

Supplementary information for: **New Journal of Chemistry, RSC**

On the energetics of binding and hydrides exchange in the $\text{RuH}_2(\text{H}_2)_2[\text{P}(\text{C}_5\text{H}_9)_3]_2$ Complex as Revealed by Inelastic Neutron Scattering and DFT Studies

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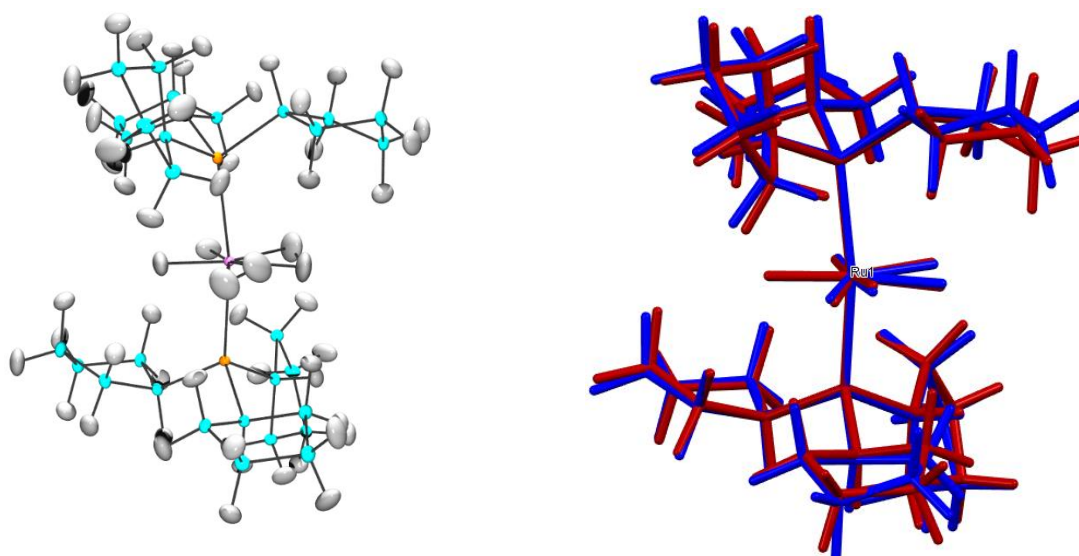


Figure S1. ORTEP drawing of the $\text{RuH}_2(\text{H}_2)_2[\text{P}(\text{C}_5\text{H}_9)_3]_2$ complex on the left, Colour codes: Ru orchid, C cyan, H Gray, and a comparison between the experimental neutron diffraction and the B3LYP/BS2 relaxed structures.

Atomic cartesian coordinates of computed final structures:

1. The fully optimized (b3lyp/BS2) $\text{RuH}_2(\text{H}_2)_2[\text{P}(\text{C}_5\text{H}_9)_3]_2$ complex, along with the used basis

P	-2.31259200	0.23031500	0.13437300
P	2.34199100	-0.30409800	-0.08405400
Ru	0.00311000	-0.22934900	0.16452800
C	-3.40456200	-0.45941500	1.50391300
C	-2.96434200	-0.04885200	2.94939200
C	-3.01971200	-1.34110200	3.80506400
C	-3.89682800	-2.31210100	2.99948200

