

Supporting Information:

S1. Additional conformations studies

S2. Nuclear magnetic resonance

- ^1H NMR spectrum of **1**
- ^{13}C { ^1H }
- NMR spectrum of **1**
- COSY NMR spectrum of **1**
- VT ^1H NMR Spectra of **1**

S3. ESI mass spectrometry (Q-Tof)

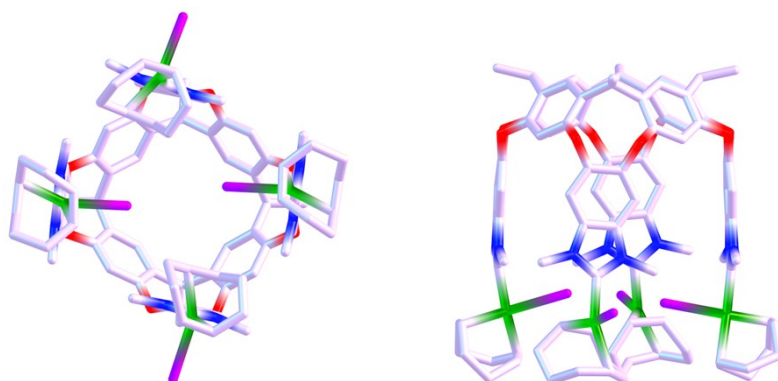
- HRMS of compound **1**

S4. Cartesian Coordinates of **1**

S1. Additional conformational studies

In addition of the conformations presented in the main text, additional conformation for the cavitant **1** were also optimized. They are shown in Figure S1. The difference between conformation in *vase_2* and *vase_5* is a subtle movement of the relative position of the metal complexes.

Vase_2 (1.3 kcal/mol)



Vase_5 (4.0 kcal/mol)

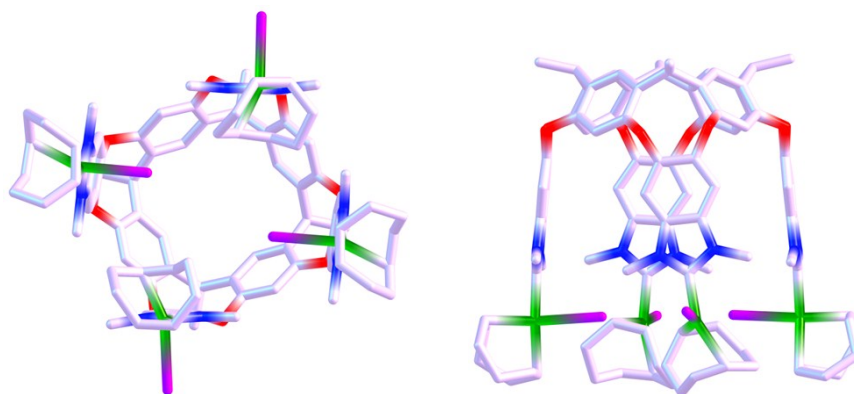


Figure S1. Top and side views of additional conformations optimized with rotation of the NHC-Rh bond. In parenthesis relative energies over *vase_1* conformation.

