Electrochemical Reduction of Carbon Dioxide with a Molecular Polypyridyl Nickel Complex

Supporting Information

Lauren E. Lieske^a, Arnold L. Rheingold^b, Charles W. Machan^{a,*}

* - machan@virginia.edu; 0000-0002-5182-1138

^a – Department of Chemistry, University of Virginia, McCormick Road PO Box 400319, Charlottesville, VA 22904-4319

^b – Department of Chemistry & Biochemistry, University of California, San Diego, La Jolla, CA 92093-0358.

The Evans Method for determining paramagnetic susceptibility was performed by making a concentration of 1 x 10^{-3} M [Ni(TPEN)](PF₆)₂ (1) in acetonitrile (MeCN). A capillary insert was then made with a 50% v/v mixture of MeCN and MeCN-*d*₃. The insert was flame sealed, and then placed in an NMR tube contain [Ni(TPEN)](PF₆)₂. ¹H NMR spectra with 64 scans were then taken using a 600 MHz Varian NMR Spectrometer.

Paramagnetic moment was then determined following the following equations^{1,2}:

$$\begin{split} \chi_{\rm D}^{\rm (TPEN) = 46.5} \chi_{\rm D}^{\rm (en)} + 49 \chi_{\rm D}^{\rm (pyr)} + 49 \chi_{\rm D}^{\rm (pyr)} + 49 \chi_{\rm D}^{\rm (pyr)} + 6 \chi_{\rm D}^{\rm (C)} + 6 \chi_{\rm D}^{\rm (C)} + 6 \chi_{\rm D}^{\rm (C)} \\ &+ 6 \chi_{\rm D}^{\rm (C)} + 6 \chi_{\rm D}^{\rm (C)} . \\ &= 267.00 \text{ x } 10^{-6} \text{ emu mol}^{-6} \\ \chi_{\rm dia}^{\rm dia} = \chi^{\rm Higand} + \chi^{\rm Ni\,2+} \\ \chi_{\rm dia}^{\rm dia} = [-267.00 + (-12.0)] \text{ x } 10^{-6} \text{ emu mol}^{-1=} \\ &- 279.00 \text{ x } 10^{-6} \text{ emu mol}^{-1} \\ \delta v_{\rm p}^{\rm p} = (2.22 - 1.99)^{*}600 \text{ Hz} \\ \chi_{\rm dia}^{\rm para} = \frac{(138 \text{ Hz})^{*}(770. \text{ g/mol})}{(600 \text{ Hz})^{*}(1.33\pi)^{*}(1.06 \text{ x } 10^{-2} \text{ g/mL})} - \chi^{\rm dia} \end{split}$$

 $=4.27 \times 10^{-3} \text{ emu mol}^{-1}$

 $\mu_{\rm eff}$ = 3.1 Bohr Magnetons



Figure S1. ¹H NMR of the TPEN ligand; *d*₃-CD₃CN; 600 MHz Varian.



S4



Figure S3. ESI-MS of TPEN.



Figure S4. ¹H NMR of [Ni(TPEN)](PF₆)₂ **1**; *d*₃-CD₃CN; 600 MHz Varian.



Figure S5. ESI-MS of [Ni(TPEN)](PF₆)₂ 1.





Figure S7. ESI-MS of TMC.







Figure S9. ESI-MS of [Ni(TMC)](PF₆)₂.



Figure S10. Linear Fit of variable scan rate data from **Figure 3** demonstrating that $[Ni(TPEN)](PF_6)_2$ **1** shows a diffusion-limited current response. Conditions: 1 mM analyte; 0.1 M TBAPF₆/MeCN, glassy carbon working electrode, Pt wire counter electrode, Ag/AgCl pseudoreference electrode; varied scan rate; referenced to internal ferrocene standard.



Figure S11. Log-log plot from data obtained from CVs of complex [Ni(TPEN)](PF₆)₂ **1**, (1 mM) with variable PhOH concentrations and CO₂ saturation at -1.93 V vs Fc/Fc⁺. Adapted from Sathrum and Kubiak *J. Phys. Chem. Lett.* **2011**, *2*, 2372.⁴ *F* is Faraday's constant, *A* is the electrode area, [*Q*] is the substrate concentration, k_{cat} is the catalytic rate, *D* is the diffusion constant of the catalyst, [*cat*] is the concentration of the catalyst, and n_{cat} is the number of electrons involved in the catalytic process. Uses data from **Figure 5** in main text.



(1) $i_{cat} = n_{cat} FA[cat] (Dk_{cat}[Q]^y)^{1/2}$

Figure S12. Plot displaying the Nernstian voltage dependence of $[Ni(TPEN)](PF_6)_2$ **1** on the concentration of PhOH in MeCN under CO₂ saturation. Conditions: 0.1 M TBAPF₆/MeCN, glassy carbon working electrode, glassy carbon counter electrode, Ag/AgCl pseudoreference electrode; scan rate 100 mV/s; referenced to internal ferrocene standard. Uses data from **Figure 5** in main text.



Figure S13. CVs of $[Ni(TPEN)](PF_6)_2$ **1**, obtained under variable CO₂ concentrations with 0.5 M PhOH. Conditions: 1 mM analyte; 0.1 M TBAPF₆/MeCN, glassy carbon working electrode, glassy carbon counter electrode, Ag/AgCl pseudoreference electrode; scan rate 100 mV/s; referenced to internal ferrocene standard.



Figure S14. Log-log plot from data obtained from CVs of complex $[Ni(TPEN)](PF_6)_2$ **1** (1 mM) under variable CO₂ concentration conditions with 0.5 M PhOH at -2.0 V vs Fc/Fc⁺.



Figure S15. CVs of complex [Ni(TPEN)](PF₆)₂ 1 at variable concentrations, obtained under CO₂ saturation and 0.5 M PhOH. Conditions: 0.1 M TBAPF₆/MeCN, glassy carbon working electrode, glassy carbon counter electrode, Ag/AgCl pseudoreference electrode; scan rate 100 mV/s; referenced to internal ferrocene standard.



Figure S16. Log-log plot from data obtained from CVs of complex $[Ni(TPEN)](PF_6)_2$ 1 under variable concentration conditions with 0.5 M PhOH and CO₂ saturation at -1.93 V vs Fc/Fc⁺.



Figure S17. CVs showing CO₂ and PhOH control responses. Conditions: 0.1 M TBAPF₆/MeCN, glassy carbon working electrode, glassy carbon counter electrode, Ag/AgCl pseudoreference electrode; scan rate 100 mV/s; referenced to internal ferrocene standard.



Figure S18. Cyclic voltammogram of [Ni(TPEN)](PF₆)₂ (1) (1 mM) under CO₂ saturation and 0.5 M PhOH. Conditions: 0.1 M TBAPF₆/MeCN; glassy carbon working electrode, glassy carbon counter electrode; Ag/AgCl pseudoreference electrode; varied scan rate; referenced to internal ferrocene standard.



Figure S19. Linear fit between peak catalytic current over non-catalytic vs the inverse square root of the scan rate from the variable scan rate data in **Figure S18**.³ This establishes the validity of using the equations for the FOWA.³



Figure S20. Linear fit plot of TOF (s⁻¹) vs scan rate of the variable scan rate data from **Figure S18** demonstrating that [Ni(TPEN)](PF₆)₂ **1** can be analyzed by FOWA using these data.³



Figure S21. A) CV overlay between catalytic current under CO₂ and 0.5 M phenol and $[Ni(TPEN)](PF_6)_2$ 1 under argon. B) Linear region from the FOWA. C) Entire region of i_c/i_p vs $1/(1+\exp(f(E-E^\circ)))$. Conditions: 1 mM analyte; 0.1 M TBAPF₆/MeCN, glassy carbon working electrode, glassy carbon counter electrode, Ag/AgCl pseudoreference electrode; scan rate 100 mV/s; referenced to internal ferrocene standard.



Figure S22. IR controls for the following with their corresponding v_{max}/cm^{-1} taken in MeCN: TBA(HCO₂⁻) 1333 cm⁻¹ and 1608 cm⁻¹,⁶ TBA(HCO₃⁻) (1676 cm⁻¹), PhO⁻ (1589 cm⁻¹) and PhOH (3408 cm⁻¹) in MeCN.



Figure S23. A comparison of the $[Ni(TPEN)(CO)]^+$ stretch with labeled CO₂ without (A) and with 0.3 M solution of PhOH (B). Conditions: 3 mM solution of (1); ¹³CO₂ and CO₂ sparged for ~ 30s; 0.1 M TBAPF₆/MeCN; referenced to internal ferrocene standard.



Figure S24. A) IR-SEC analysis of a 3 mM solution of [Ni(TPEN)](PF₆)₂ 1 with CO sparged into solution for ~30 s. **B)** Different conditions with catalyst under CO. Ni-CO stretch from [Ni(TMC)(CO)]⁺ grows in at 1967 cm⁻¹ with a shoulder associated with Ni-CO stretch from Ni(κ^4 -TPEN)(CO)]⁺ at 1984 cm⁻¹. Conditions: 0.1 M TBAPF₆/MeCN; referenced to internal ferrocene standard.



Figure S25. **A)** UV-Vis of the bulk solution before and after electrolysis. **B)** Current vs time plot of electrolysis experiment held at -2.05 V vs Fc/Fc^+ . **C)** Charge passed during electrolysis experiment. Conditions: 1 mM of $[Ni(TPEN)](PF_6)_2$ 1; 0.5 M PhOH; 0.1 M TBAPF₆/MeCN, graphite working electrode, graphite carbon counter electrode, Ag/AgCl pseudoreference electrode, and 0.5 M Fc was used as a sacrificial oxidant.



Figure S26. IR comparison between the post bulk electrolysis experiments of $[Ni(TPEN)](PF_6)_2$ 1 with and without $[Ni(TMC)]^{2+}$. $Ni(CO)_4$ appears at 2042 cm⁻¹ while the Ni-CO stretch is observed at 1981 cm⁻¹ in both solutions.