C	-3.50281000	-2.00507300	1.54639100
C	-2.81449000	2.03971900	0.14490700
C	-2.32983800	2.88201900	1.34546500
C	-2.49584600	4.32672300	0.84822500
C	-1.99834100	4.26995800	-0.60916200
C	-2.31396100	2.82782200	-1.10371400
C	-3.17502900	-0.31797400	-1.44271000
C	-4.70481200	-0.11836000	-1.56357100
C	-5.07623400	-0.98787500	-2.77547700
C	-4.24602200	-2.26713300	-2.56185500
C	-2.92777600	-1.79704200	-1.88534800
C	3.16075100	-1.97854400	-0.35036700
C	2.70956700	-2.77770300	-1.59470800
C	3.12492600	-4.21982500	-1.26433400
C	2.74247100	-4.37142300	0.21917500
C	2.95358500	-2.96351100	0.84448600
C	3.30712100	0.24825500	1.43503700
C	2.86414000	1.61013900	2.06939500
C	4.17063400	2.32651900	2.49936600
C	5.24143400	1.22332700	2.52744600
C	4.85205400	0.33209800	1.33666900
C	3.08144800	0.69612700	-1.48842900
C	2.52786000	0.32760200	-2.90659300
C	2.20329300	1.67260500	-3.60439800
C	2.99625900	2.72837200	-2.81870700
C	2.88408700	2.22839600	-1.37005600
H	-4.41329600	-0.06418400	1.33382200
H	-1.96206400	0.38703600	2.96859800
H	-3.64630000	0.71095300	3.34357900
H	-2.01240100	-1.76283800	3.90808100
H	-3.39627000	-1.15840600	4.81651600
H	-4.95969700	-2.08507300	3.15515200
H	-3.74232500	-3.36119300	3.27321800
H	-4.21380100	-2.40103300	0.81474500
H	-2.52458900	-2.45491000	1.33495500
H	-3.91276000	2.05673100	0.15121400
H	-2.89183200	2.68174700	2.26184700
H	-1.27195000	2.67295100	1.54263300
H	-3.55663000	4.60836300	0.87795400
H	-1.94999300	5.05462300	1.45783100
H	-0.91663000	4.44189700	-0.63675700

H	-2.45899000	5.03762900	-1.23901400
H	-1.41343000	2.36309300	-1.51484400
H	-3.07342300	2.82538100	-1.89225600
H	-2.70284600	0.32307900	-2.19628100
H	-5.22616000	-0.49430600	-0.67444600
H	-4.98588500	0.93226800	-1.68667400
H	-6.15121200	-1.18166700	-2.85517700
H	-4.76566000	-0.48312200	-3.69932800
H	-4.06780800	-2.81611300	-3.49179800
H	-4.78894400	-2.94629800	-1.89329400
H	-2.08090900	-1.83858000	-2.57598800
H	-2.67183400	-2.44721900	-1.04591600
H	4.23622500	-1.78599800	-0.45703000
H	3.15689100	-2.40614900	-2.52026700
H	1.62029000	-2.72373500	-1.71187400
H	2.64451500	-4.96368600	-1.90872400
H	4.20979200	-4.33082200	-1.39074900
H	1.68710800	-4.65814600	0.29757400
H	3.32136600	-5.14754500	0.72954600
H	3.82240900	-2.94481800	1.51027600
H	2.08387700	-2.68338300	1.44888300
H	3.07326300	-0.54041800	2.16077000
H	2.27633500	2.21996700	1.38203600
H	2.21824100	1.42067600	2.93252100
H	4.44736700	3.08143500	1.75306900
H	4.06861000	2.84886900	3.45588600
H	5.17050100	0.64868500	3.46027500
H	6.26368500	1.61058900	2.45902900
H	5.32929500	-0.65273000	1.36226100
H	5.16414100	0.82094900	0.40589800
H	4.15867400	0.48938500	-1.48188000
H	3.28574600	-0.23010800	-3.46641300
H	1.63509200	-0.29883300	-2.84565300
H	2.44262100	1.65937000	-4.67272000
H	1.13148500	1.88316200	-3.51171900
H	2.60899700	3.74441900	-2.95033600
H	4.04726800	2.73365100	-3.13769000
H	3.61000900	2.69477700	-0.69622600
H	1.88011000	2.44459000	-0.98854900
H	0.22709500	1.36494700	0.29652300
H	-0.07168700	0.16723000	-1.40212400

H	-0.19645500	-1.76574600	-0.65769200
H	-0.31783600	-1.98519300	0.15311200
H	0.17306900	-0.80117500	1.84920400
H	0.07752500	0.04056900	1.90047900

