Supporting Information

ONO Dianionic Pincer-type Ligand Precursors for the Synthesis of σ,π-Cyclooctenyl Iridium(III) Complexes: Formation Mechanism and Coordination Chemistry

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Coordinates and energies for metanol and compounds 1,4,and 4a-d and the related transition states. Optimized in gas phase.

Comp 1-MeOH

Sum of electronic and thermal Free Energies= -1157.117265

Ir 0.3516 -0.1255 0.3093

O -0.3186 -2.1107 0.2853

O -2.1028 -3.3586 -0.3196

O 0.1704 1.9574 0.3010

O -1.2760 3.6088 -0.2328

N -1.5209 0.1072 -0.3246

C -1.5368 -2.2858 -0.1961

C -2.2491 -0.9948 -0.5618

C -3.5451 -0.8690 -1.0518

H -4.1217 -1.7684 -1.2359

C -4.0516 0.4151 -1.2838

H -5.0587 0.5376 -1.6703

C -3.2661 1.5416 -1.0134

H -3.6206 2.5545 -1.1679

C -1.9772 1.3528 -0.5255

C -0.9780 2.4293 -0.1413

C 1.1084 -0.2311 -1.6317

H 0.2460 -0.3000 -2.3093

C 1.9007 -1.5517 -1.7176

H 2.4965 -1.5767 -2.6414

H 1.1873 -2.3767 -1.7779

C 2.8042 -1.7899 -0.4811

H 2.8441 -2.8607 -0.2632

H 3.8357 -1.4787 -0.6756

C 2.2839 -1.0687 0.7598

H 2.0844 -1.7066 1.6189

C 2.3950 0.3056 1.0242

H 2.2370 0.5892 2.0656

C 3.1128 1.3835 0.2336

H 2.5961 2.3260 0.4417

H 4.1184 1.4828 0.6703

C 3.2460 1.2187 -1.2895

H 3.9394 0.4057 -1.5274

H 3.7202 2.1291 -1.6766

C 1.9198 1.0080 -2.0378

H 1.3022 1.9049 -1.9311

H 2.1495 0.9154 -3.1109

O -0.3228 -0.3178 2.5947

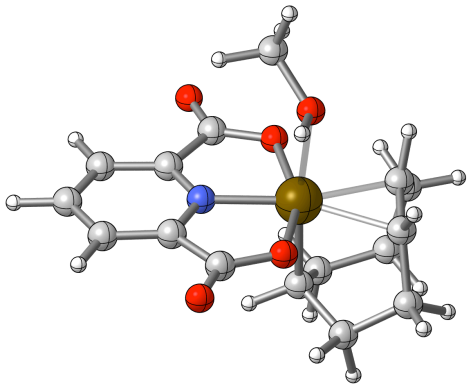
H -0.6753 -1.2204 2.5932

C -1.2489 0.5791 3.2256

H -1.3456 0.3418 4.2901

H -2.2360 0.5442 2.7508

H -0.8332 1.5804 3.1121



Comp 4

Sum of electronic and thermal Free Energies= -1041.414971

C -2.3230 -1.1278 0.7637

C -3.2994 0.0317 -1.3609

C -1.5330 1.5620 -0.3608

C -2.0506 0.9959 2.1343

C -2.4920 -1.0322 -0.6439

C -2.9834 1.4478 -0.8340

C -1.1235 1.3773 0.9890

C -2.9755 -0.1917 1.7791

H -2.0452 -2.1099 1.1447

H -4.3763 -0.1833 -1.2913

H -3.1605 2.1798 -1.6292

H -0.9159 2.2039 -0.9799

H -2.6415 1.8640 2.4624

H -3.2087 -0.7567 2.6873

H -2.3416 -1.9524 -1.2092

H -3.0436 -0.0237 -2.4247

H -3.6653 1.7199 -0.0221

H -0.2438 1.9317 1.3195

H -1.4203 0.7157 2.9857

H -3.9349 0.1662 1.3925

Ir -0.5515 -0.3422 -0.1189

N 1.6218 0.0107 -0.1480

C 2.2311 -1.1899 0.0086

C 2.3783 1.1212 0.0165

C 3.5696 -1.3166 0.3775

C 3.7053 1.0678 0.4421

C 4.3132 -0.1721 0.6317

H 3.9673 -2.3210 0.4636

H 4.2389 1.9977 0.5992

H 5.3474 -0.2356 0.9554

C 1.4103 -2.4473 -0.2553

O 1.9838 -3.5260 -0.2730

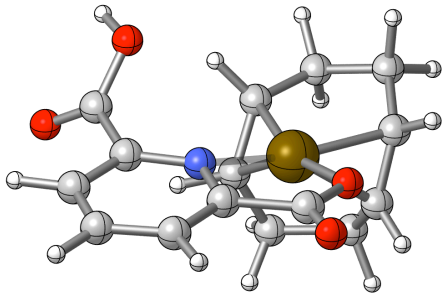
O 0.1412 -2.2379 -0.4517

C 1.8533 2.4897 -0.3105

O 2.0240 3.4583 0.3969

O 1.2833 2.5445 -1.5292

H 1.0196 3.4709 -1.6689



Comp 4a

Sum of electronic and thermal Free Energies= -1157.096687

Ir 0.6393 -0.2191 0.2310

O -2.0293 -3.5191 -0.2665

O -0.2579 -2.2907 0.4109

O -0.5760 2.6306 0.6229

O -2.5102 3.5050 -0.0320

