

Carboxylic acid-capped ruthenium nanoparticles: experimental and theoretical case study with ethanoic acid

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P17 and beyond: Cartesian coordinates of all RuNPs studied in this work by DFT.

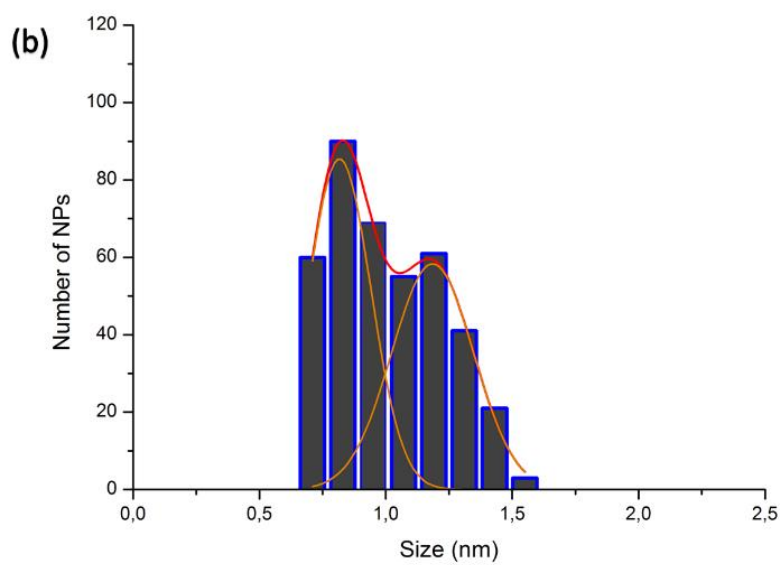
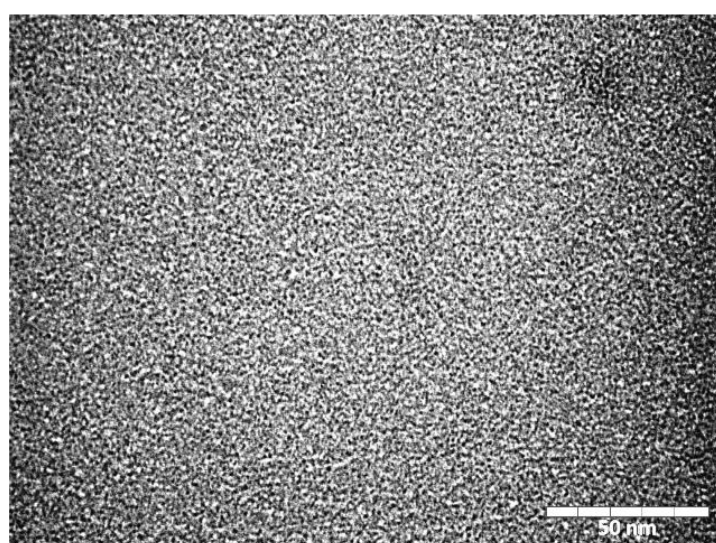
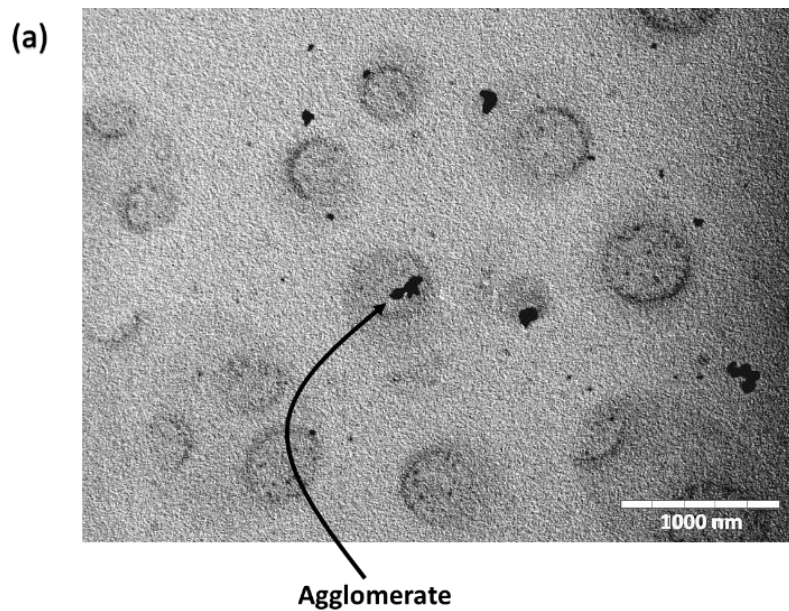


Figure SI.1. a) TEM images and b) corresponding size histogram of $\text{Ru}_x(\text{CH}_3\text{COOH})_{0.2y}$ NPs.

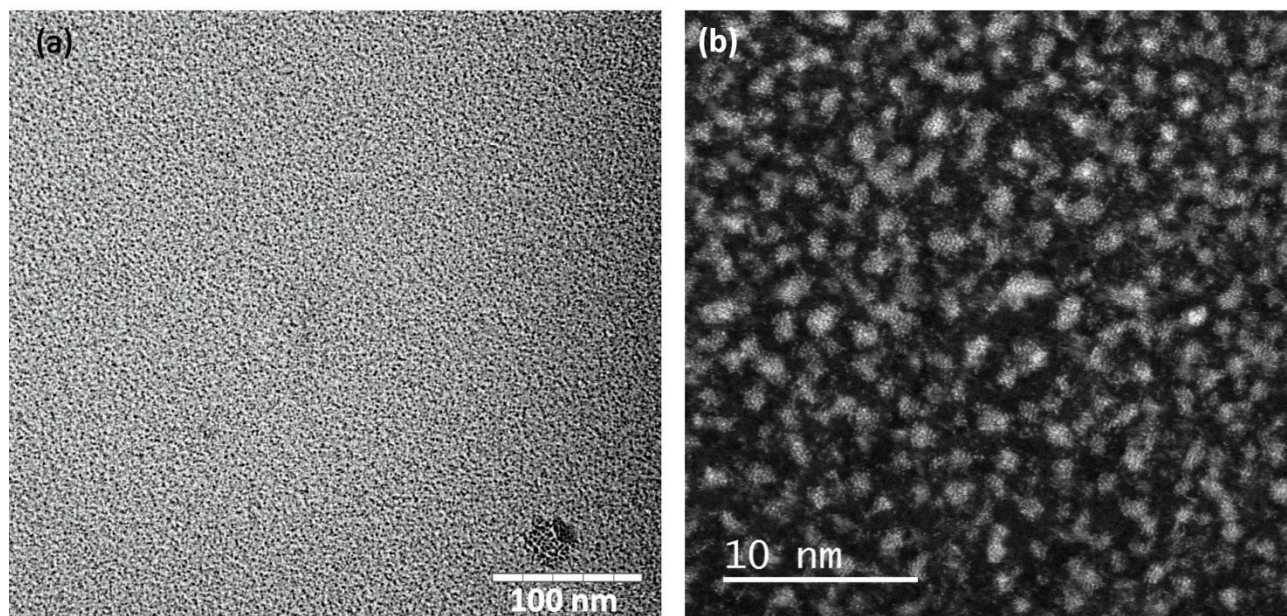
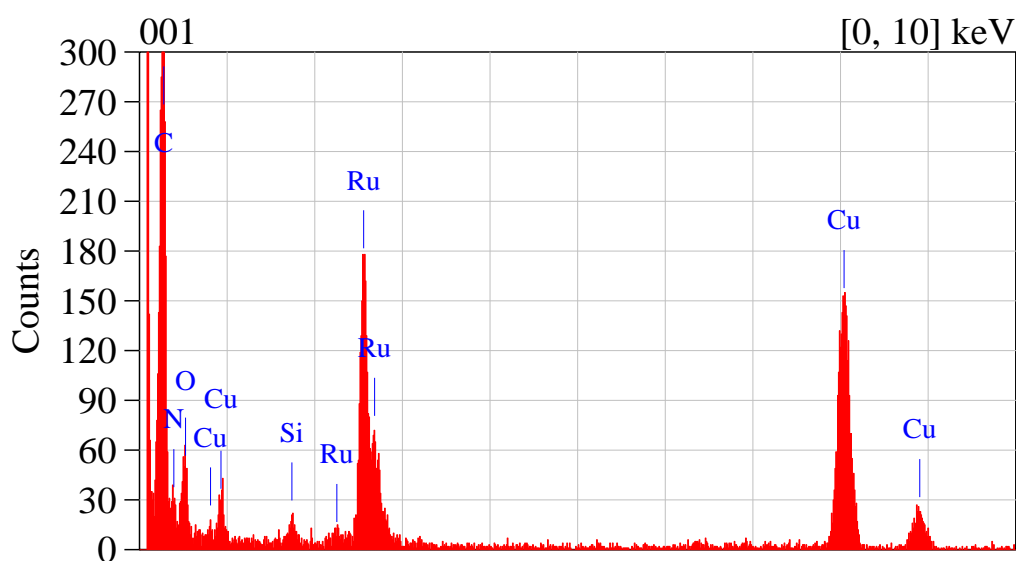
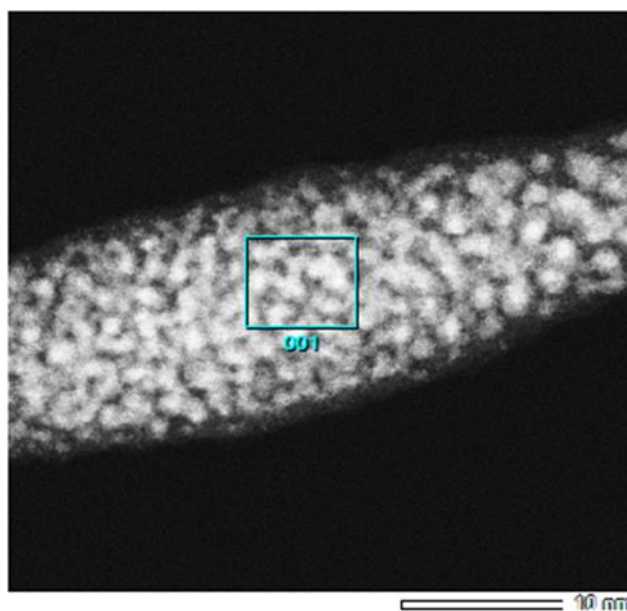


Figure SI.2. a) TEM and b) HRTEM images of Ru_x(CH₃COOH)_{0.4y} NPs.

Figure SI.3. EDX data recorded for $\text{Ru}_x(\text{CH}_3\text{COOH})_{0.4y}$ NPs.

Title : $\text{Ru}_x(\text{CH}_3\text{COOH})_{0.4y}$

 Instrument : JEM-ARM200F (URP)
 Volt : 200,00 kV
 Mag. : x 5,000,000
 Date : 2017/04/25
 Pixel : 512 x 512

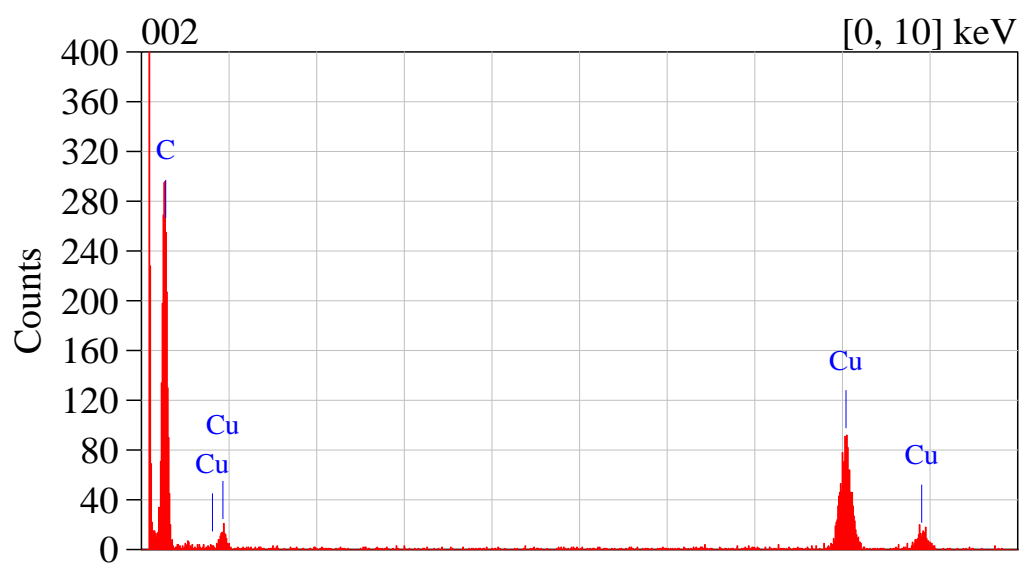
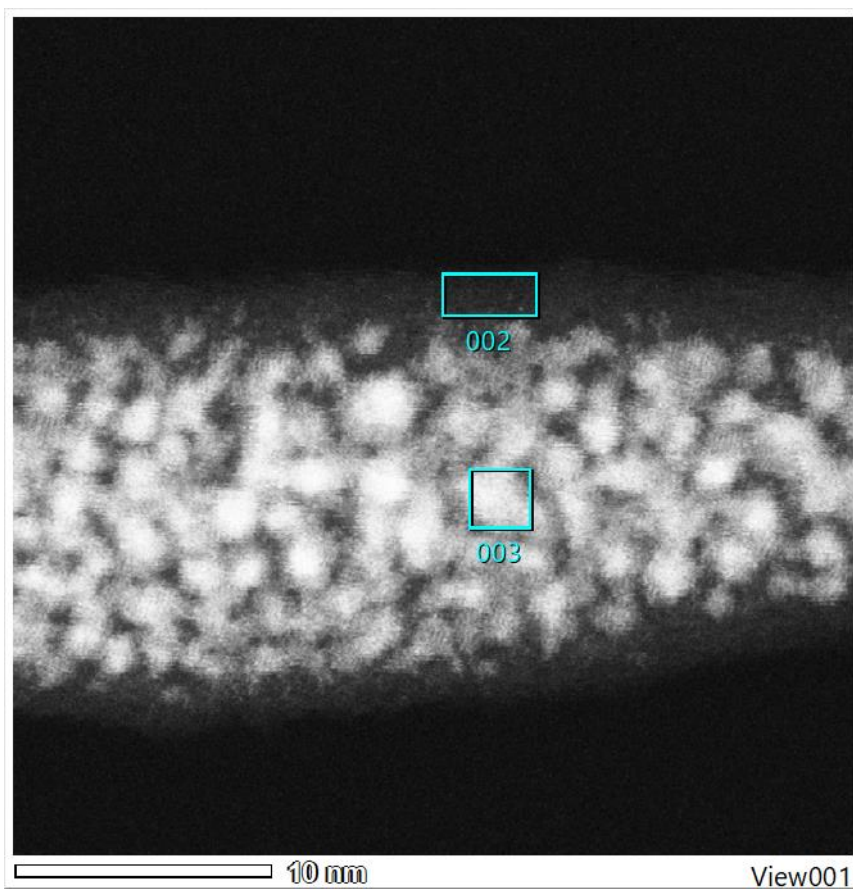
View **001** (in a group of NPs)

Thin Film Standardless Standardless Quantitative Analysis

Fitting Coefficient: 0.6664

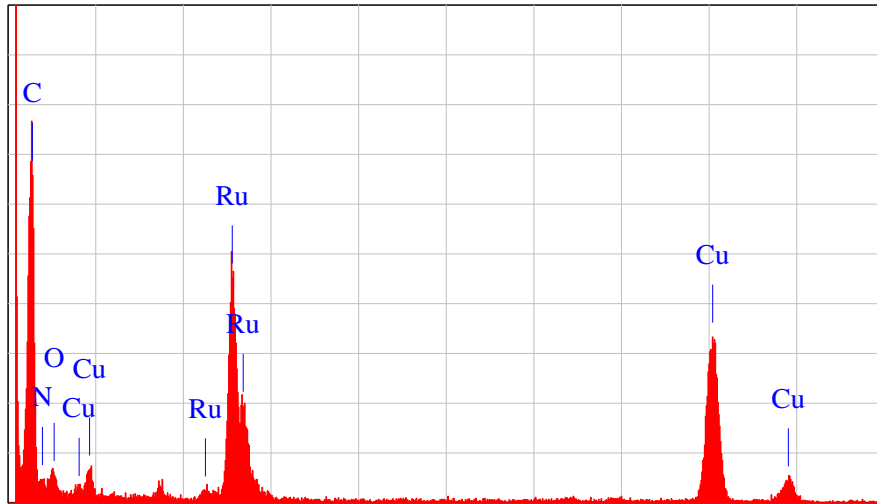
Element	(keV)	Mass%	Counts	Sigma	Atom%	Compound	Mass%	Cation	K
C K (Ref.)	0.277	56.6	2322.9	0.8	84.3				1.0000
N K !	0.392	5.2	317.1	0.4	6.7				0.6760
O K !	0.525	2.4	191.5	0.3	2.7				0.5110
Ru L	2.558	35.8	1612.6	1.2	6.3				0.9117
Total		100.0			100.0				

Views 002 (outside a group of NPs) and 003 (in a group of NPs)



003

VFS = 1000 count

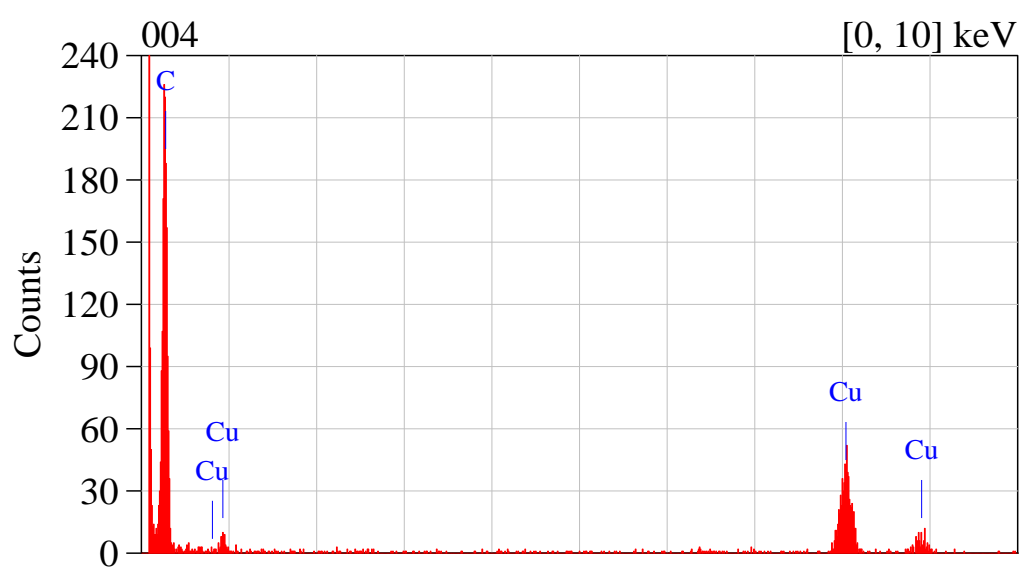
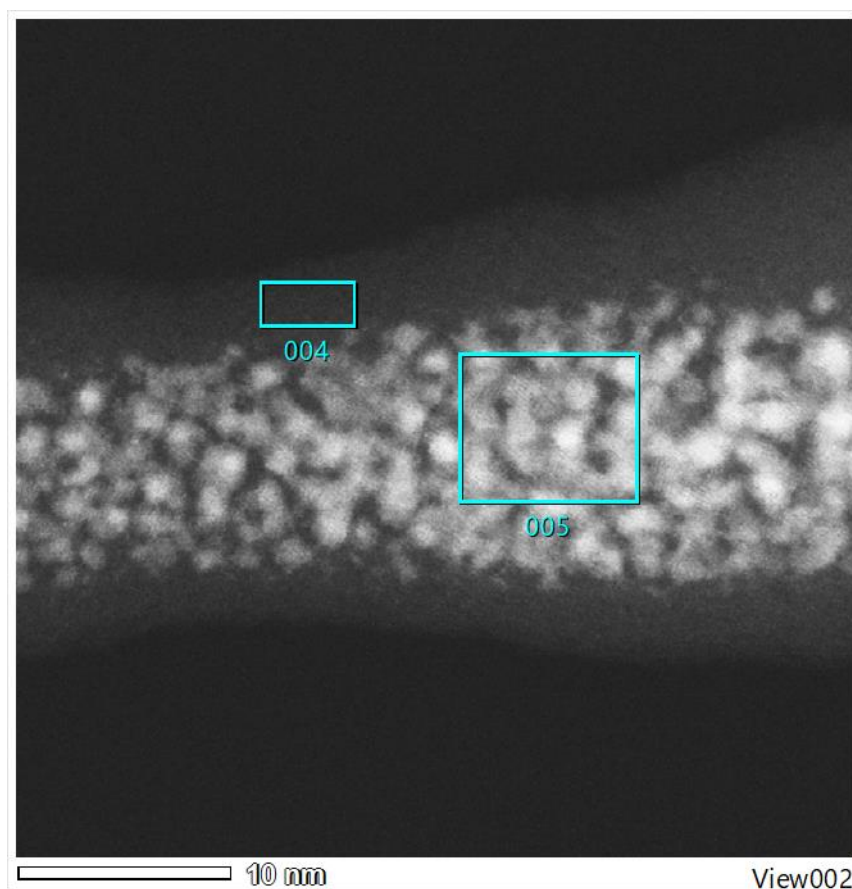