2. The transition state between the reactant (above) and the intermediate state along

Path A

P	-2.33557600	-0.20012600	-0.16379200
P	2.33196300	0.26426800	0.13572500
Ru	-0.03097500	0.27374400	0.03852300
C	-3.35593400	0.84830700	-1.34169900
C	-2.81967800	0.86698900	-2.81243500
C	-2.86629100	2.34791100	-3.27114400
C	-3.80652100	3.04496400	-2.27529900
C	-3.48329600	2.34100400	-0.94835100
C	-2.77677200	-1.93518200	-0.72675200
C	-2.20062000	-2.39060800	-2.08738700
C	-2.30939900	-3.92229700	-2.02148600
C	-1.86619400	-4.25030100	-0.58446700
C	-2.34077100	-3.04798100	0.27911700
C	-3.29628300	-0.15077500	1.44813600
C	-4.82782600	-0.35260900	1.40895200
C	-5.25786700	0.02398100	2.83593800
C	-4.40860800	1.27227500	3.15696800
C	-3.09332300	1.11236600	2.33768300
C	3.23722500	1.91253200	0.06849400
C	2.91502100	2.93503100	1.18077700
C	3.40940600	4.26616700	0.59276800
C	2.94934600	4.20211700	-0.87494600
C	3.00803000	2.69662200	-1.26218900
C	3.14842300	-0.57367000	-1.33507200
C	2.62881900	-2.00229000	-1.70642000
C	3.87658900	-2.80647500	-2.15999900
C	4.96629100	-1.75144600	-2.41730900
C	4.69309600	-0.69611600	-1.33406600
C	3.12009400	-0.53673200	1.63678500
C	2.65411100	0.06673200	3.00362900
C	2.38281800	-1.14074900	3.93913500
C	3.08131800	-2.33352900	3.26721000

C	2.86595000	-2.05849500	1.77142100
H	-4.36371500	0.41507400	-1.35114600
H	-1.80261800	0.47415900	-2.88007200
H	-3.45375500	0.23943400	-3.44649600
H	-1.86550000	2.78925600	-3.19465900
H	-3.18820700	2.45411200	-4.31200100
H	-4.85473200	2.86545800	-2.54862800
H	-3.66035200	4.12937100	-2.23054800
H	-4.24010200	2.50977900	-0.17582800
H	-2.52528500	2.71494700	-0.56710200
H	-3.87150700	-1.95380900	-0.80975900
H	-2.73606700	-1.96231600	-2.93906900
H	-1.14885100	-2.09485700	-2.16824700
H	-3.35236300	-4.22811100	-2.17762000
H	-1.70480800	-4.42739200	-2.78221300
H	-0.77323700	-4.32278000	-0.54663600
H	-2.26275600	-5.20557000	-0.22611900
H	-1.53001700	-2.70166200	0.92611900
H	-3.17914000	-3.32366100	0.92724800
H	-2.87029400	-0.99821900	1.99853100
H	-5.29724600	0.33306600	0.69259600
H	-5.11855000	-1.36998100	1.12892900
H	-6.33407500	0.20359000	2.92925000
H	-5.00432600	-0.79463000	3.52127000
H	-4.22041500	1.38161100	4.22938100
H	-4.94248600	2.17465900	2.83760000
H	-2.21771200	0.98319000	2.97838400
H	-2.91115600	2.00811600	1.73819400
H	4.30487400	1.67125600	0.14962400
H	3.38512700	2.68722400	2.13611400
H	1.83232600	2.99144900	1.35021400
H	3.02154900	5.14040700	1.12617700
H	4.50489100	4.31002600	0.64814800
H	1.91797200	4.56458400	-0.95292300
H	3.55741600	4.82797200	-1.53557400
H	3.81776900	2.49235600	-1.96987900
H	2.07344000	2.39239900	-1.74278900
H	2.87720800	0.09358100	-2.16160000
H	2.12177500	-2.49171200	-0.87393500
H	1.88860600	-1.92540900	-2.50751600
H	4.20333400	-3.47746400	-1.35601700