N -1.6020 0.0196 -0.1377

C -1.4471 -2.4579 -0.0765

C -2.2018 -1.1638 -0.3986

C -3.5031 -1.2484 -0.8944

H -3.9013 -2.2398 -1.0753

C -4.2186 -0.0799 -1.1248

H -5.2280 -0.1121 -1.5236

C -3.6215 1.1370 -0.8089

H -4.1331 2.0843 -0.9221

C -2.3169 1.1595 -0.3084

C -1.7926 2.5343 0.0955

C 1.1410 -0.5471 -1.7843

H 0.3186 -1.0574 -2.2876

C 2.4692 -1.2863 -1.8628

H 2.9208 -1.1538 -2.8571

H 2.2453 -2.3532 -1.7630

C 3.4468 -0.8698 -0.7400

H 4.1009 -1.7143 -0.5020

H 4.1095 -0.0647 -1.0758

C 2.6922 -0.4400 0.5242

H 2.8894 -1.0575 1.4011

C 2.3141 0.9330 0.7908

H 2.2488 1.2017 1.8474

C 2.6455 2.1082 -0.1176

H 2.1223 2.9895 0.2669

H 3.7194 2.3422 -0.0788

C 2.1839 1.8350 -1.5613

H 3.0012 1.4301 -2.1664

H 1.8838 2.7708 -2.0434

C 1.0024 0.8603 -1.5880

H -0.0626 1.7647 0.5458

H 0.0673 1.2939 -1.9400

C -0.6543 -0.0181 3.1984

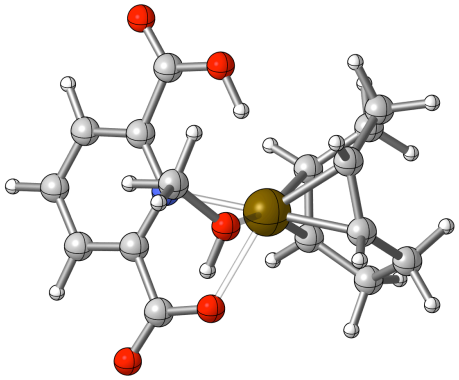
H -1.6541 -0.0648 2.7567

H -0.6648 -0.4677 4.1955

H -0.3368 1.0221 3.2690

O 0.3128 -0.7026 2.3796

H -0.0127 -1.6024 2.1506



Comp 4c

Sum of electronic and thermal Free Energies= -1157.089395

Ir -0.4898 -0.3174 -0.0405

O 1.9255 3.4982 -0.6994

O 1.0689 2.5215 1.1579

O 0.2758 -2.1024 0.5753

O 2.0206 -3.4636 0.1643

N 1.6097 0.0457 -0.2294

C 1.6961 2.5413 0.0395

C 2.3023 1.1947 -0.3718

C 3.6397 1.1624 -0.7877

H 4.1336 2.1140 -0.9450

C 4.2876 -0.0539 -0.9646

H 5.3254 -0.0860 -1.2828

C 3.5937 -1.2326 -0.6837

H 4.0458 -2.2166 -0.7244

C 2.2593 -1.1448 -0.3192

C 1.4922 -2.3668 0.1405

C -1.4994 1.7217 -0.1666

H -0.7313 2.4513 0.0633

C -2.6526 1.7263 0.8147

H -3.3367 2.5495 0.5639

H -2.2292 1.9584 1.7945

C -3.4164 0.3900 0.8986

H -3.8913 0.3091 1.8808

H -4.2287 0.3589 0.1655

C -2.5097 -0.8175 0.6932

H -2.3007 -1.4187 1.5752

C -2.3178 -1.4432 -0.5490

H -1.9837 -2.4779 -0.5327

C -2.9096 -0.9671 -1.8620

H -2.4219 -1.5288 -2.6645

H -3.9749 -1.2344 -1.9025

C -2.7273 0.5487 -2.1139

H -3.6112 1.0994 -1.7778

H -2.6561 0.7232 -3.1916

C -1.4954 1.1589 -1.4427

H -0.3497 -0.8753 -1.4910

H -0.7104 1.4987 -2.1132

C 0.5350 -0.2440 3.0102

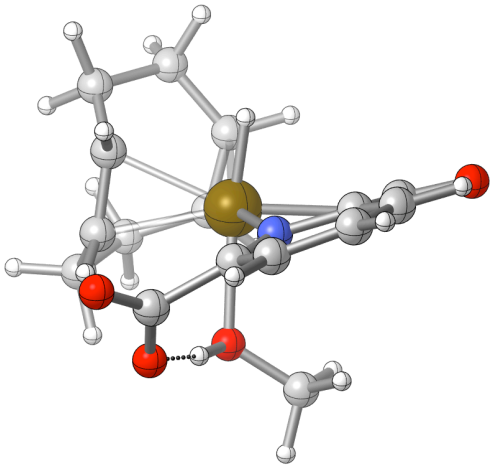
H 1.5493 -0.5147 2.6960

H 0.5912 0.3402 3.9350

H -0.0269 -1.1616 3.1929

O -0.1466 0.5257 2.0188

H 0.4315 1.3583 1.7360



Comp 4d

Sum of electronic and thermal Free Energies= -1041.410001

Ir -0.3368 0.0052 -0.4572

O 0.1088 -2.0450 -0.4772

O 1.8091 -3.4802 -0.1054

O 0.0450 2.0645 -0.3589

O 1.6954 3.5377 0.0834

N 1.6019 0.0262 0.0158

C 1.3553 -2.3505 -0.1743

C 2.2419 -1.1491 0.1001

C 3.6017 -1.1675 0.3922

H 4.1055 -2.1251 0.4593

C 4.2638 0.0516 0.5771

H 5.3253 0.0615 0.8042

C 3.5653 1.2581 0.4570

H 4.0400 2.2256 0.5753

C 2.2061 1.2138 0.1641

C 1.2811 2.3980 -0.0436

C -1.2097 -0.7052 1.7815

H -0.2826 -1.0469 2.2386

C -2.1808 -1.7992 1.3956

H -2.8229 -2.0421 2.2543

H -1.5893 -2.6911 1.1802

C -3.0614 -1.4881 0.1606