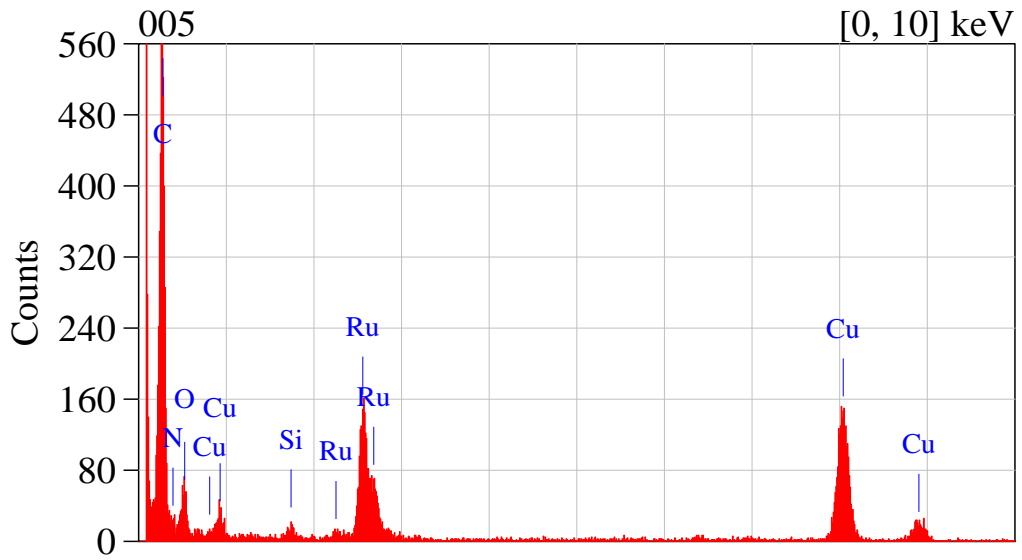
Thin Film Standardless Standardless Quantitative Analysis

Fitting Coefficient: 0.6788

Element	(keV)	Mass%	Counts	Sigma	Atom%	Compound	Mass%	Cation	K
C K (Ref.)	0.277	54.2	3284.4	0.7	85.9				1.0000
N K !	0.392	4.1	366.7	0.3	5.6				0.6760
O K !	0.525	0.7	85.4	0.1	0.9				0.5110
Ru L	2.558	41.0	2728.6	1.1	7.7				0.9117
Total		100.0			100.0				

Views 004 (outside a group of NPs) and 005 (in a group of NPs)

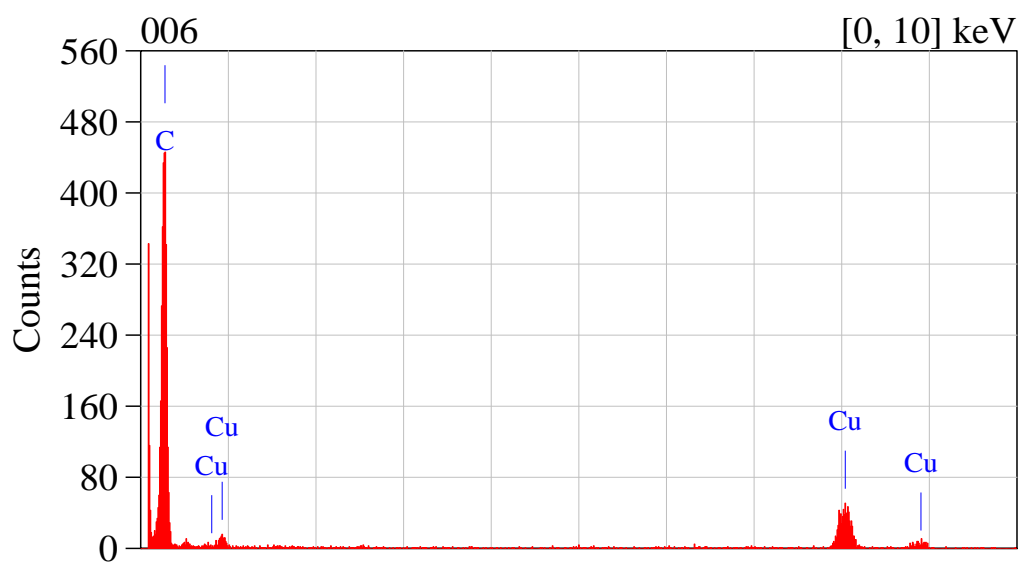
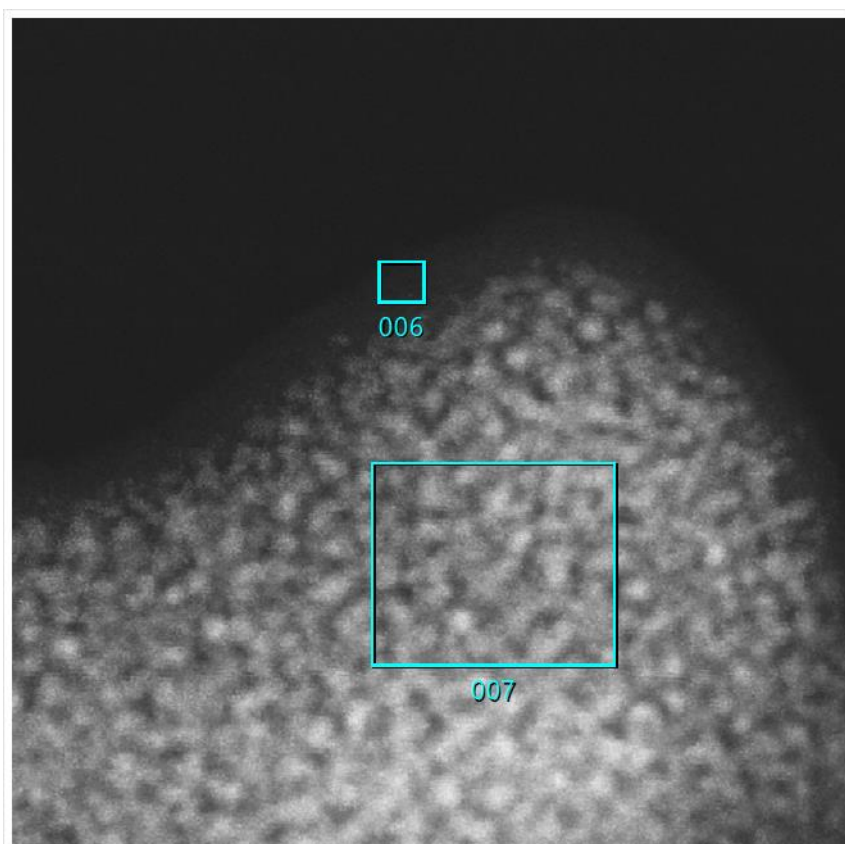




Thin Film Standardless Standardless Quantitative Analysis
 Fitting Coefficient: 0.6107

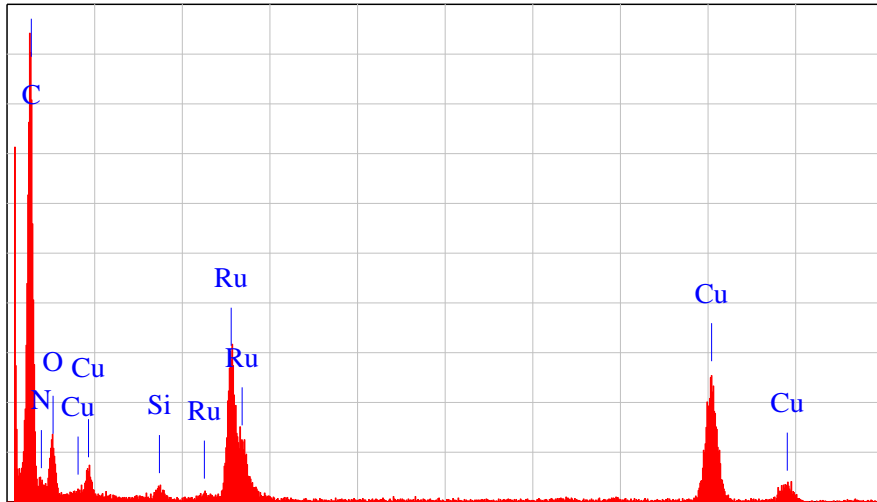
Element	(keV)	Mass%	Counts	Sigma	Atom%	Compound	Mass%	Cation	K
C K (Ref.)	0.277	71.6	3907.5	0.8	89.6				1.0000
N K !	0.392	5.4	432.4	0.4	5.7				0.6760
O K !	0.525	1.6	168.2	0.2	1.5				0.5110
Ru L	2.558	21.5	1287.5	0.9	3.2				0.9117
Total		100.0			100.0				

Views **006** (outside a group of NPs) and **007** (in a group of NPs)



007

VFS = 1000 count



Thin Film Standardless Standardless Quantitative Analysis

Fitting Coefficient : 0.5964

Element	(keV)	Mass%	Counts	Sigma	Atom%	Compound	Mass%	Cation	K
C K (Ref.)	0.277	66.3	6249.6	0.6	88.0				1.0000
N K !	0.392	5.1	705.0	0.3	5.8				0.6760
O K !	0.525	2.1	388.8	0.2	2.1				0.5110
Ru L	2.558	26.6	2746.2	0.7	4.2				0.9117
Total		100.0			100.0				

EDX data									
% Mass	View 001	View 003	View 005	View 007	\bar{X}	[mmol]		[O]/[Ru]	[CH ₃ COOH]/[Ru]
%C	56,60	54,20	71,60	66,30	62,18	51,77		0,34	0,17
%O	2,40	0,70	1,60	2,10	1,70	1,06			
%Ru	35,80	41,00	21,50	26,60	31,23	3,09			
%N	5,20	4,10	5,40	5,10	4,95	3,54			
Total	100,00	100,00	100,00	100,00					
RuNP description						Experimental quantification		Theoretical titration (300 K)	
Total number of Ru atoms ($d_{\text{mean}} = 1.5 \text{ nm}$)				147		H ^a	0.3 H/Ru _{surf}	H ^a	[0.4 - 0.6] H/Ru _{surf}
Number of Ru surface atoms (63.0 %)				92		CH ₃ COOH (L)	0.3 L/Ru _{surf}	CH ₃ COOH (L)	0.4 L/Ru _{surf}
						^a %H is not known by EDX			
[CH ₃ COOH]/[Ru _{surf}]									
0,27									

Table SI.4. Summary of EDX data for Ru_x(CH₃COOH)_{0.4y} NPs and determination of the [CH₃COOH]/[Ru_{surf}] ratio with comparison with data obtained by experimental NMR quantification and theoretical titration at 300 K.

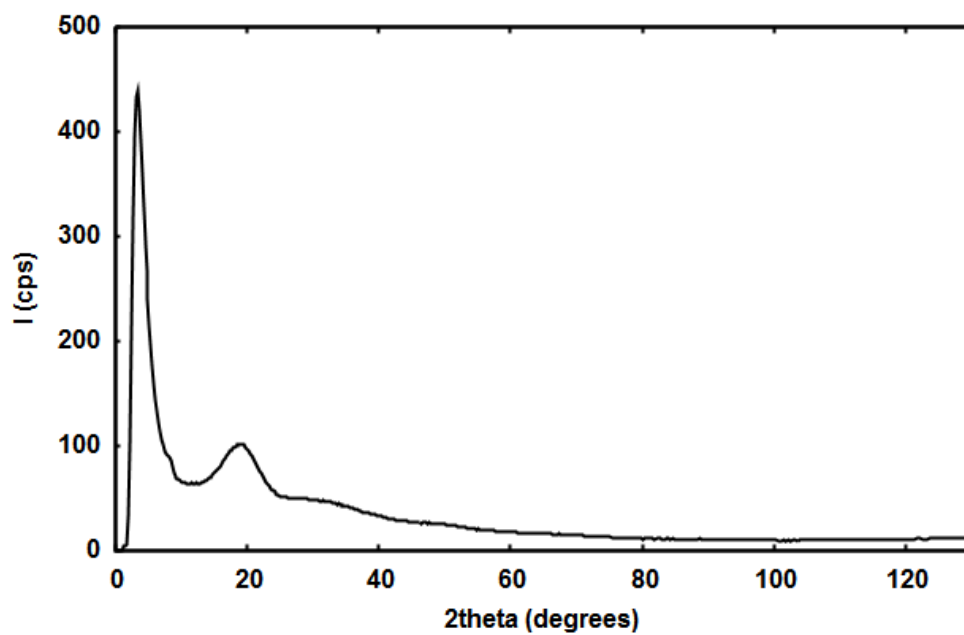


Figure SI.5. WAXS diagram of $\text{Ru}_x(\text{CH}_3\text{COOH})_{0.4y}$ NPs (experimental data obtained in solid state).

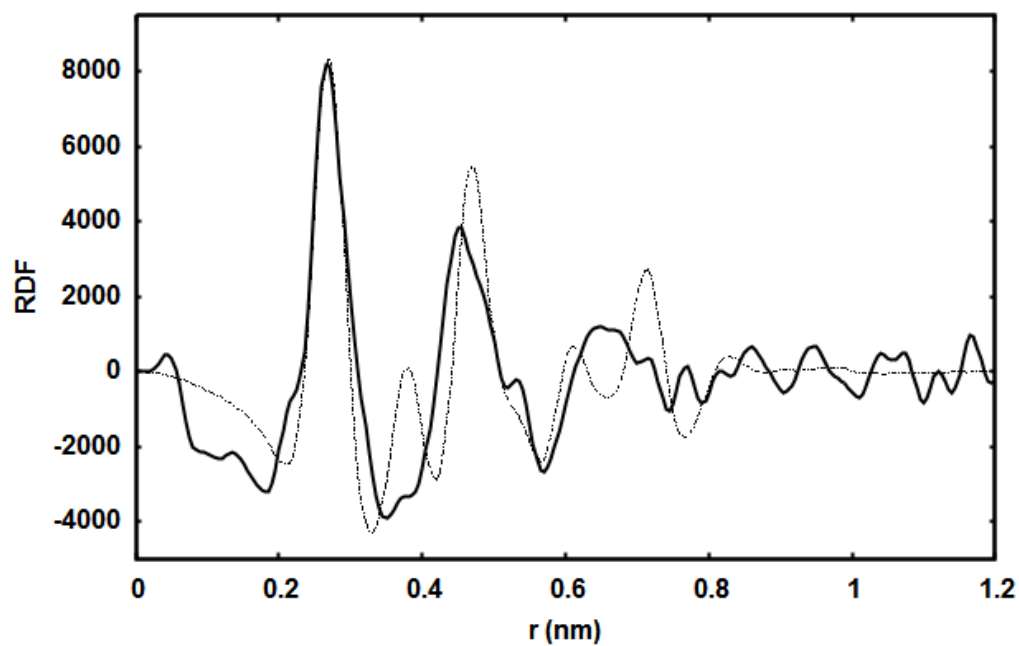


Figure SI.6. RDF of $\text{Ru}_x(\text{CH}_3\text{COOH})_{0.4y}$ NPs (plain line: experimental data obtained in solid state; dashed line: computed Ru hcp crystallite (30 atoms)).

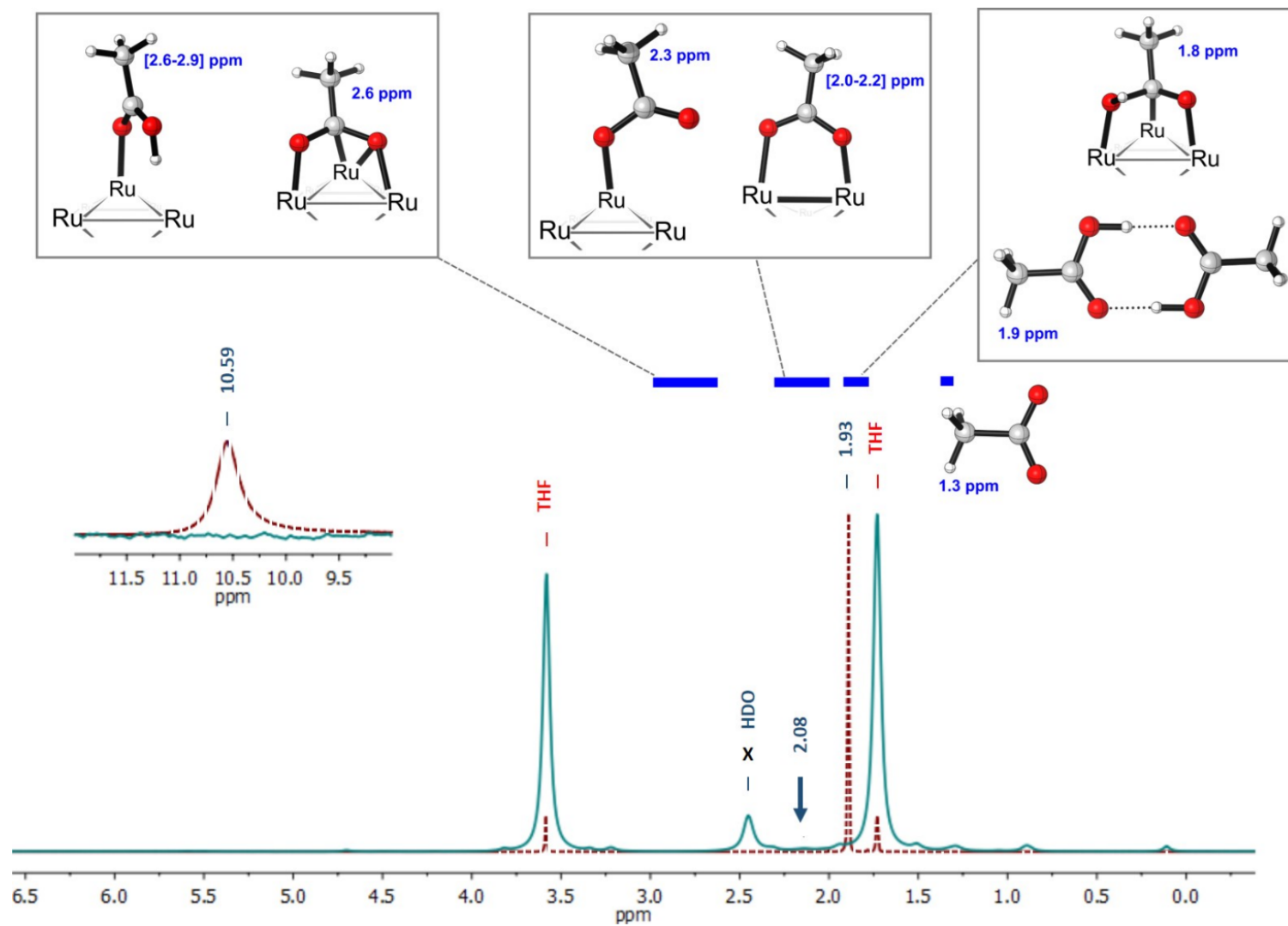


Figure SI.7. Experimental ^1H NMR spectrum (THF-d^8) of $\text{Ru}_x(\text{CH}_3\text{COOH})_{0.4y}$ NPs (in solid green) in comparison with that of free CH_3COOH (in dotted burgundy). The DFT ^1H NMR chemical shifts of the methyl group in different models ($(\text{CH}_3\text{COOH})_2$, CH_3COO^- , $[\text{Ru}_6]$ clusters) are given on top of the figure. The DFT results are positioned by the blue thick horizontal lines.