H	3.67632200	-3.43397100	-3.03416700
H	4.83469600	-1.30360000	-3.41092600
H	5.98178600	-2.15946400	-2.37496700
H	5.19277100	0.25749400	-1.53046800
H	5.06072100	-1.06608100	-0.36913000
H	4.20199200	-0.37970100	1.54448400
H	3.43566300	0.71529700	3.41203400
H	1.74982400	0.67062800	2.89340300
H	2.72635500	-0.96269900	4.96322200
H	1.30458000	-1.33194200	3.98401900
H	2.67946700	-3.30147400	3.58503000
H	4.15453800	-2.33090500	3.50015600
H	3.51977900	-2.65355600	1.12592000
H	1.82731200	-2.28380900	1.50563900
H	0.16823800	-1.28770600	-0.23651600
H	-0.11283200	-0.44909300	1.53326100
H	0.15806700	1.73560600	1.00471500
H	-0.68325600	1.67357400	0.88926100
H	-0.01790600	1.36300600	-1.19477800
H	0.11906600	0.02555500	-1.53355900

3. The trihydrogen transition state atomic coordinates along path C

P	-2.34138700	0.20683000	0.09450700
P	2.34181200	-0.29856400	-0.12942300
Ru	-0.00784100	-0.17495100	0.07435500
C	-3.26788900	-0.11434300	1.69766100
C	-2.69568300	0.65899700	2.93334900
C	-2.64242200	-0.36593200	4.09684300
C	-3.56579700	-1.51371000	3.65973000
C	-3.31630700	-1.59607000	2.14593700
C	-2.91299100	1.94379900	-0.32545300
C	-2.36937300	3.08526600	0.56442400
C	-2.58101500	4.33948400	-0.29803000
C	-2.16329800	3.87842600	-1.70571500
C	-2.56845800	2.38007100	-1.78562900
C	-3.31062700	-0.75271100	-1.19709100
C	-4.85251200	-0.61049300	-1.21972100
C	-5.30081000	-1.78920300	-2.09840600
C	-4.40705900	-2.94685500	-1.61775100

C	-3.04506900	-2.29269300	-1.25679300
C	3.06652800	-1.84601300	-0.91472800
C	2.54692800	-2.20502400	-2.32451800
C	2.93150000	-3.68524800	-2.47616700
C	2.59863200	-4.28851300	-1.09855900
C	2.83311700	-3.14024100	-0.07484400
C	3.28763400	-0.31355500	1.49545300
C	2.90281700	0.79847300	2.52616500
C	4.22269500	1.18670600	3.24736200
C	5.22744700	0.07786900	2.88620100
C	4.83544000	-0.29508100	1.44763000
C	3.16926700	1.05285200	-1.13099600
C	2.63186200	1.19443000	-2.59509300
C	2.45985000	2.71577300	-2.84491400
C	3.28133500	3.39913000	-1.73994600
C	3.06554100	2.47685600	-0.53009500
H	-4.30017100	0.21850100	1.53391000
H	-1.70396800	1.07126600	2.73216500
H	-3.35141400	1.49930100	3.18192200
H	-1.61960400	-0.74619000	4.20846000
H	-2.92877400	0.07430600	5.05715600
H	-4.61517100	-1.25411300	3.85181300
H	-3.36078500	-2.45558200	4.17962100
H	-4.07810300	-2.17311400	1.61298100
H	-2.34928800	-2.08180900	1.96714600
H	-4.00561100	1.93158900	-0.21882500
H	-2.87563600	3.14410700	1.53199300
H	-1.30071300	2.93664600	0.75405100
H	-3.64162400	4.62394200	-0.28960100
H	-2.00954700	5.20386600	0.05640000
H	-1.07644100	3.97215800	-1.81272600
H	-2.61679200	4.47789900	-2.50142500
H	-1.74726600	1.78571100	-2.19563900
H	-3.43384200	2.23193600	-2.43986600
H	-2.93185400	-0.32606500	-2.13336800
H	-5.27715000	-0.72685800	-0.21481200
H	-5.18190100	0.36046200	-1.60283600
H	-6.37077400	-2.00780400	-2.01506100
H	-5.09451700	-1.56234900	-3.15241900
H	-4.30567300	-3.74245900	-2.36256000
H	-4.85247100	-3.40404100	-0.72560200