H -3.4050 -2.4408 -0.2532

H -3.9658 -0.9482 0.4576

C -2.3683 -0.7122 -0.9612

H -2.2083 -1.2780 -1.8757

C -2.3397 0.6859 -1.0812

H -2.1907 1.0884 -2.0818

C -2.8851 1.6987 -0.0944

H -2.3387 2.6301 -0.2610

H -3.9401 1.9017 -0.3288

C -2.7511 1.3053 1.3968

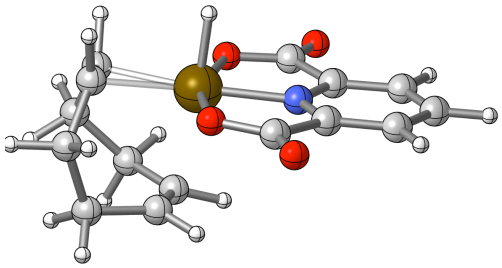
H -3.5763 0.6548 1.6972

H -2.8459 2.2150 1.9984

C -1.4353 0.6395 1.7489

H -0.6579 1.2923 2.1368

H 0.1008 0.0276 -1.9570



Comp 4e

Sum of electronic and thermal Free Energies= -1041.374794

Ir 0.3733 -0.2767 -0.0749

O -0.2721 1.6037 -1.1903

O -1.3833 3.4746 -0.5373

O -0.6796 -1.7573 -1.1043

O -2.3250 -3.2185 -0.5610

N -1.5842 0.0857 0.3749

C -1.1576 2.2730 -0.5077

C -2.0725 1.3333 0.2927

C -3.4202 1.5581 0.5624

H -3.7977 2.5732 0.5080

C -4.2519 0.4554 0.7875

H -5.3057 0.6037 1.0039

C -3.7538 -0.8371 0.5824

H -4.3945 -1.7107 0.5406

C -2.3956 -0.9866 0.3207

C -1.7683 -2.1433 -0.4551

C 1.4117 1.4655 0.9084

H 0.6304 2.1458 1.2383

C 2.3888 2.0652 -0.0800

H 3.1245 2.6817 0.4559

H 1.8120 2.7323 -0.7226

C 3.1050 1.0137 -0.9584

H 3.3861 1.4813 -1.9063

H 4.0403 0.6872 -0.4925

C 2.2426 -0.2068 -1.2630

H 1.8571 -0.2733 -2.2782

C 2.2540 -1.3893 -0.5133

H 1.8969 -2.2926 -1.0019

C 3.0549 -1.6051 0.7572

H 2.6789 -2.5174 1.2300

H 4.1080 -1.7969 0.5083

C 2.9517 -0.4321 1.7598

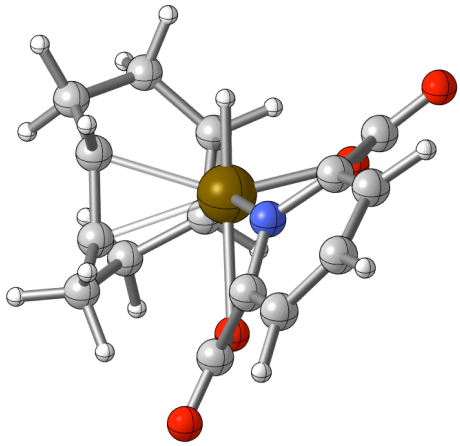
H 3.7690 0.2779 1.6032

H 3.0780 -0.8193 2.7755

C 1.6297 0.3344 1.6992

H 0.4527 -1.4875 0.9090

H 0.9749 0.2078 2.5573



TS 4-4c

TS Sum of electronic and thermal Free Energies= -1272.768218

C -2.4284 1.2690 0.3609

C -3.0896 -1.0389 1.3497

C -1.6845 -1.4813 -0.7404

C -2.4808 0.5833 -2.0944

C -2.3688 0.2932 1.3741

C -3.0077 -1.7369 -0.0249

C -1.4596 -0.4592 -1.6742

C -3.2722 1.1802 -0.9062

H -2.1229 2.2721 0.6547

H -4.1370 -0.9013 1.6551

H -3.1150 -2.8161 0.1190

H -1.0236 -2.3383 -0.7919

H -3.1675 0.1471 -2.8338

H -3.6093 2.1873 -1.1708

H -2.0505 0.6338 2.3584

H -2.6248 -1.6819 2.1025

H -3.8402 -1.4323 -0.6656

H -0.6589 -0.6389 -2.3900

H -1.9402 1.3881 -2.5977

H -4.1779 0.6008 -0.7080

Ir -0.5244 0.2205 0.1995

N 1.5426 -0.1619 -0.1604

C 2.3024 0.8206 0.4016

C 2.1482 -1.1400 -0.8686

C 3.6714 0.9009 0.2119

C 3.5291 -1.0895 -1.1159

C 4.2968 -0.0658 -0.5812

H 4.2039 1.7108 0.6964

H 3.9669 -1.8708 -1.7270

H 5.3668 -0.0244 -0.7628

C 1.5919 1.8000 1.3125

O 2.2083 2.7222 1.8239

O 0.3173 1.5475 1.4917

C 1.3468 -2.3294 -1.3923

O 1.2022 -2.3820 -2.6172

O 0.9559 -3.1445 -0.4935

H 0.4954 -2.7326 0.8732

C 1.0216 -2.2397 2.7717

H 0.5286 -1.8261 3.6544

H 1.4313 -3.2239 3.0228

H 1.8451 -1.5751 2.4825

O 0.0496 -2.3712 1.7352

H -0.3689 -1.1171 1.1779

O 0.1521 2.3227 -1.5637

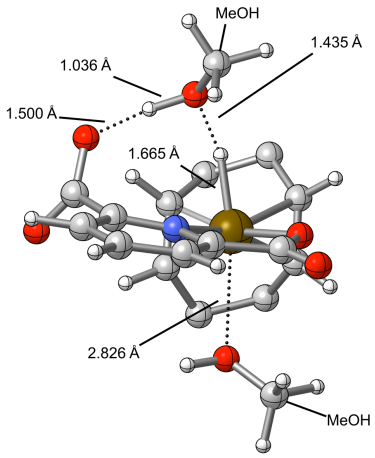
H 0.8774 1.9942 -2.1103

C 0.4198 3.6857 -1.2116

H 1.3355 3.7876 -0.6193

H 0.4843 4.3200 -2.1043

