

Supplementary Material to:

A.J. Muller, J. Conradie, W. Purcell, S.S. Basson and J.A. Venter, *S. Afr. J. Chem.*, 2010, **63**, 11–19.

Table S1 Kinetic results for the oxidative addition between CH₃I and [Ir(bpt)(cod)] in acetone.

Temperature/K	[CH ₃ I]/mol L ⁻¹	k _{obs} /10 ⁻⁴ s ⁻¹
288.9	0.0202	0.4223
	0.0370	0.6863
	0.0657	1.142
	0.0905	1.503
	0.1221	1.994
	0.1693	2.491
302.5	0.0196	0.961
	0.0338	1.633
	0.0717	3.055
	0.1224	4.64
	0.1582	5.96
311.3	0.0177	1.287
	0.0322	2.142
	0.0627	4.02
	0.0913	5.33
	0.1276	7.78

Table S2 Kinetic results for the oxidative addition between CH₃I and [Ir(bpt-NH)(cod)] in benzene.

Temperature/K	[CH ₃ I]/mol L ⁻¹	k _{obs} /10 ⁻⁴ s ⁻¹
287.9	0.0190	0.131
	0.0552	0.234
	0.0899	0.412
	0.1419	0.629
	0.2120	0.976
297.8	0.0206	0.228
	0.0364	0.372
	0.0583	0.608
	0.0917	0.912
	0.1390	1.16
	0.2100	2.0
310.6	0.0187	0.493
	0.0459	1.019
	0.0896	1.739
	0.1448	2.834
	0.1752	3.37

Table S3 Kinetic results for the oxidative addition between CH₃I and [Ir(bpt-NH)(cod)] in DMC.

Temperature/K	[CH ₃ I]/mol L ⁻¹	k _{obs} /10 ⁻⁴ s ⁻¹
288.7	0.0291	2.72
	0.0586	5.93
	0.0807	7.10
	0.1093	11.29
	0.1407	13.4
	0.1782	17.80
297.9	0.0320	6.18
	0.0554	9.61
	0.0710	10.5
	0.1429	20.9
	0.1760	27.3
304.1	0.0448	10.87
	0.0699	15.4
	0.0880	20.3
	0.1049	23.0
	0.1425	36.9
0.1778	42.2	

Table S4 Kinetic results for the oxidative addition between CH₃I and [Rh(bpt)(cod)] in acetone.

Temperature/K	[CH ₃ I]/mol L ⁻¹	k _{obs} /10 ⁻⁴ s ⁻¹
298.5?	0.0581	0.0845
	0.0782	0.1241
	0.0991	0.1332
	0.1208	0.1743
	0.1429	0.2035
	0.1606	0.2274
301.9	0.0621	0.1391
	0.0860	0.1963
	0.1197	0.263
	0.1432	0.3121
307.5	0.0599	0.2387
	0.0893	0.3282
	0.1166	0.4438
	0.1388	0.5470

Table S5 Kinetic results for the oxidative addition between CH₃I and [Rh(bpt)(cod)] in benzene.

Temperature/K	[CH ₃ I]/mol L ⁻¹	k _{obs} /10 ⁻⁴ s ⁻¹
288.9	0.0237	0.2762
	0.0380	0.5006
	0.0592	0.689
	0.0913	1.079
	0.1095	1.266
	0.1273	1.481
297.5	0.0299	0.753
	0.0530	1.223
	0.0764	1.751
	0.1102	2.394
307.7	0.0191	0.881
	0.0391	1.630
	0.0547	2.332
	0.0704	2.945
	0.1048	4.50
	0.1413	6.09

Table S6 Kinetic results for the oxidative addition between CH₃I and [Rh(bpt)(cod)] in DCM.