S2. Nuclear magnetic resonance Spectra of 1

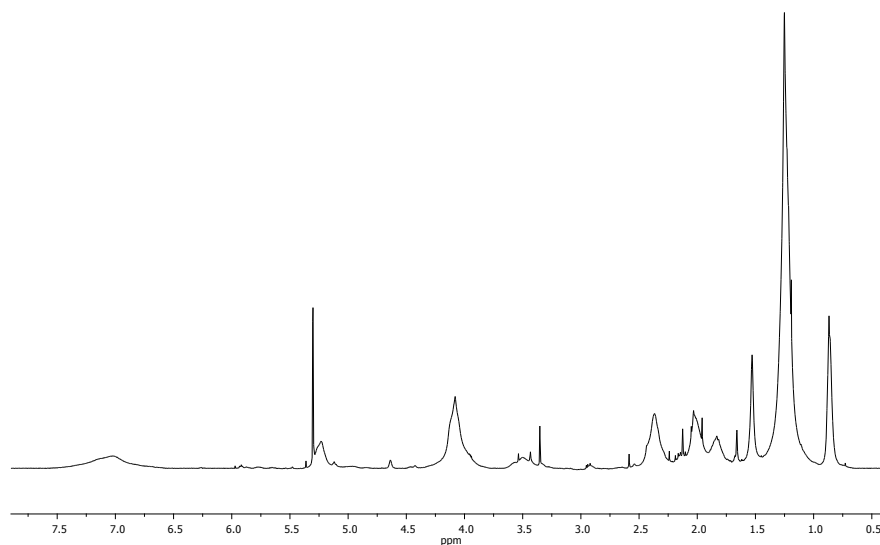


Figure S2. ^1H NMR (500 MHz, CD_2Cl_2): δ 7.5-6.7 ($\text{CH}_{\text{aromatic}}$), 5.96 (CH), 5.17 (CH_{COD}), 4.0 (CH_3), 3.5-3.35 (CH_2), 2.41 ($\text{CH}_{2,\text{COD}}$), 2.08 ($\text{CH}_{2,\text{COD}}$), 2.42-1.00 (CH_2), 0.88 (CH_3).

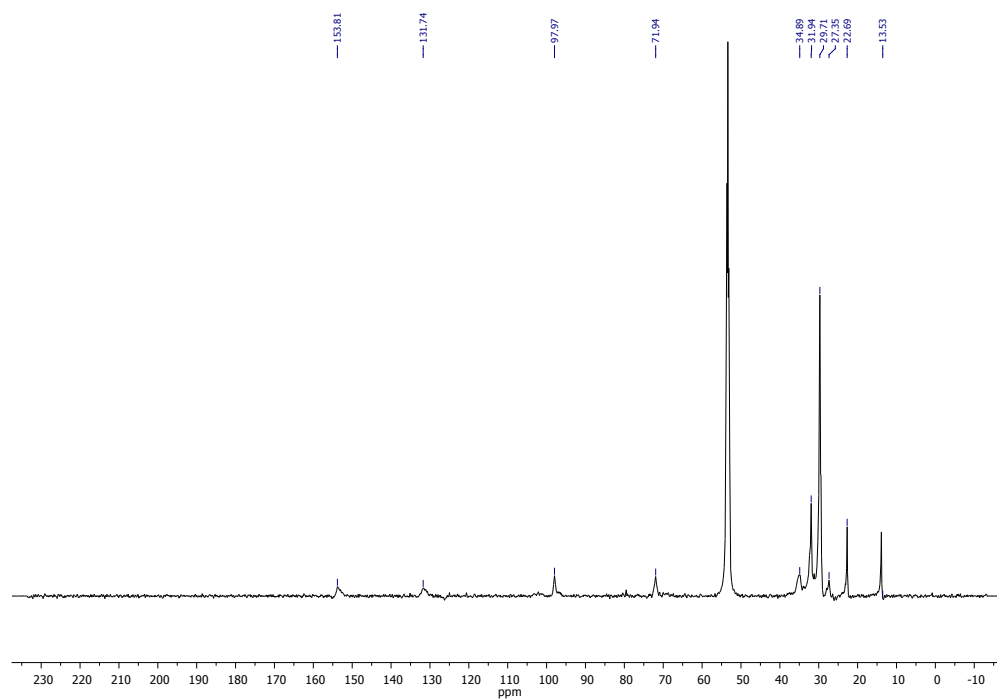


Figure S3. ^{13}C NMR (126 MHz, CD_2Cl_2) δ 153.8, 131.7, 98.0, 71.9, 34.9, 31.9, 29.7, 27.4, 22.7, 13.5.