H -0.4200 4.0223 -0.6019



TS 4c-1

Sum of electronic and thermal Free Energies= -1157.067001

Ir -0.5075 -0.2548 0.0961

O 2.0104 3.5016 -0.5843

O 0.9496 2.5496 1.1396

O 0.2921 -2.1855 0.6296

O 1.9866 -3.5166 -0.0516

N 1.5543 0.0122 -0.2544

C 1.6842 2.5148 0.0525

C 2.2525 1.1630 -0.3734

C 3.5767 1.1431 -0.8192

H 4.0805 2.0941 -0.9430

C 4.2061 -0.0739 -1.0678

H 5.2338 -0.0993 -1.4172

C 3.5111 -1.2539 -0.8129

H 3.9501 -2.2407 -0.9044

C 2.1876 -1.1788 -0.3952

C 1.4371 -2.4298 0.0673

C -1.2390 1.4928 -0.8245

H -0.4696 2.2174 -1.0848

C -2.3895 2.1427 -0.0706

H -2.9610 2.8253 -0.7162

H -1.9262 2.7632 0.7027

C -3.3159 1.1064 0.5960

H -3.7539 1.5311 1.5042

H -4.1579 0.8539 -0.0567

C -2.5599 -0.1619 0.9665

H -2.3269 -0.2852 2.0197

C -2.4629 -1.2925 0.1500

H -2.2097 -2.2399 0.6198

C -3.0680 -1.4027 -1.2424

H -2.6592 -2.3069 -1.7049

H -4.1518 -1.5621 -1.1593

C -2.7677 -0.1959 -2.1599

H -3.5404 0.5737 -2.0787

H -2.7733 -0.5278 -3.2025

C -1.4071 0.4462 -1.8434

H -0.6725 -0.7485 -1.4723

H -0.7552 0.5658 -2.7104

C 0.7039 -0.3677 2.9187

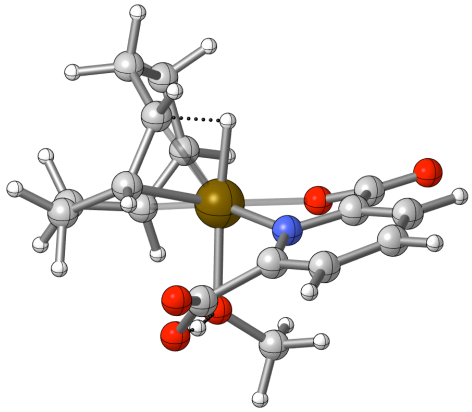
H 1.7004 -0.6644 2.5605

H 0.8299 0.2125 3.8421

H 0.1519 -1.2847 3.1522

O -0.0027 0.4411 1.9950

H 0.6271 1.6212 1.5543



TS 4a-1

Sum of electronic and thermal Free Energies= -1157.038364

Ir 0.1687 -0.1353 -0.4912

O -0.4317 1.8347 -0.6294

O -2.2429 3.1523 -0.3425

O -0.0173 -2.2242 -0.1431

O -1.4614 -3.7360 0.7481

N -1.7360 -0.3157 -0.0378

C -1.7083 2.0568 -0.3611

C -2.4943 0.7998 -0.0523

C -3.8562 0.7216 0.2041

H -4.4390 1.6359 0.1839

C -4.4257 -0.5297 0.4762

H -5.4888 -0.6122 0.6769

C -3.6191 -1.6700 0.4996

H -4.0131 -2.6547 0.7249

C -2.2576 -1.5304 0.2398

C -1.2497 -2.6298 0.3100

C 1.5727 -0.7567 1.7737

H 0.7638 -0.7968 2.5051

C 2.2287 0.6024 1.7075

H 2.9448 0.6307 2.5476

H 1.4792 1.3676 1.9238

C 2.9563 1.0107 0.4128

H 3.0902 2.0937 0.4612

H 3.9544 0.5631 0.3605

C 2.1794 0.6855 -0.8568

H 1.9815 1.5373 -1.5042

C 2.0989 -0.5818 -1.4534

H 1.8158 -0.5848 -2.5085

C 2.8392 -1.8602 -1.0795

H 2.2425 -2.7040 -1.4461

H 3.7630 -1.8742 -1.6766

C 3.2226 -2.1380 0.4006

H 4.0600 -1.4977 0.6959

H 3.6022 -3.1643 0.4450

C 2.0642 -1.9972 1.3719

H 0.8666 -2.3680 0.5906

H 1.8434 -2.8402 2.0319

O 1.1952 3.6595 0.7878

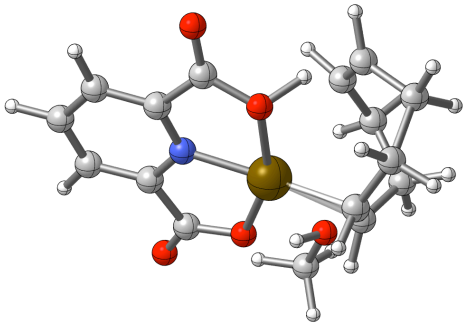
H 0.6334 3.1489 0.1773

C 0.7501 5.0037 0.7716

H -0.3329 5.0863 0.9352

H 0.9887 5.5159 -0.1741

H 1.2647 5.5350 1.5790



Methanol

Sum of electronic and thermal Free Energies= -115.693167

C 0.6612 -0.0195 0.0000

H 1.0824 0.9894 -0.0001

H 1.0385 -0.5430 0.8919

H 1.0385 -0.5431 -0.8918

O -0.7489 0.1220 0.0000

H -1.1353 -0.7621 0.0000

Coordinates and energies for metanol and compounds 1,4,and 4a-d and the related transition states. Optimized in dichloromethane solution using the SMD continuum model. Total energies