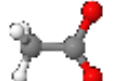
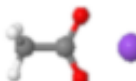
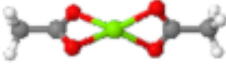
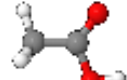
		6-31G**			cc-pvtz	
		E	¹ H	¹³ C	¹ H	¹³ C
TMS		σ	31.7	196.8	31.6	189.2
 <chem>(CH3COOH)2</chem>	CH ₃	σ	29.7	175.3	29.6	167.5
		δ	1.9	21.5	2.0	21.7
	C(OOH)	σ		24.6		4.2
		δ			172.3	185.0
 <chem>(CH3COO)^-</chem>	CH ₃	σ	30.7	169.7	30.3	163.4
		δ	0.9	27.1	1.3	25.8
	C(OO)	σ		39.4		18.2
		δ			157.4	171.0
 <chem>CH3COONa</chem>	CH ₃	σ	29.9	172.7	29.7	165.8
		δ	1.8	24.1	1.9	23.4
	C(OO)	σ		21.1		1.4
		δ			175.7	187.8
 <chem>Mg(CH3COO)2</chem>	CH ₃	σ	29.6	175.7	29.5	167.9
		δ	2.1	21.1	2.1	21.3
	C(OO)	σ		11.8		-7.2
		δ			185.0	196.4
 <chem>CH3COOH</chem>	CH ₃	σ	29.8	177.5	29.6	169.7
		δ	1.9	172.3	1.9	19.5
	C(OOH)	σ		34.3		14.7
		δ			162.5	174.4

Table SI.8. Comparison of the ¹H and ¹³C NMR chemical shieldings calculated for different carboxylic-based compounds and basis set.

Table SI.9. Energies (in eV), labelling and coordination of the surface species in the 44 models used within the *ab initio* thermodynamics method (the generation process of the geometries is explained in the “methods” section of the article).

#	E	nH (a)	nH/Ru_surf (a)	nH* (b)	nH*/Ru_surf (b)	nCH ₃ COOH	nCOO-*	nCOOH*	Name in Fig. 8	xyz name
1	-424.37	0	0.0	0	0.0	0	0	0	Ru ₅₅	Ru_55
2	-492.69	17	0.4	17	0.4	0	0	0	H ₁₇	Ru_55-H_0.4
3	-564.41	35	0.8	35	0.8	0	0	0	H ₃₅	Ru_55-H_0.8
4	-634.19	53	1.2	53	1.2	0	0	0	H ₅₃	Ru_55-H_1.2
5	-697.69	70	1.6	70	1.6	0	0	0	H ₇₀	Ru_55-H_1.6
6	-612.81	35	0.8	36	0.8	1	1	0	(CH ₃ COO) H ₃₆	CH3COOH-H_0.8
7	-682.91	53	1.2	54	1.2	1	1	0	(CH ₃ COO) H ₅₄	CH3COOH-H_1.2
8	-745.93	70	1.6	71	1.6	1	1	0	(CH ₃ COO) H ₇₁	CH3COOH-H_1.6
9	-660.00	35	0.8	37	0.8	2	2	0	(CH ₃ COO) ₂ H ₃₇	CH3COOH_2-H_0.8
10	-729.60	53	1.2	55	1.3	2	2	0	(CH ₃ COO) ₂ H ₅₅	CH3COOH_2-H_1.2
11	-793.09	70	1.6	72	1.6	2	2	0	(CH ₃ COO) ₂ H ₇₂	CH3COOH_2-H_1.6
12	-708.14	35	0.8	38	0.9	3	3	0	(CH ₃ COO) ₃ H ₃₈	CH_3COOH_3-H_0.8
13	-777.89	53	1.2	56	1.3	3	3	0	(CH ₃ COO) ₃ H ₅₆	CH_3COOH_3-H_1.2
14	-840.62	70	1.6	73	1.7	3	3	0	(CH ₃ COO) ₃ H ₇₃	CH_3COOH_3-H_1.6
15	-618.99	0	0.0	4	0.1	4	4	0	(CH ₃ COO) ₄ H ₄	CH3COOH_4
16	-670.85	13	0.3	17	0.4	4	4	0	(CH ₃ COO) ₄ H ₁₇	CH3COOH_4-H_0.4
17	-756.37	35	0.8	39	0.9	4	4	0	(CH ₃ COO) ₄ H ₃₉	CH3COOH_4-H_0.8
18	-826.00	53	1.2	57	1.3	4	4	0	(CH ₃ COO) ₄ H ₅₇	CH3COOH_4-H_1.2
19	-888.47	70	1.6	74	1.7	4	4	0	(CH ₃ COO) ₄ H ₇₄	CH3COOH_4-H_1.6
20	-814.00	0	0.0	8	0.2	8	8	0	(CH ₃ COO) ₈ H ₈	CH3COOH_8
21	-848.65	9	0.2	17	0.4	8	8	0	(CH ₃ COO) ₈ H ₁₇	CH3COOH_8-H_0.2
22	-863.98	13	0.3	21	0.5	8	8	0	(CH ₃ COO) ₈ H ₂₁	CH3COOH_8-H_0.3
23	-880.14	17	0.4	25	0.6	8	8	0	(CH ₃ COO) ₈ H ₂₅	CH3COOH_8-H_0.4
24	-947.36	35	0.8	43	1.0	8	8	0	(CH ₃ COO) ₈ H ₄₃	CH3COOH_8-H_0.8
25	-1,014.50	53	1.2	61	1.4	8	8	0	(CH ₃ COO) ₈ H ₆₁	CH3COOH_8-H_1.2
26	-1,074.53	70	1.6	78	1.8	8	8	0	(CH ₃ COO) ₈ H ₇₈	CH3COOH_8-H_1.6
27	-912.05	0	0.0	10	0.2	10	10	0	(CH ₃ COO) ₁₀ H ₁₀	CH3COOH_10
28	-976.91	17	0.4	27	0.6	10	10	0	(CH ₃ COO) ₁₀ H ₂₇	CH3COOH_10-H_0.4
29	-1,043.37	35	0.8	45	1.0	10	10	0	(CH ₃ COO) ₁₀ H ₄₅	CH3COOH_10-H_0.8
30	-1,106.51	53	1.2	63	1.4	10	10	0	(CH ₃ COO) ₁₀ H ₆₃	CH3COOH_10-H_1.2
31	-1,168.13	70	1.6	79	1.8	10	9	1	(CH ₃ COO) ₉ (CH ₃ COOH) H ₇₉	CH3COOH_10-H_1.6
32	-1,009.28	0	0.0	12	0.3	12	12	0	(CH ₃ COO) ₁₂ H ₁₂	CH3COOH_12
33	-1,072.83	17	0.4	29	0.7	12	12	0	(CH ₃ COO) ₁₂ H ₂₉	CH3COOH_12-H_0.4
34	-1,137.82	35	0.8	47	1.1	12	12	0	(CH ₃ COO) ₁₂ H ₄₇	CH3COOH_12-H_0.8
35	-1,204.67	53	1.2	65	1.5	12	12	0	(CH ₃ COO) ₁₂ H ₆₅	CH3COOH_12-H_1.2
36	-1,262.42	70	1.6	80	1.8	12	10	2	(CH ₃ COO) ₁₀ (CH ₃ COOH) ₂ H ₈₀	CH3COOH_12-H_1.6
37	-1,106.85	0	0.0	14	0.3	14	14	0	(CH ₃ COO) ₁₄ H ₁₄	CH3COOH_14
38	-1,168.63	17	0.4	31	0.7	14	14	0	(CH ₃ COO) ₁₄ H ₃₁	CH3COOH_14-H_0.4
39	-1,202.18	0	0.0	16	0.4	16	16	0	(CH ₃ COO) ₁₆ H ₁₆	CH3COOH_16
40	-1,235.95	9	0.2	25	0.6	16	16	0	(CH ₃ COO) ₁₆ H ₂₅	CH3COOH_16-H_0.2
41	-1,264.48	17	0.4	33	0.8	16	16	0	(CH ₃ COO) ₁₆ H ₃₃	CH3COOH_16-H_0.4
42	-1,326.98	35	0.8	51	1.2	16	16	0	(CH ₃ COO) ₁₆ H ₅₁	CH3COOH_16-H_0.8
43	-1,391.54	53	1.2	69	1.6	16	16	0	(CH ₃ COO) ₁₆ H ₆₉	CH3COOH_16-H_1.2
44	-1,449.19	70	1.6	84	1.9	16	14	2	(CH ₃ COO) ₁₄ (CH ₃ COOH) ₂ H ₈₄	CH3COOH_16-H_1.6

(a) Number of hydrides that come only from the dissociative adsorption of H₂

(b) Total number of hydrides, i.e. that come from the dissociative adsorption of H₂ and from CH₃COOH

63

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-./_Model_1COOH_472.13976406.xyz
Ru 11.07601281969288 9.28375286938952 9.64262095429748
Ru 12.33716817368049 11.480963622274644 9.98999971377968
Ru 12.37741601832162 6.97209759395201 9.19450598935777
Ru 13.48033116468226 13.69138026863234 10.3385896455873
Ru 13.419796925667 0.03879401580595 4.44503128712020
Ru 12.20115085269931 8.85645156408889 7.41674589131923
Ru 13.62342188231989 9.29942102125659 9.51028385621674
Ru 12.44658846730270 8.15115695372516 11.44820092847402
Ru 13.89232467892823 8.49230604120504 13.51178161910180
Ru 14.56653146246980 12.34889789322135 5.77138572239983
Ru 13.419329557739 11.16478488390854 7.710837998115
Ru 14.92820533997459 11.64592676681506 9.8430810110278
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D	17.84130	16.23630	15.52380
D	14.53270	6.52900	15.78120
D	16.43530	6.97980	14.60116
D	15.17230	10.29770	7.53060
D	12.91530	10.26430	7.40170
D	19.70550	12.63600	16.00200
D	19.90200	11.26100	14.21630
D	10.33980	7.25180	12.47270
D	10.02170	8.60880	10.69430
D	9.80180	9.30300	17.11350
D	11.05850	9.05430	18.87730
D	10.22530	13.05000	19.60530
D	11.16950	15.57080	19.71480
D	16.18300	18.45030	10.38360
D	16.18930	17.19430	8.48980
D	15.84850	17.29400	18.65400
D	15.68300	16.58650	16.79060
D	11.97630	19.30450	11.09450
D	12.92450	19.99800	13.03560
D	13.06700	15.84100	7.31510
D	13.73380	13.67150	7.19130
H	5.56400	8.93630	13.62170
H	4.05500	10.26050	12.63960
H	4.84250	10.38400	14.40320
H	15.14930	11.63750	22.45750
H	13.41730	11.26650	22.33430
H	13.92550	12.96150	22.53890
H	21.31050	12.22980	8.64370
H	20.77400	13.71450	7.80290
H	20.25000	12.13780	7.19080
H	7.19100	14.92450	7.79430
H	7.41330	16.40950	8.79090
H	6.56300	15.00980	9.46630
H	8.76730	21.02530	15.90910
H	10.43320	21.40580	16.34130
H	9.48880	20.50230	17.47770
H	19.76150	17.81550	15.06700
H	18.97000	18.62330	13.65940
H	19.76430	17.04630	13.45810
H	16.72700	4.41480	14.91360
H	15.55230	4.29830	16.27200
H	17.13000	5.11450	16.48740
H	13.22550	9.62100	4.97690
H	14.41150	8.43350	5.58170
H	14.99180	9.98780	4.95900
H	10.13230	14.58480	11.63660
H	16.22680	9.66970	10.13010
H	13.70730	17.01300	9.85060
H	10.31150	14.94830	17.31830
H	11.29680	16.93950	9.99490
H	13.25350	16.60430	18.62070
H	9.32400	12.27950	17.24610
H	10.31250	10.93170	12.02030
H	22.39180	11.48450	14.50980
H	22.10680	11.24780	16.25830
H	22.26500	12.89430	15.62550
H	17.82650	13.22030	17.70520
H	8.92820	6.61530	9.58460
H	8.00380	6.46550	11.10410
H	9.43830	5.45130	10.06300
H	9.01680	17.00450	13.28390
H	8.89480	9.35950	20.18200

H	9.53720	7.77280	19.69010
H	8.13850	8.45450	18.81360
H	11.30970	14.74230	8.59380
H	10.54820	15.55100	22.14600
H	10.16130	13.79080	22.17830
H	8.94780	14.95600	21.62060
H	14.90650	18.51970	12.71060
H	17.53500	19.03150	7.44430
H	18.38400	19.26000	9.00510
H	16.97050	20.25850	8.63560
H	11.31630	8.14430	15.44630
H	17.08080	20.27450	18.00660
H	17.82900	19.01930	19.05490
H	16.32380	19.79900	19.56010
H	10.53480	11.46800	9.76460
H	12.56830	22.33380	12.23040
H	11.03080	21.82830	11.46050
H	12.52030	21.82650	10.50630
H	16.22580	9.04230	17.40340
H	13.92580	14.04230	4.71070
H	13.81800	15.83650	4.83890
H	12.33950	14.86050	4.81600
H	12.60720	9.36200	10.45720

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./Thermo-and-HER_CH3COOH-H_1_2-Domain4.xyz

Ru	15.25553	13.23005	15.29992
Ru	15.27287	13.47170	10.90189
Ru	15.32763	11.83864	13.02533
Ru	13.74322	15.52744	15.45353
Ru	13.70818	15.85144	11.02650
Ru	12.48075	13.15444	15.30143
Ru	13.91771	14.14965	13.14282
Ru	12.50866	13.45724	10.90442
Ru	12.66197	11.80284	12.96676
Ru	12.41812	16.42222	13.30978
Ru	11.24458	14.03441	13.13171
Ru	8.49293	13.95873	13.03401
Ru	9.70901	16.18117	13.31891
Ru	9.75721	11.52486	12.99312
Ru	10.91898	18.45629	13.41055
Ru	11.10749	14.21943	8.94692
Ru	9.92786	13.17540	11.06818
Ru	9.89993	13.00552	15.05253
Ru	11.12622	13.64078	17.34120
Ru	12.32306	16.60741	9.95379
Ru	11.05319	15.65902	11.16948
Ru	11.09251	15.37607	15.34771
Ru	12.37456	16.04022	17.52508
Ru	12.30971	18.03090	11.23519
Ru	13.52390	18.07011	13.45062
Ru	12.35940	17.74097	15.54110
Ru	11.30174	9.30375	12.88662
Ru	12.56929	12.01211	8.81703
Ru	11.27131	11.07206	10.92550
Ru	11.31672	10.83291	14.90075
Ru	12.49674	11.38706	17.22893
Ru	13.75041	14.34524	8.82222
Ru	13.79170	13.73620	17.48171
Ru	14.95441	16.74774	9.02779
Ru	15.07557	16.56835	13.30377
Ru	14.98073	16.15997	17.57425
Ru	14.85144	18.10990	11.29160
Ru	14.86943	17.83641	15.51374
Ru	14.04801	9.45127	12.99504
Ru	12.55298	8.70731	15.16983
Ru	15.16196	12.18924	8.75597
Ru	14.01639	11.09526	10.86637
Ru	13.93156	10.89742	15.07888
Ru	15.20253	11.50437	17.19141
Ru	16.38522	14.51933	8.88231
Ru	16.55791	14.35048	13.16839
Ru	16.45767	13.93554	17.39301
Ru	16.38806	15.96574	11.16879
Ru	16.37200	15.66812	15.34297
Ru	16.54524	9.64382	12.82671
Ru	16.65329	11.32060	10.75392
Ru	18.01269	11.91179	12.93151
Ru	16.65629	11.04894	15.05748
Ru	17.79960	13.76291	10.99731
Ru	17.77547	13.39777	15.16882
C	12.38868	7.44750	19.33963
C	12.44858	8.42450	18.19572
O	12.36245	7.91450	17.00985
O	12.58096	9.65799	18.45285
H	6.88617	13.94333	13.10674
H	10.51151	8.01060	13.46342
H	8.00858	15.58721	13.49609
H	9.59696	17.70511	14.35706
H	8.30813	12.45526	12.07000
H	9.48552	13.24754	16.79693
H	10.57135	15.98066	9.35178
H	9.65044	17.73158	12.34891
H	9.46163	13.67014	9.42075
H	10.59736	15.42302	17.16738
H	11.79019	18.22408	9.50463
H	12.02425	19.50813	12.37493

H 11.74496 17.67882 17.23425
H 11.18970 12.74537 7.92784
H 10.51271 9.48133 11.26258
H 11.49333 10.58497 9.23673
H 9.65969 9.68478 13.26327
H 11.90799 10.70201 16.70988
H 12.95773 15.09859 7.83936
H 12.40948 14.37706 18.53288
H 13.62304 17.48708 8.12952
H 13.67734 16.86243 18.51601
H 14.82745 19.50191 12.43878
H 15.25100 18.39523 9.53336
H 16.65439 17.64783 11.61537
H 14.76700 19.40388 14.61207
H 13.94931 10.77842 8.96725
H 12.81725 9.63519 11.70277
H 14.16373 9.12992 15.48137
H 13.88024 12.09919 18.34638
H 15.11219 15.27891 7.81223
H 16.59729 12.35917 18.20869
H 18.09636 15.53238 11.35803
H 15.39093 17.85317 17.23541
H 15.44155 8.31709 13.16133
H 16.61596 11.12278 8.98323
H 15.47758 9.94588 10.88963
H 18.23721 10.22641 12.42986
H 16.46973 10.34834 16.69353
H 17.27498 9.36640 14.33292
H 18.07944 14.11504 9.26140
H 18.39428 12.01680 11.09492
H 18.46050 13.58848 13.36292
H 18.46095 11.61151 14.62500
H 8.10628 12.98862 14.36184
H 11.94005 19.34283 14.62194
H 11.12595 12.14519 18.23348
H 15.13220 14.56143 18.56043
H 12.72687 8.17915 13.42216
H 16.41908 13.12035 7.81309
H 16.77030 16.33161 9.39590
H 16.81203 15.78352 17.15340
H 18.14661 13.69141 16.90292
H 12.57130 7.95281 20.29254
H 13.12775 6.65981 19.18117
H 11.39734 6.97210 19.35623
H 16.61722 17.38545 14.97345

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./Thermo_CH3COOH_10-H_0_4.xyz