Temperature/K	[CH ₃ I]/mol L ⁻¹	k _{obs} /10 ⁻⁴ s ⁻¹
288.9	0.0292	4.83
	0.0588	8.54
	0.0722	9.97
	0.1094	15.4
	0.1436	19.0
	0.1936	25.0
297.9	0.0418	9.64
	0.0530	12.04
	0.0722	16.54
	0.1085	23.6
	0.1435	32.3
	0.1752	38.9
303.9	0.0292	9.89
	0.0588	21.26
	0.0722	23.0
	0.1094	30.8
	0.1436	43.9
	0.1036	58.1

Optimized Cartesian coordinates/Å

All compounds were optimized with B3LYP/TZP

1. [Ir(bpt)(cod)] (1)

Ir	0.562259000	0.807973000	-1.355486000
N	-1.394708000	1.624313000	-2.070795000
C	-2.152364000	1.192847000	-3.089924000
C	-3.352399000	1.795794000	-3.448561000
C	-3.787877000	2.903689000	-2.711838000
C	-3.012600000	3.362569000	-1.655508000
C	-1.813255000	2.702928000	-1.353755000
C	-0.937810000	3.123016000	-0.271083000
N	-1.101836000	4.135284000	0.580449000
C	0.016756000	4.041391000	1.340824000
N	0.833836000	3.025682000	0.982409000
N	0.212222000	2.442901000	-0.051779000
C	0.347946000	4.947510000	2.461073000
N	-0.522727000	5.927302000	2.753258000
C	-0.227521000	6.749253000	3.762907000
C	0.932735000	6.652636000	4.533971000
C	1.837232000	5.632839000	4.228603000
C	1.544326000	4.767787000	3.180346000
H	-1.779301000	0.333195000	-3.635600000
H	-3.924796000	1.405727000	-4.281483000
H	-4.719168000	3.399789000	-2.962890000
H	-3.294921000	4.215653000	-1.050299000
H	-0.956969000	7.529946000	3.969914000
H	1.116620000	7.352286000	5.342564000
H	2.753849000	5.514858000	4.797643000
H	2.212532000	3.961411000	2.904268000
C	0.410637000	-1.218367000	-2.233603000
H	-0.638543000	-1.372980000	-2.481842000
C	1.168940000	-0.430954000	-3.114533000
H	0.651062000	-0.010253000	-3.974161000
C	2.689520000	-0.515130000	-3.253315000
H	2.960147000	-0.318234000	-4.294601000
H	3.014661000	-1.538465000	-3.045710000
C	3.440329000	0.485332000	-2.338766000
H	4.466999000	0.136510000	-2.153003000
H	3.534469000	1.443983000	-2.858753000
C	2.734386000	0.753042000	-1.020753000
H	2.967919000	1.711157000	-0.561748000
C	2.146103000	-0.213963000	-0.188380000
H	1.963602000	0.083491000	0.840971000
C	2.191951000	-1.718339000	-0.450354000
H	2.243558000	-2.241755000	0.508734000
H	3.114673000	-1.967882000	-0.982311000
C	0.959635000	-2.228372000	-1.237898000
H	1.196190000	-3.173775000	-1.748154000
H	0.155957000	-2.456733000	-0.530319000

2. [Ir(bpt-NH)(cod)] (2)

Ir	3.207019000	0.652744000	2.695577000
N	2.135955000	1.759426000	1.066455000
C	2.854207000	2.615102000	0.300733000
H	3.897893000	2.718867000	0.557548000
C	2.338326000	3.342708000	-0.753596000
H	2.983749000	4.010276000	-1.311804000
C	0.979932000	3.186074000	-1.066006000
H	0.529407000	3.730405000	-1.889018000
C	0.224102000	2.322710000	-0.302771000
H	-0.829359000	2.160999000	-0.488617000
C	0.814158000	1.613517000	0.774385000
C	-0.077608000	0.761128000	1.538335000
N	0.222387000	-0.093935000	2.569267000
N	1.449260000	-0.379868000	3.068853000
H	1.303292000	-1.020566000	3.846146000

N	-1.407458000	0.730250000	1.308501000
N	-1.959490000	-0.117460000	2.167525000
C	-0.990408000	-0.627834000	2.944517000
C	-1.221990000	-1.587878000	4.018169000
C	-2.537107000	-2.034606000	4.270592000
H	-3.346384000	-1.658181000	3.657482000
C	-2.749165000	-2.940021000	5.298460000
H	-3.751023000	-3.297879000	5.512484000
C	-1.656490000	-3.384383000	6.054189000
H	-1.778732000	-4.091987000	6.866386000
C	-0.395443000	-2.890513000	5.733805000
H	0.479173000	-3.209652000	6.295188000
N	-0.170308000	-2.015995000	4.745415000
C	5.251137000	0.966173000	1.898965000
H	5.165896000	1.192747000	0.837906000
C	4.985172000	2.004821000	2.813212000
H	4.686478000	2.967687000	2.405348000
C	5.579072000	2.077313000	4.221780000
H	5.759271000	3.125589000	4.477504000
H	6.560480000	1.594464000	4.229238000
C	4.657183000	1.446530000	5.290148000
H	5.238715000	1.140046000	6.172862000
H	3.945842000	2.201035000	5.641019000
C	3.848826000	0.271635000	4.768195000
H	2.939424000	0.076025000	5.331469000
C	4.335498000	-0.774723000	3.961173000
H	3.756115000	-1.694450000	3.955789000
C	5.797634000	-0.926195000	3.542175000
H	6.040810000	-1.991434000	3.488691000
H	6.443493000	-0.507148000	4.319358000
C	6.097456000	-0.267609000	2.175767000
H	7.167077000	-0.022542000	2.093391000
H	5.888014000	-0.989898000	1.379912000

