Silver Dependent Enantiodivergent Gold(I) Catalysed Asymmetric Intramolecular Hydroamination of Alkenes: A Theoretical Study

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Level of Theory	Cat 4a → Int 1	Int 1→ Int 2a	Int 1→ Int 2b	Int 2a→ Int 3a	Int 2b→ Int 3b	Int 3a→ Pdt (S)
PBE/def-TZVP	ΔE = -17.7	ΔE = -2.9	ΔE = 1.9	ΔE = 3.6	ΔE = 1.4	ΔE = -4.3
	ΔG = -0.2	ΔG = 1.9	ΔG = 6.8	ΔG = 3.5	ΔG = 0.6	ΔG = -23.0
PBE0/def2-TZVP	ΔE = -18.8	ΔE = -1.0	ΔE = 3.3	ΔE = 1.7	ΔE = 0.2	ΔE = -6.2
	ΔG = -1.3	ΔG = 3.8	ΔG = 8.2	ΔG = 1.6	ΔG = -0.6	ΔG = -24.9

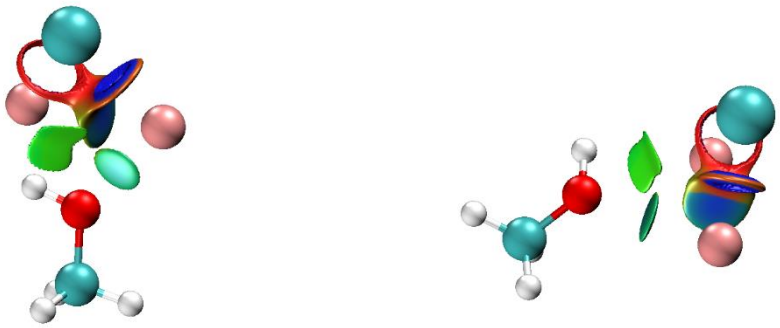
Table S1. The electronic and Gibb's free energy for each chemical step of the catalytic cycle with catalyst **4a** in toluene is provided. All values are in kcal/mol.

Level of Theory	Cat 4c → Int 1'	Int 1'→ Int 2a'	Int 1'→ Int 2b'	Int 2a'→ Int 3a'	Int 2b'→ Int 3b'	Int 3b'→ Pdt (R)
PBE/def-TZVP	ΔE = -12.2	ΔE = 0.5	ΔE = 0.0	ΔE = -4.5	ΔE = -5.0	ΔE = -1.0
	ΔG = 9.3	ΔG = 0.8	ΔG = -0.1	ΔG = 9.3	ΔG = 9.2	ΔG = -32.5
PBE0/def2-TZVP	ΔE = -17.1	ΔE = 2.1	ΔE = 1.6	ΔE = -2.8	ΔE = -4.7	ΔE = -0.3
	ΔG = 4.4	ΔG = 2.3	ΔG = 1.5	ΔG = 10.9	ΔG = 9.4	ΔG = -31.8

Table S2. The electronic and Gibb's free energy for each chemical step of the catalytic cycle with catalyst **4c** in methanol with the assistance of one molecule of methanol is provided. All values are in kcal/mol.

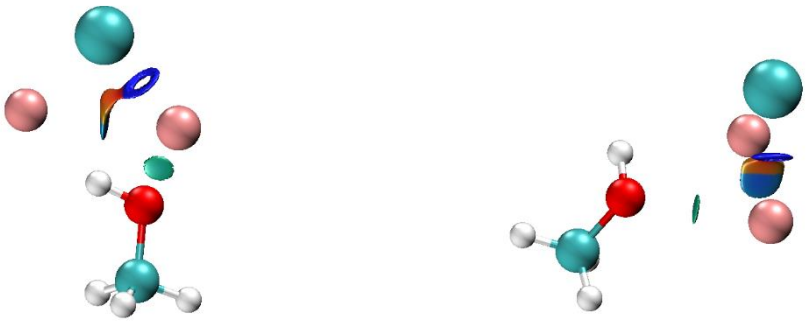
Level of Theory	Cat 4c → Int 1'	Int 1'→ Int 2a'	Int 1'→ Int 2b'	Int 2a'→ Int 3a'	Int 2b'→ Int 3b'	Int 3a'→ Pdt (S)
PBE/def-TZVP	ΔE = -12.2	ΔE = 0.5	ΔE = 0.0	ΔE = 1.6	ΔE = 7.4	ΔE = -10.2
	ΔG = 9.3	ΔG = 0.8	ΔG = -0.1	ΔG = 4.3	ΔG = 5.8	ΔG = -29.6
PBE0/def2-TZVP	ΔE = -17.1	ΔE = 2.1	ΔE = 1.6	ΔE = -0.3	ΔE = 6.4	ΔE = -7.6
	ΔG = 4.4	ΔG = 2.3	ΔG = 1.5	ΔG = 1.4	ΔG = 5.7	ΔG = -27.0

Table S3. The electronic and Gibb's free energy for each chemical step of the catalytic cycle with catalyst **4c** in methanol without the assistance of one molecule of methanol is provided. All values are in kcal/mol.