1…MeOH

E=-1157.44498117

Ir 0.3471 -0.1063 0.3159

O -0.2798 -2.1026 0.4107

O -2.0342 -3.4266 -0.0734

O 0.1352 1.9668 0.1252

O -1.3303 3.5483 -0.5207

N -1.5337 0.0455 -0.3196

C -1.5011 -2.3246 -0.0255

C -2.2502 -1.0809 -0.4558

C -3.5580 -1.0131 -0.9260

H -4.1322 -1.9264 -1.0333

C -4.0906 0.2402 -1.2460

H -5.1074 0.3170 -1.6171

C -3.3179 1.3952 -1.0827

H -3.7033 2.3820 -1.3130

C -2.0164 1.2639 -0.6090

C -1.0269 2.3759 -0.3338

C 1.1084 -0.3735 -1.6082

H 0.2480 -0.5137 -2.2769

C 1.9269 -1.6814 -1.5843

H 2.5347 -1.7651 -2.4969

H 1.2293 -2.5223 -1.5923

C 2.8214 -1.8088 -0.3244

H 2.8667 -2.8569 -0.0142

H 3.8526 -1.5097 -0.5388

C 2.2940 -0.9861 0.8481

H 2.1017 -1.5437 1.7632

C 2.3933 0.4065 0.9877

H 2.2400 0.7811 2.0004

C 3.1075 1.4106 0.1030

H 2.5983 2.3711 0.2355

H 4.1158 1.5434 0.5243

C 3.2323 1.1192 -1.4013

H 3.9289 0.2922 -1.5723

H 3.7003 1.9963 -1.8662

C 1.9047 0.8365 -2.1214

H 1.2754 1.7320 -2.0876

H 2.1304 0.6574 -3.1845

O -0.3317 0.0031 2.5948

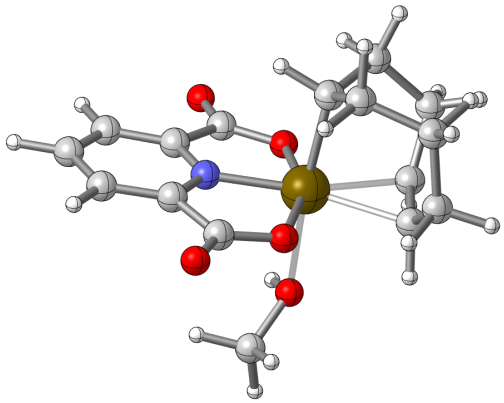
H -0.7872 -0.8321 2.7866

C -1.1083 1.0914 3.1297

H -1.2035 0.9837 4.2150

H -2.1053 1.1374 2.6790

H -0.5638 2.0086 2.9046



4…2MeOH

E=-1273.17424562

C 1.7690 -2.3665 -0.3572

C 3.3929 -1.2458 1.3514

C 2.6266 0.5335 -0.2956

C 2.5156 -1.0291 -2.3818

C 2.0858 -1.8991 0.9485

C 3.8288 -0.1549 0.3504

C 2.0511 0.1436 -1.5328

C 2.7189 -2.3173 -1.5518

H 0.9973 -3.1348 -0.4138

H 4.1802 -2.0043 1.4732

H 4.4292 0.5973 0.8726

H 2.5066 1.5743 -0.0143

H 3.4355 -0.7677 -2.9251

H 2.5381 -3.1910 -2.1857

H 1.5412 -2.3643 1.7719

H 3.2475 -0.7950 2.3399

H 4.4791 -0.5777 -0.4216

H 1.5510 0.9278 -2.1037

H 1.7504 -1.2083 -3.1458

H 3.7554 -2.3986 -1.2103

Ir 0.7493 -0.5324 0.0175

N -0.9044 0.9520 -0.1867

C -2.0848 0.2874 -0.0595

C -0.9328 2.2055 -0.6887

C -3.2992 0.8289 -0.4710

C -2.1127 2.7928 -1.1536

C -3.3106 2.0956 -1.0490

H -4.2107 0.2548 -0.3422

H -2.0722 3.7891 -1.5778

H -4.2377 2.5356 -1.4017

C -2.0332 -1.0805 0.5940

O -3.0773 -1.6736 0.8808

O -0.8508 -1.5471 0.8366

C 0.3126 3.0625 -0.7661

O 0.6002 3.6244 -1.8060

O 1.0073 3.2586 0.3464

H 0.7327 2.7200 1.1527

C -0.4326 1.8461 3.3648

H -0.2742 1.2033 4.2374

H -0.5905 2.8717 3.7052

H -1.3240 1.5068 2.8250

O 0.7325 1.8565 2.5254

H 0.8644 0.9592 2.1540

O -5.7664 -1.3732 0.2573

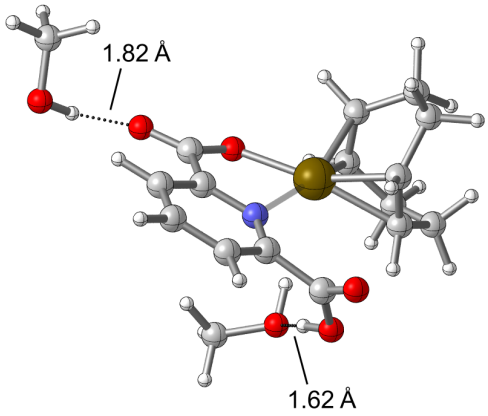
H -4.8613 -1.4784 0.6080

C -5.9279 -2.3626 -0.7476

H -5.1935 -2.2672 -1.5619

H -5.8546 -3.3843 -0.3448

H -6.9267 -2.2434 -1.1809