3. [Rh(bpt)(cod)] (3)

Rh	0.560131000	0.829027000	-1.361852000
N	-1.369177000	1.620162000	-2.091722000
C	-2.115625000	1.187014000	-3.117502000
C	-3.320219000	1.778491000	-3.482595000
C	-3.772970000	2.878011000	-2.744177000
C	-3.009256000	3.339986000	-1.680621000
C	-1.804687000	2.691413000	-1.373999000
C	-0.935394000	3.109272000	-0.286933000
N	-1.097294000	4.119414000	0.569216000
C	0.022833000	4.021223000	1.326058000
N	0.836747000	3.004280000	0.961446000
N	0.213053000	2.426557000	-0.072508000
C	0.363740000	4.923478000	2.445782000
N	-0.505676000	5.900482000	2.751838000
C	-0.199351000	6.720311000	3.760091000
C	0.970216000	6.624218000	4.516848000
C	1.872889000	5.606763000	4.197756000
C	1.569265000	4.744437000	3.150458000
H	-1.731006000	0.333760000	-3.665624000
H	-3.883578000	1.386096000	-4.320775000
H	-4.708441000	3.364939000	-2.999592000
H	-3.305880000	4.187348000	-1.074057000
H	-0.927730000	7.499297000	3.977646000
H	1.162506000	7.322135000	5.325034000
H	2.796693000	5.488770000	4.755352000
H	2.236392000	3.940885000	2.863833000
C	0.410653000	-1.177326000	-2.238993000
H	-0.644311000	-1.306715000	-2.477054000
C	1.175896000	-0.394346000	-3.106427000
H	0.665738000	0.057352000	-3.955253000
C	2.697141000	-0.473359000	-3.227817000

H	2.979261000	-0.274155000	-4.266104000
H	3.025753000	-1.495388000	-3.017688000
C	3.431585000	0.531634000	-2.303653000
H	4.459955000	0.189266000	-2.112065000
H	3.523277000	1.491132000	-2.821708000
C	2.712638000	0.791479000	-0.991088000
H	2.908711000	1.762214000	-0.540681000
C	2.121929000	-0.173041000	-0.170499000
H	1.891333000	0.129544000	0.848195000
C	2.167686000	-1.677158000	-0.431432000
H	2.205079000	-2.200504000	0.528529000
H	3.097224000	-1.930700000	-0.949644000
C	0.945139000	-2.187114000	-1.235637000
H	1.190310000	-3.133685000	-1.741122000
H	0.132672000	-2.416632000	-0.539181000

4. [Rh(bpt-NH)(cod)] (4)