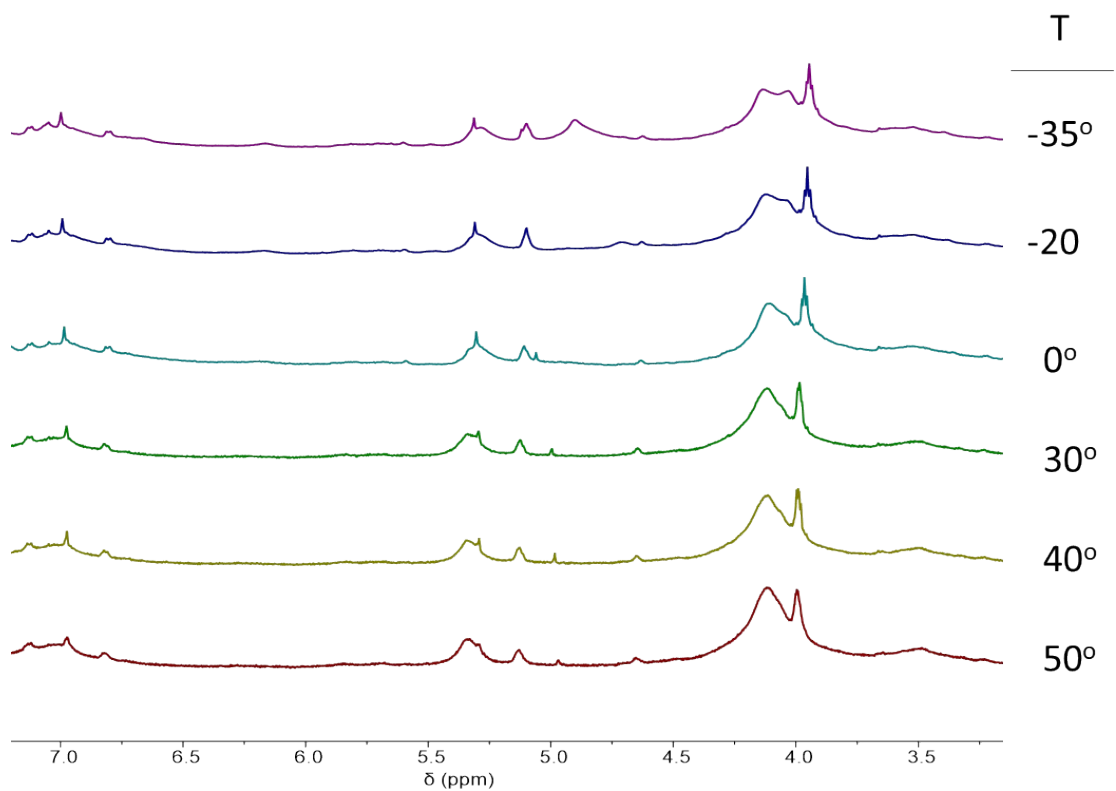


Figure S4. VT ^1H NMR spectrum of **1** (CD_2Cl_2)