Figure S27. CVs of $[Ni(TPEN)](PF_6)_2$ **1** at 1 mM, obtained under CO₂ saturation with 0.5 M PhOH and with $[Ni(TMC)]^{2+}$ titrations Conditions: 1 mM analyte; 0.1 M TBAPF₆/MeCN glassy carbon working electrode, glassy carbon counter electrode, Ag/AgCl pseudoreference electrode; scan rate 100 mV/s; referenced to internal ferrocene standard.



Figure S28. A) CV overlay between catalytic current under CO₂ with phenol (red trace) and 1 mM of [Ni(TPEN)](PF₆)₂ **1**, and 2 mM [Ni(TMC)]²⁺ under Ar (black trace) **B.)** Linear region from the FOWA. **C.)** Entire region of i_c/i_p vs $1/(1+\exp(f \text{ (E-E^o)}))$. Conditions: 1 mM **1**; 2 mM Ni(TMC)[PF₆]₂; 0.1 M TBAPF₆/MeCN, glassy carbon working electrode, glassy carbon counter electrode, Ag/AgCl pseudoreference electrode; scan rate 100 mV/s; referenced to internal ferrocene standard.



Figure S29. IR-SEC analysis of a 3 mM solution of $[Ni(TPEN)](PF_6)_2 \mathbf{1}$ with CO₂ in a solution containing 20 mM of $[Ni(TMC)](PF_6)_2$. Ni-CO stretch from $[Ni(TMC)(CO)]^+$ grows in at 1967 cm⁻¹ with a shoulder associated with Ni-CO stretch from $Ni(\kappa^4-TPEN)(CO)]^+$ at 1982 cm⁻¹. Conditions: 0.1 M TBAPF₆/MeCN; referenced to internal ferrocene standard.



Figure S30. **A)** UV-Vis of the bulk solution before and after electrolysis. **B)** Current vs time plot of control electrolysis experiment held at -2.05 V vs Fc/Fc^+ . **C)** Charge passed during control electrolysis experiment. Conditions: 1 mM of $[Ni(TPEN)](PF_6)_2$ 1; 3 mM $[Ni(TMC)]^{2+}$; 0.5 M PhOH; 0.1 M TBAPF₆/MeCN, graphite working electrode, graphite carbon counter electrode, Ag/AgCl pseudoreference electrode, and 0.5 M Fc was used as a sacrificial oxidant.



Figure S31. CVs of $[Ni(TPEN)](PF_6)_2 \mathbf{1} (1 \text{ mM})$ obtained under Ar and then Ar and CO₂ upon the addition of 1 mM of $[Ni(TMC)]^{2+}$. Conditions: 0.1 M TBAPF₆/MeCN, glassy carbon working electrode, glassy carbon counter electrode, Ag/AgCl pseudoreference electrode; scan rate 100 mV/s; referenced to internal ferrocene standard.



Figure S32. IR-SEC analysis of a 20 mM solution of $[Ni(TMC)]^{2+}$ with CO₂, without the addition of $[Ni(TPEN)](PF_6)_2$ **1**. No carbonyl-containing species are observed. Conditions: 0.1 M TBAPF₆/MeCN; referenced to internal ferrocene standard.



Figure S33. A) IR-SEC analysis of $[Ni(TMC)]^{2+1}$ with CO sparged into solution for ~30 s to show the $[Ni(TMC)(CO)]^+$ stretch at 1967 cm⁻¹. Conditions: 0.1 M TBAPF₆/MeCN; referenced to internal ferrocene standard. **B)** Linear fit of $[Ni(TMC)(CO)]^+$ absorbance.



Figure S34. A comparison of the 3 mM solution of (1) with a 3 mM solution of $[Ni(TMC)]^{2+}$ to show the catalytic activity of $[Ni(TPEN)]^{2+}$.



Figure S35. IR-SEC spectra overlaying of 3 mM Ni(TPEN)[PF₆]₂ **1** with the addition of 20 mM $[Ni(TMC)]^{2+}$ to show the loss of Ni(CO)₄ formation upon the addition of the CO scavenger. Timepoints: blue 60 s; red 30 s; green 60 s.



Figure 36. Kohn-Sham orbital representations of $[Ni(TPEN)]^{2+}$ **1** (A); SOMO-I (B); and SOMO-II (C). ORCA 4.0; B3LYP/G; ZORA; def2-TZVP; CPCM(Acetonitrile), 2S+1 = 3.



Figure S37. Calculated spin density localization of $[Ni(TPEN)]^{2+}$ 1. ORCA 4.0; B3LYP/G; def2-TZVP; CPCM(Acetonitrile), 2S+1 = 3.



Figure S38. Kohn-Sham orbital representations of the SOMO (B) and LUMO (C) of $[Ni(TPEN)(CO)]^+$ **5** (A); spin density (D). ORCA 4.0; B3LYP/G; def2-TZVP; CPCM(Acetonitrile), 2S+1 = 2.

Table S1. The peak to peak separation as well as the peak current ratio for both 1 and the internal Fc/Fc^+ reference at 100 mV/s.

Scan Rate (100mV/s)	<i>i</i> _{pa} (<i>J</i> (A/cm ²)	<i>i</i> _{pc} (<i>J</i> (A/cm ²)	E _{pa} (V)	E _{pc} (V)	ΔE (V)	<i>i</i> _{pa} / <i>i</i> _{pc} (<i>J</i> (A/cm ²)
Fc/Fc^+	4.88 x 10 ⁻⁴	-5.00 x 10 ⁻⁴	0.035	-0.032	0.067	9.76 x 10 ⁻¹
1	2.06 x 10 ⁻⁴	-2.23 x 10 ⁻⁴	-1.82	-1.89	0.07	9.26 x 10 ⁻¹

Foot-of-the-Wave Calculations⁵

$$\frac{i_c}{i_p} = \frac{2.24n_{cat}^{\circ}\sqrt{\frac{RT}{F_{\nu}}}k_{cat}C_{substrate}}{1 + \exp\left[\frac{F}{RT}(E - E^0)\right]}$$

where $n_{cat}^{\sigma} = 2$, $\frac{RT}{Fv} = 0.256796$ s, $k_{cat} = k_{obs}$ [catalyst]; $E^{\circ} = E_{1/2}(1 \text{ mM Ni(II)/Ni(I)}) = -1.86 \text{ V vs}$ Fc/Fc⁺.⁵

Table S2. FOWA analysis of 1 with PhOH titrations; k_{cat} assumes first-order concentrationdependences for [PhOH] and [CO₂] for simplicity.Phenol

Phenol Concentration (M)	TOF _{max} (s ⁻¹)	$[Ni(TPEN)](PF_6)_2 k_{cat} (M^{-2}s^{-1})$
0.24	2.18 x 10 ²	3.24 x 10 ³
0.5	2.67×10^2	3.97 x 10 ³
0.75	4.02×10^3	$6.00 \ge 10^4$
1.0	$3.60 \ge 10^4$	5.36 x 10 ⁵
1.48	1.02×10^5	1.51 x 10 ⁶
1.98	3.70 x 10 ⁵	5.51 x 10 ⁶
2.49	7.72 x 10 ⁸	$1.15 \ge 10^{10}$

Table S3. FOWA analysis of **1** with [Ni(TMC)]²⁺ titrations at 0.5 M PhOH.

	$(\mathbf{m}\mathbf{M})$	$\mathbf{TOF}_{\mathbf{max}}\left(\mathbf{s}^{-1}\right)$	$[Ni(TPEN)](PF_6)_2 k_{cat} (M^{-2}s^{-1})$
-	1	7.96 x 10 ⁵	4.02×10^9
	2	2.31 x 10 ⁴	$1.17 \ge 10^8$
	5	2.74 x 10 ⁴	1.39 x 10 ⁸

Identification code	CWM-002		
Empirical formula	C26 H28 F12 N6 Ni P2		
Formula weight	773.19		
Temperature	100.0 K		
Wavelength	0.71073 Å		
Crystal system	Monoclinic		
Space group	P 21/n		
Unit cell dimensions	a = 13.8699(6) Å	$\alpha = 90^{\circ}$.	
	b = 17.1455(7) Å	$\beta = 100.970(2)^{\circ}$.	
	c = 14.2982(8)	$\gamma = 90^{\circ}$.	
Volume	3338.1(3) Å ³		
Ζ	4		
Density (calculated)	1.539 Mg/m ³		
Absorption coefficient	0.772 mm ⁻¹		
F(000)	1568		
Crystal size	0.26 x 0.15 x 0.1 mm ³		
Theta range for data collection	2.565 to 26.027°.		
Index ranges	-11<=h<=17, -21<=k<=20	-11<=h<=17, -21<=k<=20, -17<=l<=12	
Reflections collected	15877		
Independent reflections	6314 [R(int) = 0.0550]		
Completeness to theta = 25.242°	96.1 %		
Absorption correction	Semi-empirical from equi	valents	
Max. and min. transmission	0.4293 and 0.3852		
Refinement method	Full-matrix least-squares	on F ²	
Data / restraints / parameters	6314 / 0 / 424		
Goodness-of-fit on F ²	1.011		
Final R indices [I>2sigma(I)]	R1 = 0.0471, $wR2 = 0.09$	06	
R indices (all data)	R1 = 0.0902, $wR2 = 0.1046$		
Extinction coefficient	n/a		
Largest diff. peak and hole	0.516 and -0.424 e.Å ⁻³	0 516 and -0 424 e Å ⁻³	
SQUEEZE	154e/unit cell (roughly four hexane)		
		/	