Rh	3.197962000	0.633250000	2.669430000
N	2.154551000	1.770202000	1.066311000
C	2.881765000	2.602266000	0.285429000
H	3.930000000	2.689154000	0.531483000
C	2.371006000	3.330823000	-0.772840000
H	3.024195000	3.979829000	-1.344217000
C	1.007950000	3.199717000	-1.072950000
H	0.562561000	3.744756000	-1.898767000
C	0.241648000	2.357236000	-0.295059000
H	-0.816057000	2.213323000	-0.471987000
C	0.829125000	1.648079000	0.781829000
C	-0.064809000	0.822235000	1.570894000
N	0.263891000	-0.097271000	2.532539000
N	1.515729000	-0.500249000	2.878372000
H	1.394160000	-1.136336000	3.663874000
N	-1.405941000	0.886329000	1.450619000
N	-1.940935000	0.033962000	2.319460000
C	-0.946563000	-0.570641000	2.989378000
C	-1.153755000	-1.555174000	4.046616000
C	-2.470861000	-1.926760000	4.393276000
H	-3.300079000	-1.478766000	3.860186000
C	-2.658659000	-2.851068000	5.409268000
H	-3.661281000	-3.152350000	5.695332000
C	-1.540407000	-3.388127000	6.060350000
H	-1.643442000	-4.113402000	6.859646000
C	-0.279585000	-2.963726000	5.651527000
H	0.614385000	-3.355718000	6.130814000
N	-0.077936000	-2.073123000	4.672611000
C	5.262261000	1.033792000	2.005334000
H	5.203469000	1.243695000	0.939162000
C	4.900712000	2.049028000	2.898158000
H	4.551132000	2.989880000	2.479520000
C	5.393239000	2.139837000	4.342554000
H	5.518707000	3.193838000	4.609191000
H	6.387384000	1.690428000	4.420230000
C	4.417625000	1.476313000	5.342264000
H	4.943914000	1.198437000	6.268681000
H	3.653997000	2.204416000	5.632688000
C	3.696915000	0.267996000	4.769795000
H	2.746883000	0.049349000	5.251860000
C	4.274721000	-0.752151000	4.001384000
H	3.724779000	-1.687676000	3.930874000
C	5.765168000	-0.848873000	3.675981000
H	6.049790000	-1.904505000	3.634771000
H	6.346867000	-0.412533000	4.493257000
C	6.127898000	-0.174298000	2.331585000
H	7.193175000	0.103311000	2.317398000
H	5.991912000	-0.900145000	1.523635000

5. [Ir(bpt)(cod)(CH₃)I] (5)

Ir	0.077166000	0.918947000	-1.030857000
N	-1.970377000	1.716717000	-1.376959000
C	-2.982664000	1.114795000	-2.027704000
C	-4.228756000	1.710508000	-2.187211000
C	-4.448738000	2.982499000	-1.650119000
C	-3.409673000	3.614182000	-0.982647000
C	-2.178035000	2.958453000	-0.865292000
C	-1.054538000	3.540996000	-0.164263000
N	-1.027488000	4.652664000	0.572651000
C	0.225877000	4.620156000	1.078122000
N	0.945125000	3.549242000	0.673870000
N	0.121369000	2.874945000	-0.138517000
C	0.774710000	5.623066000	2.017907000
N	0.068917000	6.749920000	2.204293000
C	0.541035000	7.651390000	3.068154000
C	1.726126000	7.493122000	3.789925000
C	2.460443000	6.321894000	3.592882000
C	1.981403000	5.372612000	2.696032000
H	-2.780680000	0.119946000	-2.405311000
H	-5.009035000	1.174640000	-2.714240000
H	-5.413895000	3.467692000	-1.749221000
H	-3.509381000	4.595961000	-0.536418000
H	-0.058257000	8.550954000	3.193433000
H	2.056344000	8.260733000	4.481535000
H	3.385747000	6.149623000	4.133148000
H	2.511044000	4.444824000	2.518307000
C	0.900177000	1.029161000	-3.497418000
H	-0.085319000	1.005256000	-3.956149000
C	1.336985000	2.198646000	-2.965537000
H	0.676026000	3.060962000	-2.985676000
C	2.769826000	2.430283000	-2.519974000
H	3.020617000	3.481308000	-2.689465000
H	3.430817000	1.848965000	-3.168745000
C	3.061107000	2.104855000	-1.031262000
H	4.135651000	1.903500000	-0.907687000
H	2.834224000	2.977106000	-0.419685000
C	2.308133000	0.933813000	-0.431795000
H	2.219834000	0.966332000	0.650842000
C	2.077295000	-0.284914000	-1.050433000
H	1.829515000	-1.121426000	-0.407728000
C	2.596403000	-0.652776000	-2.440283000
H	2.693155000	-1.740395000	-2.476007000
H	3.610315000	-0.247947000	-2.526543000
C	1.748776000	-0.215542000	-3.672888000
H	2.420698000	-0.071077000	-4.529914000
H	1.080509000	-1.035861000	-3.935299000
I	-0.823901000	-1.730941000	-1.734299000
C	-0.506885000	0.311961000	0.924644000
H	-0.225911000	1.105884000	1.616411000
H	-1.585510000	0.157699000	0.937613000
H	-0.003419000	-0.620167000	1.180152000