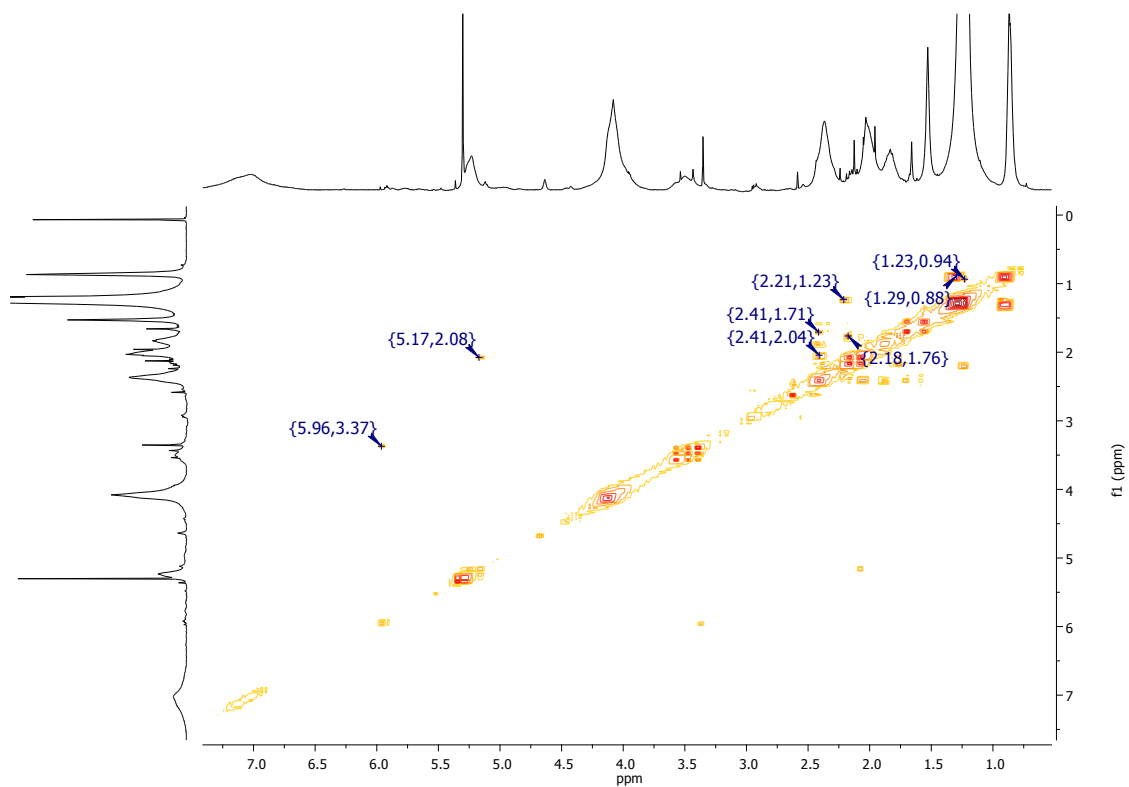


Figure S5. COSY NMR spectrum of **1** (CD_2Cl_2)

S3. ESI mass spectrometry

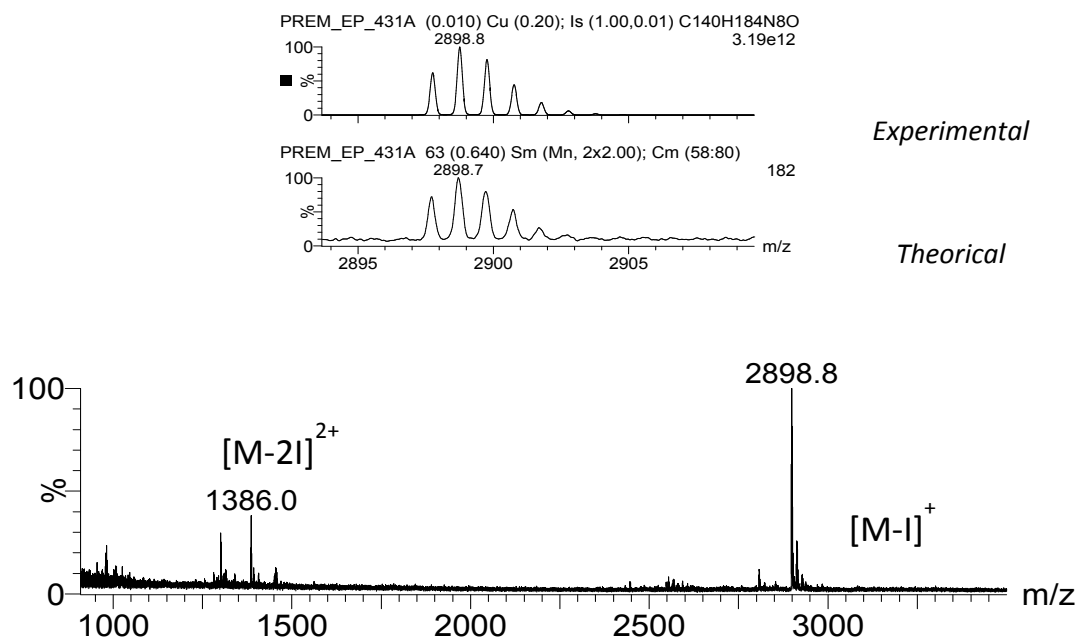


Figure S6. Time-Of-Flight Mass Spectrum (TOF-MS) of **1**

S4. Cartesian Coordinates of A1 and A2 (1 conformational forms)