Front View **Side View**

Figure S1. The NCI plot for non-covalent interaction between oxygen (of methanol) and Ag metal unit of **int_3b'** has been shown. The rest part of the **int 3b'** has been omitted for the purpose of clarity. The isosurface value is 0.5 and the color scale is $-0.04 < \rho < 0.04$ a.u. for each figure.

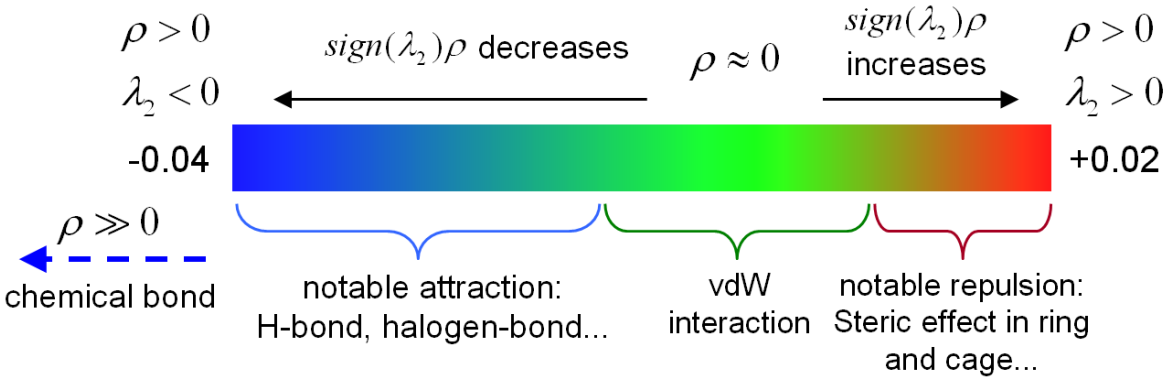


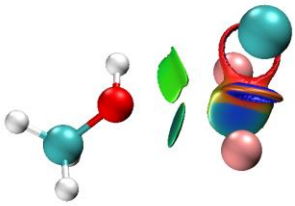
Front View **Side View**

Figure S2. The NCI plot for non-covalent interaction between oxygen (of methanol) and Ag metal unit of **int_3b'** has been shown. The rest part of the **int 3b'** has been omitted for the purpose of clarity. The isosurface value is 0.3 and the color scale is $-0.04 < \rho < 0.04$ a.u. for each figure.

Front View **Side View**

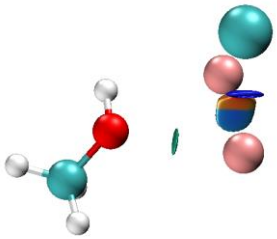
Figure S3. The NCI plot for non-covalent interaction between oxygen (of methanol) and Ag metal unit of **int_3b'** has been shown. The rest part of the **int 3b'** has been omitted for the purpose of clarity. The isosurface value is 1.0 and the color scale is -0.04 < ρ < 0.04 a.u. for each figure.



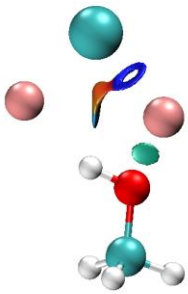


Side View (isosurface = 0.5)

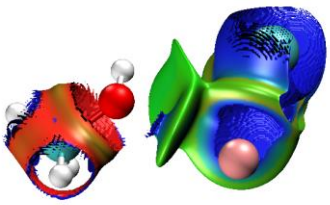
Front View (isosurface = 0.5)



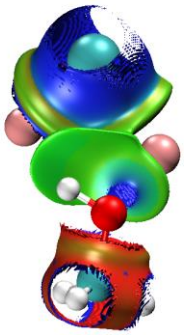
Side View (isosurface = 0.3)



Front View (isosurface = 0.3)



Side View (isosurface = 1.0)



Front View (isosurface = 1.0)

Figure S4. Summary of the NCI plots for non-covalent interaction between oxygen (of methanol) and Ag metal unit of **int_3b'** has been shown. The rest part of the **int 3b'** has been omitted for the purpose of clarity.

