Supporting Information

for

Iridium-catalyzed hydroacylation reactions of C1-substituted oxabenzonorbornadienes with salicylaldehyde: an experimental and computational study

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Beilstein J. Org. Chem. 2022, 18, 251–261. doi:10.3762/bjoc.18.30

Cartesian coordinates and selected energy values for all calculated structures
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Cartesian Coordinates and Selected Raw Output

Cat (Ir[COD]OH)₂

Electronic energy at 338.15 K (1,4-dioxane): -984.346550 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -984.009733 au

KOH

Electronic energy at 338.15 K (1,4-dioxane): -675.763153 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -675.778517 au

Salicylaldehyde-K

Electronic energy at 338.15 K (1,4-dioxane): -1020.007902 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1020.007902 au

MeOB Coordinates

Half cat Ir[COD]OH

Electronic energy at 338.15 K (1,4-dioxane): -492.125033 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -491.971714 au

KOH

Electronic energy at 338.15 K (1,4-dioxane): -675.763153 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -675.778517 au

Salicylaldehyde-K

Electronic energy at 338.15 K (1,4-dioxane): -1020.007902 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1020.007902 au

MeOB Coordinates
Main Path

MeOBD

Electronic energy at 338.15 K (1,4-dioxane) - 500.168186 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane) - 500.029150 au

1b

Electronic energy at 338.15 K (1,4-dioxane) - 1336.604994 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane) - 1336.203866 au
1ats2a

Electronic energy at 338.15 K (1,4-dioxane): -1336.591381 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.193023 au

Imaginary frequency (at Def2SVP): -186.12 cm⁻¹

1bts2b

Electronic energy at 338.15 K (1,4-dioxane): -1336.594620 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.195914 au

Imaginary frequency (at Def2SVP): -176.30 cm⁻¹
2a

Electronic energy at 338.15 K (1,4-dioxane): -1336.607761 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.205945 au

2b

Electronic energy at 338.15 K (1,4-dioxane): -1336.608532 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.206909 au
### 2ats3a

**Electronic energy at 338.15 K (1,4-dioxane):** -1336.593325 au

**Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane):** -1336.188694 au

**Imaginary frequency (at Def2SVP):** -199.36 cm⁻¹

| C      | -0.67522000 2.44021800 -0.92280000 |
|--------|-------------------------------------|
| C      | 0.76625900 3.71038500 0.51211320  |
| C      | -0.31896500 2.36798600 0.44820100  |
| C      | -0.55446400 4.85409900 -0.76007700  |
| C      | -1.03143700 3.77148200 0.58026700  |
| C      | -0.13251000 2.55275800 1.02015700  |
| C      | -0.24772400 7.47679400 0.60597900  |
| C      | -0.61803000 7.85365400 -1.23763800 |
| H      | 0.11523800 2.34014800 -2.26240100 |
| H      | -0.09761300 5.68774300 1.19516100 |
| C      | 1.29013900 6.26775900 1.23096600 |
| C      | 2.25373100 7.83443600 0.88554500 |
| C      | 3.61877800 -1.16149400 -0.71667800 |
| C      | 5.27260200 -0.50320200 0.50780100 |
| C      | 2.12378600 -0.79383400 1.02719200 |
| C      | 1.20688800 0.12749600 0.14418000 |
| H      | 1.65009500 0.03738600 -0.03001100 |
| H      | 2.11684100 -2.67103400 -1.52993500 |
| H      | 1.70842300 1.09572500 -0.01654900 |
| H      | -3.11130000 1.33592800 -0.09047800 |
| C      | -0.30968900 0.26098600 0.12698900 |
| C      | -3.39097800 -0.11252500 1.53830400 |
| C      | -0.90601000 -0.61245800 -1.00889800 |
| C      | -2.42638900 -3.02465600 -0.72266500 |
| C      | -3.55852900 -2.04536700 -0.92657900 |
| H      | -3.21617100 -0.11509100 -1.98099600 |
| C      | -1.30030700 -2.44647200 0.09622100 |
| C      | -2.76925400 -1.44081400 1.97141700 |
| C      | -1.44782600 -1.70949300 1.27972500 |
| H      | -0.31797800 -2.91869000 -0.04643500 |
| C      | -0.95228800 2.92147000 3.05546500 |
| O      | -0.94940900 1.34019600 -1.58646800 |
| C      | -0.09925500 1.02621100 1.05163200 |