H	-2.28139900	-2.50460100	-2.00957000
H	-2.65864600	-2.68706600	-0.31478700
H	4.14880600	-1.67640700	-0.99129500
H	2.97378200	-1.57268100	-3.10748100
H	1.45753000	-2.09163900	-2.36088600
H	2.40579100	-4.18269700	-3.29794000
H	4.00721100	-3.77056100	-2.67849700
H	1.54698800	-4.59628800	-1.07619100
H	3.19519300	-5.17775000	-0.87174100
H	3.69367800	-3.34027600	0.57126000
H	1.96164600	-3.03843400	0.58014300
H	2.99186600	-1.27560700	1.93210000
H	2.44170200	1.66528500	2.05015200
H	2.15908100	0.41158700	3.22810700
H	4.58958600	2.14760000	2.86627900
H	4.09148500	1.30506600	4.32750800
H	5.08782900	-0.79055900	3.54309400
H	6.27169800	0.39424600	2.98088300
H	5.26048400	-1.24887500	1.11936700
H	5.20073200	0.47901700	0.76176700
H	4.23218800	0.78706200	-1.18444100
H	3.35070300	0.76103900	-3.29776000
H	1.68411600	0.66967200	-2.73201500
H	2.76643600	3.01197300	-3.85325600
H	1.40418800	2.99064900	-2.73389200
H	2.97171200	4.43231700	-1.54994600
H	4.34512500	3.42025900	-2.01182000
H	3.78848600	2.64693300	0.27400800
H	2.06235000	2.64007000	-0.12092200
H	0.08045200	1.12116100	-0.86713100
H	-0.13949800	-0.56342200	-1.49667300
H	-0.22738500	-1.86915200	0.05532500
H	-0.10010000	-1.56448100	1.07954800
H	0.03997500	-0.69069300	1.70352600
H	0.19622000	1.18510100	0.93456800

4. Optimized (mPW1/PW91/BS2) RuH₂(H₂)₂[P(C₅H₉)₃]₂ complex coordinates

P	-2.27196200	0.26136900	0.13303100
P	2.29038800	-0.35170500	-0.06881800

Ru	-0.00935000	-0.26607700	0.23933400
C	-3.40813600	-0.26468700	1.51721000
C	-2.97149400	0.23638800	2.92400900
C	-3.04380500	-0.98785300	3.85755400
C	-3.96139500	-1.97338400	3.13501800
C	-3.56001100	-1.79030000	1.67176400
C	-2.68304800	2.07047400	-0.02299600
C	-2.21769000	2.97011700	1.13355800
C	-2.18242700	4.36332500	0.50413900
C	-1.55798400	4.10719700	-0.86910000
C	-2.07355700	2.71601000	-1.29711000
C	-3.11850100	-0.37279400	-1.40135700
C	-4.63397900	-0.16014000	-1.55148500
C	-4.98790700	-1.07232800	-2.72637200
C	-4.18938700	-2.34733600	-2.43265400
C	-2.89228500	-1.87072000	-1.73791800
C	3.07539900	-2.01766700	-0.36911100
C	2.59455400	-2.77766000	-1.61569100
C	2.96487500	-4.22862400	-1.30934600
C	2.57556200	-4.38647200	0.16291600
C	2.85024600	-3.00760300	0.80533800
C	3.28219200	0.17391300	1.42313200
C	2.84295800	1.51101800	2.08749200
C	4.14615300	2.23049000	2.48968800
C	5.21897300	1.14028000	2.47983400
C	4.81352200	0.27436300	1.28583600
C	2.99943800	0.65027400	-1.46739200
C	2.40611100	0.31048700	-2.86574800
C	2.04893300	1.66105900	-3.51425000
C	2.88334400	2.69143800	-2.75439500
C	2.82117000	2.17291700	-1.31808300
H	-4.39514200	0.15677000	1.29358500
H	-1.96580500	0.66499500	2.91754000
H	-3.64769700	1.02578800	3.26297500
H	-2.04868200	-1.43355300	3.96275700
H	-3.38998800	-0.73030300	4.86194600
H	-5.01128700	-1.68926400	3.27414500
H	-3.85021200	-3.00355000	3.48474000
H	-4.27930300	-2.21571300	0.96691500
H	-2.59559300	-2.28408200	1.50100700
H	-3.77690300	2.13567100	-0.08130800