HPLC chromatograms

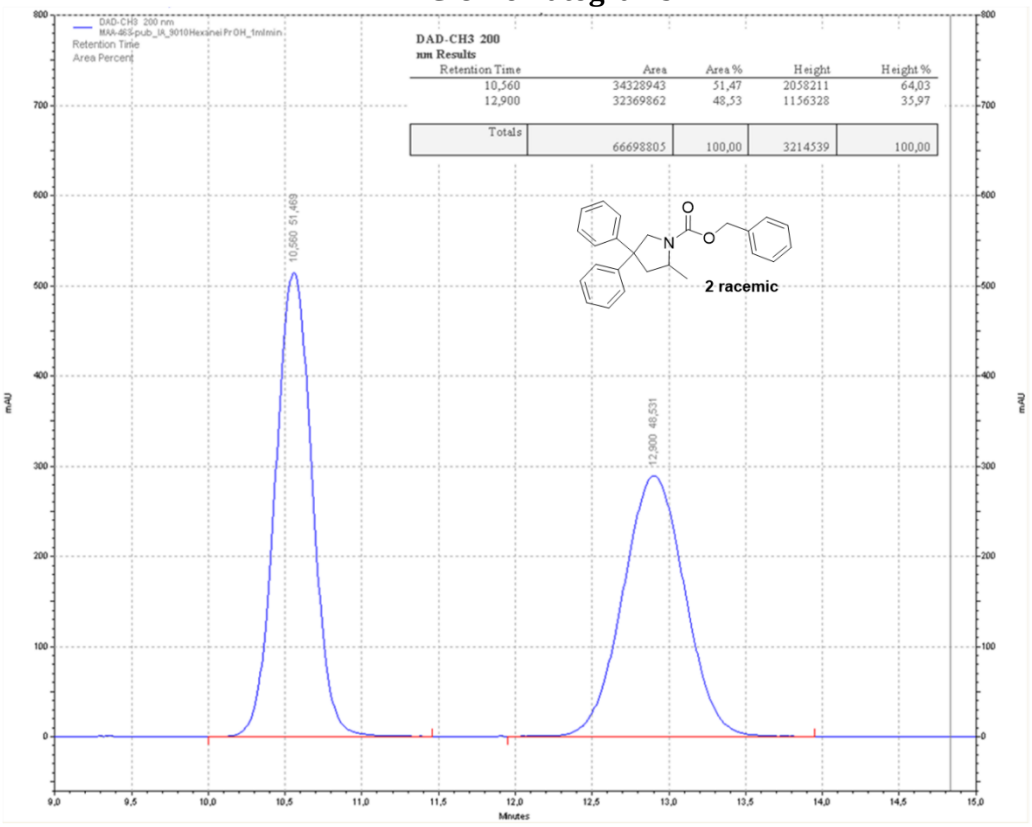


Figure S5. Chiral HPLC analysis of racemic 2. Daicel Chiralpak™ IA chiral stationary phase (at 25°C) with (90/10) *n*-hexane/*i*PrOH, 1.0 mL/min, λ = 200 nm

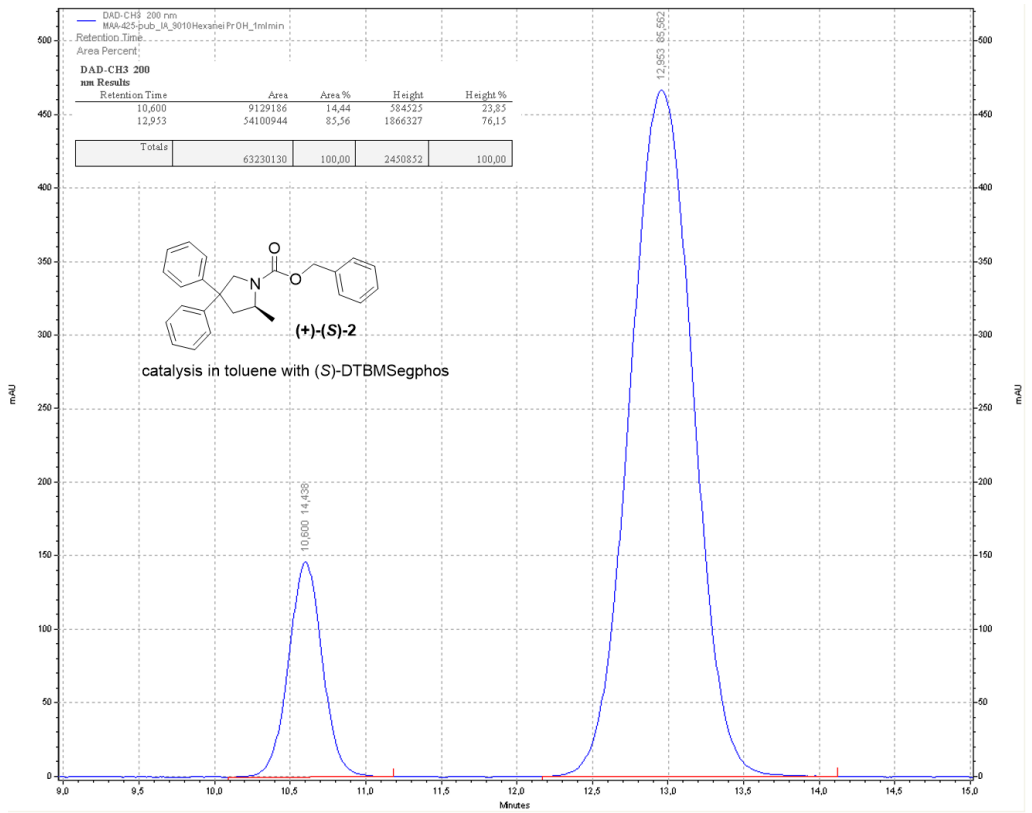


Figure S6. Chiral HPLC analysis of (+)-(*S*)-2. Daicel Chiralpak™ IA chiral stationary phase (at 25°C) with (90/10) *n*-hexane/*i*PrOH, 1.0 mL/min, λ = 200 nm