Comp 4c…MeOH

E=-1273.15920614

C -2.8601 -0.5886 0.1758

C -2.8307 0.6993 -2.0758

C -1.0811 1.8305 -0.5519

C -2.4293 1.4544 1.6382

C -2.6102 -0.5191 -1.2034

C -2.2907 2.0115 -1.4646

C -1.1626 1.6157 0.8239

C -3.4837 0.5425 0.9820

H -2.9501 -1.5857 0.6019

H -3.9023 0.7951 -2.2976

H -2.0058 2.6861 -2.2771

H -0.1341 2.2172 -0.9255

H -2.8523 2.4477 1.8433

H -4.1156 0.1064 1.7611

H -2.5384 -1.4631 -1.7388

H -2.3311 0.5122 -3.0309

H -3.0777 2.5224 -0.9024

H -0.2953 1.8837 1.4156

H -2.1398 1.0327 2.6039

H -4.1478 1.1222 0.3345

Ir -0.6757 -0.3968 -0.1278

N 1.4649 -0.6311 -0.0338

C 1.8304 -1.7509 -0.7079

C 2.4194 0.1943 0.4407

C 3.1532 -2.0292 -1.0202

C 3.7659 -0.0130 0.1214

C 4.1385 -1.1231 -0.6288

H 3.3790 -2.9448 -1.5537

H 4.4991 0.6953 0.4894

H 5.1804 -1.2953 -0.8798

C 0.7302 -2.7466 -0.9909

O 0.9765 -3.8204 -1.5239

O -0.4544 -2.3888 -0.5565

C 2.0565 1.2750 1.4533

O 1.3921 0.8736 2.4548

O 2.4944 2.4274 1.2468

H 2.2823 2.9633 -0.4261

C 1.7623 4.6841 -1.1676

H 1.4346 5.0733 -2.1379

H 0.9788 4.9161 -0.4296

H 2.6711 5.2335 -0.8755

O 1.9934 3.2929 -1.3058

H -0.4328 -0.1428 -1.6414

O -0.5055 -0.8722 2.1096

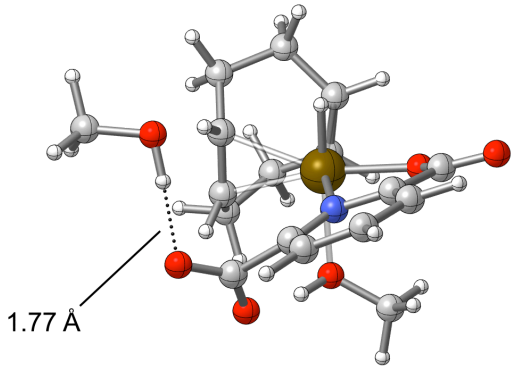
H 0.2720 -0.2672 2.3349

C -0.2225 -2.2025 2.5654

H 0.6904 -2.6080 2.1162

H -0.1100 -2.1884 3.6550

H -1.0659 -2.8429 2.3027



Comp 4a

E=-1157.41871089

Ir 0.6341 -0.2141 0.2419

O -2.0006 -3.5536 -0.1983

O -0.2650 -2.2912 0.4836

O -0.5672 2.6352 0.4614

O -2.4988 3.4889 -0.2020

N -1.6125 -0.0046 -0.1399

C -1.4437 -2.4703 -0.0067

C -2.2188 -1.1965 -0.3373

C -3.5349 -1.3016 -0.7884

H -3.9469 -2.2939 -0.9259

C -4.2623 -0.1457 -1.0415

H -5.2842 -0.1952 -1.4036

C -3.6544 1.0819 -0.8001

H -4.1779 2.0177 -0.9472

C -2.3346 1.1251 -0.3434

C -1.7917 2.5114 -0.0326

C 1.1570 -0.6635 -1.7530

H 0.3406 -1.2131 -2.2235

C 2.4954 -1.3886 -1.7815

H 2.9558 -1.2944 -2.7760

H 2.2876 -2.4546 -1.6391

C 3.4567 -0.9071 -0.6711

H 4.1104 -1.7348 -0.3782

H 4.1183 -0.1186 -1.0453

C 2.6876 -0.4087 0.5585

H 2.8851 -0.9689 1.4738

C 2.3010 0.9770 0.7362

H 2.2291 1.3155 1.7723

C 2.6364 2.0914 -0.2448

H 2.1187 2.9978 0.0856

H 3.7113 2.3228 -0.2192

C 2.1773 1.7328 -1.6706

H 3.0002 1.3009 -2.2489

H 1.8706 2.6378 -2.2047

C 1.0032 0.7496 -1.6496

H -0.0562 1.7576 0.4411

H 0.0646 1.1517 -2.0277

C -0.5263 0.3575 3.2225

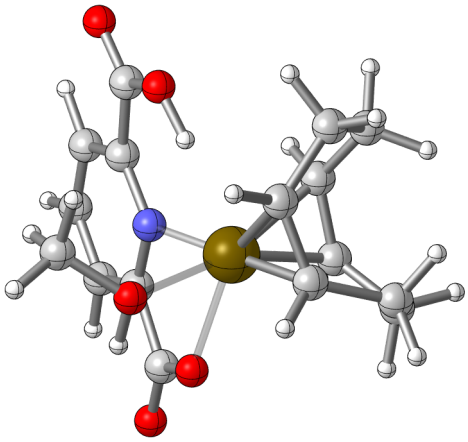
H -1.5272 0.4818 2.8001

H -0.5954 -0.0609 4.2304

H -0.0153 1.3191 3.2630

O 0.2848 -0.5193 2.4065