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### 2bts3b

**Electronic energy at 338.15 K (1,4-dioxane):** -1336.602791 au

**Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane):** -1336.197620 au

**Imaginary frequency (at Def2SVP):** -179.71 cm⁻¹

| C      | -0.93969200 2.34694300 -1.05524900 |
|--------|-------------------------------------|
| C      | -1.19937000 3.55077900 -1.74125300 |
| C      | -0.58779900 2.42039500 0.31333100 |
| C      | -1.15710000 4.76012600 -1.06232000 |
| H      | -1.45922400 4.39744700 -2.80243900 |
| C      | -0.57176200 3.64531000 0.98750200 |
| C      | -0.85643200 4.82166100 0.30609800 |
| C      | -1.37614000 5.68412800 -1.60764500 |
| C      | -0.31675650 3.64913500 2.05196900 |
| C      | -0.84066950 5.78319800 0.82612300 |
| C      | 1.41345100 -1.51754000 -1.10557800 |
| C      | 2.45553000 -1.54049000 -0.59041100 |
| C      | 3.73428700 -0.77400300 -0.31203000 |
| C      | 3.47315400 0.04575200 0.85418700 |
| C      | -2.94566800 -0.40143100 -1.19562600 |
| C      | -1.17571200 0.36001600 0.16947100 |
| C      | 1.76000800 0.09247100 -1.95315700 |
| C      | 1.61269900 1.34538200 -0.05978200 |
| C      | -3.22836500 1.07845600 -1.19750700 |
| C      | -0.30239300 0.04932300 0.13928900 |
| C      | -3.37112200 -0.19735100 1.58564100 |
| C      | -0.30529800 -0.94882400 -0.88966900 |
| C      | -2.11160600 -3.23549100 -0.34293900 |
| C      | -3.35872400 -2.40510400 -0.64854300 |
| C      | -3.16903800 -0.57772100 -1.91148900 |
| C      | -1.05438700 -2.45496400 0.40052100 |
| C      | -2.62254900 -1.39992600 -2.16214600 |
| C      | -1.27721200 -1.63134100 1.49664100 |
| C      | -0.03032600 -2.84226800 0.31031300 |
| C      | -0.46066700 -1.39769500 2.12554500 |
| C      | -0.10516100 1.17838800 -1.64173000 |
| C      | -0.16990700 1.17498000 1.00983900 |
| C      | 0.13772400 1.06981100 2.21903200 |
| H      | 1.71645400 -0.29586500 2.23736800 |
Electronic energy at 338.15 K (1,4-dioxane): -1336.66158 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.257114 au
Electronic energy at 338.15 K (1,4-dioxane): -1520.066060 au

Electronic energy at 338.15 K (1,4-dioxane): -1520.296221 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1520.066060 au

Imaginary frequency (at Def2SVP): --198.93 cm⁻¹

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.752949 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.170875 au

Proda

Electronic energy at 338.15 K (1,4-dioxane): -1520.296221 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1520.066060 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1520.070629 au

Prodb

Electronic energy at 338.15 K (1,4-dioxane): -1520.300902 au
C 2.98026500 0.12541800 0.47404500
C 3.17115700 -2.26507300 1.33868100
C 2.67078500 -0.84108700 1.40361100
H 2.82560900 1.17129200 0.79353300
H 2.25717400 -0.49964100 2.35988100
H 1.51435000 -3.66665800 1.37277200
H 2.78559100 -4.09982900 2.27607000
H 3.35465800 -2.62056500 3.34683700
H 4.15983800 -2.71515600 0.48735200
H 4.84472400 -0.08948000 -0.57010400
H 3.58739500 -0.79378800 -1.43471200
H 3.61943400 -1.20908300 -2.62821800
H 3.99824100 -2.21018300 -1.23944500
O -2.11644700 -1.48602200 1.18252800
C -4.76379800 0.77281000 0.25283600
C -5.70361900 0.50785800 -0.72889600
C -5.56772700 -0.54568700 -1.62530200
C -4.43316800 -1.36949800 -1.57350200
H -4.89278600 1.60430300 0.95372900
H -6.62542100 1.13423500 -0.79892900
H -6.33743300 -0.73478800 -2.37941300
H -4.39653700 -2.19665700 -1.20613700
H -1.93623100 -2.72817900 -0.48795400
Tr 0.78786600 -0.59047000 -0.04674600
C -0.00522700 1.30575000 1.14221500
H 0.33774500 -1.55585900 1.11989600
C 0.55663900 2.43253800 0.38000800
O 0.00439900 1.22503000 2.35105000
C 0.69711000 3.68503000 0.99708000
C 0.96442600 2.22854700 -0.96904900
C 1.16919100 4.77167500 0.28052400
H 0.40643500 3.77836300 2.08459600
C 1.42039000 3.36116900 -1.68792000
O 0.96519800 1.04218800 -1.49482000
C 1.51960300 4.59534400 -1.07017500
H 1.26344900 5.75307900 0.75270000
H 1.72217100 3.21713000 -2.73071500
H 1.89082200 5.45080800 -1.64452500
C -2.64295600 0.40555100 2.60203700
H -2.73553000 1.50197400 2.61654600
H -3.57836600 -0.03586300 2.98700000
H -1.81255000 0.12943900 3.26519100