Geometry-Optimized DFT Coordinates

[Ni(κ⁶-TPEN)]²⁺; 2S+1=3

Ni	6.271361	12.877217	12.070347
Ν	4.546489	11.748955	11.624644
N	7.936293	14.087427	12.527486
N	5.058258	13.480623	13./1508/
	7.024973	12.010/00	10.120020
N	6,833000	11.040093	13 501538
C	3 576296	11 831845	12 538833
Ň	5.618725	14.697368	11.155956
С	6.406484	13.416597	9.239812
С	5.907552	13.213023	14.886690
Н	5.349323	13.281472	15.823029
Н	6.692694	13.968886	14.918500
С	5.297967	14.290995	9.778850
н	5.142508	15.150513	9.123087
п С	7 000220	15.722437	9.797555
č	3 819018	12 675347	13 761941
Ĥ	2.958269	13.324167	13.932900
н	3.864995	12.003809	14.620573
С	9.017743	13.702631	13.221490
Н	9.002092	12.699586	13.619779
С	8.011045	11.815257	9.715605
Н	8.488527	11.207445	10.472294
C L	4.460657	15.107491	11.977819
п	3.000320 1 101151	14.492730	11.095541
С	8 417213	11 759507	8 393091
H	9.219919	11.097748	8.101392
С	4.784874	14.910118	13.453637
Н	5.672241	15.480456	13.725282
Н	3.959857	15.273811	14.070922
С	6.702182	15.703772	11.177287
Н	6.314867	16.659921	11.534054
Н	7.044122	15.880644	10.156783
н	2.303279	11.130242	12.402149
C	4.375841	10.952721	10.559385
Ĥ	5.191496	10.911660	9.852024
С	7.394720	10.248139	13.308788
Н	7.597290	9.967393	12.284144
С	6.808396	11.045282	15.848836
Н	6.547165	11.387638	16.840315
С	3.224207	10.217993	10.358707
н С	3.130969 6.763036	9.589368	9.484939
н	6 257644	14 082718	7 211899
С	7.704542	9.399007	14.357726
Ĥ	8.159670	8.439790	14.159227
С	7.408749	9.808994	15.651119
Н	7.631720	9.170171	16.494747
С	2.203276	10.314367	11.299258
Н	1.283476	9.759379	11.174035
С Ц	8.949450	16.212301	12.1/39/3
C	7 777435	12 575479	7 469279
й	8.072253	12.563805	6.428770
С	10.101926	14.532456	13.426588
Н	10.952441	14.179189	13.991381
С	10.063463	15.817502	12.894195
Н	10.891159	16.498708	13.038750

[Ni(κ⁵-TPEN)]⁺; 2S+1=2

Ni	6.498403	12.830453	12.138965
Ν	4.779259	11.681902	11.833517
Ν	8.131724	13.971546	12.345123
N	5.026442	13.663898	13.802202
IN C	6 302302	12.497202	9.102100
N	6.900211	11.562878	13.788527
С	3.813609	11.734480	12.758405
Ν	5.773472	14.606858	11.017891
С	6.298621	13.697707	8.761356
С	5.841937	13.407138	14.975108
н	5.296003 6 680947	14 106113	14 963860
С	5.254938	14.297484	9.666689
Н	4.841067	15.196920	9.196696
Н	4.444847	13.580913	9.796498
С	8.010086	15.244017	11.927687
С Ц	3.799992	12.889507	13.746113
н	3 554091	12 492016	14 735126
С	9.169738	13.661847	13.143815
С	7.720005	11.948849	8.333776
Н	8.084334	10.975020	8.642128
С	4.665175	15.122519	11.851073
н	3.780032	14.533299	11.012820
С	8.224510	12.557747	7,189704
Ĥ	8.989629	12.068675	6.602352
С	4.922775	15.044128	13.351952
Н	5.853231	15.554358	13.602070
Н	4.114879	15.587747	13.861264
н	0.097207	15.554525	10.961550
н	7.333364	15.518926	9.962572
С	2.806738	10.774710	12.815549
Н	2.044702	10.844316	13.581382
C	4.759607	10.690254	10.930272
C	7.395730 6.365880	10.323970	13.720540
н	5 933875	11 564696	16 999847
С	3.792498	9.700944	10.923720
С	6.736842	14.374668	7.626548
С	7.406612	9.457452	14.803552
C	0.880621	9.900726	16.009249
c	2.795540	16 234631	12 314413
Ĥ	8.756657	17.249010	11.968569
С	7.714619	13.795822	6.826875
С	10.106862	14.589581	13.557753
С	9.9/0891	15.909695	13.139354
н	6.322001	14.305205	5.942007 7 381318
н	9.227701	12.632115	13.464528
Н	10.676090	16.667421	13.453091
Н	10.919834	14.282204	14.200860
Н	7.812591	8.461554	14.696671
п	0.000492	9.202910	10.0/0022
Н	5.549988	10.724976	10.193507
Н	3.823092	8.917869	10.178457
н	2.024007	8.983956	11.925911

[Ni(κ⁵-TPEN)(CO₂)]⁺; 2S+1=2

Ni	6.651240	12.675429	12.287086
N	5.006555	11.488279	11.828454
N	8.074521	14.085183	12.746304
IN N	5.250869	13.482674	13.772450
	0.154590	12.223007	0.000470
N	7 060067	11.907004	10.101011
C	2 20/212	11.402233	14.023737
N	5 868106	1/ 276602	12.317400
C	6 12/21/	12 555880	8 6/1062
ĉ	5 02/525	13.333000	15 065960
й	5.924525	13 /00372	15.005900
н	6 703498	14 0008072	15 135244
Ċ	5 238747	14 138491	9 708197
н	4 825373	15 087520	9 350582
н	4 413266	13 451088	9 873179
c	7.980223	15,234278	12.066394
č	4.009896	12.693254	13,714629
Ĥ	3.136264	13.346734	13.768191
н	3.963137	12.054386	14.598336
С	9.012716	13.956323	13.692328
Č	6.913952	11.666494	7.609032
н	6.915583	10.581988	7.572558
С	4.793233	14.970624	11.888383
Н	3.873422	14.434027	11.660225
Н	4.631769	16.014660	11.604034
С	7.672941	12.401218	6.706965
Н	8.274005	11.898867	5.961234
С	5.057158	14.884017	13.376531
н	5.947807	15.443250	13.652231
н	4.213368	15.336156	13.908992
С	7.011641	15.295150	10.920679
Н	6.673642	16.324181	10.766962
Н	7.580921	15.000265	10.040948
С	2.666720	11.215992	12.204790
Н	1.789009	11.496089	12.770828
С	4.936667	10.575306	10.849776
C	7.646515	10.256883	14.053628
C	6.614463	11.2/2606	16.360422
Н	6.177930	11.703904	17.250494
C	3.754748	9.946815	10.501123
C	6.830351	14.372406	7.760213
C	7.747780	9.507032	15.215268
C	7.223414	10.023727	10.390001
Ĉ	2.392410	10.200070	11.100744
ц	8 700131	17 232356	12.340000
\hat{C}	7 621028	13 786238	6 782383
č	9 889524	14 976007	14 012625
č	9 780879	16 181061	13 329514
č	8 045688	11 838936	10.020014
õ	8 023349	10 624314	11 013539
õ	8.642920	12,700869	10.307075
н	8.183821	14.399795	6.090323
H	6,755909	15,448950	7.837450
H	9.051212	13.005119	14.201938
H	10.439961	17.008146	13.560055
н	10.632078	14.826135	14.783191
н	8.221518	8.536314	15.190101
н	7.275885	9.465202	17.314525
н	8.025869	9.898217	13.108368
Н	5.858095	10.361017	10.339625
Н	3.750312	9.217652	9.703273
н	1.646631	9.829020	10.922196