H	-2.87174300	2.91143200	2.00657400
H	-1.20779700	2.67815000	1.44288700
H	-3.20360300	4.74762500	0.39300100
H	-1.62352200	5.08933500	1.10144900
H	-0.46816100	4.07867400	-0.77012500
H	-1.79518600	4.88660600	-1.59806800
H	-1.25072700	2.10896100	-1.68434600
H	-2.82902000	2.79003300	-2.08472200
H	-2.62857900	0.20978000	-2.19050300
H	-5.17094800	-0.49642700	-0.65692500
H	-4.90212800	0.88595200	-1.72219600
H	-6.06188700	-1.25178600	-2.82829600
H	-4.64216200	-0.61524700	-3.66077300
H	-3.99208700	-2.93760100	-3.33113300
H	-4.76401300	-2.98761700	-1.75483500
H	-2.01802700	-1.97600900	-2.38389800
H	-2.68693400	-2.46854700	-0.84804600
H	4.15277400	-1.84248300	-0.48105900
H	3.04568700	-2.40531600	-2.53768000
H	1.50697500	-2.68557300	-1.72112600
H	2.46574400	-4.94792000	-1.96467500
H	4.04532200	-4.36774900	-1.43353500
H	1.50842700	-4.62133300	0.23387300
H	3.11367100	-5.19678000	0.66145500
H	3.72771400	-3.03348100	1.45739500
H	2.00040500	-2.70145100	1.42417300
H	3.07263300	-0.63177500	2.13740000
H	2.22616700	2.12103000	1.42674900
H	2.22440900	1.30039100	2.96373500
H	4.39931300	2.99332500	1.74506000
H	4.06400300	2.74253400	3.45195300
H	5.16599900	0.54805300	3.40114800
H	6.23638700	1.53391500	2.40153900
H	5.30112600	-0.70425900	1.27681600
H	5.09424000	0.78822000	0.35957900
H	4.07299700	0.42800200	-1.48874900
H	3.14984600	-0.22399800	-3.46361800
H	1.52312300	-0.32764600	-2.78958500
H	2.22667800	1.66919100	-4.59303300
H	0.98624100	1.87172500	-3.35558100
H	2.50532000	3.71269000	-2.85611900

H	3.91914000	2.68605600	-3.11536500
H	3.57088900	2.62194200	-0.66056100
H	1.83142900	2.38546800	-0.89958900
H	0.25253600	1.32519200	0.29028400
H	-0.09956200	0.02708500	-1.34480400
H	-0.16590700	-1.83687500	-0.43815200
H	-0.48008500	-1.93547500	0.37777300
H	0.38352000	-0.69582200	1.88105700
H	-0.06594700	0.05238900	1.93810300

5. Optimized (mPW1/PW91/BS4) $\text{RuH}_2(\text{H}_2)_2[\text{P}(\text{C}_5\text{H}_9)_3]_2$ complex coordinates

P	-2.27022000	0.26521600	0.13276800
P	2.28903200	-0.35698700	-0.06468400
Ru	-0.00960400	-0.26686600	0.24357600
C	-3.41415900	-0.25828200	1.51079200
C	-2.98186100	0.23848700	2.91825000
C	-3.06187600	-0.98531500	3.84909200
C	-3.97769400	-1.96677900	3.12174600
C	-3.57261700	-1.78164900	1.66137500
C	-2.67566900	2.07509500	-0.02140100
C	-2.21114500	2.97004500	1.13696700
C	-2.15565400	4.36166600	0.50892600
C	-1.52833500	4.09948900	-0.86023900
C	-2.06029800	2.71783100	-1.29197000
C	-3.11562100	-0.36196100	-1.40501500
C	-4.62797000	-0.14253400	-1.55677200
C	-4.98590300	-1.05445400	-2.72880200
C	-4.19233100	-2.33079300	-2.43455900
C	-2.89442100	-1.85854200	-1.74205000
C	3.07115100	-2.02351400	-0.36515100
C	2.59035700	-2.78027700	-1.61168900
C	2.94258500	-4.23344600	-1.30218600
C	2.54854900	-4.38456300	0.16793700
C	2.84201600	-3.01089600	0.80848100
C	3.28531800	0.16636000	1.42511800
C	2.85288700	1.50571100	2.08546800
C	4.15799100	2.22941500	2.46548100
C	5.22797200	1.13859000	2.46323700
C	4.81506600	0.25904400	1.28352300