Ru 15.10700 13.54560 15.81830
Ru 15.17560 13.44090 11.48590
Ru 15.19070 11.97180 13.68476
Ru 13.61070 15.67670 15.08690
Ru 13.55450 15.73720 11.44610
Ru 12.28960 13.36390 15.77660
Ru 13.76380 14.20150 13.65560
Ru 12.39440 13.32500 11.55140
Ru 12.40380 11.74500 13.67040
Ru 12.27640 16.47350 13.63380
Ru 11.03730 14.04920 13.59340
Ru 8.39840 14.12960 13.50410
Ru 9.54990 16.21780 13.65250
Ru 9.44270 11.66620 13.63430
Ru 10.71120 18.48850 13.63180
Ru 11.02630 13.91260 9.45950
Ru 9.79780 13.14710 11.59760
Ru 9.65660 13.31750 15.63630
Ru 10.99740 13.96760 17.83120
Ru 12.36220 16.40300 9.36540
Ru 10.89400 15.55690 11.50240
Ru 10.99670 15.59090 15.67940
Ru 12.21130 16.28340 17.88860
Ru 12.14410 17.90510 11.58090
Ru 13.37340 18.80630 13.68360
Ru 12.13330 17.92310 15.79280
Ru 11.24040 9.41870 13.76870
Ru 12.48910 11.78630 9.44590
Ru 11.13640 10.97960 11.62170
Ru 10.88940 11.02300 15.64890
Ru 12.30340 11.62730 17.70970
Ru 13.64820 14.05130 9.42560
Ru 13.61800 14.05080 17.94270
Ru 14.90540 16.29040 9.37890
Ru 14.91210 16.67250 13.71190
Ru 14.74310 16.43220 17.98270
Ru 14.74930 17.99440 11.56930
Ru 14.55460 18.04550 15.98210
Ru 13.93360 9.60170 13.79310
Ru 12.56690 9.34360 16.23800
Ru 15.05030 11.91560 9.37660
Ru 13.85560 11.07270 11.56430
Ru 13.96900 11.13990 15.76620
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Ru 16.26530 14.31490 9.36990
Ru 16.42520 14.31840 13.67690
Ru 16.27700 14.27950 17.90490
Ru 16.24430 15.81770 11.57350
Ru 16.23400 15.91350 15.83650

Ru 16.40390 9.72410 13.74860
Ru 16.48270 11.16450 11.54690
Ru 17.79950 11.94450 13.62650
Ru 16.49570 11.34190 15.77270
Ru 17.73040 13.70890 11.57040
Ru 17.75010 13.59400 15.79650
C 5.08010 11.37050 14.04840
C 6.44870 11.97210 13.87010
C 13.73900 12.41490 22.04800
C 13.97630 12.64110 20.57920
C 20.49110 14.53190 8.27690
C 19.23620 14.20070 9.04010
C 7.52170 16.40140 8.75560
C 8.79310 15.83930 9.33020
C 9.71950 21.40340 16.74340
C 10.29780 20.22000 16.01940
C 18.80520 18.97480 14.05150
C 17.67260 18.01740 14.30550
C 15.50530 6.04030 15.93510
C 14.65940 7.21310 15.49580
C 13.69170 9.49510 5.96960
C 13.70390 10.31510 7.22990
C 21.63730 11.53870 15.70440
C 20.26950 12.00040 15.30480
C 8.74450 7.34370 10.86570
C 9.63600 8.37410 11.50800
O 6.53910 13.24860 13.85970
O 7.43390 11.15880 13.72140
O 13.65420 13.76760 20.07960
O 14.47710 11.66160 19.90350
O 18.11670 14.48580 8.47590
O 19.34520 13.68230 10.19820
O 9.22270 16.33500 10.42440
O 9.37280 14.88650 8.69370
O 11.02570 19.40600 16.69950
O 10.06130 20.09390 14.77140
O 16.76510 17.90020 13.41560
O 17.66120 17.37990 15.42040
O 13.62340 7.49250 16.18260
O 15.02770 7.86160 14.43740
O 14.82650 10.54510 7.78820
O 12.57580 10.74380 7.68210
O 19.69600 12.87790 16.05100
O 19.73000 11.47450 14.26660
O 10.15580 8.07250 12.64310
O 9.82960 9.47840 10.90320
H 8.98670 17.92130 13.53040
H 12.35490 14.86570 8.33200
H 8.17830 13.78400 11.63740
H 9.45950 11.75550 16.43660
H 10.40110 12.03120 12.03120
H 14.55300 19.50260 14.93020
H 12.40060 10.17360 10.66350
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H 12.17240 9.81940 17.94690
H 16.02290 17.53600 10.41570
H 12.59000 8.32900 13.45790
H 15.95320 13.00400 8.21300
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H 16.54260 12.64570 18.62060
H 16.62610 16.08040 17.69940
H 18.24770 13.73650 14.01120
H 17.20930 9.65870 15.28520
H 5.15270 10.34880 14.43570
H 4.57650 11.33890 13.07040
H 4.47690 11.99800 14.71510
H 14.43660 11.66860 22.44340
H 12.71400 12.03710 22.18270
H 13.82590 13.35960 22.59570
H 21.33240 13.93580 8.64390
H 20.72200 15.59680 8.43420
H 20.34150 14.37780 7.20160
H 7.40020 16.09660 7.71120
H 7.52110 17.49470 8.84380
H 6.67220 16.02050 9.34190
H 8.08760 21.83520 16.17810
H 10.50600 22.16540 16.85430
H 9.39740 21.11160 17.74950
H 19.62870 18.79820 14.75070
H 18.43700 20.00320 14.18340
H 19.15080 18.07810 13.01470
H 16.36200 5.90760 15.26870
H 14.89190 5.13860 15.95550
H 15.85470 6.22760 16.96160
H 12.66650 9.32850 5.62520
H 14.19120 8.53360 6.19050
H 14.26460 10.01860 5.19150
H 17.99470 15.45240 11.52090
H 15.33360 9.90200 11.26720
H 13.62660 17.14580 8.34850
H 10.43820 15.72530 17.52910
H 11.71720 17.98610 9.79360
H 13.45490 17.23790 18.87450
H 9.26690 13.73660 17.32280
H 18.19040 11.86730 11.77200
H 22.13060 11.02900 14.87050

H 21.54410 10.83540 16.54580
H 22.23720 12.38900 16.05040
H 9.69110 10.01650 14.52220
H 8.47940 7.64400 9.84760
H 7.82970 7.23280 11.46520
H 9.24990 6.36930 10.85560
H 17.99120 14.06940 17.50480

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./Thermo_CH3COOH_10-H_0.8.xyz

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Ru 15.04520 11.71910 13.63240
Ru 13.67950 15.63250 15.78560
Ru 13.72190 15.58710 11.39070
Ru 12.24260 13.32690 15.76120
Ru 13.72030 14.07130 13.62420
Ru 12.30170 13.31420 11.45820
Ru 12.20320 11.73880 13.54670
Ru 12.40020 15.45600 13.62940
Ru 10.97090 14.11290 13.59040
Ru 8.33380 14.14560 13.50410
Ru 9.57770 16.37470 13.60970
Ru 9.51160 11.77340 13.61220
Ru 11.04270 18.55310 13.40890
Ru 11.00440 14.63240 9.28930
Ru 9.74350 13.27080 11.53070
Ru 9.62930 13.39630 15.69340
Ru 10.97680 14.10320 17.80070
Ru 12.63110 16.33580 9.25990
Ru 10.97420 15.73260 11.53770
Ru 10.92800 15.73800 15.63600
Ru 12.36200 15.36340 17.81860
Ru 12.60870 17.87750 11.40220
Ru 13.71060 18.76010 13.59200
Ru 12.23320 18.10320 15.73570
Ru 10.95440 9.46860 13.66880
Ru 12.26530 11.78930 9.24530
Ru 10.90800 11.03710 11.45450
Ru 10.87750 11.02250 15.70720
Ru 12.26040 11.74360 17.82090
Ru 13.69660 13.90180 9.38590
Ru 13.62420 14.01490 17.99810
Ru 15.19130 16.11600 9.39400
Ru 15.14460 16.34690 13.06150
Ru 14.96150 16.27160 17.89340
Ru 15.10430 17.75010 11.48700
Ru 15.08060 17.87430 15.83460
Ru 13.59210 9.53070 13.67440
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Ru 14.91560 11.72500 9.29070
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Ru 16.39170 13.83700 9.36490
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C 15.42270 7.65020 16.42030
C 19.53960 17.55970 13.45040
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C 13.56100 9.13240 5.98190
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C 8.20750 19.21480 14.50850
C 20.70120 13.59800 8.49690
C 19.40250 13.51780 9.25820
C 7.55730 16.80890 8.84830
C 0.77550 15.09200 9.37830
C 5.09600 11.23660 13.69980
C 6.45350 11.88270 13.58310
C 15.21600 12.90600 21.98030
C 14.96100 13.13710 20.52090
C 21.86870 12.41220 14.97270
C 20.36370 12.34520 14.88540
C 10.01270 6.93930 10.19930
C 10.45220 8.09920 11.05270
O 9.02880 18.38810 13.78270
O 8.52550 20.36990 14.72320
O 12.45190 10.59050 7.56030
O 14.71010 10.41040 7.67620
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O 18.18530 16.43950 15.06760
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O 9.15460 16.41630 10.56240
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O 6.49840 13.16330 13.64080
O 15.84500 12.64840 19.67730
O 13.93040 13.75490 20.14800
O 19.70680 13.13200 15.65870
O 19.85930 11.50170 14.06830
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H 14.92510 19.29310 12.44320
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H 9.66650 10.17660 12.64400
H 10.92340 12.60170 8.29750
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H 13.96790 16.93330 8.29060
H 13.63720 17.06780 18.86700
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H 15.21690 19.08010 14.55130
H 16.10500 15.45100 19.00300
H 15.60220 17.80490 9.71630
H 15.73320 17.85940 17.47260
H 10.87090 10.66820 17.49330
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H 17.67340 14.63810 16.80310
H 18.09950 14.89750 11.61380
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H 18.08300 13.21730 13.48620
H 17.94020 9.68460 13.71610
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H 15.46590 5.64760 17.21720
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H 17.05780 6.26290 16.62190
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H 20.31970 17.41150 14.20330
H 19.42460 18.63030 13.23200
H 19.82310 17.06050 12.51260
H 10.51840 15.85640 17.44710
H 14.38100 8.45990 6.06120
H 13.70950 9.76590 5.06100
H 12.59440 8.67210 5.91280
H 13.57530 18.52610 16.69300
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H 7.12040 17.64150 15.50720
H 6.33530 18.26960 14.05910
H 9.33690 13.56890 17.46610
H 21.55220 13.49780 9.17780
H 20.75650 14.54270 7.94300
H 20.73570 12.78020 7.76240
H 19.61720 17.50220 15.98630
H 7.24090 16.37930 7.89290
H 7.79840 17.87270 8.71360
H 6.74540 16.74460 9.58410
H 9.10410 11.62210 15.42600
H 4.31570 11.90400 13.31820
H 4.09300 11.94410 14.76410
H 5.08220 10.27700 13.17180
H 12.43810 14.75470 8.24770
H 14.64670 13.61660 22.58680
H 16.28990 12.97780 22.19360
H 14.89270 11.88490 22.23400
H 12.21800 18.02660 9.67120
H 22.32170 11.83110 14.16940
H 22.18640 12.01010 15.94540
H 22.19560 13.45870 14.92930
H 16.91040 15.70510 9.83560
H 10.22250 7.13180 9.14230
H 8.92700 6.08010 10.32360
H 14.80960 6.01520 10.53250
H 14.80060 8.19560 13.28990

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./Thermo_CH3COOH_10-H_1.2.xyz

Ru 15.29330 13.39200 15.62620
Ru 15.10920 13.50510 11.29550
Ru 15.37050 11.91400 13.46580
Ru 13.64800 15.52180 15.80800
Ru 13.37880 15.74210 11.46630
Ru 12.52990 12.99810 15.70020
Ru 13.74350 14.06840 13.57550
Ru 12.32200 13.20300 11.30900
Ru 12.57610 11.57900 13.45990
Ru 12.94520 16.23350 13.70610
Ru 11.00890 13.77970 13.65080

Ru	8.28790	13.41310	13.54110
Ru	9.35470	15.90330	13.63460
Ru	9.81500	11.21720	13.65920
Ru	10.40360	18.22090	13.93500
Ru	10.84130	13.82240	9.36260
Ru	9.83450	12.75290	11.61660
Ru	9.88790	12.72000	15.75360
Ru	11.30710	13.42440	17.92870
Ru	11.95720	16.32850	9.37830
Ru	10.67690	15.31900	11.51220
Ru	10.80730	15.19340	15.95780
Ru	12.35550	15.82420	18.81300
Ru	11.72560	17.76840	11.76780
Ru	12.99380	18.63220	13.89780
Ru	11.81710	17.74330	16.11200
Ru	11.49770	9.07580	13.55450
Ru	12.41490	11.77960	9.12600
Ru	11.22900	10.66850	11.30530
Ru	11.46580	10.65500	15.59070
Ru	12.75260	11.30760	17.81640
Ru	13.48490	14.20850	9.33690
Ru	13.93770	13.76060	17.83740
Ru	14.47790	16.59720	9.33830
Ru	14.91590	16.55560	13.69400
Ru	14.93050	16.19650	17.90490
Ru	14.43970	18.05460	11.59620
Ru	14.57950	17.92450	15.94400
Ru	14.23490	9.45700	13.41030
Ru	13.61080	8.54980	15.69680
Ru	15.11060	12.13620	9.03360
Ru	13.99980	11.04080	11.24200
Ru	14.16530	10.88610	15.62060
Ru	15.51740	11.64290	17.78000
Ru	16.15360	14.51600	9.15820
Ru	16.35040	14.41800	13.48260
Ru	16.52430	14.11800	17.70380
Ru	16.94850	16.04260	11.41870
Ru	16.39440	15.90790	15.74940
Ru	16.80400	9.82940	13.30080
Ru	16.66030	11.36050	11.21540
Ru	18.13270	12.09870	13.34280
Ru	16.82400	11.25090	15.49880
Ru	17.66560	13.94870	11.34530
Ru	17.95420	13.67170	15.40930
C	9.38280	7.56650	19.74840
C	12.65460	8.41430	18.73260
C	14.08100	9.17650	5.96850
C	13.93980	10.12500	7.13100
C	8.81330	20.81810	17.05230
C	9.04660	19.79400	16.22850
C	19.12410	18.74610	13.95880
C	17.92150	17.88720	14.25980
C	20.40470	15.14940	8.11130
C	19.16080	14.77220	8.87800
C	7.32650	16.28020	8.69060
C	8.55200	15.61900	9.26180
C	5.55660	10.03430	14.05490
C	6.77240	10.89340	13.81740
C	15.88550	9.87550	21.69720
C	15.43350	10.84750	20.62340
C	22.17750	13.53940	14.27640
C	20.68550	13.32340	14.29370
C	10.36500	6.49970	10.17550
C	10.81270	7.67020	11.01180
O	10.69900	19.36250	16.90160
O	9.22430	19.40250	15.17800
O	15.02550	10.57750	7.64430
O	12.75970	10.42630	7.51300
O	12.90290	7.91290	17.49100
O	12.90380	9.69460	18.96020
O	17.99600	17.16340	15.32190
O	16.91870	17.91940	13.49180
O	18.04030	14.98340	8.29670
O	19.31660	14.27900	10.04840
O	8.94730	16.90590	10.41320
O	9.14090	14.73230	8.55680
O	7.91100	10.30890	13.83090
O	6.59150	12.14350	13.63290
O	14.78140	11.85890	20.89530
O	15.83170	10.48730	19.40680
O	20.21330	12.47530	13.46240
O	20.00460	13.99220	15.15220
O	11.06000	7.46550	12.24360
O	10.89260	8.80900	10.41400
H	7.37610	14.09800	12.29540
H	11.47850	7.92830	14.85340
H	7.83080	15.18240	13.98660
H	8.70670	17.47250	13.67320
H	8.01660	13.54810	11.79330
H	9.82400	12.54100	17.54700
H	10.71060	16.90420	8.51900
H	8.36510	16.18680	12.43000
H	9.54910	12.74480	9.86360
H	10.60400	15.28230	17.78030
H	11.42370	17.89720	9.94700
H	12.89570	19.23560	12.18560

H	11.96450	17.53160	17.85280
H	11.18990	12.44110	8.12530
H	10.13500	9.79370	12.50700
H	10.99120	10.96420	9.47380
H	10.19840	9.67090	14.77700
H	11.29570	10.50760	17.39020
H	11.95210	14.90480	8.26980
H	12.49100	14.30460	19.04110
H	13.16200	17.26250	8.37560
H	13.60310	16.70680	18.97870
H	14.68750	18.66210	13.20280
H	14.41920	18.29410	9.82770
H	16.07770	17.85400	11.37220
H	14.26440	19.38550	15.06060
H	13.36960	10.33370	9.84870
H	12.62630	9.68950	12.29590
H	14.60780	9.01910	15.15330
H	14.15990	12.21530	18.85440
H	14.97200	15.38500	8.08390
H	16.76400	12.65810	18.62980
H	17.78650	15.74420	11.42230
H	15.24990	17.95340	17.56720
H	15.70020	8.44720	13.17680
H	16.70970	11.34270	9.44940
H	15.47370	10.27730	10.55130
H	18.55760	10.42900	13.34680
H	16.99190	10.78760	17.19260
H	16.96570	9.55290	15.12030
H	17.10640	13.18250	9.87780
H	18.35890	12.09520	11.53850
H	18.17880	13.99220	13.18880
H	18.50850	11.94520	15.13220
H	8.25150	13.00940	15.27290
H	11.60540	19.57660	14.27270
H	11.43340	12.06580	18.95430
H	15.26420	14.63020	18.92910
H	13.20960	8.04680	14.00980
H	16.04400	13.26080	7.94060
H	16.35770	16.38330	9.69530
H	16.74570	15.99640	17.63470
H	18.13590	13.46440	17.22560
H	12.18050	6.50540	19.54900
H	12.15650	7.95610	20.75220
H	15.95130	18.67000	15.63160
H	9.25340	15.68480	15.46270
H	13.16470	8.59360	5.83240
H	14.94530	8.51900	6.11800
H	14.26250	9.76560	5.05710
H	13.13150	18.63490	16.78150
H	7.90640	20.32610	17.43390
H	8.49530	21.60510	16.35790
H	9.36900	21.24330	17.89340
H	9.35600	14.24600	16.43400
H	19.05580	19.16490	12.95000
H	20.04100	18.15350	14.06940
H	19.16870	19.56560	14.69050
H	10.30870	16.86300	16.30470
H	21.29190	14.69750	8.56550
H	20.51060	16.24400	8.12870
H	20.30670	14.84350	7.06270
H	10.30160	18.74560	12.19930
H	6.90930	15.68110	7.87470
H	7.62070	17.26380	8.29500
H	6.57960	16.44620	9.47580
H	18.04460	15.15890	16.27980
H	4.65670	10.52140	13.66570
H	5.43700	9.89230	15.13930
H	5.69350	9.04610	13.60160
H	14.71180	10.18010	17.13380
H	16.38710	8.99720	21.27860
H	15.01090	9.56850	22.28490
H	16.57040	10.40390	22.37510
H	17.13280	9.62930	11.55920
H	22.43860	14.46310	14.80220
H	22.54420	13.56020	13.24340
H	22.66630	12.69270	14.78620
H	14.39860	9.37630	11.62140
H	10.60640	6.66360	9.12020
H	9.27290	6.40280	10.26900
H	10.82050	5.57360	10.54340
H	13.68680	12.75290	8.11830

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Ru	15.43540	12.99290	15.40250
Ru	15.00170	13.34180	11.06000
Ru	15.13730	11.61780	13.13480
Ru	14.09750	15.33740	15.78020
Ru	13.63010	15.78100	11.41620
Ru	12.62440	13.01910	15.62710
Ru	13.87560	13.98220	13.45120
Ru	12.17890	13.43360	11.41220
Ru	12.32150	11.68260	13.37530
Ru	12.49180	16.34420	13.81910
Ru	11.03730	14.11210	13.72480
Ru	8.13190	14.08910	14.02970
Ru	9.84660	16.55340	13.99640