Ni6.71918012.56072812.224117N4.93297311.42493111.818142N8.11260314.14869512.757103N5.27160413.42553713.768801N6.08872412.2235918.546930C6.58622211.90744715.173465N7.11929011.39919814.052880C3.84092911.78834812.499591N5.87213614.39110211.026507C6.11285813.5556418.637482C5.94445613.26748915.063029H5.26012613.42828515.901076H6.72276214.02785915.135227C5.23747814.1735829.694441H4.85511015.1335709.328424H4.39097813.5110439.855463C7.97398715.28568112.068729C4.01803012.65304713.722507H3.15582313.31450313.835366H3.99846211.98047414.582261C9.03283114.07043813.722294C6.83607611.6343537.618855H6.79291010.5506277.580185C7.6370312.3353056.726366H8.22559711.8076335.985445S5.08898214.83373913.387822H5.98269115.33577510.898544H6.7149016.31237310.678928H7.618857<				
N 4.932973 11.424931 11.818142 N 8.112603 14.148695 12.757103 N 5.271604 13.425537 13.768801 C 6.586222 11.907447 15.173465 N 7.119290 11.399198 14.052880 C 3.840929 11.788348 12.499591 N 5.872136 14.391102 11.026507 C 6.112858 13.555641 8.637482 C 5.944456 13.267489 15.063029 H 5.260126 13.428285 15.901076 H 6.722762 14.027859 15.13527 C 5.237478 14.17352 9.69441 H 4.855110 15.135570 9.328424 H 4.390978 13.514043 9.855633 C 7.973987 15.285681 12.068729 C 4.018030 12.653047 13.722507 H 3.998462 11.980474 14.582261 C 9.032	Ni	6.719180	12.560728	12.224117
N 8.112603 14.148695 12.757103 N 5.271604 13.425537 13.768801 N 6.088724 12.223591 8.546930 C 6.586222 11.907447 15.173465 N 7.119290 11.389198 14.052880 C 3.840929 11.788348 12.499591 N 5.872136 14.391102 11.026507 C 6.112858 13.555641 8.637482 C 5.944456 13.267489 15.063029 H 5.260126 13.428285 15.901076 H 6.722762 14.027859 15.135227 C 5.237478 14.173582 9.694441 H 4.855110 15.13527 9.328424 H 4.390978 13.511043 9.855463 C 7.973987 15.285681 12.068729 C 4.018030 12.653047 13.722507 H 3.198462 11.804353 7.615865 H 6.792	Ν	4.932973	11.424931	11.818142
N 5:71604 13.425537 13.768801 N 6.088724 12.223591 8.546930 C 6.586222 11.907447 15.173465 N 7.119290 11.38348 12.499591 N 5.872136 14.391102 11.026507 C 6.112858 13.555641 8.637482 C 5.944456 13.267489 15.063029 H 5.260126 13.428285 15.901076 H 6.722762 14.027859 15.35227 C 5.237478 14.173582 9.694441 H 4.855110 15.135279 9.328424 H 4.390978 13.511043 9.855463 C 7.973987 15.285681 12.068729 C 4.018030 12.653047 13.722507 H 3.155823 13.314503 13.835366 H 3.998462 11.804333 7.615865 G 6.792910 10.550627 7.580185 C 4.819447	N	8 112603	14 148695	12 757103
N 5.271004 13.723037 13.763030 C 6.586222 11.907447 15.173465 N 7.119290 11.399198 14.052880 C 3.840929 11.788348 12.499591 N 5.872136 14.391102 11.026507 C 6.112858 13.555641 8.637482 C 5.944456 13.267489 15.063029 H 5.260126 13.428285 15.901076 H 6.722762 14.027859 15.135227 C 5.237478 14.173582 9.694441 H 4.855110 15.133570 9.328424 H 4.390978 13.511043 9.855463 C 7.973987 15.285681 12.068729 C 4.018030 12.653047 13.722507 H 3.15833 13.314503 13.835366 G 8.36076 11.634353 7.615865 C 9.032831 14.070438 13.722294 C 6.360	N	5 271604	13 425537	12 768801
N 6.088/24 12.223591 8.546930 C 6.586222 11.907447 15.173465 N 7.119290 11.389198 14.052880 C 3.840929 11.788348 12.499591 N 5.872136 14.391102 11.026507 C 6.112858 13.555641 8.637482 C 5.944456 13.267489 15.063029 H 5.260126 13.428285 15.901076 H 6.722762 14.027859 15.135227 C 5.237478 14.173582 9.694441 H 4.855110 15.133570 9.328424 H 4.390978 13.511043 9.855463 C 7.973987 15.285681 12.068729 C 4.018030 12.653047 13.722507 H 3.155823 13.314503 13.835366 H 3.998462 11.804333 7.615865 H 6.792910 10.550627 7.580185 C 4.839	IN .	5.271004	13.423337	13.700001
C6.58622211.90744715.173465N7.11929011.38919814.052880C3.84092911.78834812.499591N5.87213614.39110211.026507C6.11285813.5556418.637482C5.94445613.26748915.063029H5.26012613.42828515.901076H6.72276214.02785915.135227C5.23747814.1735829.694441H4.85511015.1335709.328424H4.39097813.5110439.855463C7.97398715.28568112.068729C4.01803012.65304713.722507H3.15582313.31450313.835366H3.99846211.98047414.58261C9.03283114.07043813.72294C6.83607611.6343537.615865H6.79291010.5506277.580185C4.81944714.96638311.901140H3.88956614.45047711.665411H4.66621416.02365011.634394H5.98269115.38154213.673394H4.24856215.28199513.929779C7.03048515.28797510.898544C5.08898214.83373913.387822H5.98269115.38154213.673394H4.24856215.28199513.929779C7.03048515.28797510.8985445C5.088982 <td>N</td> <td>6.088724</td> <td>12.223591</td> <td>8.546930</td>	N	6.088724	12.223591	8.546930
N 7.119290 11.399198 14.052880 C 3.840929 11.788348 12.499591 N 5.872136 14.391102 11.026507 C 6.112858 13.555641 8.637482 C 5.944456 13.267489 15.063029 H 5.260126 13.428285 15.901076 H 6.722762 14.027859 15.135227 C 5.237478 14.173582 9.694441 H 4.855110 15.133570 9.328424 H 4.390978 13.511043 9.855463 C 7.973987 15.285681 12.068729 C 4.018030 12.653047 13.722507 H 3.15823 13.314503 13.835366 H 3.998462 11.980474 14.582261 C 9.032831 14.070438 13.722597 H 3.889566 14.450477 11.665411 H 4.666214 16.023650 11.658980 C 7.6	С	6.586222	11.907447	15.173465
1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.	N	7.119290	11.399198	14.052880
C 3.647925 11.760346 12.495951 N 5.872136 14.391102 11.026507 C 6.112858 13.555641 8.637482 C 5.944456 13.267489 15.063029 H 5.260126 13.428285 15.901076 H 6.722762 14.027859 15.135227 C 5.237478 14.173582 9.694441 H 4.855110 15.133570 9.328424 H 4.390978 13.511043 9.855463 C 7.973987 15.285681 12.068729 C 4.018030 12.653047 13.722507 H 3.155823 13.314503 13.835366 H 3.998462 11.980474 14.582261 C 6.836076 11.634353 7.615865 H 7.92910 10.550627 7.580185 C 4.819447 14.966383 11.901140 H 3.889566 14.450477 11.655411 H 6.662	Ĉ	3 840020	11 7993/9	12 /00501
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C 6.112858 13.555641 8.637482 C 5.944456 13.267489 15.0603029 H 5.260126 13.428285 15.901076 H 6.722762 14.027859 15.135227 C 5.237478 14.173582 9.694441 H 4.855110 15.133570 9.328424 H 4.390978 13.511043 9.855463 C 7.973987 15.285681 12.068729 C 4.018030 12.653047 13.722507 H 3.155823 13.314503 13.835366 H 3.998462 11.980474 14.582261 C 6.836076 11.634353 7.615855 H 6.792910 10.550627 7.580185 C 4.819447 14.966383 11.901140 H 3.889566 14.450477 11.665411 H 4.666214 16.023650 11.658980 C 7.637030 12.335305 6.723636 H 2.61	N	5.872136	14.391102	11.026507
C5.94445613.26748915.063029H5.26012613.42828515.901076H6.72276214.02785915.135227C5.23747814.1735829.694441H4.85511015.1335709.328424H4.39097813.5110439.855463C7.97398715.28568112.068729C4.01803012.65304713.722507H3.15582313.31450313.835366H3.99846211.98047414.582261C9.03283114.07043813.722294C6.83607611.6343537.615865H6.79291010.5506277.580185C4.81944714.96638311.901140H3.88956614.45047711.665411H4.66621416.02365011.658980C7.63703012.3353056.723636H8.22559711.8076335.985445C5.08898214.83373913.387822H5.98269115.38154213.673394H4.24856215.28797510.898544H6.71149016.31237310.678928H7.61985714.93867510.050474C2.57926911.31586412.157179H1.71281411.64533712.714177C4.82002310.55001510.812272C7.72682710.2103114.092154C6.64913311.22485416.380605H6.198588 <td>С</td> <td>6.112858</td> <td>13.555641</td> <td>8.637482</td>	С	6.112858	13.555641	8.637482
H5.26012613.42828515.901076H6.72276214.02785915.135227C5.23747814.1735829.694441H4.85511015.1335709.328424H4.39097813.5110439.855463C7.97398715.28568112.068729C4.01803012.65304713.722507H3.15582313.31450313.835366H3.99846211.98047414.582261C9.03283114.07043813.722294C6.83607611.6343537.615865H6.79291010.5506277.580185C4.81944714.96638311.901140H3.8856614.45047711.665411H4.66621416.02365011.658980C7.63703012.3353056.723636H8.22559711.8076335.985445C5.08898214.8373913.387822H5.98269115.38154213.673394H4.24856215.28199513.929779C7.03048515.28797510.898544H6.71149016.31237310.678928H7.61985714.93867510.050474C2.57926911.31586412.157179H1.7281411.64533712.714177C4.82002310.55001510.812272C7.2682710.21033114.092154C6.64913311.22485416.380605H6.198588 <t< td=""><td>С</td><td>5.944456</td><td>13.267489</td><td>15.063029</td></t<>	С	5.944456	13.267489	15.063029