C	3.00000700	0.64220300	-1.46377600
C	2.40569600	0.30277700	-2.85976300
C	2.04979400	1.65163200	-3.50865600
C	2.88352800	2.68130800	-2.74987200
C	2.82560900	2.16333300	-1.31477600
H	-4.39495200	0.16935600	1.27881100
H	-1.97610900	0.66297100	2.91551300
H	-3.65567400	1.02883400	3.25573100
H	-2.06967800	-1.43305400	3.95943200
H	-3.41304100	-0.72730800	4.85028500
H	-5.02671800	-1.68195700	3.25831800
H	-3.86864000	-2.99678100	3.46891600
H	-4.29165300	-2.20180200	0.95530400
H	-2.61093100	-2.27818100	1.49160700
H	-3.76797900	2.13831700	-0.08256600
H	-2.87262400	2.91859000	2.00312100
H	-1.20815800	2.66818800	1.45450300
H	-3.17047500	4.75853300	0.39340800
H	-1.59071900	5.07888500	1.10898200
H	-0.44082800	4.05638900	-0.75649000
H	-1.75263700	4.88161300	-1.58861000
H	-1.24684700	2.10273300	-1.68195000
H	-2.81487400	2.80516900	-2.07735900
H	-2.62011400	0.22008300	-2.18902400
H	-5.16626600	-0.47444800	-0.66278500
H	-4.89016500	0.90313500	-1.73034200
H	-6.05947800	-1.23044300	-2.82828700
H	-4.64024300	-0.60027000	-3.66343200
H	-3.99694200	-2.92125200	-3.33179800
H	-4.76822500	-2.96798800	-1.75675800
H	-2.02304400	-1.96589600	-2.38900200
H	-2.68967900	-2.45594800	-0.85363500
H	4.14675600	-1.84526600	-0.47466600
H	3.05101600	-2.41466900	-2.53004100
H	1.50586500	-2.67647000	-1.72421900
H	2.43639300	-4.94671500	-1.95669600
H	4.02059700	-4.38551700	-1.42363200
H	1.47931000	-4.60379800	0.23727300
H	3.07443600	-5.20044900	0.66778600
H	3.72273800	-3.04835900	1.45345100
H	2.00131800	-2.69545200	1.43244900

H	3.07085000	-0.63686400	2.13829200
H	2.22589400	2.10844600	1.43022200
H	2.24915600	1.29954700	2.97137100
H	4.40578100	2.98008800	1.70845500
H	4.08330400	2.75448000	3.41990800
H	5.17935600	0.55880800	3.39152300
H	6.24431300	1.52926700	2.37361800
H	5.29791200	-0.72041700	1.28703500
H	5.09473500	0.75898700	0.35077700
H	4.07091000	0.41422100	-1.48109300
H	3.14706200	-0.23260100	-3.45750400
H	1.52350300	-0.33356700	-2.78147800
H	2.22961400	1.65810500	-4.58587200
H	0.98820200	1.86252400	-3.35252600
H	2.50407000	3.70090000	-2.85014100
H	3.91775900	2.67752300	-3.11246900
H	3.57787000	2.61071400	-0.66146900
H	1.83911800	2.37726000	-0.89283500
H	0.25420900	1.32480900	0.28771700
H	-0.10105100	0.01375000	-1.34316800
H	-0.16397800	-1.84460700	-0.42166700
H	-0.48655000	-1.93450300	0.39051400
H	0.38538700	-0.68725100	1.88796600
H	-0.06659200	0.05837100	1.94234300