H -0.1428 -1.3959 2.3403



Comp 4b

E=1157.40536698

Ir 0.5201 -0.0814 0.2805

O -0.0173 -2.1858 0.2189

O -1.7424 -3.5404 -0.2651

O -1.2930 2.8132 1.0338

O -1.4999 3.2241 -1.1915

N -1.5216 0.0222 -0.1916

C -1.2480 -2.4232 -0.1391

C -2.1035 -1.1943 -0.3830

C -3.4309 -1.3178 -0.7589

H -3.8398 -2.3131 -0.8847

C -4.1841 -0.1599 -0.9681

H -5.2238 -0.2253 -1.2741

C -3.5779 1.0742 -0.7848

H -4.1209 1.9977 -0.9523

C -2.2384 1.1550 -0.3745

C -1.6030 2.5367 -0.1518

C 1.0137 -0.2984 -1.8046

H 0.0899 -0.5222 -2.3369

C 2.0898 -1.3570 -1.9547

H 2.5582 -1.2632 -2.9440

H 1.5906 -2.3290 -1.9319

C 3.1571 -1.3133 -0.8400

H 3.5903 -2.3106 -0.7222

H 3.9808 -0.6494 -1.1165

C 2.5885 -0.8729 0.5052

H 2.4831 -1.6548 1.2544

C 2.5892 0.4485 0.9649

H 2.4894 0.5986 2.0377

C 3.0983 1.6472 0.1874

H 2.7573 2.5453 0.7103

H 4.1963 1.6617 0.2217

C 2.6024 1.6939 -1.2744

H 3.3164 1.2039 -1.9429

H 2.5453 2.7379 -1.5949

C 1.2269 1.0603 -1.4726

H 0.5273 1.4426 0.6289

H 0.4284 1.7507 -1.7310

O 0.0534 -0.4624 2.3761

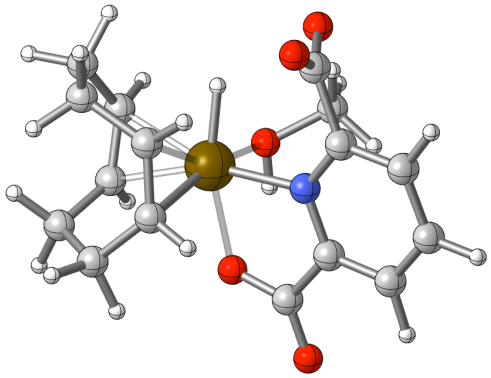
H -0.0402 -1.4296 2.4417

C -1.0803 0.1765 3.0373

H -0.8765 0.1995 4.1108

H -1.9980 -0.3834 2.8421

H -1.1596 1.1828 2.6242



TS' 4-4c

E=-1273.13904951

C -2.4152 1.3183 0.3096

C -3.1966 -0.9819 1.2221

C -1.7090 -1.4306 -0.8056

C -2.3865 0.6772 -2.1579

C -2.4313 0.3218 1.3043

C -3.0710 -1.6604 -0.1582

C -1.4128 -0.3981 -1.7104

C -3.2065 1.2803 -0.9933

H -2.0951 2.3077 0.6327

H -4.2523 -0.8074 1.4737

H -3.2170 -2.7384 -0.0394

H -1.0687 -2.3042 -0.8372

H -3.0566 0.2678 -2.9271

H -3.4947 2.3035 -1.2524

H -2.1536 0.6308 2.3114

H -2.7993 -1.6508 1.9913

H -3.8621 -1.3176 -0.8306

H -0.5862 -0.5779 -2.3965

H -1.8038 1.4714 -2.6307

H -4.1379 0.7275 -0.8453

Ir -0.5392 0.2125 0.2031

N 1.5430 -0.2044 -0.1172

C 2.2978 0.7821 0.4414

C 2.1564 -1.1638 -0.8438

C 3.6633 0.8865 0.2299

C 3.5292 -1.0877 -1.1182

C 4.2906 -0.0555 -0.5873

H 4.2011 1.6947 0.7108

H 3.9755 -1.8566 -1.7387

H 5.3554 0.0071 -0.7897

C 1.5880 1.7299 1.3810

O 2.2065 2.6256 1.9450

O 0.3154 1.4825 1.5559

C 1.3959 -2.3914 -1.3417

O 1.3673 -2.5656 -2.5676

O 0.9284 -3.1558 -0.4322

H 0.4309 -2.7104 0.9152

C 0.8335 -2.1897 2.8506

H 0.2856 -1.7206 3.6708

H 1.1918 -3.1717 3.1756

H 1.6923 -1.5631 2.5860

O -0.0698 -2.3540 1.7474

H -0.4443 -1.1599 1.1943

O 0.2797 2.3410 -1.5099

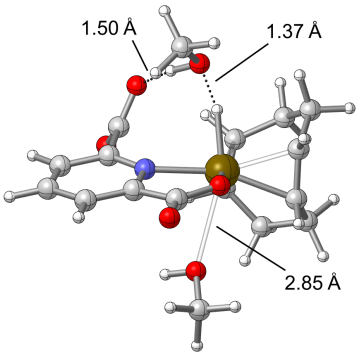
H 0.8892 1.9921 -2.1768

C 0.6293 3.7051 -1.2548

H 1.6360 3.8015 -0.8303

H 0.5684 4.3088 -2.1693