In3.20012013.420285915.135227C5.23747814.1735829.694441H4.85511015.1335709.328424H4.39097813.5110439.855463C7.97398715.28568112.068729C4.01803012.65304713.722507H3.15582313.31450313.835366H3.99846211.98047414.582261C9.03283114.07043813.722294C6.83607611.6343537.615865H6.79291010.5506277.580185C4.81944714.96638311.901140H3.88956614.45047711.665411H4.66621416.02365011.658980C7.63703012.3353056.723636H8.22559711.8076335.985445C5.08898214.8337913.387822H5.98269115.38154213.673394H4.24856215.28199513.929779C7.03048515.28797510.898544H6.71149016.31237310.678928H7.61885710.95001510.812272C7.72682710.21033114.092154C6.64913311.22485416.380605H6.19858811.65416817.264741C3.60232910.01245710.433096C6.86542114.3411897.765793C7.2851779.99191216.425875C2.457906 <td>й</td> <td>5 260126</td> <td>13 / 28285</td> <td>15 001076</td>	й	5 260126	13 / 28285	15 001076
H 6.722762 14.027839 15.133277 C 5.237478 14.173582 9.694441 H 4.855110 15.133570 9.328424 H 4.390978 15.285681 12.068729 C 4.018030 12.653047 13.722507 H 3.155823 13.314503 13.835366 H 3.998462 11.980474 14.582261 C 9.032831 14.070438 13.722294 C 6.836076 11.634353 7.615865 H 6.792910 10.550627 7.580185 C 4.819447 14.966383 11.901140 H 3.889566 14.450477 11.665411 H 6.66214 16.023650 11.658980 C 7.637030 12.335305 6.723636 H 8.225597 11.807633 5.985445 C 5.088982 14.833739 13.387822 H 5.982691 15.312373 10.678928 H 7.619857 14.938675 10.050474 C 2.579269 1		0.200120	13.420203	15.301070
C5.23747814.1735829.694441H4.85511015.1335709.328424H4.39097813.5110439.855463C7.97398715.28568112.068729C4.01803012.65304713.722507H3.15582313.31450313.835366H3.99846211.98047414.582261C9.03283114.07043813.722294C6.83607611.6343537.615865H6.79291010.5506277.580185C4.81944714.96638311.901140H3.88956614.45047711.665411H4.66621416.02365011.658980C7.63703012.3353056.723636H8.22559711.8076335.985445C5.08898214.83373913.387822H5.98269115.38154213.673394H4.24856215.28797510.898544H6.71149016.31237310.678928H7.61985714.93867510.050474C2.57926911.31586412.157179H1.71281411.64533712.714177C4.82002310.55001510.812272C7.72682710.21033114.092154C6.64913311.22485416.380605H6.19858811.65416817.264741C3.60232910.01245710.433096C7.8351079.4728415.261029C7.285177	н	6.722762	14.027859	15.135227
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H4.39097813.5110439.855463C7.97398715.28568112.068729C4.01803012.65304713.722507H3.15582313.31450313.835366H3.99846211.98047414.582261C9.03283114.07043813.722294C6.83607611.6343537.615865H6.79291010.5506277.580185C4.81944714.96638311.901140H3.88956614.45047711.665411H4.66621416.02365011.658980C7.63703012.3353056.723636H8.22559711.8076335.985445C5.08898214.83373913.387822H5.98269115.38154213.673394H4.24856215.28199513.929779C7.03048515.28797510.898544H6.71149016.31237310.678928H7.61985714.93867510.050474C2.57926911.31586412.157179H1.71281411.64533712.714177C4.82002310.55001510.812272C7.72682710.21033114.092154C6.64913311.22485416.380605H6.19858811.65416817.264741C3.60232910.01245710.433096C7.8351079.47288415.261029C7.2851779.99191216.425875C2.457906 <td>н</td> <td>4.855110</td> <td>15.133570</td> <td>9.328424</td>	н	4.855110	15.133570	9.328424
11.000000000000000000000000000000000000	н	4 390978	13 511043	9 855463
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$\begin{array}{llllllllllllllllllllllllllllllllllll$		2.379209	11.313004	12.13/1/9
C4.82002310.55001510.812272C7.72682710.21033114.092154C6.64913311.22485416.380605H6.19858811.65416817.264741C3.60232910.01245710.433096C6.86542114.3411897.765793C7.8351079.47288415.261029C7.2851779.99191216.425875C2.45790610.41618611.109112C8.74641516.40569312.358422H8.60032217.31816211.797145C7.64353713.7214546.798082C9.85015015.13534414.059185C9.69511916.33037313.366021C8.08925410.40482710.748888O8.92402412.40465510.273540H8.23923214.3105146.113001H6.83540115.4200117.841829H9.10668913.12283514.238018H10.30444717.19094213.607803H10.58048515.02896014.848608H8.3318988.51346215.251280H7.3416569.44133317.355362H8.1259809.85140713.153086H5.73600910.29593810.305670H3.5550599.3065079.615931H1.48626310.0322710.826925H8.79643210.18653010.111160	н	1.712814	11.645337	12./141//
C7.72682710.21033114.092154C6.64913311.22485416.380605H6.19858811.65416817.264741C3.60232910.01245710.433096C6.86542114.3411897.765793C7.8351079.47288415.261029C7.2851779.99191216.425875C2.45790610.41618611.109112C8.74641516.40569312.358422H8.60032217.31816211.797145C7.64353713.7214546.798082C9.85015015.13534414.059185C9.69511916.33037313.366021C8.08156511.78365410.904251O8.0825410.40482710.748888O8.92402412.40465510.273540H8.23923214.3105146.113001H6.83540115.4200117.841829H9.10668913.12283514.238018H10.30444717.19094213.607803H10.58048515.02896014.848608H8.3318988.51346215.251280H7.3416569.44133317.355362H8.1259809.85140713.153086H5.73600910.29593810.305670H3.5550599.3065079.615931H1.48626310.0322710.826925H8.79643210.18653010.111160	С	4.820023	10.550015	10.812272
C 6.649133 11.224854 16.380605 H 6.198588 11.654168 17.264741 C 3.602329 10.012457 10.433096 C 6.865421 14.341189 7.765793 C 7.835107 9.472884 15.261029 C 7.285177 9.991912 16.425875 C 2.457906 10.416186 11.109112 C 8.746415 16.405693 12.358422 H 8.600322 17.318162 11.797145 C 7.643537 13.721454 6.798082 C 9.850150 15.135344 14.059185 C 9.695119 16.330373 13.366021 C 8.081565 11.783654 10.904251 O 8.089254 10.404827 10.748888 O 8.924024 12.404655 10.273540 H 8.239232 14.310514 6.113001 H 6.835401 15.420011 7.841829 H 9.10	С	7.726827	10.210331	14.092154
H 6.19858 11.62168 17.264741 C 3.602329 10.012457 10.433096 C 6.865421 14.341189 7.765793 C 7.835107 9.472884 15.261029 C 7.835107 9.472884 15.261029 C 7.835107 9.472884 15.261029 C 7.835107 9.991912 16.425875 C 2.457906 10.416186 11.109112 C 8.746415 16.405693 12.358422 H 8.600322 17.318162 11.797145 C 7.643537 13.721454 6.798082 C 9.850150 15.135344 14.059185 C 9.695119 16.30373 13.366021 C 8.081565 11.783654 10.904251 O 8.08254 10.404827 10.748888 O 8.024024 12.404655 10.273540 H 8.1028042 13.122835 14.238018 H 10.3044	С	6 649133	11 224854	16 380605
Image: Non-State State Image: Non-State State Image: Non-State Image	ŭ	6 100500	11 65/160	17 264741
C 3.602329 10.012457 10.433096 C 6.865421 14.341189 7.765793 C 7.835107 9.472884 15.261029 C 7.285177 9.991912 16.425875 C 2.457906 10.416186 11.109112 C 8.746415 16.405693 12.358422 H 8.600322 17.318162 11.797145 C 7.643537 13.721454 6.798082 C 9.850150 15.135344 14.059185 C 9.695119 16.330373 13.366021 C 8.081565 11.783654 10.904251 O 8.924024 12.404655 10.273540 H 8.239232 14.310514 6.113001 H 6.835401 15.420011 7.841829 H 9.106689 13.122835 14.238018 H 10.304447 17.190942 13.607803 H 10.580485 15.028960 14.848608 H 8.	П	0.190000	11.004100	17.204741
C 6.865421 14.341189 7.765793 C 7.835107 9.472884 15.261029 C 7.285177 9.991912 16.425875 C 2.457906 10.416186 11.109112 C 8.746415 16.405693 12.358422 H 8.600322 17.318162 11.797145 C 7.643537 13.721454 6.798082 C 9.850150 15.135344 14.059185 C 9.695119 16.330373 13.366021 C 8.081565 11.783654 10.904251 O 8.089254 10.404827 10.748888 O 8.924024 12.404655 10.273540 H 8.239232 14.310514 6.113001 H 6.835401 15.420011 7.841829 H 9.106689 13.122835 14.238018 H 10.304447 17.190942 13.607803 H 10.580485 15.028960 14.848608 H 8.	C	3.602329	10.012457	10.433096
C 7.835107 9.472884 15.261029 C 7.285177 9.991912 16.425875 C 2.457906 10.416186 11.109112 C 8.746415 16.405693 12.358422 H 8.600322 17.318162 11.797145 C 7.643537 13.721454 6.798082 C 9.850150 15.135344 14.059185 C 9.695119 16.30373 13.366021 C 8.081565 11.783654 10.904251 O 8.08254 10.404827 10.748888 O 8.924024 12.404655 10.273540 H 8.389232 14.310514 6.113001 H 6.835401 15.420011 7.841829 H 9.106689 13.122835 14.238018 H 10.304447 17.190942 13.607803 H 10.304447 17.190942 13.607803 H 10.304447 17.190942 13.607803 H 8.	С	6.865421	14.341189	7.765793