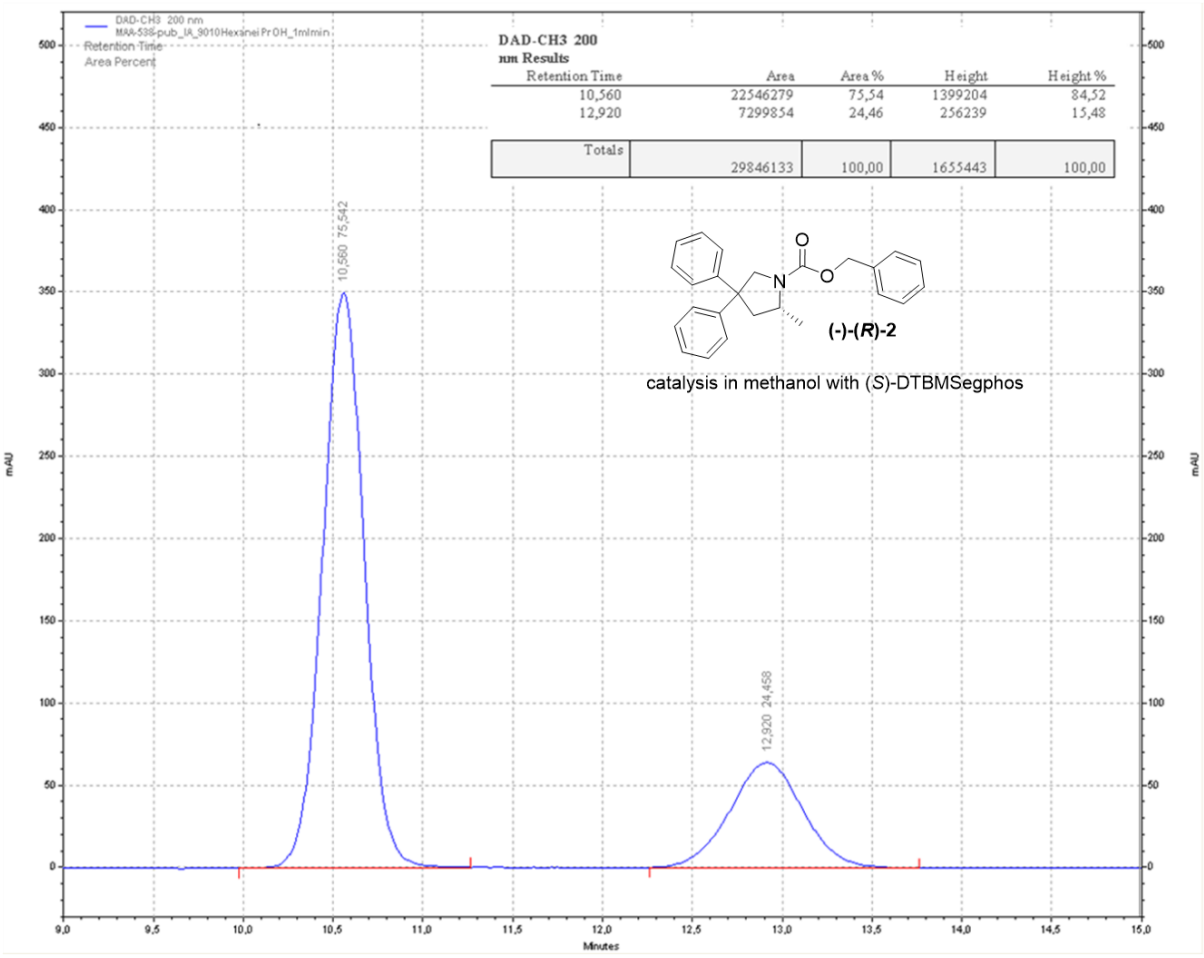


Figure S7. Chiral HPLC analysis of (-)-(*R*)-2. Daicel Chiralpak™ IA chiral stationary phase (at 25°C) with (90/10) *n*-hexane/*i*PrOH, 1.0 mL/min, λ = 200 nm

XYZ Coordinate

Catalytic cycle in Toluene

1. Catalyst 4a

C -0.0969404 0.4472033 0.1789876
C -0.0807546 -0.0418512 1.5121796
C 1.1769515 -0.2847512 2.0733595
C 2.3518377 -0.1288462 1.3346695
C 2.2818376 0.1496261 -0.0330086
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C 6.7068972 -0.2155568 -0.8586500
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C 7.2035656 -3.9830610 0.0712411
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Cl 4.5964551 -4.4423241 5.6361157
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2. Int 1

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6. Int 3b

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7. Product (S)

C -2.6420978 20.6513644 9.5893324
C -4.0911998 20.9005926 9.1827905
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C -7.7757668 22.0965845 6.6027723
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H -4.1666495 20.9302960 8.0833050
H -2.3158962 19.6644764 9.2277660