Ru 9.54720 11.54280 13.65700
Ru 11.36670 18.64380 14.14700
Ru 10.63500 14.50360 9.40350
Ru 9.64490 13.45950 11.66870
Ru 9.97600 13.08100 15.85360
Ru 11.61000 13.61420 17.92500
Ru 12.16110 15.66090 9.51920
Ru 10.95470 15.80310 11.73230
Ru 11.24790 15.52010 16.05210
Ru 12.99860 15.80090 18.03980
Ru 12.42350 18.10780 11.82660
Ru 13.98470 18.74690 13.90120
Ru 12.96000 17.67450 16.13020
Ru 11.14370 9.25610 13.35880
Ru 11.86250 12.26750 9.05100
Ru 10.79460 11.10830 11.26830
Ru 11.26680 10.77080 15.50890
Ru 12.72730 11.25950 17.64110
Ru 13.41390 14.39130 9.25570
Ru 14.22820 13.47600 17.78700
Ru 14.74250 16.63250 9.26410
Ru 15.15860 16.27800 13.51730
Ru 15.59600 15.78070 17.78530
Ru 15.16320 18.04250 11.50720
Ru 15.61140 17.62700 15.85250
Ru 13.78920 9.33850 13.12110
Ru 12.69030 8.42850 15.51560
Ru 14.56810 12.10170 8.76340
Ru 13.50920 11.07680 11.05580
Ru 13.92040 10.69980 15.30650
Ru 15.56010 11.14400 17.50500
Ru 15.97400 14.25300 8.82310
Ru 16.51320 13.89280 13.17930
Ru 16.86200 13.53480 17.40790
Ru 16.33720 15.67130 11.21010
Ru 16.81800 15.30250 15.49240
Ru 16.26200 9.34630 12.74390
Ru 16.13900 10.96800 10.77240
Ru 17.94740 11.42990 12.74200
Ru 16.69870 10.58890 15.03990
Ru 17.59400 13.34610 10.80880
Ru 18.09490 12.93730 15.16620
C 12.54450 7.35780 19.78960
C 12.66250 8.21710 18.62920
C 19.89010 18.56600 15.91910
C 18.56710 17.84110 15.83200
C 12.76590 9.03180 6.19140
C 12.89840 10.16740 7.17330
C 7.65480 19.63980 16.26830
C 8.72800 18.90780 15.50700
C 20.18280 14.59050 7.47960
C 18.97670 14.26190 8.32550
C 7.27380 16.00320 7.09740
C 8.01770 15.40730 8.27790
C 5.15730 10.79970 14.17050
C 6.47220 11.53520 14.02830
C 15.02540 11.63130 21.93830
C 15.37650 11.88730 20.46440
C 22.49130 14.17770 15.19170
C 21.05220 13.98110 14.83190
C 8.72050 7.32940 10.22840
C 9.55210 8.33680 10.98470
D 9.03420 19.51480 15.29720
D 8.48150 17.70530 15.13850
D 14.08970 10.49220 7.52470
D 11.83250 10.72040 7.59860
D 18.60460 16.57960 15.64390
D 17.50980 18.55360 15.96670
D 12.54370 9.55610 18.08660
D 12.90950 7.78220 17.48600
D 17.84190 14.67050 7.89290
D 19.18130 13.61480 9.41000
D 9.29480 15.18240 8.01420
D 7.45850 15.20240 9.36350
D 7.51730 10.80890 13.93200
D 6.41840 12.81070 14.01760
D 14.76170 12.95080 20.15130
D 15.80850 10.97420 19.66160
D 20.29560 13.25750 15.50580
D 20.67150 14.62730 13.73460
D 9.76000 9.46650 10.41430
H 10.01460 7.97660 12.12120
H 7.20140 15.16510 13.05560
H 13.78190 20.27210 13.19080
H 11.44720 7.83190 14.40880
H 15.99350 19.38630 11.21600
H 8.77850 15.43080 14.80840
H 8.40450 12.74700 12.88250
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H 7.57860 14.63720 12.43700
H 9.07470 14.31160 10.25280
H 8.23960 13.45840 15.64500
H 9.30450 16.02210 12.45440
H 11.20420 15.53360 17.09900
H 12.64920 17.55970 17.86290
H 10.82270 17.63560 11.51720

H 12.17480 18.37970 10.10350
H 11.55110 19.52370 12.65520
H 12.77750 19.36630 15.12670
H 9.62930 9.81640 14.04590
H 11.91320 9.92930 11.97870
H 10.29270 11.80900 9.63650
H 11.70450 12.13730 18.06790
H 11.10190 10.80220 17.31770
H 13.38580 17.53650 8.55510
H 14.41530 16.40360 18.97500
H 15.20420 18.31110 9.80590
H 14.31460 20.41390 13.94320
H 15.96160 17.47870 17.59830
H 13.17840 12.93000 7.94330
H 13.68120 9.36220 11.33440
H 14.73340 10.18580 10.09460
H 15.68050 9.57100 17.77690
H 16.50810 16.07720 9.48470
H 15.66760 13.02000 7.61910
H 17.14150 11.89940 17.95840
H 15.54900 18.87680 12.96620
H 15.03090 8.08870 12.81080
H 16.09470 11.15780 9.01070
H 16.34090 9.13010 11.00540
H 18.12870 9.83650 12.31970
H 16.83960 10.16500 16.83640
H 16.93040 8.96540 14.53960
H 16.90880 12.88360 9.23580
H 17.95040 11.49740 10.90180
H 19.47590 11.02030 12.52160
H 18.43590 13.03000 16.94390
H 19.02550 14.40960 14.20240
H 19.02580 12.28150 13.75420
H 18.21610 11.30270 15.77070
H 9.15440 11.29820 11.96220
H 9.42350 11.42180 15.52820
H 9.96080 12.98750 17.63860
H 10.39150 16.26450 10.04140
H 12.02070 15.34460 8.30700
H 12.84360 14.26650 19.06740
H 13.79780 19.11740 11.19300
H 10.76710 13.12790 8.09340
H 12.13600 10.61880 10.02850
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H 15.81710 14.29540 18.73090
H 16.80100 17.47300 11.41730
H 12.40570 8.21100 12.79940
H 14.14040 10.09040 17.03950
H 7.66470 7.22640 14.69190
H 14.15750 11.79470 18.52000
H 17.36530 15.26800 17.30290
H 17.99040 15.08110 11.08130
H 16.91150 15.77770 12.84140
H 19.70900 14.45610 13.59880
H 11.05730 6.54190 19.53170
H 12.20240 7.87830 20.68920
H 13.53080 6.91070 19.97910
H 16.51210 16.98520 14.44410
H 19.74890 19.64520 15.80180
H 20.57750 18.18260 15.15660
H 20.33690 18.36970 16.90470
H 7.15500 15.02090 14.89680
H 11.74040 8.96540 5.81450
H 13.02830 8.09220 6.69870
H 13.47350 9.16730 5.36400
H 14.40670 18.48280 16.81850
H 6.06360 19.26560 15.99000
H 7.73010 20.71850 16.09300
H 7.80080 19.45760 17.34350
H 9.72430 14.70800 16.43630
H 21.02360 13.93880 7.73810
H 20.47220 15.63380 7.67560
H 19.93570 14.50660 6.41540
H 18.72290 13.03210 12.05820
H 7.39560 17.09670 7.12940
H 6.20570 15.77310 7.17640
H 7.68200 15.64730 6.14460
H 14.09290 7.36160 15.44280
H 4.31490 11.49040 14.06940
H 5.12120 10.32500 15.16170
H 5.09350 10.00190 13.42070
H 11.21230 17.29620 16.01040
H 16.32150 10.79890 22.08140
H 14.66640 11.39270 22.41930
H 16.01320 12.54340 22.40950
H 18.27630 10.42000 14.07590
H 23.11790 13.60910 14.48890
H 22.67330 13.81940 16.20860
H 22.76610 15.23560 15.09590
H 15.37250 9.56210 15.32970
H 8.29120 6.59310 10.91550
H 9.37010 6.80270 9.51360
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H 9.99320 16.21350 16.76500

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 Ru 15.06760 13.40690 11.64130
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 Ru 13.69410 14.18010 13.79620
 Ru 12.34950 13.30670 11.68720
 Ru 12.29900 11.69910 13.77570
 Ru 12.13970 16.45900 13.75780
 Ru 10.98580 14.04700 13.71830
 Ru 8.37950 13.97760 13.62540
 Ru 9.52700 16.17810 13.77260
 Ru 9.56850 11.59520 13.80790
 Ru 10.67120 18.48260 13.65870
 Ru 10.97310 13.86640 9.56060
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 Ru 9.61280 13.26590 15.75200
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 Ru 13.37150 18.78280 13.68160
 Ru 12.05790 17.95550 15.87850
 Ru 11.11780 9.42810 13.89980
 Ru 12.41950 11.77120 9.55330
 Ru 11.06700 10.99360 11.65080
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 Ru 12.26180 11.82630 17.91780
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 Ru 14.62000 16.50290 18.07150
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 Ru 13.85990 9.59820 13.84380
 Ru 12.51690 8.83280 15.77440
 Ru 15.01550 11.71400 9.66700
 Ru 13.73520 11.07000 11.69000
 Ru 13.65880 11.02930 15.94460
 Ru 14.86590 11.90650 17.96030
 Ru 16.17540 14.30190 9.52620
 Ru 16.40470 14.19420 13.86310
 Ru 16.04580 14.46800 18.04260
 Ru 16.17990 15.70920 11.64940
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 Ru 16.34260 9.69270 13.97260
 Ru 16.36770 11.12430 11.79860
 Ru 17.70770 11.92270 13.84490
 Ru 16.30420 11.25310 15.93420
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 C 6.54100 11.69670 13.65950
 C 14.32890 12.66170 22.21580
 C 14.31590 12.81560 20.71720
 C 20.13200 13.58830 8.10320
 C 10.99720 13.61770 9.01320
 C 7.60080 16.47840 8.70210
 C 8.81330 15.85280 9.33770
 C 9.56530 21.43850 16.69530
 C 10.20410 20.27210 15.99110
 C 10.94090 18.47150 14.03000
 C 17.76440 17.76090 14.30700
 C 15.89950 6.04180 15.68030
 C 14.87730 7.07100 15.29440
 C 13.77410 9.79100 5.93740
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C 15.31100 7.06830 14.59590
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C 22.09300 12.62000 14.95290
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C 9.48450 9.20630 18.89420
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C 10.25420 15.70900 21.26900
C 10.79680 15.49650 19.87990
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O 17.10920 17.84150 13.05850
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O 15.60600 7.89480 13.63670
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H 13.75530 12.01630 21.94430
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H 20.80630 14.67680 7.25270
H 20.21400 13.14600 6.58710
H 7.72000 16.10680 7.21320
H 7.81950 17.48230 8.37330
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H 9.72130 21.30930 17.14410
H 19.98600 18.59200 14.44820
H 19.15580 19.44880 13.09520
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H 15.83380 5.17480 15.45930
H 17.05830 6.45500 15.63640
H 13.22100 9.86180 4.90490
H 14.53650 8.82680 5.52990
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H 10.67270 10.65000 9.55450
H 13.86280 17.26450 7.99270

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H 9.52750 13.20800 16.95670
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H 22.50480 13.61900 15.14600
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H 8.46930 7.27800 10.39900
H 9.91300 6.25450 10.32800
H 9.27500 17.87130 13.00600
H 9.35900 9.74280 19.84220
H 9.97900 8.24780 19.11490
H 8.51350 8.99980 18.43300
H 12.68380 14.87030 7.87590
H 10.76400 16.54320 21.76250
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H 14.64250 19.63450 11.96600
167
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Ru 13.49350 15.22380 15.42760
Ru 13.60880 15.28300 11.06950
Ru 12.26150 12.77550 15.38060
Ru 13.71930 13.71480 13.24800
Ru 12.40980 12.90700 11.06270
Ru 12.37200 11.26980 13.21140
Ru 12.22380 15.92300 13.25170
Ru 11.06200 13.53380 13.15260
Ru 8.40400 13.33480 13.05280
Ru 9.46450 15.54030 13.26990
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Ru 10.55780 17.86900 13.00840
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Ru 9.80600 12.62500 11.13320
Ru 9.65050 12.62780 15.13250
Ru 10.76480 13.44630 17.31810
Ru 12.36700 15.98130 9.02930
Ru 10.80800 15.06730 11.00350
Ru 10.80430 14.95500 15.25520
Ru 11.97500 15.90350 17.48140
Ru 12.14380 17.42500 11.18940
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Ru 11.86430 17.38330 15.32860
Ru 11.37300 8.91650 13.16510
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Ru 11.16480 10.33030 15.28490
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Ru 14.94600 16.10200 9.05870
Ru 14.82000 16.16630 13.29250
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Ru 13.85330 10.71120 11.12640
Ru 13.73230 10.54330 15.36260
Ru 14.88030 11.47530 17.48660
Ru 16.28180 14.11530 9.14710
Ru 16.45250 13.75780 13.37180
Ru 16.02900 14.00030 17.50970
Ru 16.34780 15.36630 11.29750
Ru 16.16100 15.36850 15.47990
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Ru 16.45450 10.71650 11.36380
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Ru 16.30250 10.85650 15.49760
Ru 17.71550 13.17300 11.21410
Ru 17.56680 13.04650 15.59380
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C 6.68430 10.97430 13.16280
C 14.26380 12.32180 21.71550
C 14.27330 12.46050 20.21550
C 20.14850 13.03820 7.50960
C 19.00800 13.17150 8.48350
C 7.64030 16.11180 8.24900
C 8.86800 15.48750 8.89550
C 9.63950 21.10630 15.06810
C 10.18130 19.83730 15.26770
C 19.13330 17.78480 13.34550
C 17.85100 17.07580 13.67290
C 16.24430 5.23330 15.49550
C 15.66000 6.54870 15.04670
C 14.08430 9.69600 5.26660
C 14.00000 10.30130 6.64070
C 21.79930 12.12550 15.03160
C 20.31250 12.19780 14.80960

C 9.32830 6.70000 10.02480
C 10.11400 7.76500 10.74019
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C 9.97800 9.64150 17.99540
C 9.99850 15.08550 21.31510
C 10.59630 14.90030 19.90820
C 17.20900 19.75450 8.40290
C 16.36950 18.72180 8.99830
C 16.88000 19.69320 18.42050
C 16.08250 18.61400 17.73880
D 6.63980 12.26400 13.16590
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O 15.01130 11.63350 19.55720
O 17.89100 13.61880 8.00670
O 19.18780 12.85150 9.69770
O 9.14670 15.79250 10.06820
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D 10.09500 19.08000 16.01760
D 9.92180 19.59350 14.03670
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O 17.68650 16.61480 14.84890
O 14.46950 6.82830 15.42660
D 16.41150 7.28580 14.31590
D 15.09330 10.59300 7.23640
D 12.83800 10.46800 7.10250
O 19.63180 12.94600 15.60160
O 19.80180 11.50100 13.86920
O 10.47800 7.52330 11.94860
D 10.35900 8.85580 10.12650
O 9.75430 9.58230 16.74878
D 11.01350 10.21230 18.51930
O 10.21950 13.80780 19.31510
O 11.16880 15.87230 19.39110
O 15.88250 18.97000 10.15900
O 16.13630 17.66000 8.33220
D 15.86000 17.53400 18.37478
D 15.05330 18.94830 16.54610
H 5.50830 9.17250 13.26830
H 4.78980 10.49550 12.29360
H 4.77320 10.61020 14.05820
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H 7.62450 17.18800 8.46200
H 6.74660 15.67830 8.71318
H 8.74250 11.43380 15.33220
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H 9.42750 20.96280 16.93350
H 19.74470 17.92030 14.24330
H 18.91050 18.75450 12.88140
H 19.08930 17.18630 12.60840
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H 15.49300 4.62600 16.00980
H 17.08930 5.42480 16.17230
H 13.12880 9.79620 4.74140
H 14.32180 8.62600 5.36350
H 14.89330 10.16530 4.69400
H 18.05580 14.90600 10.94520
H 16.15900 9.99200 9.76090
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H 10.25350 15.20450 17.02690
H 11.53250 17.52580 9.52950
H 13.23400 16.89250 18.32320
H 9.28250 12.54700 15.92160
H 18.22250 11.36800 11.61730
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H 22.19830 13.12700 15.23500
H 17.75630 13.54500 17.33290
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H 8.28050 6.75930 19.35580
H 9.70430 5.70450 10.28850
H 8.90850 17.28900 12.96650
H 8.77000 9.69830 19.76600
H 9.46970 8.11230 19.39730
H 8.99130 8.70730 18.42460
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H 10.07680 14.14220 21.86890
H 8.93400 15.36050 21.27450
H 14.29580 19.23800 12.21320
H 17.49870 19.52830 7.35280
H 18.23380 19.75830 8.96710
H 16.84600 20.75330 8.50120
H 11.25550 8.40350 14.99910
H 17.14400 20.48800 17.71560
H 17.78450 19.26080 18.86720
H 16.28100 20.11880 19.23820
H 9.82680 12.37800 9.33110

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Ru 15.15030 13.02070 11.09840
Ru 15.08480 11.52250 13.34760
Ru 13.68250 15.31350 15.46980
Ru 13.65230 15.39680 11.10170
Ru 12.36030 12.91700 15.43050
Ru 13.75650 13.85050 13.25530
Ru 12.37650 12.96200 11.16880
Ru 12.38600 11.34680 13.24910
Ru 12.32530 16.08550 13.29350
Ru 11.04130 13.64230 13.25900
Ru 8.43600 13.70780 13.24520
Ru 9.66800 15.84170 13.37180
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Ru 10.75620 18.11850 13.21530
Ru 11.03330 13.64030 9.06310
Ru 9.67450 12.84930 11.24060
Ru 9.71450 12.91150 15.32750
Ru 10.92450 13.74130 17.49670
Ru 12.32180 16.02100 9.02540
Ru 10.91730 15.17530 11.19480
Ru 10.96300 15.22630 15.33190
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Ru 12.12380 17.51280 11.20000
Ru 13.44800 18.37030 13.23140
Ru 12.18280 17.60800 15.39300
Ru 11.16800 9.05300 13.31430
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Ru 10.99580 10.56030 15.45600
Ru 12.27050 11.42580 17.52610
Ru 13.69000 13.74400 9.03580
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Ru 14.96150 16.04720 9.00560
Ru 14.96850 16.26220 13.31230
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Ru 14.64050 17.71500 15.51080
Ru 13.96450 9.15530 13.27220
Ru 12.63450 8.49080 15.33950
Ru 15.11230 11.49300 8.96090
Ru 13.77400 10.66230 11.08150
Ru 13.77680 10.60280 15.43980
Ru 14.99830 11.59250 17.55220
Ru 16.31530 13.90420 9.02170
Ru 16.39380 13.83880 13.28730
Ru 16.27150 13.89400 17.53050
Ru 16.29850 15.39180 11.10880
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Ru 16.39530 9.31700 13.39990
Ru 16.43800 10.75180 11.17350
Ru 17.73580 11.52350 13.25840
Ru 16.43380 10.91600 15.42810
Ru 17.72500 13.24600 11.18030
Ru 17.71980 13.09950 15.48090
C 5.22630 10.81670 13.42350
C 6.58000 11.46090 13.41240
C 13.87450 12.40430 21.73650
C 14.05180 12.52230 20.24390
C 20.56200 13.99130 7.92450
C 19.28030 13.78500 8.68870
C 7.54230 16.22300 8.52750
C 8.81350 15.62600 9.05500
C 10.03050 21.32950 16.10100
C 10.52280 20.06050 15.46120
C 19.05630 18.22200 13.55590
C 17.83450 17.41480 13.90580
C 16.01080 5.66850 15.18890
C 14.98530 6.70120 14.81560
C 13.61150 9.67230 5.22310
C 13.67380 10.34550 6.56860
C 21.65000 11.16380 15.19670
C 20.24030 11.58630 14.87850
C 8.54080 7.23630 10.26840
C 9.46850 8.19550 10.97120
C 10.28780 15.64370 21.39890
C 10.70630 15.38800 19.97580
C 10.40430 7.70930 18.90150
C 10.95950 8.84430 18.08300
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C 15.22230 18.93500 8.39960
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C 16.30650 18.75300 17.76480
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D 19.34680 13.23000 9.83890
D 9.22530 16.01900 10.20210
D 9.41880 14.75530 8.33250
D 11.27800 19.29850 16.16680
D 10.17550 19.81330 14.25550
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D 17.88700 16.66130 14.94010
D 13.96500 6.84530 15.55550

