4.60156490839308	3.91602249354007	0.33900052539732
Н	-2.78867182796523	3.62930308740733	2.06634217493257
Н	1.91318837024058	2.13054553837888	2.60925746065989
Н	0.84330330125434	3.25130401987971	1.74396113516773
Н	2.60920088274402	3.44243601722960	1.62157286097456
Н	-1.33586383796193	1.61919835457098	2.04048136584389
Н	0.01423854800639	0.88138350824965	-3.14811675870542
Н	1.44364227793286	-0.04325871959651	-3.60666251866207
Н	1.43163575284467	1.72496320948543	-3.80305994571855
Н	-4.88211167893794	2.13681671703737	-1.40897009939481
С	0.61388213429756	-0.48587983526294	2.41731535898566
Н	1.55724982987487	-0.89264311393225	2.83643968965728
Н	0.35379090655967	0.41341639118542	3.01384954374164
Н	-0 17852078834293	-1 23556665439822	2 58569335777329

17.96819115568152 10.96531247876784