1dts2d

Electronic energy at 338.15 K (1,4-dioxane): -1336.578080 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.176122 au

Imaginary frequency (at Def2SVP): -177.57 cm⁻¹

-1.24416700 0.71359400 0.29400900
-3.63037100 0.46393800 0.55850000
-3.64550500 -0.64373800 -0.29474400
-2.34799800 -1.38271000 0.00770300
-1.24465200 -0.49893500 -0.62186000
-1.43883400 1.63900700 -2.68685000
-1.37629700 -0.28592400 -1.69390000
H 0.28590800 -1.32712600 -0.81184300
1.21340000 -2.62661500 -0.51062700
1.97608000 -3.33701600 0.57397600
1.78222800 -1.74499400 -1.45782700
3.72433600 -0.23563500 -0.74282900
3.26477500 -1.44834100 -1.56070900
1.20620100 -1.85952800 -1.79627200
2.94914300 -0.02010500 0.52511500
2.97098600 -2.44536400 1.31423400

2c

Electronic energy at 338.15 K (1,4-dioxane): -1336.589749 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.187326 au
Electronic energy + thermal free energy correction

Imaginary frequency (at Def2SVP):

Electronic energy at 338.15 K (1,4-dioxane): -1336.580487 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.179770 au

Imaginary frequency (at Def2SVP): -681.13 cm⁻¹

C -1.40305200 0.75679000 0.29987000
C -2.49410400 0.15424100 1.25107900
C 0.37400400 0.03367300 0.38835900
C -3.51394400 -1.07092600 -0.43605800
C -2.12402600 -1.51881700 -0.05216200
C -1.16490900 -0.47256500 -0.66437900
C -1.83427700 1.57859500 -0.29935500
C -1.48826600 -0.18415000 -1.67787700
C 0.17352200 -1.62463100 1.88088300
C 1.12317900 -1.77285300 1.35079100
C 2.77532500 2.63796500 2.67572900
C 2.95412500 3.58904700 1.09353900
C 2.86647200 1.55826900 -0.65382900
C 3.09587300 2.56066200 -1.03674100
C 2.15296800 -1.67814000 -1.86745600
C 1.82866800 -2.64161500 -1.33553100
C 1.20420500 -1.60319500 -2.42058300
C 2.97994200 -1.67788000 -2.59456000

2cts3c

Electronic energy at 338.15 K (1,4-dioxane): -1336.580487 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.179770 au

Imaginary frequency (at Def2SVP): -681.13 cm⁻¹
Imaginary frequency (at Def2SVP):

| Mode | Imaginary Frequency (cm⁻¹) |
|------|---------------------------|
| 1    | -653.88                    |

2dts3d

Electronic energy at 338.15 K (1,4-dioxane): -1336.579845 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.195904 au

| Path | Electronic energy at 338.15 K (1,4-dioxane): -1336.579845 au |
|------|-------------------------------------------------------------|
| 1e   | -1336.579845 au                                            |

Endo Path

Electronic energy at 338.15 K (1,4-dioxane): -1336.597344 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.195904 au

| Path | Electronic energy at 338.15 K (1,4-dioxane): -1336.597344 au |
|------|-------------------------------------------------------------|
| 1e   | -1336.597344 au                                            |
Electronic energy at 338.15 K (1,4-dioxane): -1336.578695 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.195032 au

Imaginary frequency (at Def2SVP): -172.02 cm⁻¹
Electronic energy at 338.15 K (1,4-dioxane): -1336.578513 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.179952 au

Imaginary frequency (at Def2SVP): -184.03 cm⁻¹

Electronic energy at 338.15 K (1,4-dioxane): -1336.604435 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.201054 au
Electronic energy at 338.15 K (1,4-dioxane): -1336.599637 au

Electronic energy + thermal free energy correction at 338.15 K (1,4-dioxane): -1336.196060 au