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O	14.81850	10.66730	7.02440
O	12.56000	10.53300	7.18950
O	19.68800	12.43400	15.66710
O	19.67450	11.06250	13.85880
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O	9.75230	9.29420	10.38210
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O	10.32330	14.30230	19.42510
O	10.72850	8.81450	16.80820
O	11.59850	9.77250	18.66460
O	15.14830	19.18220	9.64650
O	15.12630	17.76130	7.87960
O	15.98830	17.72950	18.45010
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H	9.93350	17.54800	13.23090
H	12.26180	14.53980	7.94920
H	8.11080	13.52250	11.27360
H	9.57200	11.32230	16.17360
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H	13.73500	10.23830	17.23880
H	16.35220	17.00350	10.25130
H	12.57680	8.23180	12.59520
H	16.39450	12.33830	8.10780
H	16.58130	10.53350	9.39430
H	16.51320	12.25650	18.21140
H	16.66080	15.65500	17.21510
H	18.11940	13.31730	13.74900
H	17.12720	9.22150	14.98380
H	5.30850	9.75400	13.67420
H	4.78500	10.90700	12.41940
H	4.56350	11.33380	14.12710
H	14.52730	11.62650	22.14550
H	12.82930	12.13130	21.94450
H	14.07230	13.36930	22.21800
H	21.28850	13.21350	8.18510
H	20.98950	14.96580	8.20350
H	20.36930	13.99730	6.84610
H	7.44230	16.03680	7.45320
H	7.51080	17.29330	8.74090
H	6.69630	15.75350	9.05130
H	9.25380	21.79730	15.48850
H	10.87630	22.02450	16.20970
H	9.65100	21.11580	17.10830
H	19.84650	18.07350	14.29870
H	18.79100	19.28580	13.49430
H	19.41650	17.91350	12.56420
H	16.19200	5.47650	14.36390
H	15.50980	4.74200	15.49520
H	16.58000	6.03800	16.05500
H	12.68100	9.93320	4.70650
H	13.62280	8.58230	5.37420
H	14.48450	9.94500	4.62050
H	15.93650	14.99000	11.33730
H	15.16680	9.44850	11.52350
H	12.76200	16.71350	7.63780
H	10.47980	15.50800	17.08950
H	12.01380	17.69680	9.32910
H	13.50180	17.09880	18.25900
H	9.18150	13.61030	16.82850
H	18.17700	11.39730	11.42990
H	22.12180	10.70380	14.32260
H	21.62480	10.42900	16.01500
H	22.23180	12.02600	15.54360
H	9.73830	9.58000	14.21970
H	8.26780	7.61780	9.27970
H	7.63600	7.09530	10.87550
H	9.02780	6.25680	10.17200
H	17.98680	13.56200	17.17560
H	9.41850	15.03130	21.66190
H	10.07450	16.70800	21.55040
H	11.12490	15.37280	22.06200
H	14.16230	19.44230	9.44230
H	10.08100	7.67080	19.08610
H	10.53500	6.75900	18.37000
H	9.32330	7.86650	19.03300
H	15.18250	14.68480	7.80180
H	15.90500	19.74150	6.42250
H	16.11950	20.65330	7.74070
H	14.56500	20.77550	7.54550
H	11.14700	7.75830	14.41280
H	17.12280	20.74350	17.87270
H	18.22750	19.43680	18.37840
H	16.90980	19.91900	19.46260
H	9.80100	12.43230	9.46350

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Ru	15.13748345270525	12.57194677183878	11.41311827654457
Ru	15.14782882988457	11.05853766969584	13.60179578977617
Ru	13.3393963286583	14.90564533039370	15.79119205137872
Ru	13.63925320742796	14.87517983973913	11.43183624188325
Ru	12.44687526669081	12.4706957840538	15.71233626519266

Ru	13.81688036021416	13.35511897862926	13.57823916017713
Ru	12.40791888953592	12.51073946407655	11.44705992386166
Ru	12.40972384326653	10.86110093990432	13.59952409121808
Ru	12.40281201559974	15.66004000326605	13.60541734866298
Ru	11.14493305116458	13.19845092184726	13.58525864548294
Ru	8.52647963505332	13.20804346858589	13.58975523110284
Ru	9.7172202647451	15.3656035597000	13.05308102049616
Ru	9.74872089608850	10.80058861202382	13.67724483384270
Ru	10.84230120691303	17.65187556485589	13.58780214135146
Ru	10.91310554756047	13.08716222344401	9.41328395756144
Ru	9.78750150168086	12.34066022139069	11.63014883708531
Ru	9.76758581767382	12.45862796828230	15.6655416200979
Ru	11.02369386649516	13.21847816592022	17.72346959727557
Ru	12.35212478999565	15.62233941462259	9.37544463439074
Ru	10.97838531862291	14.71360367365977	11.46095740616690
Ru	11.07044816874741	14.7335515416612	15.66902978123972
Ru	12.31618343958078	15.51946596837577	17.91254208437154
Ru	12.16240363498203	17.17203498716747	11.48683882109873
Ru	13.57522552360809	16.01110341053601	13.60109255250123
Ru	12.33951120442216	17.09083495093758	15.715335201625
Ru	11.24467692447534	8.60128769073732	13.70838357658061
Ru	12.44334348788755	11.01863067796681	9.35518600755847
Ru	11.15686873133470	10.14313471753741	11.50536436032684
Ru	11.19257228582321	10.12384063809233	15.77870873909795
Ru	12.5930994621615	10.99366772514760	17.34659619207646
Ru	13.70894739337041	13.35195157973482	9.28758094863981
Ru	13.75218789978233	13.3285959238003	17.84162777110367
Ru	15.04150774283235	15.59029718044247	9.19951651830943
Ru	15.00664242077525	15.66371943757792	13.51387955453077
Ru	15.08490013073613	15.61311832179096	17.84194520589376
Ru	14.95489815152481	17.11701106400362	11.39323140249573
Ru	14.96681394719408	17.16477297213591	15.62595387060177
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Ru 10.47028 13.69483 17.15868
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Ru 10.62669 15.24589 10.92192
Ru 10.40108 15.26301 15.05250
Ru 11.70954 15.97939 17.22597
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Ru 10.09218 10.66157 10.86527
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Ru 11.68736 11.44936 17.24737
Ru 13.31922 13.70586 8.81242
Ru 13.06407 13.78622 17.34035
Ru 14.61911 15.95834 8.86387
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Ru 14.30158 16.08696 17.30220
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Ru 14.37618 17.67033 15.13630
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Ru 12.22022 8.45140 15.26268
Ru 14.63752 11.53765 8.82861
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Ru 13.21249 10.64146 15.17710
Ru 14.31864 11.48283 17.27370
Ru 15.90321 13.82075 8.91402
Ru 15.92662 13.81593 13.14739
Ru 15.64412 13.08033 17.34576
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Ru 15.99801 10.73985 11.02090
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H 7.85339 12.19559 11.87906
H 7.47615 12.93139 14.34329
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H 9.92489 15.45189 16.95560
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Ru 12.35760 12.81470 15.30590
Ru 13.62390 13.91030 13.10150
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Ru 12.49020 11.45160 12.99840
Ru 11.96510 16.05810 13.28150
Ru 10.96520 13.63010 13.18550
Ru 8.18940 13.33670 13.16390
Ru 9.23430 15.70440 13.41620
Ru 9.61960 10.96730 13.12810
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Ru 10.69710 13.67410 9.92100
Ru 9.65010 12.60910 11.07090
Ru 9.74670 12.53200 15.14100
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Ru 11.75720 16.15870 9.05020
Ru 10.55030 15.19270 11.18380
Ru 10.76330 14.98200 15.37310
Ru 12.11660 15.76390 17.40750
Ru 11.69340 17.60280 11.22160
Ru 13.08390 18.56170 13.31430
Ru 11.80090 17.44490 15.43860
Ru 11.32840 8.90860 13.04240
Ru 12.26500 11.57610 8.85220
Ru 11.09520 10.60670 10.95560
Ru 11.28090 10.45930 15.00320
Ru 12.49420 11.12980 17.28800
Ru 13.29430 13.95850 8.79170
Ru 13.66850 13.55560 17.43080
Ru 14.32540 16.44250 8.89700
Ru 14.68060 16.45050 13.22440
Ru 14.66450 16.02480 17.48520
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Ru 14.82520 11.90230 8.69060
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Ru 11.49500 9.58090 17.14720
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Ru 16.20810 14.25080 13.04020
Ru 16.30040 13.92000 17.29170
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D 12.59180 7.64470 17.09370
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H 11.48360 6.80240 19.48350
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Ru 13.60560 13.75080 13.01780

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Ru 9.47430 16.05060 13.30110
Ru 9.35090 11.30860 13.17290
Ru 10.85350 18.23860 13.27310
Ru 10.71630 13.84160 8.95750
Ru 9.43600 13.03310 11.12130
Ru 9.61280 13.01820 15.27790
Ru 11.04570 13.63230 17.39220
Ru 12.06600 16.13510 8.92050
Ru 10.78600 15.34940 11.09950
Ru 10.97680 15.28560 15.29890
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Ru 12.13970 17.65970 11.08550
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Ru 12.39410 17.58790 15.37140
Ru 10.73090 9.08270 13.14380
Ru 11.99100 11.55410 8.82500
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Ru 10.86860 10.70490 15.18270
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Ru 12.21860 8.53570 15.48230
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Ru 13.43570 10.60180 10.90240
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Ru 10.79010 13.92530 9.26300
Ru 9.12900 13.14700 11.22320
Ru 9.22370 13.09190 15.51930
Ru 10.54500 13.88970 17.64250
Ru 12.05900 16.21240 9.29260
Ru 10.65260 15.52320 11.42930
Ru 10.45010 15.48630 15.56520
Ru 11.79360 16.14770 17.74390
Ru 11.98310 17.76830 11.34250
Ru 12.99270 18.77920 13.51080
Ru 11.57650 17.90360 15.65760
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Ru 12.02740 11.69740 9.17640
Ru 10.03640 10.97640 11.27450
Ru 10.54670 10.82260 15.48990
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Ru 12.23400 8.65510 15.62400
Ru 14.62730 11.80330 9.15070
Ru 13.36770 10.92710 11.33470
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Ru 12.49970 11.54510 13.35710
Ru 11.95400 16.18070 13.76140
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Ru 9.21890 15.77790 13.87620
Ru 9.68110 11.05970 13.47580
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O 12.45510 11.06460 7.18650
O 17.77110 16.77120 15.29360
O 16.62530 17.90940 13.71020
O 12.57230 7.66980 17.35190
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H 6.58310 13.22150 13.68780
H 11.16590 7.93730 14.71400
H 7.60180 15.01750 14.03440
H 8.60600 17.45840 14.10780
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H 8.92780 15.89830 12.12790
H 9.10360 13.22330 9.96320
H 10.33070 15.03890 17.64920
H 11.11480 17.91210 9.97560
H 11.41880 19.23220 12.93820
H 11.40400 17.38030 17.75930
H 10.75490 12.37060 8.47980
H 10.57640 9.11740 11.69950
H 11.31190 10.18520 9.69610
H 9.61500 9.23070 13.58780
H 11.07410 10.35460 17.16150
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H 12.26200 14.12460 18.94090
H 12.93300 17.27630 8.48370
H 13.31860 16.60860 18.98290
H 13.83860 19.49700 12.59690
H 14.42480 18.32050 9.82660
H 16.06200 17.74330 11.45620
H 14.56870 18.93430 14.63040
H 13.79400 10.63670 9.43260
H 12.73480 9.41190 12.14280
H 14.34590 9.15150 16.08040
H 13.89690 11.94850 18.68940
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H 16.42820 11.09190 9.28140
H 15.43100 9.94130 11.35790
H 18.26870 10.37710 12.82480
H 16.73950 10.67250 17.06040
H 17.24060 9.42670 14.65350
H 17.63260 14.18860 9.50040
H 18.18320 12.18360 11.31480
H 18.19070 13.83550 12.99090
H 18.40700 11.88080 14.87670
H 7.94050 12.40030 14.90410
H 10.55350 18.80180 15.35490
H 11.15020 11.79660 18.69670
H 14.95960 14.46880 18.93750
H 13.04940 7.96570 13.80760
H 16.12900 13.10960 8.17320
H 16.23240 16.30700 9.61860
H 16.51510 15.83040 17.57980
H 17.98520 13.81710 17.16650
H 12.87710 7.69340 20.62120
H 13.28590 6.35440 19.48600
H 11.59300 6.79440 19.75960
H 15.71700 18.61310 16.24170
H 9.13460 15.71680 15.67220
H 18.83060 19.03140 13.17010
H 19.79880 17.88850 14.17280
H 18.98510 19.26820 14.93380
H 12.60550 9.98200 4.92630
H 14.39420 9.76420 4.99630
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H 12.76990 18.95690 15.66260

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Ru 14.85680 11.55280 13.30220
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Ru 15.41850 15.53910 11.23500
Ru 12.27420 13.10650 15.62620
Ru 13.61640 13.94470 13.38540
Ru 12.04610 13.19120 11.28200
Ru 12.16540 11.64980 13.39320
Ru 12.22700 16.30200 13.53740
Ru 10.89610 13.98480 13.55090
Ru 8.12860 14.07370 13.57920
Ru 9.48510 16.25110 13.71160
Ru 9.34850 11.60140 13.54050
Ru 10.87990 18.43660 13.64890
Ru 10.67980 14.00330 9.33160
Ru 9.40730 13.26130 11.50910
Ru 9.63820 13.23110 15.64720
Ru 11.09540 13.78580 17.75000
Ru 12.03630 16.28850 9.27160
Ru 10.77760 15.53830 11.47300
Ru 11.02760 15.49680 15.69200
Ru 12.47560 16.03640 17.77690
Ru 12.14950 17.84450 11.42260
Ru 13.59500 18.78940 13.50750
Ru 12.40700 17.79940 15.74920
Ru 10.72390 9.29310 13.48030
Ru 11.89490 11.72130 9.10170
Ru 10.70390 10.90510 11.37330
Ru 10.06750 10.90930 15.53440
Ru 12.26500 11.43590 17.69850
Ru 13.31020 13.99010 9.10780
Ru 13.75790 13.73050 17.71220
Ru 14.63590 16.22800 9.08740
Ru 14.88810 16.26410 13.37670
Ru 15.11800 16.00120 17.70660
Ru 14.85110 17.85600 11.23920
Ru 15.12490 17.74140 15.67050
Ru 13.38820 9.22570 13.43130
Ru 12.23510 8.75740 15.80290
Ru 14.61290 11.61900 8.92500
Ru 13.40150 10.84060 11.21260
Ru 13.58400 10.78250 15.43700
Ru 14.96580 11.38500 17.61260
Ru 15.95320 13.92410 8.96640
Ru 16.29290 13.92050 13.26860
Ru 16.38710 13.72310 17.53250
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Ru 16.47730 15.43910 15.49270
Ru 16.05660 9.32880 13.20510
Ru 16.07550 10.78660 11.11940
Ru 17.66690 11.50520 13.17400
Ru 16.26510 10.68710 15.34760
Ru 17.38290 13.13320 11.03510
Ru 17.59240 12.99240 15.34200
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C 19.39190 18.78640 15.85080
C 18.09650 18.02190 15.73570
C 12.99650 9.05490 5.76440
C 13.09770 9.96350 6.96220
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O 12.01660 10.26800 7.57510
O 18.17800 16.75080 15.63020
O 17.01190 18.70110 15.76930
O 12.19020 9.80820 19.06860
O 12.50100 8.93500 17.67360
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H 7.74120 15.74760 13.78190
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H 11.08020 17.71660 17.41770
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H 11.72370 17.98890 9.68350
H 12.21620 19.70540 13.18410
H 10.86830 18.67280 15.42860
H 9.04070 9.79770 13.69170
H 10.13420 9.14760 11.89130
H 10.45470 10.88860 9.56200
H 11.08320 12.33620 18.74490
H 10.74410 10.71020 17.32840
H 13.28160 17.04560 8.23200
H 13.86960 16.78760 18.69500
H 14.87620 17.97290 9.50180
H 13.81290 19.40680 14.95960
H 15.44860 17.69380 17.43640

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H 13.68710 9.19000 11.64160
H 13.80780 10.18410 9.65410
H 15.12160 10.45910 18.90760
H 16.47400 15.69450 9.35450
H 15.55710 12.46300 7.95000
H 16.38040 12.11510 18.38620
H 15.30660 18.69590 12.64000
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H 16.29880 9.03680 11.42790
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H 16.20840 10.27150 17.14520
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H 17.58190 13.34600 9.24560
H 17.63100 11.41660 10.57840
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H 18.09350 13.46620 16.97160
H 17.77760 14.52170 14.39980
H 18.84250 11.94880 14.32140
H 17.68660 11.43860 16.14760
H 8.95510 11.39520 11.76000
H 9.04580 11.42960 15.30140
H 9.39550 13.45630 17.42750
H 10.24680 15.83230 9.70510
H 11.91240 14.81700 8.14520
H 12.47080 14.50520 18.85460
H 13.61850 19.10810 11.64600
H 10.59370 12.53950 8.24630
H 12.01150 9.86010 10.76800
H 10.53890 8.85890 15.18990
H 14.61480 14.77990 7.94950
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H 15.16560 14.47770 18.75300
H 16.53720 17.28950 11.18940
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H 14.10590 9.99930 17.21800
H 12.90970 7.84270 14.55240
H 13.77140 12.08240 18.73870
H 16.88720 15.46240 17.34240
H 17.84620 14.88050 11.16080
H 16.68330 15.74400 12.80720
H 18.53230 12.79580 12.39730
H 11.65810 6.79970 19.83440
H 12.18810 8.14880 20.93950
H 13.36500 7.18490 20.10040
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H 19.23640 19.84400 15.61560
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H 17.75970 18.70170 16.88370
H 9.44220 15.27230 15.49320
H 11.95130 8.92510 5.46700
H 13.42950 8.07650 6.01610
H 13.58320 9.47070 4.93560
H 13.76140 18.45500 16.61940

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Ru 15.66944 11.63980 13.56787
Ru 14.96747 15.32040 15.73430
Ru 14.01704 15.37960 11.31413
Ru 12.77892 13.01273 15.67423
Ru 14.19194 13.84020 13.50851
Ru 12.80417 12.98852 11.39228
Ru 12.89323 11.43685 13.59543
Ru 12.68702 16.04213 13.49289
Ru 11.47304 13.69844 13.49952
Ru 8.86835 13.09756 13.42001
Ru 10.03880 15.87033 13.61980
Ru 10.04242 11.26602 13.54814
Ru 11.22228 18.14665 13.60790
Ru 11.43256 13.64943 9.31900
Ru 10.20720 12.78698 11.50771
Ru 10.14618 12.98418 15.58280
Ru 11.48022 13.60526 17.69546
Ru 12.69443 16.06130 9.34272
Ru 11.30943 15.20595 11.39450
Ru 11.38563 15.22927 15.61550
Ru 12.62373 16.00770 17.66301
Ru 12.56259 17.58012 11.52427
Ru 13.96402 18.45782 13.59926
Ru 12.56825 17.52227 15.59231
Ru 11.71207 9.15628 13.67060
Ru 12.88110 11.42750 9.45236
Ru 11.58774 10.62291 11.56849
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Ru 12.79508 11.30025 17.62526
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Ru 14.10467 13.73218 17.81741
Ru 15.34809 16.02051 9.28642
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Ru 15.22530 16.12153 17.79432
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Ru 15.12810 17.65956 15.77699
Ru 14.38628 9.26415 13.67398