C7.2851779.99191216.425875C2.45790610.41618611.109112C8.74641516.40569312.358422H8.60032217.31816211.797145C7.64353713.7214546.798082C9.85015015.13534414.059185C9.69511916.33037313.366021C8.08156511.78365410.904251O8.08925410.40482710.748888O8.92402412.40465510.273540H8.23923214.3105146.113001H6.83540115.4200117.841829H9.10668913.12283514.238018H10.30444717.19094213.607803H10.58048515.02896014.848608H8.3318988.51346215.251280H7.3416569.44133317.355362H8.1259809.85140713.153086H5.73600910.29593810.305670H3.5550599.3065079.615931H1.48626310.0322710.826925H8.79643210.18653010.111160	С	7.835107	9.472884	15.261029
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C 2.437300 10.410180 11.103112 C 8.746415 16.405693 12.358422 H 8.600322 17.318162 11.797145 C 7.643537 13.721454 6.798082 C 9.850150 15.135344 14.059185 C 9.695119 16.330373 13.366021 C 8.081565 11.783654 10.904251 O 8.089254 10.404827 10.748888 O 8.924024 12.404655 10.273540 H 8.239232 14.310514 6.113001 H 6.835401 15.428011 7.841829 H 9.106689 13.122835 14.238018 H 10.304447 17.190942 13.607803 H 10.304447 17.190942 13.607803 H 10.304447 17.190942 13.607803 H 10.304447 17.190942 13.607803 H 10.580485 15.028960 14.848608 H	č	2 457006	10 / 16 1 86	11 100112
C8.74641516.40569312.338422H8.60032217.31816211.797145C7.64353713.7214546.798082C9.85015015.13534414.059185C9.69511916.33037313.366021C8.08156511.78365410.904251O8.08925410.40482710.748888O8.92402412.40465510.273540H8.23923214.3105146.113001H6.83540115.4200117.841829H9.10668913.12283514.238018H10.30444717.19094213.607803H10.58048515.02896014.848608H8.3318988.51346215.251280H7.3416569.44133317.355362H8.1259809.85140713.153086H5.73600910.29593810.305670H3.5550599.3065079.615931H1.48626310.03328710.826925H8.79643210.18653010.111160	2	2.437300	10.410100	10.050400
H8.60032217.31816211.797145C7.64353713.7214546.798082C9.85015015.13534414.059185C9.69511916.33037313.366021C8.08156511.78365410.904251O8.08925410.40482710.748888O8.92402412.40465510.273540H8.23923214.3105146.113001H6.83540115.4200117.841829H9.10668913.12283514.238018H10.30444717.19094213.607803H10.58048515.02896014.848608H8.3318988.51346215.251280H7.3416569.44133317.355362H8.1259809.85140713.153086H5.73600910.29593810.305670H3.5550599.3065079.615931H1.48626310.03328710.826925H8.79643210.18653010.111160	C	8.746415	16.405693	12.358422
C 7.643537 13.721454 6.798082 Q.850150 15.135344 14.059185 Q.9850150 15.135344 14.059185 C 9.695119 16.330373 13.366021 C 8.081565 11.783654 10.904251 O 8.089254 10.404827 10.748888 O 8.924024 12.404655 10.273540 H 8.239232 14.310514 6.113001 H 6.835401 15.420011 7.841829 H 9.106689 13.122835 14.238018 H 10.304447 17.190942 13.607803 H 10.580485 15.028960 14.848608 H 8.331898 8.513462 15.251280 H 7.341656 9.441333 17.355362 H 8.125980 9.851407 13.153086 H 5.736009 10.295938 10.305670 H 3.555059 9.306507 9.615931 H 1.486263 10.033287	Н	8.600322	17.318162	11.797145
C9.85015015.13534414.059185C9.69511916.33037313.366021C8.08156511.78365410.904251O8.08925410.40482710.748888O8.92402412.40465510.273540H8.23923214.3105146.113001H6.83540115.4200117.841829H9.10668913.12283514.238018H10.30444717.19094213.607803H8.3318988.51346215.251280H7.3416569.44133317.355362H8.1259809.85140713.153086H5.73600910.29593810.305670H3.5550599.3065079.615931H1.48626310.03328710.826925H8.79643210.18653010.111160	С	7.643537	13.721454	6.798082
C9.69511916.33037313.366021C8.08156511.78365410.904251O8.08925410.40482710.748888O8.92402412.40465510.273540H8.23923214.3105146.113001H6.83540115.4200117.841829H9.10668913.12283514.238018H10.30444717.19094213.607803H10.58048515.02896014.848608H8.3318988.51346215.251280H7.3416569.44133317.355362H8.1259809.85140713.153086H5.73600910.29593810.305670H3.5550599.3065079.615931H1.48626310.03328710.826925H8.79643210.18653010.111160	С	9.850150	15.135344	14.059185
C 8.0831565 11.783654 10.904251 C 8.081565 11.783654 10.904251 O 8.089254 10.404827 10.748888 O 8.924024 12.404655 10.273540 H 8.239232 14.310514 6.113001 H 6.835401 15.420011 7.841829 H 9.106689 13.122835 14.238018 H 10.304447 17.190942 13.607803 H 10.580485 15.028960 14.848608 H 8.331898 8.513462 15.251280 H 7.341656 9.441333 17.355362 H 8.125980 9.851407 13.153086 H 5.736009 10.295938 10.305670 H 3.555059 9.306507 9.615931 H 1.486263 10.033287 10.826925 H 8.796432 10.186530 10.111160	č	0.605110	16 330373	13 366021
C 8.081565 11.783654 10.904251 O 8.089254 10.404827 10.748888 O 8.924024 12.404655 10.273540 H 8.239232 14.310514 6.113001 H 6.835401 15.420011 7.841829 H 9.106689 13.122835 14.238018 H 10.304447 17.190942 13.607803 H 10.580485 15.028960 14.848608 H 8.331898 8.513462 15.251280 H 7.341656 9.441333 17.355362 H 8.125980 9.851407 13.153086 H 5.736009 10.295938 10.305670 H 3.555059 9.306507 9.615931 H 1.486263 10.033287 10.826925 H 8.796432 10.186530 10.111160	č	9.095119	10.330373	10.000021
O 8.089254 10.404827 10.748888 O 8.924024 12.404655 10.273540 H 8.239232 14.310514 6.113001 H 6.835401 15.420011 7.841829 H 9.106689 13.122835 14.238018 H 10.304447 17.190942 13.607803 H 8.331898 8.513462 15.251280 H 8.331898 8.513462 15.251280 H 8.125980 9.851407 13.153086 H 5.736009 10.295938 10.305670 H 3.555059 9.306507 9.615931 H 1.486263 10.03287 10.826925 H 8.796432 10.186530 10.111160	C	8.081565	11.783654	10.904251
O 8.924024 12.404655 10.273540 H 8.239232 14.310514 6.113001 H 6.835401 15.420011 7.841829 H 9.106689 13.122835 14.238018 H 10.304447 17.190942 13.607803 H 10.580485 15.028960 14.848608 H 8.331898 8.513462 15.251280 H 7.341656 9.441333 17.355362 H 8.125980 9.851407 13.153086 H 5.736009 10.295938 10.305670 H 3.555059 9.306507 9.615931 H 1.486263 10.033287 10.826925 H 8.796432 10.186530 10.111160	0	8.089254	10.404827	10.748888
H8.23923214.3105146.113001H6.83540115.4200117.841829H9.10668913.12283514.238018H10.30444717.19094213.607803H10.58048515.02896014.848608H8.3318988.51346215.251280H7.3416569.44133317.355362H8.1259809.85140713.153086H5.73600910.29593810.305670H3.5550599.3065079.615931H1.48626310.03328710.826925H8.79643210.18653010.111160	0	8.924024	12.404655	10.273540
H 6.835401 15.420011 7.841829 H 9.106689 13.122835 14.238018 H 10.304447 17.190942 13.607803 H 10.580485 15.028960 14.848608 H 8.331898 8.513462 15.251280 H 7.341656 9.441333 17.355362 H 8.125980 9.851407 13.153086 H 5.736009 10.295938 10.305670 H 3.555059 9.306507 9.615931 H 1.486263 10.033287 10.826925 H 8.796432 10.186530 10.111160	н	8.239232	14.310514	6.113001
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H 10.30444/ 17.190942 13.607803 H 10.580485 15.028960 14.848608 H 8.331898 8.513462 15.251280 H 7.341656 9.441333 17.355362 H 8.125980 9.851407 13.153086 H 5.736009 10.295938 10.305670 H 3.555059 9.306507 9.615931 H 1.486263 10.033287 10.826925 H 8.796432 10.186530 10.111160		9.100089	13.122835	14.230018
H10.58048515.02896014.848608H8.3318988.51346215.251280H7.3416569.44133317.355362H8.1259809.85140713.153086H5.73600910.29593810.305670H3.5550599.3065079.615931H1.48626310.03328710.826925H8.79643210.18653010.111160	н	10.304447	17.190942	13.607803
H8.3318988.51346215.251280H7.3416569.44133317.355362H8.1259809.85140713.153086H5.73600910.29593810.305670H3.5550599.3065079.615931H1.48626310.03328710.826925H8.79643210.18653010.111160	Н	10.580485	15.028960	14.848608
H 7.341656 9.441333 17.355362 H 8.125980 9.851407 13.153086 H 5.736009 10.295938 10.305670 H 3.555059 9.306507 9.615931 H 1.486263 10.033287 10.826925 H 8.796432 10.186530 10.111160	Н	8.331898	8.513462	15.251280
H 8.125980 9.851407 13.153086 H 8.125980 9.851407 13.153086 H 5.736009 10.295938 10.305670 H 3.555059 9.306507 9.615931 H 1.486263 10.033287 10.826925 H 8.796432 10.186530 10.111160	н	7 341656	9 441333	17 355362
n 0.120900 9.851407 13.153086 H 5.736009 10.295938 10.305670 H 3.555059 9.306507 9.615931 H 1.486263 10.033287 10.826925 H 8.796432 10.186530 10.111160	L	0 105000	0.051107	12 152000
H5.73600910.29593810.305670H3.5550599.3065079.615931H1.48626310.03328710.826925H8.79643210.18653010.111160	п	0.125980	9.001407	13.153086
H3.5550599.3065079.615931H1.48626310.03328710.826925H8.79643210.18653010.111160	н	5.736009	10.295938	10.305670
H1.48626310.03328710.826925H8.79643210.18653010.111160	Н	3.555059	9.306507	9.615931
H 8.796432 10.186530 10.111160	Н	1.486263	10.033287	10.826925
	Н	8.796432	10.186530	10.111160