Vase_1

E =	-1324,4269090621		
C	11.2119265301	13.1651665111	20.5412309861
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C	12.8019286906	10.8142324900	20.6499987501
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C	10.6478004833	15.5198652280	19.6445699250
C	10.2234955140	15.5358285103	18.3060494679
C	10.4890975669	16.5611782786	17.3814591228
C	10.1213041536	16.3022986004	15.9214940888
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H	18.7681433979	13.9734828591	19.7097156945
H	17.8200314071	13.3430551860	21.0767201670
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C	18.5323008502	10.4737525850	23.1441709723
H	18.1838927610	9.5032916818	23.5259755370
H	19.5965507358	10.6154072013	23.3804956265
H	17.9569158042	11.2882334920	23.6082886344

Vase_2

E =	-1324,4248870152		
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C	11.8873306276	14.5817421090	20.8907798614
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C	13.8252833982	15.3825844642	22.1328529506
C	13.2003837016	14.3997574885	21.3610544605
C	11.1900915321	18.2165948616	21.9504016933
C	11.7013201618	19.1590893591	20.8558469815
C	10.9728025788	19.2478525098	19.6588541536

C	11.3246264771	20.0469336053	18.5565416359
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C	11.0306452738	18.9195419208	16.3182678941
C	10.4372752478	17.6479503988	16.2705843616
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C	12.1038440479	19.1401949103	15.4347858015
C	12.4708215454	18.1659280821	14.5016606528
C	11.8259206733	16.9261328517	14.4705848833
C	12.8708804282	19.9368776258	20.9271050024
C	13.2316996348	20.7839752493	19.8777711701
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C	14.8732950270	19.3531929458	22.1445476500
C	14.9698999322	18.1090946298	22.8169718678
C	16.2097446127	17.5152876525	23.0840471280
C	16.0176537323	19.9938237095	21.6506507686
C	17.3420053818	18.1581864112	22.5852238441
C	17.2438822584	19.3605995387	21.8591684631
O	13.7982139978	17.5164183221	23.2685437687
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C	20.8401123950	9.0843008726	18.7803602404
H	19.8605220480	8.6401965986	18.9811158137
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H	20.1847087061	10.8610741894	19.7752410496
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C	22.8642430951	10.6309192851	17.0793316349
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C	12.7191837335	10.7440162299	20.2768851508
C	10.0841037728	14.2238166914	20.1508368737
C	10.5113149299	15.4176990787	19.2921594117
C	10.1093946699	15.4305824863	17.9470806260
C	10.3808192561	16.4578588013	17.0257966979
C	10.0229919626	16.1940131384	15.5636769361
C	11.1743772060	15.4371497780	14.8988782609
C	10.9967563625	14.0993021174	14.5310611296
C	11.9757623448	13.3122772565	13.9042927261
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C	11.2450304126	16.5364807203	19.7276519302
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C	13.3255134317	18.1633403783	15.5963610769
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C	14.8522653175	9.7941380477	20.0768059842
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C	15.3865141356	12.7821191306	13.2072609507
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C	12.5908794410	14.2997127026	21.5005737190
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H	17.6798009736	23.9681671822	13.3559863068
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C	15.8661098401	21.0842010339	21.8866498521
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H	16.9252416622	20.8952392605	21.6580336415
C	13.7368179187	17.7347059863	24.8480533273
H	13.6247037446	18.5111667110	25.6192765385
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H	14.4290994931	16.9615226897	25.2124933573
C	18.8296678787	11.4287211761	17.5203977147
H	18.7544151700	10.6728148962	18.3158445724
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2 arms up 2 down alternatively (b)