6. [Ir(bpt-NH)(cod)(CH₃)I] (6)

Ir	2.949905000	0.746801000	2.429859000
N	1.800014000	1.741247000	0.778756000
C	2.483275000	2.443341000	-0.148183000
H	3.555576000	2.478513000	-0.019937000
C	1.874163000	3.139706000	-1.182970000
H	2.487240000	3.697087000	-1.880694000
C	0.481620000	3.122141000	-1.276836000
H	-0.033662000	3.667702000	-2.060110000
C	-0.232700000	2.376071000	-0.353546000
H	-1.312017000	2.298530000	-0.382168000
C	0.449438000	1.679406000	0.659078000
C	-0.348716000	0.875325000	1.573996000

N	0.111872000	-0.192174000	2.284201000
N	1.383530000	-0.727471000	2.161841000
H	1.394062000	-1.459945000	2.868339000
N	-1.647849000	1.064761000	1.815449000
N	-2.038827000	0.126800000	2.692896000
C	-0.980751000	-0.633465000	2.993954000
C	-1.018547000	-1.742507000	3.949069000
C	-2.223343000	-2.025218000	4.623121000
H	-3.098672000	-1.424671000	4.409708000
C	-2.244442000	-3.060532000	5.546636000
H	-3.158019000	-3.297020000	6.082115000
C	-1.072711000	-3.789427000	5.778572000
H	-1.044669000	-4.605037000	6.492109000
C	0.070248000	-3.438834000	5.064647000
H	0.999553000	-3.981788000	5.217739000
N	0.109822000	-2.443616000	4.170026000
C	4.133339000	-1.040435000	0.904334000
H	3.505002000	-0.858809000	0.036038000
C	5.157841000	-0.190041000	1.148340000
H	5.302983000	0.654685000	0.481877000
C	6.232651000	-0.428481000	2.193397000
H	7.167458000	0.009859000	1.832728000
H	6.410401000	-1.504833000	2.267246000
C	5.942217000	0.160396000	3.600854000
H	6.523546000	-0.397372000	4.350870000
H	6.295183000	1.191477000	3.635965000
C	4.496143000	0.154859000	4.056712000
H	4.275037000	0.867480000	4.845306000
C	3.600514000	-0.892052000	3.878846000
H	2.750495000	-0.921140000	4.552753000
C	3.959214000	-2.227639000	3.219050000
H	3.309052000	-2.995910000	3.646847000
H	4.975202000	-2.488572000	3.529452000
C	3.840988000	-2.316769000	1.668902000
H	4.502165000	-3.117913000	1.312229000
H	2.825870000	-2.620539000	1.409944000
I	4.499695000	3.236889000	2.575860000
C	1.736791000	1.675001000	3.902258000
H	1.090776000	2.409859000	3.420095000
H	1.132638000	0.912520000	4.397997000
H	2.371611000	2.185185000	4.625146000

7. [Rh(bpt)(cod)(CH₃)I] (7)

Rh	-0.020309000	0.945058000	-0.972972000
N	-2.032810000	1.724379000	-1.337515000
C	-3.038827000	1.121196000	-1.996486000
C	-4.274982000	1.727792000	-2.193900000
C	-4.491094000	3.012267000	-1.686940000
C	-3.458460000	3.646091000	-1.010474000
C	-2.236893000	2.979045000	-0.855793000
C	-1.114917000	3.556996000	-0.149250000
N	-1.081886000	4.668597000	0.587825000
C	0.166216000	4.619323000	1.105809000
N	0.875601000	3.540060000	0.706422000
N	0.052301000	2.876520000	-0.114438000
C	0.717797000	5.607531000	2.058384000
N	0.023353000	6.740315000	2.250969000
C	0.497060000	7.625228000	3.131065000
C	1.672786000	7.443868000	3.863123000
C	2.395785000	6.266935000	3.658335000
C	1.915243000	5.334928000	2.744582000
H	-2.842616000	0.116792000	-2.351013000
H	-5.049680000	1.189928000	-2.727364000
H	-5.448160000	3.506528000	-1.816926000
H	-3.556736000	4.638510000	-0.587539000
H	-0.093364000	8.529845000	3.261847000