Catalytic Cycle in Methanol

1. Catalyst 4c

C 3.7516884 0.9503777 1.9844037
C 2.6940756 0.2429877 1.4197755
C 2.3522529 -1.0155170 1.9263606
C 3.1177654 -1.6214738 2.9283998
C 4.2591064 -0.9112315 3.4021934
C 4.5224051 0.4308842 3.0317072
P 1.7818176 1.0025634 0.0273930
Au 1.0485348 -0.5826671 -1.4514572
Cl 0.4998896 -2.2870335 -3.0798593
Ag 1.6302985 -3.4818598 -1.0704162
O 3.6887419 -3.9450119 -0.2995821
Cl 4.8460159 -3.0194424 -0.8568927
O 5.4806933 -2.3082303 0.3092619
C 2.6987935 -2.9910084 3.5075792
C 1.3981223 -3.4946817 2.8606585
O 5.1082891 -1.5764238 4.2684719
C 6.3341993 -2.0199217 3.6430113
C 5.5562556 1.3986359 3.6608721
C 6.1042635 0.9613526 5.0343447
C 0.5365971 2.1568446 0.7426663
C 0.7749312 2.6743933 2.0231154
C -0.0172418 3.6919080 2.5798645
C -1.0493408 4.1719326 1.7967554
C -1.3067906 3.6518261 0.5240996
C -0.5532737 2.6359309 -0.0404008

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C -1.4055973 1.3118195 -4.1114785
C -2.0839642 0.7439292 -3.0217185
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C -6.5285269 -1.2414872 -0.8206853
C -7.1681418 -0.0941858 -1.3743246
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C -7.2908111 -2.5405256 -0.4807521
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O 0.0326924 -2.4243780 8.3699003
C 1.1748975 -1.8301333 9.0215428
C 0.5633845 -4.0418381 6.0099160
C 0.7461562 -4.6043181 4.5853555
C -0.0442401 6.4197725 4.9272144
C 0.7428468 4.9176209 6.8030448
C 3.7202483 2.4715984 0.8922416
C 4.9565893 2.9270797 2.9804931
C -0.5129006 -4.8992446 6.7154691
C 1.9178662 -4.1990709 6.7365044
C -0.7938185 1.3982865 8.6547756
C -3.0062089 0.6307097 7.7488160
O 5.0230071 -0.4686249 -0.5704087
Cl 5.7296774 -1.5149961 -1.4900195
O 6.8676395 -0.8063167 -2.1896191
C -2.2668577 4.2553204 -4.1167152
C -4.5924962 4.3760979 -3.1685000
C -5.7926893 -1.5469537 -5.6773555
C -3.5611627 -2.6208402 -5.4673956
O 4.7260042 -2.0399732 -2.4996275
O 6.2411593 -2.6495450 -0.6238159
O 2.7574759 -0.2837605 4.5718524
O 3.5934719 -2.5630581 4.0071296
H -5.8804683 -2.9530090 3.6284077
H -6.6656227 -1.4876453 2.9592849
H -7.6015499 -3.0077253 3.1437726
H 1.3718688 -2.4379188 9.9129963
H 2.0544730 -1.8449933 8.3597806
H 0.9752087 -0.7917874 9.3251079
H 3.5994592 5.9991004 5.8722986

H 3.7441314 4.2224005 5.6642014
H 4.6426738 5.3434682 4.5816614
H -6.8689031 0.9533857 -4.7327539
H -6.4375231 2.6875690 -4.6414435
H -7.1006563 2.0132657 -6.1646392
H -1.4741682 -4.8308879 6.1836639
H -0.2012782 -5.9552962 6.7195556
H -0.6637459 -4.5773316 7.7533226
H 1.5436465 -4.0824055 4.0368465
H 1.0278392 -5.6648685 4.6591900
H 2.6710669 -3.5254141 6.3032939
H 1.8301496 -4.0026746 7.8099650
H 2.2772310 -5.2329438 6.6137670
H -3.6100467 -0.2213047 7.4013682
H -3.5427593 1.1174322 8.5764581
H -2.9454764 1.3595825 6.9291935
H -0.9922591 -0.9584029 10.0615578
H -2.5571610 -0.1403825 10.1663448
H -2.4023834 -1.6449860 9.2271536
H 0.1955652 1.1231519 9.0472304
H -0.6350897 2.0679381 7.7966585
H -1.3254538 1.9653153 9.4342914
H 0.8074487 3.8853922 7.1777948
H 0.2225310 5.5248927 7.5597283
H 1.7599852 5.3091798 6.7023072
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H -1.9154310 5.3888600 6.4560127
H -1.6063158 3.6543663 6.3028052
H -0.7261230 6.5132670 4.0693612
H 0.9541714 6.7519723 4.6238724
H -0.4152176 7.0961534 5.7126956
H 5.0958320 3.5170160 3.8909808
H 5.8646414 3.0355890 2.3663881
H 4.8621547 1.8695567 3.2632425
H 3.0052472 5.1064619 1.0416571
H 4.7711888 4.8860970 1.0105258
H 3.9798804 5.5469854 2.4591579
H 2.8357414 2.6431039 0.2622188
H 3.7784809 1.4018224 1.1409126
H 4.6177322 2.6992260 0.3007176
H -5.6382417 4.0410344 -3.2315824
H -4.5785780 5.4697324 -3.2935090
H -4.2256253 4.1422691 -2.1581283
H -3.6409385 3.6301025 -6.4455439