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C	12.7770550792	15.4661747193	18.9902227296
C	14.2511086866	17.0802680328	20.8230875132
C	14.5216491870	15.7222923301	20.6855804437
C	13.8250668048	14.9250457540	19.7685813102
C	13.0790221440	19.2139362924	19.9005663041
C	14.1543728969	19.7134039665	18.9289767402
C	13.8194478040	19.8117124540	17.5709759290
C	14.7126535769	20.0405802998	16.5052930983
C	14.0586431187	20.0856478222	15.1141428507
C	14.3798142613	18.9337685244	14.1445970427
C	13.2979309539	18.0575056297	13.9165729360
C	13.2986353610	16.9199122815	13.0991333401
C	15.5666421147	18.5980706459	13.4536116202
C	15.6060679020	17.4876028247	12.5983079678
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C	16.4435233594	20.1384658057	18.2330810991
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C	11.8348137974	14.7886846159	17.9801369965
C	12.4318570996	14.3527710717	16.6308605561
C	12.0768906121	15.9956220309	13.1534235930
C	12.3983468711	14.9120634121	14.1860654781
C	12.0127862837	15.1139757034	15.5195423764
C	13.3379499763	13.3113328053	16.3284508359
C	13.6932749824	13.0282229874	15.0032340982
C	13.2192305811	13.8012303101	13.9461817906
O	17.1500829182	20.2636930559	16.0104535961
O	16.8093462983	19.2252075622	13.5513814163
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C	17.0758237622	21.1468063821	14.9481129538
C	17.2171893825	22.5248592382	15.1477807244
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C	16.8529796487	21.4080975140	12.5209958446
O	15.9026418043	20.0189393841	20.5853067703
C	16.8061581193	19.1005248718	21.1038266972
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C	17.1157088395	17.0582530461	22.4322672829
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C	19.0053093432	18.4767627452	21.7901296534
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O	14.3577962456	13.6392837817	19.6866354522
C	13.5503547284	12.5223225448	19.5870175989
C	13.3889830303	11.9398378483	18.3152818801
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C	13.0084423976	11.9376448372	20.7371677343
C	12.3082215509	10.7441667520	20.5619329285
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O	13.4993047991	13.4324415805	12.6240225006
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C	14.8247033475	13.3771253828	12.2174346587
C	16.6860973533	14.5304032313	11.1089266513
C	17.3839378587	13.3208286699	11.1551675335
C	16.8037713169	12.1560591660	11.6966318684
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H	14.8491597814	21.9449895869	14.1351629518
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H	13.8076693800	19.9802649095	21.8355595720
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H	10.6157678144	14.9116881404	11.9609488926
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H	11.2067236056	15.6385246600	17.6712181474
C	10.7877558506	13.8181203029	18.5863673406
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C	18.7549955471	26.7018807183	10.7229994304
H	19.0401412399	25.6452446161	10.6700617638
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C	19.2687221504	28.8534807057	12.1043501159
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H	19.6897268599	27.5663805231	8.9697521256
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H	19.7796072202	29.2171547167	11.2003688656
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I	22.8697450239	15.6311513716	21.0568517660
C	22.5809798573	18.4884956540	24.8047947695
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H	17.3748424509	23.0804212438	9.9304666399
C	19.6159730616	13.8536495084	10.0991637291
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C	17.2716136710	25.6714421876	14.9355539070
H	18.1138213793	25.4397800206	15.6029298135
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1 arm up 3 arms down

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C	15.7159391082	14.4563250238	17.8680166359
C	15.2290701816	18.7961504093	18.1011413426
C	16.2496554074	19.4033614803	17.1244428823
C	15.7474427926	19.7110618604	15.8463582614
C	16.4746286780	20.0755722830	14.6958859168
C	15.6270140419	20.1990586404	13.4172207553
C	15.8096751670	19.0703586043	12.3852128153