H	2.004339000	8.198489000	4.568362000
H	3.313322000	6.076254000	4.205728000
H	2.435740000	4.403234000	2.560345000
C	0.799240000	1.045517000	-3.488705000
H	-0.205409000	1.011566000	-3.904044000
C	1.247970000	2.216055000	-2.981597000
H	0.581712000	3.075105000	-2.974730000
C	2.683574000	2.443182000	-2.549549000
H	2.944528000	3.488866000	-2.736924000
H	3.338096000	1.845854000	-3.190115000
C	2.975976000	2.141664000	-1.056022000
H	4.054920000	1.964540000	-0.929693000
H	2.733070000	3.016954000	-0.455064000
C	2.252289000	0.961743000	-0.437448000
H	2.157940000	1.013896000	0.643869000
C	2.021950000	-0.256790000	-1.036331000
H	1.760725000	-1.085792000	-0.389824000
C	2.501819000	-0.637410000	-2.435662000
H	2.592988000	-1.725781000	-2.464272000
H	3.515800000	-0.238640000	-2.546974000
C	1.635134000	-0.208164000	-3.659880000
H	2.296811000	-0.080956000	-4.527955000
H	0.958971000	-1.027823000	-3.901938000
I	-0.902733000	-1.694083000	-1.642912000
C	-0.565188000	0.370886000	0.972274000
H	-0.210773000	1.147746000	1.648636000
H	-1.651219000	0.287106000	1.002640000
H	-0.109096000	-0.593029000	1.191266000

8. [Rh(bpt-NH)(cod)(CH₃)I] (8)

Rh	2.877344000	0.797436000	2.400565000
N	1.753113000	1.776168000	0.775785000
C	2.444979000	2.475392000	-0.147476000
H	3.516614000	2.507140000	-0.013914000
C	1.845143000	3.176010000	-1.185450000
H	2.465388000	3.732187000	-1.878127000
C	0.453071000	3.166225000	-1.287146000
H	-0.054591000	3.717791000	-2.071394000
C	-0.270150000	2.418575000	-0.371888000
H	-1.349530000	2.342726000	-0.409860000
C	0.403615000	1.715825000	0.642594000
C	-0.394337000	0.901957000	1.546182000
N	0.079219000	-0.158855000	2.258613000
N	1.360828000	-0.670082000	2.151935000
H	1.376515000	-1.397151000	2.864377000
N	-1.697842000	1.071432000	1.778759000
N	-2.079407000	0.128501000	2.654856000
C	-1.011185000	-0.614547000	2.964068000
C	-1.035418000	-1.715135000	3.928592000
C	-2.233726000	-1.999192000	4.613732000
H	-3.114827000	-1.407283000	4.399814000
C	-2.240377000	-3.023321000	5.549797000
H	-3.148348000	-3.259460000	6.094907000
C	-1.061627000	-3.740675000	5.782895000
H	-1.022496000	-4.547120000	6.506396000
C	0.073852000	-3.389886000	5.057361000
H	1.008571000	-3.923395000	5.211364000
N	0.099608000	-2.405464000	4.150367000
C	4.132716000	-1.008961000	0.846817000
H	3.491456000	-0.793657000	-0.005046000
C	5.175258000	-0.188578000	1.090970000
H	5.324104000	0.674278000	0.447951000
C	6.228943000	-0.439968000	2.150283000
H	7.179459000	-0.025524000	1.801636000
H	6.383062000	-1.518301000	2.242232000
C	5.929132000	0.177020000	3.543707000

H	6.521909000	-0.356359000	4.303065000
H	6.269102000	1.212630000	3.555733000
C	4.489380000	0.159516000	4.016723000
H	4.264746000	0.894499000	4.782733000
C	3.589317000	-0.869069000	3.843619000
H	2.729237000	-0.881573000	4.505390000
C	3.917196000	-2.200421000	3.161441000
H	3.251073000	-2.960429000	3.579247000
H	4.926423000	-2.486326000	3.472031000
C	3.804966000	-2.278652000	1.608275000
H	4.451486000	-3.094168000	1.256549000
H	2.785467000	-2.560749000	1.343494000
I	4.445829000	3.255818000	2.561600000
C	1.700356000	1.703063000	3.869718000
H	1.083947000	2.460357000	3.384564000
H	1.079895000	0.937644000	4.338607000
H	2.353469000	2.180013000	4.598198000