[Ni(κ⁵-TPEN)(CO₂H)]⁺; 2S+1=3

Ni(κ⁵-TPEN)(CO)]⁺; 2S+1=2

Ni6.70951612.55469011.854048N4.90352711.51584211.580364N5.50165013.24407913.679174N6.62704612.5498958.584806C6.72804411.94073715.423525N7.70495911.37768414.704833C3.94890511.67890112.501354N5.76363314.40681210.903894C6.14611313.7951638.508895C6.22954013.28734814.969032H5.58750213.71542915.747850H7.07860813.95496414.835667C5.15650614.2143149.564670H4.65556315.1357909.245891H4.39700513.4413899.666565C7.91999515.25717211.843463C4.32233312.37251613.781647H4.53857611.58451714.503385C9.18022213.80180713.119627C7.52124612.1552677.680526H7.89025811.1402947.780535C4.69277514.7401111.859440H3.84438114.10243111.659055H4.35112215.78238411.690309C7.97627912.9711286.650661H8.7053712.6019405.942363C5.11921014.62167913.308755H4.29793914.97347213.945341C6.799207<				
N 4.903527 11.515842 11.580364 N 8.138192 14.022629 12.305718 N 5.501650 13.244079 13.679174 N 6.627046 12.549895 8.584806 C 6.728044 11.940737 15.423525 N 7.704959 11.377684 14.704833 C 3.948905 11.678901 12.501354 N 5.763633 14.406812 10.903894 C 6.146113 13.795163 8.508895 C 6.29540 13.287348 14.969032 H 5.587502 13.715429 15.747850 H 7.078608 13.954964 14.835667 C 5.156506 14.214314 9.564655 C 7.91995 15.257172 11.84363 C 4.322333 12.372516 13.781647 H 3.458604 12.921575 14.171762 H 4.538576 11.584517 14.503385 C 9.18	NI	6.709516	12.554690	11.854048
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N7.70495911.37768414.704833C3.94890511.67890112.501354N5.76363314.40681210.903894C6.14611313.7951638.508895C6.22954013.28734814.969032H5.58750213.71542915.747850H7.07860813.95496414.835667C5.15650614.2143149.564670H4.65556315.1357909.245891H4.39700513.4413899.666565C7.91999515.25717211.843463C4.32233312.37251613.781647H3.45860412.92157514.171762H4.53857611.58451714.503385C9.18022213.80180713.119627C7.52124612.1552677.680526H7.89025811.1402947.780535C4.69277514.75401111.859440H3.84438114.10243111.690309C7.97627912.9711286.650661H8.70553712.6019405.942363C5.11921014.62167913.308755H5.97125715.26872213.507952H4.29793914.97347213.945341C6.6625416.4588910.983471H7.25779215.434289.870141C2.66671411.16792812.325205H1.91506211.33422313.085163C4.623974 <td< td=""><td>С</td><td>6.728044</td><td>11.940737</td><td>15.423525</td></td<>	С	6.728044	11.940737	15.423525
1.1.0100 11.07801 12.501354 N 5.763633 14.406812 10.903894 C 6.146113 13.795163 8.508895 C 6.229540 13.287348 14.969032 H 5.587502 13.715429 15.747850 H 7.078608 13.954964 14.835667 C 5.156506 14.214314 9.564670 H 4.655563 15.135790 9.245891 H 4.397005 13.441389 9.666565 C 7.919995 15.257172 11.843463 C 4.322333 12.372516 13.781647 H 3.458604 12.921575 14.171762 H 4.538576 11.584517 14.503385 C 9.180222 13.801807 13.119627 C 7.521246 12.15267 7.680526 H 7.890258 11.40294 7.780535 C 4.692775 14.754011 11.859440 H 3.844381 14.102431 11.690309 C 7.976279 12.971128	N	7 704959	11 377684	14 704833
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b) 5.587502 13.715429 15.747850 H 7.078608 13.954964 14.835667 C 5.156506 14.214314 9.564670 H 4.655563 15.135790 9.245891 H 4.397005 13.441389 9.666565 C 7.919995 15.257172 11.843463 C 4.322333 12.372516 13.781647 H 3.458604 12.921575 14.171762 H 5.38576 11.584517 14.503385 C 9.180222 13.801807 13.119627 C 7.521246 12.155267 7.680526 H 7.890258 11.140294 7.780535 C 4.692775 14.754011 11.859440 H 3.844381 14.102431 11.659055 H 4.351122 15.782384 11.690309 C 7.976279 12.971128 6.650661 H 8.705537 12.601940 5.942363 C 5.667	С	6 229540	13 287348	14 969032
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1.3.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1	н	4 397005	13 441389	9 666565
C 1.3.19993 13.237172 11.043403 C 4.322333 12.372516 13.781647 H 3.458604 12.921575 14.171762 H 4.538576 11.584517 14.503385 C 9.180222 13.801807 13.119627 C 7.521246 12.155267 7.680526 H 7.890258 11.140294 7.780535 C 4.692775 14.754011 11.859440 H 3.844381 14.102431 11.659055 H 4.351122 15.782384 11.690309 C 7.976279 12.971128 6.650661 B 8.705537 12.601940 5.942363 C 5.119210 14.621679 13.308755 H 5.971257 15.268722 13.507952 H 4.297939 14.973472 13.945341 C 6.799207 15.449066 10.859065 H 6.362854 16.445889 10.983471 H 7.257792 15.434328 9.870141 C 2.666714 <t< td=""><td>C</td><td>7 010005</td><td>15 257172</td><td>11 9/3/63</td></t<>	C	7 010005	15 257172	11 9/3/63
C 4.32233 12.372516 13.781647 H 3.458604 12.921575 14.171762 H 4.538576 11.584517 14.503385 C 7.521246 12.155267 7.680526 H 7.890258 11.140294 7.780535 C 4.692775 14.754011 11.859440 H 3.844381 14.102431 11.669055 H 4.351122 15.782384 11.690309 C 7.976279 12.971128 6.650661 H 8.705537 12.601940 5.942363 C 5.119210 14.621679 13.308755 H 5.971257 15.268722 13.507952 H 4.297939 14.973472 13.945341 C 6.799207 15.449066 10.859065 H 6.362854 16.445889 10.983471 H 7.257792 15.434328 9.870141 C 2.666714 11.367928 12.325205 H 1.915062 11.334223 13.085163 C 4.623974	č	1.313333	10.201112	11.040400
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H4.53857611.58451714.503385C9.18022213.80180713.119627C7.52124612.1552677.680526H7.89025811.1402947.780535C4.69277514.75401111.859440H3.84438114.10243111.690055H4.35112215.78238411.690099C7.97627912.9711286.650661H8.70553712.6019405.942363C5.11921014.62167913.308755H5.97125715.26872213.507952H4.29793914.97347213.945341C6.79920715.44906610.859065H6.36285416.44588910.983471H7.25779215.4343289.870141C2.66671411.16792812.325205H1.91506211.33422313.085163C4.62397410.82172010.468176C8.15573310.17969115.072393C6.18786611.32165616.547997H5.40084111.80932917.107178C3.37935910.26771210.222222C6.53552014.6758477.502735C7.6705009.48598916.175608C2.37722110.45082611.176114C8.73747416.32476312.201465H8.52315217.31443511.822000C7.46466014.2576106.558376C10.045760 <td>Н</td> <td>3.458604</td> <td>12.921575</td> <td>14.171762</td>	Н	3.458604	12.921575	14.171762
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C0.13920713.44900610.639005H6.36285416.44588910.983471T.25779215.4343289.870141C2.66671411.16792812.325205H1.91506211.33422313.085163C4.62397410.82172010.468176C8.15573310.17969115.072393C6.18788611.32165616.547997H5.40084111.80932917.107178C3.37935910.26771210.229222C6.53552014.6758477.502735C7.6705009.48598916.175608C2.37722110.45082611.176114C8.73747416.32476312.201465H8.52315217.31443511.822000C7.46466014.2576106.558376C10.04576014.80814813.507736C9.81560816.09826113.041176C7.86960711.27695911.292266O8.63697510.51276310.920372H7.78479614.9262225.770140H6.12066215.6740767.467621H9.27999012.78988613.484293H10.46389816.91421513.331398H10.87202514.58557514.168057H8.0730718.51593316.431749H6.2633369.57640117.801916H8.9454839.75528014.461607H5.42508710.	\hat{c}	6 700207	15 440066	10.040041
H6.36285416.44588910.9834/1H7.25779215.4343289.870141C2.66671411.16792812.325205H1.91506211.33422313.085163C4.62397410.82172010.468176C8.15573310.17969115.072393C6.18788611.32165616.547997H5.40084111.80932917.107178C3.37935910.26771210.229222C6.53552014.6758477.502735C7.6705009.48598916.175608C2.37722110.45082611.176114C8.73747416.32476312.201465H8.52315217.31443511.822000C7.46466014.2576106.558376C10.04576014.80814813.507736C9.81560816.09826113.041176C7.86960711.27695911.292266O8.63697510.51276310.920372H7.78479614.9262225.770140H6.12066215.6740767.467621H9.27999012.78988613.484293H10.46389816.91421513.331398H10.87202514.58557514.168057H8.0730718.51593316.431749H6.2633369.57640117.801916H8.9454839.75528014.461607H5.42508710.7537119.746280H3.199698 <td></td> <td>0.799207</td> <td>15.449066</td> <td>10.659065</td>		0.799207	15.449066	10.659065
H7.25779215.4343289.870141C2.66671411.16792812.325205H1.91506211.33422313.085163C4.62397410.82172010.468176C8.15573310.17969115.072393C6.18788611.32165616.547997H5.40084111.80932917.107178C3.37935910.26771210.229222C6.53552014.6758477.502735C7.6705009.48598916.175608C6.66810210.07595816.931802C2.37722110.45082611.176114C8.73747416.32476312.201465H8.52315217.31443511.822000C7.46466014.2576106.558376C10.04576014.80814813.507736C9.81560816.09826113.041176C7.86960711.27695911.292266O8.63697510.51276310.920372H7.78479614.9262225.770140H6.12066215.6740767.467621H9.27999012.78988613.484293H10.46389816.91421513.331398H10.87202514.58557514.168057H8.0730718.51593316.431749H6.2633369.57640117.801916H8.9454839.75528014.461607H5.42508710.7537119.746280H3.199698 </td <td>н</td> <td>6.362854</td> <td>16.445889</td> <td>10.983471</td>	н	6.362854	16.445889	10.983471
C 2.666714 11.167928 12.325205 H 1.915062 11.334223 13.085163 C 4.623974 10.821720 10.468176 C 8.155733 10.179691 15.072393 C 6.187886 11.321656 16.547997 H 5.400841 11.809329 17.107178 C 3.379359 10.267712 10.229222 C 6.535520 14.675847 7.502735 C 7.670500 9.485989 16.175608 C 6.668102 10.075958 16.931802 C 2.377221 10.450826 11.176114 C 8.737474 16.324763 12.201465 H 8.523152 17.314435 11.822000 C 7.464660 14.257610 6.558376 C 10.045760 14.808148 13.507736 C 9.815608 16.098261 13.041176 C 7.869607 11.276959 11.292266 O	н	7.257792	15.434328	9.870141
H1.91506211.33422313.085163C4.62397410.82172010.468176C8.15573310.17969115.072393C6.18788611.32165616.547997H5.40084111.80932917.107178C3.37935910.26771210.229222C6.53552014.6758477.502735C7.6705009.48598916.175608C2.37722110.45082611.176114C8.73747416.32476312.201465H8.52315217.31443511.822000C7.46466014.2576106.558376C10.04576014.80814813.507736C9.81560816.09826113.041176C7.86960711.27695911.292266O8.63697510.51276310.920372H7.78479614.9262225.770140H6.12066215.6740767.467621H9.27999012.78988613.484293H10.46389816.91421513.331398H10.87202514.58557514.168057H8.0730718.51593316.431749H6.2633369.57640117.801916H8.9454839.75528014.461607H5.42508710.7537119.746280H3.1996989.3170669.317066H1.38740910.04370711.019303	С	2.666714	11.167928	12.325205