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Ru 15.40750 11.59887 9.32437
Ru 14.28320 10.74285 11.48199
Ru 14.42886 10.74999 15.64009
Ru 15.55933 11.57618 17.73728
Ru 16.67868 13.85367 9.20774
Ru 16.80277 13.98106 13.53764
Ru 16.76007 13.90371 17.76270
Ru 16.58099 15.50546 11.47219
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C 19.57585 14.57018 9.20602
C 7.83427 16.04739 8.80417
C 9.16189 15.53227 9.28755
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O 8.09946 10.62805 13.66770
O 14.24855 13.46947 19.93276
O 15.17087 11.40530 19.77911
O 18.50031 14.60741 8.52390
O 19.64493 14.11575 10.41138
O 9.68431 16.10145 10.30947
O 9.69169 14.54069 8.65628
H 9.51937 17.65946 13.65422
H 12.71886 14.56019 8.16256
H 8.69385 13.56342 11.39476
H 10.08089 11.45896 16.51875
H 13.82193 19.01833 11.87215
H 14.89417 19.25053 14.91206
H 11.89537 9.98832 9.90774
H 11.69894 12.20481 18.81374
H 12.81143 9.42697 17.80128
H 16.62911 17.19929 10.46992
H 13.10196 8.01682 14.45353
H 16.55113 12.43904 8.13372
H 16.72651 10.39271 9.88614
H 17.22384 12.21132 18.16765
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H 19.37553 12.34250 14.71062
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H 5.84217 9.67992 14.27195
H 5.18415 10.70301 13.04214
H 5.13610 11.26968 14.74825
H 15.15215 11.39039 22.29959
H 13.46264 11.95319 22.16049
H 14.74632 13.14079 22.44852
H 21.71796 14.73954 9.12441
H 20.81941 16.20791 8.65750
H 20.88243 14.84082 7.52918
H 7.53798 15.54892 7.87617
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Ru 15.04220 11.41610 13.37700
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Ru 13.66930 15.20170 11.20220
Ru 12.13840 12.88570 15.50000
Ru 13.60770 13.70660 13.41620
Ru 12.29850 12.96020 11.18070
Ru 12.22970 11.35260 13.23220
Ru 12.37410 16.14000 13.35800
Ru 10.89040 13.63920 13.29270
Ru 8.37040 13.70920 13.08580
Ru 9.53670 15.91780 13.40560
Ru 9.61550 11.33550 13.21400
Ru 10.80110 18.13410 12.92820
Ru 11.10780 13.67190 9.06300
Ru 9.70950 12.84910 11.03980
Ru 9.51210 12.06810 15.27960
Ru 10.77080 13.66890 17.45910
Ru 12.45920 15.88950 9.09220
Ru 11.00390 15.28150 11.29270
Ru 10.84560 15.25340 15.34120
Ru 12.10060 15.97090 17.50730
Ru 12.47640 17.45620 11.11960
Ru 13.40360 18.52400 13.33330
Ru 11.85540 17.72460 15.40780
Ru 10.96850 9.09590 13.28540
Ru 12.40080 11.40320 9.02780
Ru 11.00300 10.68210 11.10790
Ru 10.85670 10.57100 15.31430
Ru 12.07470 11.37790 17.50840
Ru 13.71570 13.59410 9.11480
Ru 13.46440 13.68290 17.68370

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Ru	14.74010	15.98490	17.60390
Ru	14.93130	17.49710	11.29800
Ru	14.77760	17.54140	15.50420
Ru	13.67600	9.14020	13.35210
Ru	12.49700	8.40960	15.59140
Ru	15.01200	11.46810	9.02690
Ru	13.70930	10.63340	11.20310
Ru	13.51400	10.60650	15.40560
Ru	14.68020	11.38060	17.54370
Ru	16.28890	13.69470	9.25230
Ru	16.29230	13.71870	13.47190
Ru	16.03830	13.74230	17.67220
Ru	16.41570	15.20970	11.32800
Ru	16.31770	15.27190	15.59630
Ru	16.01910	9.06790	13.27870
Ru	16.29720	10.62000	11.31140
Ru	17.60590	11.14490	13.53600
Ru	16.08230	10.30310	15.61080
Ru	17.61450	12.90550	11.50580
Ru	17.40690	12.75200	15.67640
C	15.96080	6.09370	17.01000
C	15.29790	7.30920	16.40830
C	19.42870	17.36160	13.22590
C	18.11620	16.75490	13.66150
C	13.81240	8.84450	5.76970
C	13.78220	9.75510	6.96420
C	7.52110	18.78500	15.66460
C	8.88080	18.43600	15.14040
O	8.92670	18.02100	13.88160
O	9.09330	18.52940	15.07800
O	12.64520	10.16810	7.37970
O	14.89750	10.09640	7.49500
O	17.15230	16.77060	12.79260
O	17.99710	16.27420	14.82990
D	16.08660	8.23900	16.00230
D	14.02220	7.31530	16.37100
H	7.87640	15.30510	13.67460
H	10.83290	19.58360	13.61020
H	11.82440	17.67370	17.20260
H	10.77060	12.17100	18.46100
H	8.21850	12.16080	12.11220
H	7.00600	12.06970	14.49500
H	9.32070	13.29870	9.39200
H	10.66640	15.47650	9.42450
H	12.01390	14.51040	18.62220
H	12.04550	19.06330	12.05430
H	14.65340	19.04320	12.19540
H	12.55450	19.24970	14.70500
H	9.77860	9.54720	12.04170
H	11.08780	12.26390	8.02560
H	11.52170	9.76470	9.78150
H	10.78190	8.66310	15.16310
H	13.81000	16.56160	8.06960
H	13.45250	16.78790	18.50040
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H	10.66990	10.39580	17.10660
H	12.47750	7.76790	13.87150
H	16.48970	12.23610	8.22160
H	15.08810	9.56090	10.54840
H	16.19700	10.45740	17.38410
H	17.67610	14.34370	16.46760
H	17.90070	14.38800	10.50420
H	17.37060	12.57000	17.46560
H	18.09110	12.93520	13.98800
H	17.96930	9.49330	13.46210
H	18.14480	11.12290	11.82050
H	18.01520	11.07180	15.30760
H	15.33650	5.20410	16.87310
H	16.00070	6.25590	18.09000
H	16.09560	5.94470	16.59190
H	16.28720	17.97480	15.20040
H	20.18030	17.22160	14.03950
H	19.28290	18.43490	13.06930
H	19.76890	16.90810	12.31550
H	10.33910	15.49520	17.19590
H	14.70530	5.79400	5.79400
H	13.85400	9.46170	4.85940
H	12.90090	8.23820	5.72770
H	13.28270	18.16210	16.26270
H	7.60320	19.32120	16.61490
H	6.95550	17.85410	15.82420
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H	9.14730	13.14610	17.03440

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Ru 15.20809 11.06074 13.32735
Ru 13.44356 15.40222 15.83952
Ru 13.24724 15.66889 11.45330

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Ru	13.60890	14.01521	13.55688
Ru	12.20256	13.21505	11.37355
Ru	12.49960	11.54517	13.35704
Ru	11.95402	16.18079	13.76137
Ru	10.94714	13.71325	13.60647
Ru	9.17719	13.30952	13.58241
Ru	9.21900	15.77791	13.87614
Ru	9.68114	11.09596	13.47590
Ru	10.25177	18.06037	13.82094
Ru	10.70141	13.85993	9.44878
Ru	9.65574	12.75609	11.59246
Ru	9.74549	12.56259	15.54135
Ru	11.02998	13.28463	17.78790
Ru	11.75916	16.32535	9.50365
Ru	10.57604	15.33113	11.64571
Ru	10.74126	15.01741	15.83934
Ru	12.07885	15.76419	17.94144
Ru	11.68446	17.75020	11.67847
Ru	12.93079	16.65383	13.84611
Ru	11.69179	17.47637	15.95463
Ru	11.35564	9.02666	13.33405
Ru	12.28233	11.73942	9.15490
Ru	11.10436	10.77360	11.29819
Ru	11.29572	10.53970	15.35795
Ru	12.52925	11.14478	17.63943
Ru	13.32180	14.12392	9.22410
Ru	13.65605	13.60020	17.83941
Ru	14.31984	16.62284	9.36305
Ru	14.70668	16.55490	13.69309
Ru	14.65637	16.04208	17.96919
Ru	14.23348	16.01504	11.59170
Ru	14.34105	17.82862	15.94105
Ru	14.10402	9.34113	13.31170
Ru	12.76464	8.50452	15.50818
Ru	14.80993	12.07965	8.99253
Ru	13.86611	11.01934	11.23244
Ru	13.99514	10.75020	15.43241
Ru	15.29911	11.55752	17.52433
Ru	15.93240	14.54053	9.18319
Ru	16.21157	14.37392	13.47771
Ru	16.29277	13.96880	17.71949
Ru	15.90317	16.00132	11.41983
Ru	16.06064	15.72507	15.74757
Ru	16.55771	9.73471	13.10647
Ru	16.47545	11.42622	11.00267
Ru	17.84884	12.04479	13.15878
Ru	16.64925	11.10793	15.31207
Ru	17.49127	13.91106	11.20032
Ru	17.58703	13.51756	15.43464
C	12.61290	7.19850	19.68105
C	12.66027	8.17296	18.53424
C	18.90133	18.51774	14.13420
C	17.67255	17.68186	14.37765
C	13.56243	10.45959	5.15826
C	13.57486	10.96139	6.57617
O	14.70900	11.27665	7.08102
O	12.45503	11.06458	7.18642
O	17.77104	16.77107	15.29359
O	16.62512	17.90932	13.71034
O	12.57241	7.66969	17.35187
O	12.77617	9.40993	18.80404
H	6.58305	13.22139	13.68608
H	11.16588	7.93733	14.71408
H	7.60186	15.01749	14.03437
H	8.60610	17.45847	14.10786
H	8.10951	11.85761	12.68691
H	9.41270	12.71682	17.30949
H	10.04086	15.55692	9.84070
H	8.92793	15.89840	12.12806
H	9.10346	13.22228	9.96312
H	10.33077	15.03891	17.64938
H	11.11485	17.91212	9.97554
H	11.41881	19.23508	12.93815
H	11.40388	17.38016	17.75929
H	10.75489	12.37057	8.47869
H	10.57636	9.11742	11.69954
H	11.31202	10.18506	9.69602
H	9.61485	9.23055	13.58795
H	11.07415	10.35447	17.16152
H	11.85033	14.79620	8.29600
H	12.26278	14.12466	18.94089
H	12.93297	17.27622	8.48381
H	13.31844	16.60849	18.98291
H	13.83859	19.49707	12.59688
H	14.42472	18.32042	9.82674
H	16.06290	17.74322	11.45621
H	14.56859	18.93426	14.63839
H	13.79404	10.63678	9.43272
H	12.73473	9.41188	12.14269
H	14.34601	9.15144	16.08036
H	13.89693	11.94856	18.68933
H	14.54651	15.16719	8.15663
H	16.57376	12.40668	18.53568
H	17.65646	15.70274	11.49230
H	14.68660	17.78135	17.69142

H 15.56643 8.30927 13.43623
H 16.42828 11.09198 9.28155
H 15.43094 9.94120 11.35885
H 18.26883 10.37706 12.82482
H 16.73950 10.67249 17.06043
H 17.24053 9.42669 14.65347
H 17.63267 14.18951 9.59038
H 18.18305 12.18350 11.31480
H 18.19076 13.83555 12.99095
H 18.40711 11.88078 14.87679
H 7.94844 12.40039 14.90420
H 10.55337 18.98188 15.35486
H 11.15022 11.79074 18.69666
H 14.95964 14.46888 18.93753
H 13.04938 7.96574 13.80769
H 16.12893 13.10989 8.17321
H 16.23233 16.30693 9.61869
H 16.51519 15.83945 17.57979
H 17.99525 13.81716 17.16648
H 12.87704 7.69333 20.62124
H 13.28580 6.35429 19.48608
H 11.59306 6.79451 19.75963
H 15.71686 18.61305 16.24173
H 9.13451 15.71692 15.67211
H 18.83063 19.03131 13.17014
H 19.79890 17.88835 14.17270
H 18.98500 19.26807 14.93389
H 12.60544 9.98197 4.92629
H 14.39432 9.76425 4.99644
H 13.70747 11.31463 4.48099
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C 8.88671 20.84016 17.03974
C 9.66471 19.83198 16.24269
O 9.35908 19.69046 15.00206
O 10.57117 19.14815 16.83958
H 9.31903 20.96844 18.03639
H 7.85073 20.48213 17.13788
H 8.84922 21.79899 16.50816
H 9.19268 14.17528 16.05499

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Ru 15.10380 11.34160 13.05580
Ru 14.03680 15.16870 15.53580
Ru 13.67580 15.42310 11.17760
Ru 12.55740 12.84140 15.49600
Ru 13.86800 13.74480 13.26280
Ru 12.24590 13.08890 11.18380
Ru 12.41840 11.46040 13.22660
Ru 12.48880 15.10260 13.52940
Ru 11.08300 13.81570 13.47000
Ru 8.25630 13.72250 13.71270
Ru 9.79880 16.19170 13.76340
Ru 9.64680 11.38140 13.44000
Ru 11.25360 18.30870 13.84660
Ru 10.85530 13.98430 9.25260
Ru 9.65030 13.15130 11.44110
Ru 9.92120 12.91920 15.60640
Ru 11.46640 13.44310 17.69940
Ru 12.24480 16.22450 9.21280
Ru 10.99090 15.47010 11.43070
Ru 11.30600 15.19570 15.69400
Ru 12.83800 15.68770 17.73970
Ru 12.38520 17.75780 11.47800
Ru 13.90420 18.48630 13.55620
Ru 12.81880 17.47870 15.79370
Ru 10.99820 9.07800 13.22190
Ru 12.05390 11.72440 8.94150
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Ru 11.21630 10.57130 15.36500
Ru 12.62680 11.11220 17.53140
Ru 13.49350 13.94200 9.00030
Ru 14.09720 13.36450 17.58820
Ru 14.94270 16.17000 9.02470
Ru 15.15560 16.05040 13.29080
Ru 15.45510 15.64200 17.60560
Ru 15.13840 17.72490 11.19050
Ru 15.46400 17.44990 15.64140
Ru 13.66690 9.02440 13.12420
Ru 12.57470 8.42000 15.48990
Ru 14.78410 11.67510 8.71420
Ru 13.58530 10.74780 10.96450
Ru 13.87800 10.51050 15.21210
Ru 15.31950 11.03770 17.38830
Ru 16.13410 13.86580 8.79840
Ru 16.55210 13.68430 13.07820
Ru 16.70900 13.35650 17.33510
Ru 16.41900 15.38050 11.01460
Ru 16.76000 15.13740 15.36420
Ru 16.26050 9.08930 12.91390
Ru 16.22890 10.61580 10.80970
Ru 17.91960 11.25270 12.86260
Ru 16.56600 10.43020 15.07300
Ru 17.61180 13.00040 10.80910
Ru 17.91290 12.71770 15.13180

C 12.74430 7.19700 19.67870
C 12.70970 8.18510 18.54440
C 19.73510 18.43790 15.79090
C 18.42430 17.70090 15.66630
C 13.16680 8.44970 6.22240
C 13.23020 9.66090 7.18230
C 7.98040 18.09310 16.69390
C 8.91510 18.28530 15.68640
O 9.92360 18.97720 15.30510
O 8.67650 17.09450 15.28180
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O 12.14240 10.09190 7.62360
O 18.48100 16.44090 15.46300
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O 12.56310 9.41270 18.81430
O 12.84040 7.68850 17.35300
H 6.65710 13.67960 13.64750
H 13.71060 20.02910 12.84580
H 10.32890 7.61750 13.11660
H 15.93680 19.07730 10.86900
H 8.07000 15.35990 13.38200
H 7.93880 12.01810 13.43050
H 9.75110 17.86430 13.08580
H 8.00040 13.77120 11.97310
H 9.21620 13.52530 9.73310
H 8.04630 13.17830 15.31460
H 9.42410 15.79410 12.09240
H 11.02870 15.32110 17.54370
H 12.38760 17.40060 17.51150
H 10.76630 17.29150 11.20620
H 12.16730 17.95860 9.72500
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H 11.08130 10.42200 17.14860
H 13.50380 17.03190 8.21720
H 14.25110 16.38860 18.66560
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H 14.18880 20.17400 13.61390
H 15.77310 17.34810 17.39780
H 13.36960 12.43170 7.83080
H 13.61040 9.05600 11.34290
H 14.85970 9.76110 10.13630
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H 16.67490 15.68660 9.26580
H 16.01020 12.55650 7.64460
H 16.74160 11.73780 18.17900
H 13.46590 18.61150 12.64230
H 14.99090 7.89390 12.70220
H 16.34960 10.91040 9.04320
H 16.65330 8.88060 11.20280
H 18.03220 9.58050 13.28740
H 16.52020 9.91180 16.82180
H 16.23260 8.76260 14.73420
H 17.72930 13.21490 8.98970
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H 19.41060 10.78390 12.52640
H 18.42670 13.13240 16.75490
H 18.01660 14.26840 14.19070
H 19.05280 11.64540 14.06100
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H 9.43380 11.14330 15.26390
H 9.80180 12.89390 17.39700
H 10.44280 15.78670 9.68130
H 12.05770 14.82090 8.05480
H 12.84230 14.09020 18.78100
H 13.75810 18.77430 10.86430
H 10.75570 12.61070 8.08640
H 12.17030 9.86480 10.32390
H 10.86780 8.60830 14.95900
H 14.79820 14.77690 7.84200
H 15.17450 18.94260 14.67900
H 15.53720 14.10010 18.60880
H 16.80640 17.18780 11.19440
H 12.22640 8.86470 12.53780
H 14.40610 9.69350 16.93330
H 13.30610 7.59000 14.19260
H 14.14840 11.71200 18.57100
H 17.22380 15.10910 17.18670
H 18.09380 14.70870 10.95110
H 16.88980 15.51720 12.72880
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H 12.00720 6.40280 19.50140
H 12.54720 7.69560 20.63180
H 13.73570 6.72240 19.70580
H 16.40390 16.88010 14.24610
H 19.59150 19.51070 15.62740
H 20.46470 18.02980 15.08160
H 20.13040 18.28340 16.80560
H 7.43800 14.69080 14.67200
H 12.13600 8.28250 5.89620
H 13.54290 7.54660 6.72360