H -4.0116283 5.2279117 -5.7547275
H -5.2646581 3.9809866 -5.8187974
H -1.5946633 3.7664286 -4.8374130
H -1.8413020 4.1091819 -3.1147301
H -2.2645306 5.3363914 -4.3206653
H -2.4646329 -2.5172843 -5.4742382
H -3.8318728 -3.3355613 -6.2577555
H -3.8595840 -3.0639978 -4.5054600
H -4.3622183 0.0991085 -7.4553614
H -4.1956709 -1.6218194 -7.8921646
H -2.7946602 -0.7272070 -7.2661777
H -6.3715102 -0.6896476 -6.0376861
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H -6.0424861 -2.4109751 -6.3121905
H -6.3179206 -0.3032943 -2.4792034
H -7.9956221 0.0596093 -2.0263453
H -6.6649479 0.9424006 -1.2541980
H -7.5179474 -3.2515904 -0.4540929
H -8.4670263 -2.2862852 -1.6161277
H -6.7882804 -2.7453662 -2.0024238
H -8.1944060 -1.4792625 1.2572774
H -7.5798894 0.1903517 1.1104159
H -8.9124160 -0.3742981 0.0731825
H -3.9940593 -3.0580225 4.0336053
H -2.8126510 -4.3809858 4.1445538
H -2.3177576 -2.7931732 3.5187166
H -4.8430460 -5.4200488 1.1397762
H -4.0605317 -6.0136584 2.6249800
H -5.4134656 -4.8750649 2.7290476
H -2.3175150 -4.9025180 0.4544808
H -1.3046218 -3.9891534 1.6010739
H -1.9592022 -5.5570560 2.0725394
H -0.1811324 -4.5485633 3.9967792
H 0.2911351 -2.4084846 3.8418005
H -1.3796859 1.0362506 5.7590111
H -1.1639841 2.7121558 4.4694971
H 2.0427933 1.2546881 2.0616179
H -2.7559650 -1.5860701 -3.4832407
H -2.5807011 2.4844699 -2.1862965
H -4.6655708 0.1476368 -1.2433994
H -1.8414955 -2.3279518 0.7828616
H 1.1936332 3.5940733 -1.8412343
H -1.0333197 6.3967040 1.4235872
H 0.2660507 5.4366081 2.2826271

H 0.2637573 1.3204259 -2.1847271
H -5.3943651 0.3580902 4.0573397
H -5.8003795 4.0616291 1.3679925
H -6.4492026 2.9490463 0.0733173
H -3.0296129 -0.3580892 4.3756756
H 0.8066383 -3.3969584 -3.7440145
H 5.1752922 -1.9215904 -10.4218276
H 4.6167663 -1.0492307 -8.1862633
H 4.6119940 4.1902124 -1.6141061
H 4.3937378 1.5147661 -1.9619992
H 2.2770092 -2.7409361 -3.0046383
H 5.5503799 2.0878400 -3.1905950
H 3.2823167 6.2555728 -1.9192204
H 4.0759940 -1.6070095 -6.0113586
H 3.0027639 1.2964286 -7.9058678
H 3.4252569 -3.0187367 -11.8237720
H 1.7775187 3.4152971 -8.1904722
H -0.5936324 -0.5676627 -6.4040961
H -0.6362832 3.5723831 -7.5622884
H 3.8568263 0.1564920 -6.1987495
H -1.8036244 1.5468551 -6.6707225
H 1.5469638 6.3795160 -3.7127571
H 2.5066777 2.3620525 -4.9197373
H 1.0948059 -3.2250281 -10.9459497
H 0.5259540 -2.3439445 -8.7081587
H 1.1743377 4.4083644 -5.2018751
H 2.0027141 -3.0763585 -6.0315938
H 0.3997332 -2.3863593 -6.3327032
H 1.7678031 -0.5083081 -2.4019377
H 0.6400554 -0.7581308 -4.5944266

7. Int 3a’ with one molecule of methanol

C -2.9995719 5.0108161 0.1427615
C -2.7820842 4.8243482 -1.2311215
C -2.9653848 5.9061295 -2.1057074
C -3.3680987 7.1511277 -1.6160598
C -3.5778126 7.3345791 -0.2443469
C -3.3879048 6.2622161 0.6336617
C -2.3814791 3.4841314 -1.8022011
O -1.7349560 2.6363062 -0.8002226
C -0.4839120 2.9700162 -0.4441898
O 0.2374614 3.6503305 -1.2479786
N -0.1063679 2.4898465 0.7355812
C 1.2847802 2.3035813 1.2700266