In <td>Ĥ</td> <td>1 915062</td> <td>11 334223</td> <td>13 085163</td>	Ĥ	1 915062	11 334223	13 085163
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	\hat{c}	4 602074	10.004220	10.000100
C 8.155733 10.179691 15.072393 C 6.187886 11.321656 16.547997 H 5.400841 11.809329 17.107178 C 3.379359 10.267712 10.229222 C 6.535520 14.675847 7.502735 C 7.670500 9.485989 16.175608 C 6.668102 10.075958 16.931802 C 2.377221 10.450826 11.176114 C 8.737474 16.324763 12.201465 H 8.523152 17.314435 11.822000 C 7.464660 14.257610 6.558376 C 10.045760 14.808148 13.507736 C 9.815608 16.098261 13.041176 C 7.869607 11.276959 11.292266 Ø 8.63975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.2	č	4.023974	10.021720	10.400170
C 6.187886 11.321656 16.547997 H 5.400841 11.809329 17.107178 C 3.379359 10.267712 10.229222 C 6.535520 14.675847 7.502735 C 7.670500 9.485989 16.175608 C 2.377221 10.450826 11.176114 C 8.737474 16.324763 12.201465 H 8.523152 17.314435 11.822000 C 7.464660 14.257610 6.558376 C 10.045760 14.808148 13.507736 C 9.815608 16.098261 13.041176 C 7.869607 11.276959 11.292266 O 8.636975 10.512763 10.920372 T 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 1	C	8.155733	10.179691	15.072393
H5.40084111.80932917.107178C3.37935910.26771210.229222C6.53552014.6758477.502735C7.6705009.48598916.175608C6.66810210.07595816.931802C2.37722110.45082611.176114C8.73747416.32476312.201465H8.52315217.31443511.822000C7.46466014.2576106.558376C10.04576014.80814813.507736C9.81560816.09826113.041176C7.86960711.27695911.292266O8.63697510.51276310.920372H7.78479614.9262225.770140H6.12066215.6740767.467621H9.27999012.78988613.484293H10.46389816.91421513.331398H10.87202514.58557514.168057H8.0730718.51593316.431749H6.2633369.57640117.801916H8.9454839.75528014.461607H5.42508710.7537119.746280H3.1996989.7166009.317066H1.38740910.04370711.019303	С	6.187886	11.321656	16.547997
C 3.379359 10.267712 10.229222 C 6.535520 14.675847 7.502735 C 7.670500 9.485989 16.175608 C 6.668102 10.075958 16.931802 C 2.377221 10.450826 11.176114 C 8.737474 16.324763 12.201465 H 8.523152 17.314435 11.822000 C 7.464660 14.257610 6.558376 C 10.045760 14.808148 13.041176 C 7.869607 11.276959 11.292266 O 8.636975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H <td< td=""><td>Н</td><td>5.400841</td><td>11.809329</td><td>17.107178</td></td<>	Н	5.400841	11.809329	17.107178
C 6.535520 14.675847 7.502735 C 7.670500 9.485989 16.175608 C 6.668102 10.075958 16.931802 C 2.377221 10.450826 11.176114 C 8.737474 16.324763 12.201465 H 8.523152 17.314435 11.822000 C 7.464660 14.257610 6.558376 C 10.045760 14.808148 13.507736 C 9.815608 16.098261 13.041176 C 7.869607 11.276959 11.292266 Ø 8.636975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6	С	3 379359	10 267712	10 229222
C 0.33520 14.073047 1.352133 C 7.670500 9.485989 16.175608 C 6.668102 10.075958 16.931802 C 2.377221 10.450826 11.176114 C 8.737474 16.324763 12.201465 H 8.523152 17.314435 11.822000 C 7.464660 14.257610 6.558376 C 10.045760 14.808148 13.507736 C 9.815608 16.098261 13.041176 C 7.869607 11.276959 11.292266 O 8.636975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 <td< td=""><td>ĉ</td><td>6 535520</td><td>1/ 6758/7</td><td>7 502735</td></td<>	ĉ	6 535520	1/ 6758/7	7 502735
C 7.670500 9.485989 10.175008 C 6.668102 10.075958 16.931802 C 2.377221 10.450826 11.176114 C 8.737474 16.324763 12.201465 H 8.523152 17.314435 11.822000 C 7.464660 14.257610 6.558376 C 10.045760 14.808148 13.507736 C 9.815608 16.098261 13.041176 C 7.869607 11.276959 11.292266 O 8.636975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 <t< td=""><td>č</td><td>0.000020</td><td>0.405000</td><td>1.302133</td></t<>	č	0.000020	0.405000	1.302133
C 6.668102 10.075958 16.931802 C 2.377221 10.450826 11.176114 C 3.737474 16.324763 12.201465 H 8.523152 17.314435 11.822000 C 7.464660 14.257610 6.558376 C 10.045760 14.808148 13.041176 C 7.869607 11.276959 11.292266 O 8.636975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 3.199698 9.716600 9.317066 H 3.8	C	7.670500	9.485989	16.175608
C 2.377221 10.450826 11.176114 C 2.377474 16.324763 12.201465 H 8.523152 17.314435 11.822000 C 7.464660 14.257610 6.558376 C 10.045760 14.808148 13.507736 C 9.815608 16.098261 13.041176 C 7.869607 11.276959 11.292266 O 8.638975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.	С	6.668102	10.075958	16.931802
C 8.737474 16.324763 12.201465 H 8.523152 17.314435 11.822000 C 7.464660 14.257610 6.558376 C 10.045760 14.808148 13.507736 C 9.815608 16.098261 13.041176 C 7.869607 11.276959 11.292266 O 8.636975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.317066 1.387409	С	2.377221	10.450826	11.176114
H8.52315217.31443511.822000C7.46466014.2576106.558376C10.04576014.80814813.507736C9.81560816.09826113.041176C7.86960711.27695911.292266O8.63697510.51276310.920372H7.78479614.9262225.770140H6.12066215.6740767.467621H9.27999012.78988613.484293H10.46389816.91421513.331398H10.87202514.58557514.168057H8.0730718.51593316.431749H6.2633369.57640117.801916H8.9454839.75528014.461607H5.42508710.7537119.746280H3.1996989.7166009.317066H1.38740910.04370711.019303	С	8.737474	16.324763	12.201465
Instruct Instruct Instruct C 7.464660 14.257610 6.558376 C 10.045760 14.808148 13.507736 C 9.815608 16.098261 13.041176 C 7.869607 11.276959 11.292266 O 8.636975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.716600 9.317066 H 1.387409 10.043707 11.019303	Ĥ	8 523152	17 314435	11 822000
C 7.464600 14.237610 6.536376 C 10.045760 14.808148 13.507736 C 9.815608 16.098261 13.041176 C 7.869607 11.276959 11.292266 O 8.636975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.716600 9.317066 H 1.387409 10.043707 11.019303	2	7 464660	14.057640	6 550076
C 10.045760 14.808148 13.507736 C 9.815608 16.098261 13.041176 C 7.869607 11.276959 11.292266 O 8.636975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.317066 1.387409 10.043707	Č	7.404000	14.257610	0.000370
C 9.815608 16.098261 13.041176 C 7.869607 11.276959 11.292266 O 8.636975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.716600 9.317066 H 1.387409 10.043707 11.019303	C	10.045760	14.808148	13.507736
C 7.869607 11.276959 11.292266 O 8.636975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.716600 9.317066 H 1.387409 10.043707 11.019303	С	9.815608	16.098261	13.041176
O 8.636975 10.512763 10.920372 H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.716600 9.317066 H 1.387409 10.043707 11.019303	С	7.869607	11.276959	11.292266
H 7.784796 14.926222 5.770140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.716600 9.317066 H 1.387409 10.043707 11.019303	0	8 636975	10 512763	10 920372
H 7.184796 14.320222 3.176140 H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.716600 9.317066 H 1.387409 10.043707 11.019303	ŭ	7 784706	14 026222	5 770140
H 6.120662 15.674076 7.467621 H 9.279990 12.789886 13.484293 H 10.463898 16.914215 13.331398 H 10.872025 14.585575 14.168057 H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.716600 9.317066 H 1.387409 10.043707 11.019303		1.104190	14.920222	3.770140
H9.27999012.78988613.484293H10.46389816.91421513.331398H10.87202514.58557514.168057H8.0730718.51593316.431749H6.2633369.57640117.801916H8.9454839.7528014.461607H5.42508710.7537119.746280H3.1996989.7166009.317066H1.38740910.04370711.019303	н	6.120662	15.674076	7.467621
H10.46389816.91421513.331398H10.87202514.58557514.168057H8.0730718.51593316.431749H6.2633369.57640117.801916H8.9454839.75528014.461607H5.42508710.7537119.746280H3.1996989.7166009.317066H1.38740910.04370711.019303	Н	9.279990	12.789886	13.484293
H10.87202514.58557514.168057H8.0730718.51593316.431749H6.2633369.57640117.801916H8.9454839.75528014.461607H5.42508710.7537119.746280H3.1996989.7166009.317066H1.38740910.04370711.019303	Н	10.463898	16.914215	13.331398
H 8.073071 8.515933 16.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.716600 9.317066 H 1.387409 10.043707 11.019303	н	10.872025	14.585575	14,168057
H 5.073071 5.35335 10.431749 H 6.263336 9.576401 17.801916 H 8.945483 9.755280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.716600 9.317066 H 1.387409 10.043707 11.019303	н	8 073071	8 515032	16 4317/0
H 8.945483 9.75280 14.461607 H 5.425087 10.753711 9.746280 H 3.199698 9.716600 9.317066 H 1.387409 10.043707 11.019303	н Ц	6 262220	0.576404	17 001016
H8.9454839.75528014.461607H5.42508710.7537119.746280H3.1996989.7166009.317066H1.38740910.04370711.019303		0.203330	9.5/0401	17.001910
H5.42508710.7537119.746280H3.1996989.7166009.317066H1.38740910.04370711.019303	н	8.945483	9.755280	14.461607
H3.1996989.7166009.317066H1.38740910.04370711.019303	Н	5.425087	10.753711	9.746280
H 1.387409 10.043707 11.019303	Н	3.199698	9.716600	9.317066
	Н	1.387409	10.043707	11.019303

IR Frequencies Calibration: 2077 cm⁻¹ by calculation, 2043 cm⁻¹ by experiment, 0.983

[Ni(CO)₄]⁰; 2S+1=1

Ni	-6.263080	7.635617	-0.398814
0	-6.238815	6.641085	-3.200318
0	-9.015277	8.467393	0.356204
0	-4.466348	9.989314	-0.124617
0	-5.346613	5.462036	1.410211
С	-6.247694	7.023147	-2.131169
С	-7.965909	8.146801	0.065024
С	-5.149117	9.088720	-0.232440
С	-5.698459	6.293252	0.721472

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