H 13.81780 8.64130 5.35950
H 14.17880 18.32000 16.54600
H 6.97980 18.45800 16.59870
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Ru 12.01199 12.79740 15.64910
Ru 13.44418 13.72127 13.61384
Ru 12.25892 12.92602 11.37710
Ru 12.28602 11.30502 13.44756
Ru 11.91703 15.97203 13.53575
Ru 10.71983 13.46749 13.44404
Ru 8.20595 13.35026 13.24454
Ru 9.33763 15.66186 13.42662
Ru 9.51631 11.09218 13.39434
Ru 10.27422 17.94176 13.39114
Ru 10.91156 13.45219 9.31318
Ru 9.63218 12.61353 11.30208
Ru 9.42947 12.66087 15.46130
Ru 10.57925 13.50864 17.58349
Ru 12.10938 15.94563 9.38274
Ru 10.67130 15.03562 11.38124
Ru 10.54360 14.99322 15.54229
Ru 11.77113 15.82614 17.65964
Ru 11.00767 17.40862 11.45058
Ru 12.96832 18.35230 13.53798
Ru 11.63230 17.43914 15.66669
Ru 11.12891 8.96717 13.39502
Ru 12.39792 11.41264 9.20714
Ru 11.10996 10.54701 11.35304
Ru 10.93056 10.42942 15.30543
Ru 12.04172 11.25128 17.61286
Ru 13.54529 13.73658 9.35759
Ru 13.20115 13.61939 17.77518
Ru 14.60871 16.12709 9.40542
Ru 14.51095 16.26203 13.65251
Ru 14.26314 16.02365 17.85098
Ru 14.31961 17.65961 11.53417
Ru 14.09736 17.56878 15.79604
Ru 13.85193 9.22209 13.47825
Ru 12.68089 8.41884 15.41285
Ru 15.00784 11.59259 9.36043
Ru 13.72297 10.73080 11.30078
Ru 13.53695 10.64925 15.61508
Ru 14.66656 11.50744 17.71959
Ru 16.10681 14.15102 9.55790
Ru 16.18929 13.86080 13.69824
Ru 15.74153 14.02506 17.83923
Ru 16.07931 15.51009 11.70699
Ru 15.94141 15.44121 15.75377
Ru 16.27798 9.35346 13.35833
Ru 16.34362 10.93797 11.45474
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Ru 16.13489 10.68354 15.67972
Ru 17.43663 13.13350 11.58751
Ru 17.25267 13.05089 15.81925
C 15.99661 6.72775 17.81743
C 15.30005 7.73991 16.93402
C 19.16262 17.84400 13.85895
C 17.91132 17.00182 13.81216
C 14.03912 9.30118 5.78478
C 13.92302 10.07038 7.06913
C 8.63209 20.52513 16.48118
C 9.50206 19.53845 15.75385
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O 15.00115 10.40452 7.62663
O 17.47039 16.72029 12.64119
O 17.39098 16.66837 14.93418
O 15.96187 8.80506 16.68304
O 14.11158 7.43087 16.54676
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H 19.90035 17.45118 13.14767
H 13.27836 11.98624 18.87966
H 14.90940 8.75755 5.74903
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H 13.19155 8.61616 5.67024
H 17.89359 13.80697 10.00197
H 9.15103 20.92365 17.35921
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H 7.82157 11.47929 13.46822

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Ru 15.34918 11.56625 13.68103
Ru 13.81258 15.32971 15.84624
Ru 13.83677 15.27497 11.45853
Ru 12.51207 12.97613 15.78604
Ru 13.94193 13.83000 13.69452
Ru 12.55850 12.96664 11.53953
Ru 12.66117 11.40982 13.68075
Ru 12.46706 16.00624 13.56908
Ru 11.21111 13.69451 13.61431
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Ru 9.75862 15.84148 13.68568
Ru 9.56608 11.28988 13.68848
Ru 10.90298 18.10285 13.47257
Ru 11.16825 13.55472 9.46555
Ru 9.93362 12.77389 11.65399
Ru 9.09470 12.98346 15.69129
Ru 11.22431 13.57737 17.81669
Ru 12.50747 15.91515 9.44983
Ru 11.06465 15.17198 11.49760
Ru 11.12583 15.20893 15.69920
Ru 12.33431 15.87890 17.80439
Ru 12.34244 17.50858 11.52494
Ru 13.65573 18.39452 13.62413
Ru 12.22810 17.52996 15.73555
Ru 11.42158 9.14012 13.69511
Ru 12.55250 11.30075 9.58524
Ru 11.23861 10.63332 11.74825
Ru 11.12754 10.69626 15.56746
Ru 12.46506 11.21525 17.71372
Ru 13.83828 13.66434 9.41154
Ru 13.84174 13.72700 17.98034
Ru 15.15863 15.88350 9.42630
Ru 15.13068 16.30623 13.74736
Ru 14.91639 16.05267 17.97681
Ru 14.92242 17.56189 11.44643
Ru 14.69870 17.66785 15.98605
Ru 14.07055 9.20705 13.76105
Ru 12.71469 8.91654 16.23288
Ru 15.12478 11.43521 9.40166
Ru 13.97675 10.66410 11.58698
Ru 14.10691 10.72410 15.76048
Ru 15.18936 11.52909 17.87335
Ru 16.45847 13.70428 9.40019
Ru 16.62642 13.90112 13.73633
Ru 16.45577 13.87425 17.92886
Ru 16.37543 15.35633 11.62533
Ru 16.42054 15.50310 15.89509
Ru 16.61330 9.33542 13.85179
Ru 16.62503 10.85329 11.56692
Ru 17.97566 11.58254 13.66747
Ru 16.62590 10.90403 15.78039
Ru 17.82302 13.14960 11.69189
Ru 17.83678 13.18323 15.77962
C 5.29991 10.94068 14.33692
C 6.65817 11.55342 14.10925
C 14.15955 12.09978 22.07642
C 14.34765 12.30885 20.59719
C 20.71004 14.76857 8.87751
C 19.40568 14.31401 9.47363
C 7.63516 16.01708 8.81593
C 8.92413 15.46693 9.36309
C 10.06149 21.25638 16.38467
C 10.57708 20.00445 15.72950
C 19.13144 18.35529 13.96017
C 17.92454 17.51194 14.27460
C 15.90023 5.79105 15.95319
C 14.97804 6.90670 15.54667
C 13.64827 9.41554 5.80505
C 13.68861 10.09440 7.14727
O 6.76056 12.82692 14.09129
O 7.63532 10.72748 13.92185
O 13.97718 13.42488 20.00041
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O 18.35644 14.35600 8.75916
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O 15.32897 7.61565 14.50295
O 14.83713 10.30293 7.67127
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H 21.54563 14.20685 9.30958
H 20.85642 15.83252 9.11859
H 20.68967 14.66183 7.78797
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Ru 12.41900 12.99800 15.80620
Ru 13.85530 13.84700 13.69710
Ru 12.53350 12.94720 11.56710
Ru 12.55760 11.39900 13.65910
Ru 12.43350 16.11800 13.65730
Ru 11.13130 13.68500 13.61620
Ru 8.51470 13.78050 13.58630
Ru 9.67930 15.86750 13.73890
Ru 9.69700 11.30600 13.66790
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Ru 11.09100 13.49050 9.50530
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Ru 9.81150 13.00950 15.69910
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Ru 12.47550 15.93720 9.39610
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Ru 12.39150 15.96280 17.82900
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Ru 11.29800 9.18900 13.78990
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Ru 11.09150 10.71300 15.65410
Ru 12.43730 11.24930 17.75830
Ru 13.74400 13.67700 9.42290
Ru 13.78630 13.70980 17.95850
Ru 15.01830 15.87200 9.39300
Ru 15.09180 16.34750 13.76130
Ru 14.92750 16.04600 17.97040
Ru 14.88850 17.60830 11.56790
Ru 14.67430 17.66200 16.02850
Ru 13.96280 9.15730 13.86790
Ru 12.64080 8.84050 16.18710
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Ru 16.40730 13.82850 17.90280
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Ru 16.64330 10.96680 11.50400
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C 5.37800 10.81230 14.21940
C 6.71330 11.48330 14.03840
C 14.08750 12.05970 22.04670
C 14.24830 12.27100 20.56470
C 20.60750 14.58230 8.57090
C 19.32650 14.14330 9.22400

C 7.65100 16.09220 8.81430
C 8.93180 15.51920 9.35770
C 10.05050 21.29300 16.46790
C 10.53880 20.02500 15.82310
C 19.16470 18.34330 14.09430
C 17.94230 17.51500 14.39460
C 15.99480 5.83000 16.02540
C 15.03880 6.94730 15.66940
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C 13.68550 9.93320 7.22640
C 6.74830 12.76250 14.07460
O 7.72980 10.72050 13.83670
O 13.90730 13.40300 20.08270
O 14.70180 11.28680 19.87130
O 18.24330 14.23750 8.56470
O 19.39030 13.71900 10.43900
O 9.43250 16.07000 10.40030
O 9.44220 14.50950 8.75860
O 11.23600 19.22500 16.54740
O 10.25880 19.82130 14.59380
O 16.92330 17.64950 13.64400
O 17.99180 16.72400 15.40600
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O 15.23930 7.55780 14.53400
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H 19.09100 12.46480 14.68510
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H 14.29400 12.99150 22.58620
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H 7.70470 17.18780 8.79760
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H 10.89170 21.99930 16.53630
H 9.70650 21.09000 17.48890
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H 18.90770 19.40950 14.16220
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Ru 13.71400 15.31600 11.40280
Ru 12.39250 12.97150 15.78300
Ru 13.84980 13.82700 13.65550
Ru 12.51250 12.93200 11.52010
Ru 12.54100 11.36180 13.57070
Ru 12.47080 16.10930 13.62040
Ru 11.12880 13.64050 13.56470
Ru 8.54380 13.76730 13.53740
Ru 9.70630 15.86130 13.67130
Ru 9.74530 11.30500 13.57690
Ru 10.89750 18.11000 13.54520
Ru 11.08580 13.49180 9.45200
Ru 9.82680 12.86880 11.50110
Ru 9.79620 12.92800 15.67100
Ru 11.14280 13.63520 17.82820
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Ru 11.05080 15.20300 11.50920
Ru 11.06130 15.22600 15.64110
Ru 12.39170 15.91100 17.84350

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Ru 13.63400 18.39300 13.61260
Ru 12.29230 17.56080 15.76220
Ru 11.30430 9.15030 13.70850
Ru 12.50950 11.40930 9.40910
Ru 11.20330 10.69730 11.55050
Ru 11.13600 10.65750 15.60520
Ru 12.42150 11.27750 17.74400
Ru 13.76280 13.63550 9.38390
Ru 13.76300 13.66000 17.95140
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Ru 15.10700 16.28930 13.72280
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Ru 14.68700 17.63580 15.98950
Ru 13.93430 9.13000 13.82650
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Ru 16.40980 15.41450 15.81030
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Ru 16.59630 10.85200 11.48760
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C 20.61430 14.47230 8.47650
C 19.35030 14.02350 9.15640
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D 9.48330 14.56450 8.68580
D 11.21650 19.11050 16.58900
D 10.26200 19.75850 14.64110
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D 17.96720 16.71420 15.39300
D 14.15650 7.16730 16.43430
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H 12.52780 7.92830 14.51270
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H 16.79180 15.57650 17.66310
H 19.02350 12.47030 14.69990
H 17.99650 9.77200 14.57530
H 5.94700 9.76820 14.53040
H 4.88950 10.79620 13.23480
H 4.81100 11.37050 14.91330
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H 13.02130 11.74180 22.24510
H 14.26550 12.96550 22.56850
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H 20.56500 14.26330 7.40220
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H 9.62880 20.88950 17.58120

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H 14.08050 8.08030 6.14430
H 14.26280 9.53600 5.15660
H 17.78850 14.78850 12.52320
H 14.88130 9.16780 12.27360
H 13.79100 16.75150 8.36710
H 10.59730 15.39580 17.47100
H 11.85430 17.56550 9.77910
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Ru 12.49180 11.41380 13.48460
Ru 12.76200 16.12650 13.55820
Ru 11.22680 13.77550 13.48020
Ru 8.54100 13.68480 13.29690
Ru 9.71250 15.94500 13.65210
Ru 9.81800 11.40030 13.48590
Ru 11.20550 18.08800 13.25950
Ru 11.27300 13.66000 9.18710
Ru 9.99000 12.91280 11.42180
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Ru 12.92970 16.02750 9.17460
Ru 11.20880 15.47180 11.48710
Ru 11.17130 15.40620 15.54510
Ru 12.59230 16.05400 17.71690
Ru 12.85680 17.56300 11.31360
Ru 13.05680 18.48770 13.47370
Ru 12.42680 17.78930 15.61720
Ru 11.19950 9.15700 13.59330
Ru 12.58350 11.41250 9.27520
Ru 11.20500 10.70250 11.41740
Ru 11.09230 10.67580 15.62050
Ru 12.46630 11.45050 17.71740
Ru 13.90580 13.60040 9.29580
Ru 13.87500 13.71150 17.92340
Ru 15.46700 15.75780 9.40780
Ru 15.38230 16.00730 13.56290
Ru 15.20130 15.98530 17.76590
Ru 15.35980 17.46300 11.45090
Ru 15.28300 17.55930 15.67720
Ru 13.83630 9.17250 13.56370
Ru 12.72650 8.51730 15.80540
Ru 15.15200 11.39370 9.23520
Ru 13.89230 10.66430 11.40360
Ru 13.78400 10.65430 15.63020
Ru 15.06000 11.41480 17.72860
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Ru 16.58750 13.66200 13.62170
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Ru 16.70230 15.27850 15.76540
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C 7.12920 18.27200 14.87980
C 8.42050 18.85950 14.39670
C 20.91750 13.28030 8.41750
C 19.63100 13.23830 9.20060
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C 9.08250 15.78470 9.28490
C 5.51500 10.52230 13.33640
C 6.81000 11.27350 13.31360
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D 18.44730 16.13330 14.95420

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Ru 8.04180 13.02620 13.15830
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H 11.77250 11.68470 18.65190
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H 5.91630 8.41950 13.36870
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H 17.62680 9.78200 11.44210

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./Thermo_CH3COOH_8-H_1.6.xyz

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Ru 15.34300 11.37600 13.19290
Ru 14.16580 15.18880 15.68940
Ru 13.80930 15.46050 11.35210
Ru 12.78300 12.84380 15.59060
Ru 14.05630 13.75400 13.41180
Ru 12.43950 13.12600 11.30920
Ru 12.59930 11.46350 13.34160
Ru 12.59780 16.13500 13.58110
Ru 11.31350 13.85450 13.57430
Ru 8.14150 13.86400 13.83490
Ru 9.95350 16.17200 13.88920
Ru 9.73780 11.22900 13.49610
Ru 11.40550 18.36750 13.94280
Ru 11.01500 14.01400 9.31140
Ru 9.86850 13.08300 11.55390
Ru 10.09470 12.85850 15.61720
Ru 11.63900 13.44050 17.77310
Ru 12.45700 16.29130 9.22318
Ru 11.06520 15.48830 11.48420
Ru 11.45150 15.22500 15.82700
Ru 12.98770 15.66400 17.90720
Ru 12.52950 17.81730 11.63420
Ru 14.01100 18.55020 13.72980
Ru 12.97780 17.48350 15.97130
Ru 11.25730 8.98900 13.24520
Ru 12.26030 11.77720 9.04640
Ru 11.17450 10.81050 11.30090
Ru 11.43820 10.54600 15.41620
Ru 12.76880 11.07150 17.58900
Ru 13.71700 14.02600 9.17700
Ru 14.30380 13.38800 17.00710
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Ru 15.29100 16.09150 13.45110

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Ru 12.70200 8.35500 15.54800
Ru 14.95750 11.72850 8.81350
Ru 13.86800 10.80120 11.00250
Ru 14.09730 10.53230 15.34420
Ru 15.64930 11.03380 17.56920
Ru 16.31280 13.91700 8.86440
Ru 16.70850 13.69530 13.20330
Ru 16.95080 13.46080 17.45770
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Ru 16.88650 15.17700 15.48560
Ru 16.50500 9.14780 12.96700
Ru 16.49680 10.70700 10.90100
Ru 18.23100 11.24850 12.93530
Ru 16.86000 10.50250 15.14290
Ru 17.87100 13.93000 10.87030
Ru 18.12300 12.80450 15.25290
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C 12.85100 8.18900 18.63000
C 19.89880 18.43950 15.93200
C 18.57550 17.72700 15.78950
C 13.36180 8.53000 6.25730
C 13.41850 9.68930 7.29390
C 7.68050 19.32000 16.03780
C 8.74930 18.59980 15.25860
C 20.54730 14.48080 7.69340
C 19.31430 14.07750 8.46530
C 7.48400 16.55070 8.98660
C 8.76560 15.90150 9.44090
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H 18.32030 11.28480 11.02840
H 19.74280 10.79500 12.72990

H 18.63800 13.23530 16.89690
H 18.19630 14.31600 14.32570
H 19.26900 12.20400 13.92870
H 18.28830 11.23200 16.00090
H 9.42430 11.19200 11.66230
H 9.63630 11.11000 15.36780
H 10.94250 12.75500 17.40310
H 11.10750 16.99000 8.77210
H 12.21620 14.92350 8.17910
H 12.79250 14.13150 18.96210
H 13.92170 18.93430 11.06200
H 11.08300 12.59720 8.87740
H 12.48430 9.96330 10.34510
H 10.89700 8.77780 14.99890
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H 15.33530 18.99100 14.81920
H 15.84380 14.25450 18.74110
H 16.89730 17.29230 11.37730
H 12.54930 8.19130 12.30670
H 14.30480 9.94400 17.09530
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H 14.21780 11.73000 18.40310
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H 19.77000 19.52830 15.81530
H 20.61580 18.05070 15.19990
H 20.30100 18.23700 16.93560
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H 14.09630 8.67200 5.46490
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H 5.31150 9.92330 14.91520
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H 15.96000 10.70680 22.18320
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H 18.58880 10.27580 14.23500

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Ru 12.44580 13.00970 15.90940
Ru 13.92000 13.84080 13.81300
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Ru 12.60080 11.41730 13.78580
Ru 12.48030 16.10220 13.73810
Ru 11.19350 13.71580 13.71320
Ru 8.59130 13.66780 13.69160
Ru 9.80150 15.86800 13.70330
Ru 9.76120 11.22580 13.77220
Ru 11.01530 18.21950 13.70540
Ru 11.19900 13.49300 9.55160
Ru 9.96700 12.80550 11.71590
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Ru 12.53370 15.96600 9.47540
Ru 11.07700 15.17230 11.56870
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Ru 12.55950 9.59870 9.59870
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Ru 12.47780 11.46830 17.89630
Ru 13.82800 13.63830 9.55890
Ru 13.71200 13.76150 18.07650
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Ru 13.93000 10.71120 11.69090
Ru 13.85330 10.60800 15.90970
Ru 15.09400 11.56320 17.95690
Ru 16.41050 13.92280 9.52020
Ru 16.60180 13.87320 13.84320
Ru 16.31250 14.07050 18.04220
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Ru 16.53950 10.87350 15.97700
Ru 17.84600 13.16480 11.74130
Ru 17.69600 13.08500 16.04750
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C 14.53380 12.31280 22.21750
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C 19.26500 13.31530 9.06540
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C 9.02730 15.47430 9.34100
C 9.45700 20.77780 16.82540
C 10.18980 19.68450 16.09890
C 19.30600 18.14250 14.06960
C 18.04630 17.38020 14.30420
C 16.04850 5.60950 15.80750
C 15.05430 6.71170 15.35770
C 13.82400 9.35150 5.96750
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O 9.87650 19.46250 14.86890
O 17.07200 17.45300 13.56550
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H 10.04620 21.70450 16.74890
H 9.35480 20.53200 17.88800
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H 19.07150 19.20830 13.94430
H 19.71350 17.78250 13.11470
H 16.76920 5.45330 15.01530
H 15.52800 4.77130 16.13140
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H 14.20130 8.32700 6.10190
H 14.50430 9.86200 5.27410
H 9.55160 14.93300 11.79200
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H 13.80650 16.69150 8.42090
H 10.59820 15.51450 17.72210
H 11.83600 17.57300 9.86050
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Ru 12.29287 16.46490 12.97655
Ru 10.81693 13.97438 13.02764

Ru 8.28822 14.09464 12.92350
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 Ru 14.69852 11.87409 17.27478
 Ru 16.14613 13.97150 8.86222
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 Ru 16.02675 14.19051 17.31887
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