C 1.0202216 2.0303425 2.7735840
C -0.5171129 1.8473317 2.9717314
C -0.9828135 1.6059250 1.5212005
C 2.3634063 3.3411945 0.9782584
Au 2.4625404 5.1992174 1.9874960
P 2.6459790 7.2400888 3.2275228
C 4.3579613 7.6972839 3.7234343
C 5.4349062 7.3768949 2.8994657
C 6.7684823 7.5399151 3.3130575
C 6.9737772 8.0826556 4.6078016
C 5.9014041 8.2766356 5.5242994
C 4.6045064 8.1148217 5.0366752
C -0.8273576 0.6790119 3.9090335
C -0.2439203 0.6647009 5.1877336
C -0.5228069 -0.3560899 6.0971134
C -1.3998434 -1.3900888 5.7447673
C -1.9904265 -1.3857032 4.4788613
C -1.7076637 -0.3581793 3.5689387
C -1.2661334 3.0915933 3.5014890
C -2.6590951 2.9927174 3.6904081
C -3.4095243 4.0759746 4.1464558
C -2.7798987 5.2924571 4.4388165
C -1.4023986 5.4044089 4.2591042
C -0.6560648 4.3163600 3.7877025
C 7.8681876 7.0651565 2.3271819
C 7.4362083 5.7108625 1.7063016
O 8.2524552 8.3725485 5.0555525
C 8.7703019 9.6264761 4.5706097
C 6.1224551 8.5233839 7.0346912
C 6.8732945 9.8392343 7.3332427
C 1.6243339 8.5892471 2.4788224
C 1.9434022 9.9742999 2.3679048
C 0.8713465 10.8084367 2.0598434
C -0.4192800 10.3341788 1.7966063
C -0.7250540 8.9892413 1.8501610
C 0.3278635 8.1301715 2.1941653
O 0.8738452 12.1778607 2.0228028
C -0.4204486 12.5547517 1.4948925
O -1.2662838 11.3792801 1.5516138
C 3.2799664 10.5679389 2.6520697
C 4.3602021 10.6625822 1.7205920
C 5.5961207 11.1893466 2.1164416
C 5.8175793 11.7050739 3.4049043
C 4.7466043 11.6713883 4.2743048

C 3.5198914 11.1097183 3.9034694
O 4.6979886 12.0669206 5.5860745
C 3.2962117 11.9885983 5.9444883
O 2.6647375 11.1152379 4.9797945
P 4.1188847 10.1687275 -0.0426994
Au 3.9765463 7.8984390 -0.3822473
Cl 4.4943395 5.5869749 -0.9294734
Ag 3.0256827 6.4317900 -2.8130073
O 1.8965932 4.6473698 -3.9520818
Cl 0.5787846 4.9694027 -4.7107894
O -0.2948419 3.7274425 -4.6890687
C 5.6328906 10.6897084 -0.9564751
C 6.3810069 9.7437510 -1.6623700
C 7.4753973 10.1045489 -2.4509722
C 7.7983078 11.4869000 -2.5184424
C 7.1767158 12.4471370 -1.6787246
C 6.0468975 12.0213818 -0.9660961
C 7.6444533 13.9040135 -1.4269893
C 6.6452167 14.8954480 -2.0603509
O 8.7696939 11.8749092 -3.4265502
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C 8.3005519 9.0123264 -3.1664844
C 9.7663795 9.0971550 -2.6820032
C 2.8016685 11.2858684 -0.6585757
C 1.8510334 10.8751515 -1.5889523
C 0.9302150 11.7794744 -2.1473990
C 1.1050116 13.1568039 -1.8268776
C 2.0258037 13.5923621 -0.8297930
C 2.8434090 12.6220290 -0.2485146
C -0.2058083 11.2100925 -3.0356297
C -0.4999095 9.7422114 -2.6470453
O 0.3115900 14.1398678 -2.3894879
C 0.5505844 14.5086042 -3.7633257
C 2.1576136 15.0663414 -0.3769282
C 0.8156775 15.6118045 0.1626126
C 0.2130384 11.1925697 -4.5237664
C -1.5377108 11.9681538 -2.8386038
C 2.6395204 15.9511248 -1.5496193
C 3.1895498 15.2179418 0.7599820
C 7.6646679 14.1419742 0.1072881
C 9.0716507 14.2280247 -1.9150376
C 8.2457719 9.1578061 -4.7037949
C 7.7763227 7.6007650 -2.8326340
C 1.8352308 7.0161127 4.8678429

C 1.0210508 7.9824679 5.4477703
C 0.4582964 7.8129939 6.7254360
C 0.8605730 6.6645257 7.4496603
C 1.5921384 5.6031407 6.8413745
C 2.0757283 5.8185478 5.5497935
C -0.5694479 8.8843014 7.1725147
C -1.5793114 9.0983664 6.0129175
O 0.5169230 6.5206081 8.7846545
C 1.3383038 7.3116956 9.6684606
C 1.7786249 4.2269071 7.5155620
C 2.5947561 4.3126832 8.8244057
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C -1.4246216 8.5092855 8.4004927
C 2.5216938 3.2452271 6.5891923
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O 2.4605331 8.2773189 -4.0472528
Cl 3.6903864 8.9816172 -4.7198179
O 3.2755608 9.3936458 -6.1180611
C 8.0028079 8.0937202 1.1846405
C 9.2528118 6.8106889 2.9596793
C 4.7820584 8.5781681 7.7969663
C 6.9239238 7.3283175 7.6044311
O 4.8307197 7.9748402 -4.7757443
O 4.0734877 10.1861503 -3.9001148
O 0.9128341 5.3474151 -6.1395231
O -0.1208663 6.1173183 -4.0082055
O 1.1326222 5.8311346 -0.7921792
C 0.1215499 6.8822098 -0.8305954
H 8.8081641 9.6531542 3.4717621
H 8.1566354 10.4675752 4.9274805
H 9.7864856 9.7171182 4.9727212
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H 7.4958190 11.8716611 -5.1000931
H 7.7375982 13.4759014 -4.3428024
H 0.4227720 15.5975302 -3.8293262
H 1.5687467 14.2390234 -4.0772348
H -0.1819535 14.0302295 -4.4294860
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H 1.2598491 8.3861084 9.4431525
H 0.9700848 7.1239971 10.6841237
H 9.8249666 8.9507479 -1.5922856
H 10.3635573 8.3078876 -3.1644283
H 10.2120755 10.0692950 -2.9280836
H 6.7522659 7.4473187 -3.2038172