C	14.7171699952	18.1845579708	12.2686090549
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C	16.8618083624	17.6784143331	10.6702535364
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C	17.6485452206	19.5332915554	17.2502405794
C	18.4205500709	19.9406273529	16.1607238412
C	17.8677495660	20.1879852188	14.9009030747
C	13.5284702208	14.5735890735	16.3085923478
C	13.9726566712	14.2025660131	14.8837925768
C	13.4302140813	16.1290628807	11.5732492930
C	13.8210723516	14.9713069778	12.4979953962
C	13.5341688995	15.0781510455	13.8679443115
C	14.7782559108	13.1320867814	14.4386293618
C	15.0380322673	12.9492928858	13.0749379350
C	14.5658838303	13.8445555260	12.1172767658
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N	17.6019870791	21.7727233825	22.4945170924
C	17.1254673363	21.3603866752	23.7189314060
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H	12.9450294527	15.9425716412	14.1825179520
H	15.6342296596	12.0886031731	12.7797811634
H	13.7642839397	17.0290642292	16.9850023884
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C	15.6474741357	16.8367273800	3.7660437909
H	16.6720574588	16.7573385467	3.3896254272
C	13.6852081144	15.9424615493	6.2205047760
H	13.5070533309	15.4669253307	7.1916477487
C	14.3017978554	17.2283195500	6.2527310137
H	14.5648984706	17.6099083627	7.2440269022
C	13.3196930723	15.7229010124	3.6959128311
C	12.7879587325	15.4157836613	5.1177546015
C	14.0996693485	18.3029867346	5.1870872581
C	15.1754754633	18.2427344302	4.0745241726
H	13.0926137326	18.2072002548	4.7551228924
H	14.1272483661	19.2953874203	5.6631283650
H	12.7149698181	14.3235788584	5.2442121345
H	11.7587684216	15.8041548372	5.2380849515
H	12.9437262295	16.6955707096	3.3480403138
H	12.9223548807	14.9755481387	2.9915705809
H	16.0554907407	18.8224528189	4.3951337615
H	14.8087539162	18.7350392408	3.1541962614
C	14.1601722192	7.6427596139	18.7525777167
H	14.8709363100	7.1381819162	18.0823206846
H	13.5210090913	6.9031072257	19.2556907773
H	13.5223272531	8.3286791405	18.1759484662
C	15.1794485983	13.0362246872	7.7412659788
H	14.9499499347	13.2635023238	6.6897504554
H	15.8154595791	12.1400929487	7.7828673657
H	14.2496559521	12.8606726260	8.3019137817
C	19.2212105259	22.2981717035	10.1761865370
H	18.2599119719	21.7682007090	10.2501276482
H	19.1458105778	23.0560753015	9.3831840695
H	20.0273628960	21.5865250651	9.9458650568

C	17.5896469612	17.3484702004	8.0569103651
H	18.6844293855	17.2394842150	8.0554335499
H	17.2526125553	17.5949280444	7.0389106175
H	17.2914992578	18.1439662039	8.7556690361
C	19.6958361830	25.9226039047	13.5108788802
H	20.5656052429	26.0453854349	14.1720082150
H	19.7290096678	26.6622996769	12.6973650499
H	18.7658010966	26.0637313272	14.0817068494
C	20.4439125257	22.8773993490	23.7328348396
H	19.7850853044	23.2281713139	22.9253238578
H	20.4325504037	23.5899624811	24.5701940063
H	21.4753806168	22.7830024686	23.3617942124
C	19.1582983984	19.2660136508	26.8631225546
H	19.1190189537	20.0066412716	27.6755096281
H	18.2010764366	18.7294022977	26.7935669785
H	19.9729943271	18.5551127299	27.0648977073
C	15.4560140347	9.4341481686	23.1795816023
H	14.9670008775	10.3960464474	23.3932087584
H	14.8833553437	8.6281745895	23.6617180079
H	16.4883488973	9.4446312654	23.5574538294