H 8.4244189 6.8602548 -3.3237619
H 7.2034975 9.1983536 -5.0516761
H 8.7792416 10.0491924 -5.0500689
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H 8.3350831 13.4256316 0.6057061
H 8.0317379 15.1579954 0.3142329
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H 9.3553617 15.2136376 -1.5162920
H 9.7982038 13.4895734 -1.5486242
H 6.6052469 14.7925275 -3.1543460
H 5.6285784 14.7336842 -1.6737407
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H 3.5312801 15.5221901 -2.0291917
H 2.9036668 16.9502821 -1.1706586
H 1.8655852 16.0794218 -2.3127557
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H 3.2150260 16.2707498 1.0750549
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H 0.0062976 15.4921977 -0.5664210
H 0.9238724 16.6830152 0.3925433
H 0.4521182 12.1882374 -4.9125251
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H -0.5700836 10.9937021 7.7316312
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H -2.3177833 9.8569859 6.3102912
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H 2.8273609 3.2954619 9.1749782
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H 4.9884682 8.7070907 8.8691004
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H 6.8691464 10.0210462 8.4192769
H 8.3271956 9.0787626 1.5490381
H 8.7429124 7.7468983 0.4477117
H 7.0440349 8.2314311 0.6640953
H 9.1787307 6.1574557 3.8402406
H 9.8831834 6.3056405 2.2118783
H 9.7715491 7.7272354 3.2572531
H 7.2466711 4.9608762 2.4885295
H 6.5396509 5.7878300 1.0782469
H 8.2460899 5.3384609 1.0615701
H 7.7939597 7.3922055 -1.7532161
H 6.0730603 8.6998754 -1.6312067
H 5.4931689 12.7565154 -0.3851020
H 3.5246977 12.9064356 0.5496277
H 1.8231575 9.8275241 -1.8851898
H 2.6662874 5.0468348 5.0556608
H 0.8061129 8.8938522 4.8915128
H 3.7599829 8.2812522 5.6993993
H 5.2305147 6.9549986 1.9146282
H -1.7276886 8.6153672 1.6463576
H -0.8522165 13.3421277 2.1236376
H -0.3078364 12.8638395 0.4438833
H 0.1134421 7.0626181 2.2868813
H 6.7817652 12.1211045 3.6941478
H 2.8490459 12.9937951 5.8758188
H 3.2004584 11.5571868 6.9471437
H 6.4141927 11.2263602 1.3985880
H 3.3027376 2.8667382 1.3151252
H -2.6788383 -2.1832588 4.1917594
H -2.1920672 -0.3781789 2.5911463
H -2.7662134 5.7789367 -3.1718855

H -1.7203707 3.6003917 -2.6718032
H 2.4911152 3.4752177 -0.1044216
H -3.2600088 2.8934395 -2.0932168
H -3.5020343 7.9860833 -2.3063901
H -0.7909493 0.5663750 1.2081670
H -3.1660689 2.0461038 3.4875322
H -1.6215141 -2.1899108 6.4539655
H -4.4878743 3.9683967 4.2810406
H 0.4163997 4.4523112 3.6434843
H -3.3630123 6.1400108 4.8054027
H -2.0358109 1.8392920 1.3466755
H -0.8898875 6.3388386 4.4928599
H -3.8861460 8.3101417 0.1371337
H -2.8635297 4.1828064 0.8406718
H -0.0567915 -0.3444971 7.0849097
H 0.4311872 1.4710207 5.4788523
H -3.5435030 6.3914363 1.7068599
H 1.5449291 1.1158869 3.0759930
H 1.4269630 2.8489570 3.3801585
H 1.5878636 5.7904338 0.1088135
H -0.6955643 6.6585119 -0.1349021
H -0.2461808 6.9044801 -1.8579681
H 0.6045434 7.8285460 -0.5682725
H 0.6845697 4.6898366 -0.9824924
H 1.6101929 1.3537909 0.8050414

8. Int 3b’ with one molecule of methanol

C -3.432519500 3.997729400 -1.005928400
C -2.779509900 3.754337000 -2.217726500
C -2.772653300 4.750337100 -3.192465400
C -3.359990100 6.005437000 -2.981023900
C -3.842863800 6.269788800 -1.673885600
C -3.979736400 5.245436600 -0.699189600
P -1.933190800 2.142311200 -2.497992200
C -0.270273600 2.579558800 -3.130904700
C 0.864851300 2.502129900 -2.329449100
C 2.118468600 2.948471700 -2.782092800
C 2.144977400 3.618627100 -4.038496000
C 1.015568300 3.642689800 -4.908353300
C -0.173154300 3.089467100 -4.429544500
C 3.363042900 2.642042400 -1.909180600
C 3.655337300 3.795652500 -0.921559800
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C 3.757381600 5.421011200 -3.926426800

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9. Product (R)

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