H -0.0916 4.0946 -0.5327



TS' 4a-4b

E=-1157.40370028

Ir 0.5487 -0.1004 0.2505

O -0.0366 -2.2546 0.3846

O -1.7499 -3.6008 -0.1729

O -0.7264 2.6797 0.6395

O -2.3654 3.4193 -0.7124

N -1.5208 -0.0332 -0.1842

C -1.2408 -2.4889 -0.0350

C -2.0885 -1.2580 -0.3394

C -3.4162 -1.4074 -0.7198

H -3.8083 -2.4120 -0.8214

C -4.1842 -0.2698 -0.9535

H -5.2225 -0.3539 -1.2595

C -3.5963 0.9771 -0.7794

H -4.1418 1.8971 -0.9444

C -2.2594 1.0876 -0.3791

C -1.7204 2.5257 -0.1416

C 1.0414 -0.4205 -1.7999

H 0.1439 -0.7491 -2.3236

C 2.2012 -1.3976 -1.8873

H 2.6634 -1.3360 -2.8824

H 1.7797 -2.4031 -1.7985

C 3.2549 -1.1940 -0.7772

H 3.7660 -2.1430 -0.5910

H 4.0256 -0.4883 -1.0993

C 2.6318 -0.7084 0.5300

H 2.6126 -1.4342 1.3412

C 2.5136 0.6486 0.8913

H 2.4122 0.8633 1.9537

C 2.9566 1.8256 0.0424

H 2.5444 2.7309 0.4974

H 4.0504 1.9224 0.0855

C 2.4723 1.7278 -1.4176

H 3.2236 1.2441 -2.0485

H 2.3367 2.7358 -1.8203

C 1.1486 0.9735 -1.5487

H 0.3120 1.4647 0.4859

H 0.3060 1.5788 -1.8725

O 0.1322 -0.3944 2.3900

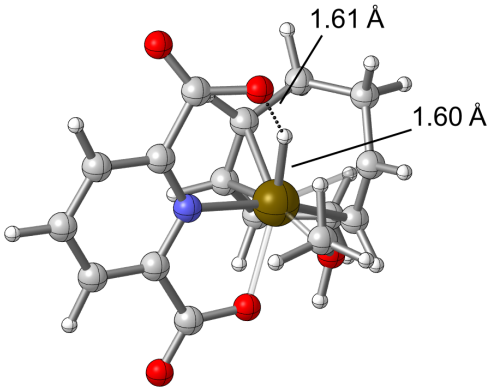
H -0.0622 -1.3486 2.4360

C -0.9037 0.3461 3.0907

H -0.7176 0.2684 4.1650

H -1.8932 -0.0504 2.8511

H -0.8289 1.3804 2.7582



TS' 4c-1

E=-1157.39496738

Ir -0.5072 -0.2432 0.1282

O 1.9233 3.5049 -0.6111

O 1.0304 2.4960 1.1926

O 0.3282 -2.1897 0.6793

O 1.9892 -3.5207 -0.0583

N 1.5494 0.0128 -0.2484

C 1.6584 2.5114 0.0745

C 2.2320 1.1696 -0.4022

C 3.5409 1.1506 -0.8945

H 4.0439 2.0991 -1.0403

C 4.1700 -0.0615 -1.1585

H 5.1856 -0.0835 -1.5413

C 3.4901 -1.2461 -0.8773

H 3.9449 -2.2232 -0.9886

C 2.1836 -1.1773 -0.4133

C 1.4519 -2.4218 0.0774

C -1.2151 1.4416 -0.8907

H -0.4316 2.1465 -1.1645

C -2.3918 2.1391 -0.2279

H -2.9405 2.7662 -0.9447

H -1.9610 2.8203 0.5130

C -3.3392 1.1509 0.4797

H -3.7911 1.6311 1.3527

H -4.1656 0.8625 -0.1765

C -2.6026 -0.0972 0.9424

H -2.4141 -0.1738 2.0097

C -2.4881 -1.2696 0.1935

H -2.2678 -2.1915 0.7269

C -3.0405 -1.4558 -1.2117

H -2.6115 -2.3800 -1.6119

H -4.1246 -1.6197 -1.1498

C -2.7231 -0.3010 -2.1858

H -3.4916 0.4757 -2.1593

H -2.7078 -0.6907 -3.2072

C -1.3639 0.3492 -1.8808

H -0.6728 -0.7225 -1.4736

H -0.7067 0.4564 -2.7467

C 0.7599 -0.2968 3.0032

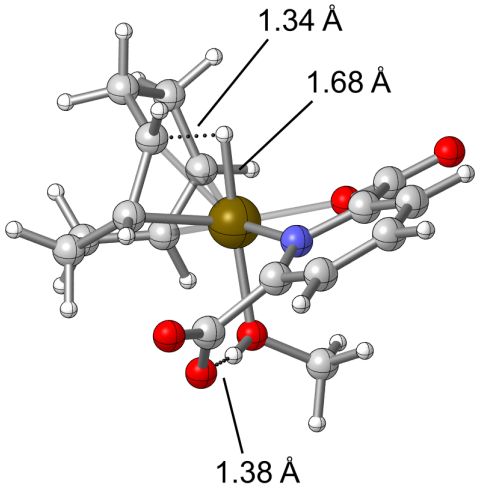
H 1.7230 -0.6081 2.5870

H 0.9328 0.3301 3.8844

H 0.1943 -1.1820 3.2980

O -0.0173 0.4665 2.0692

H 0.5060 1.3526 1.7564



TS' 4b-1

E=-1157.39249877

Ir 0.5165 -0.2080 0.1871

O -0.1276 -2.2006 0.2243

O -1.8759 -3.4984 -0.3171

O -0.8453 2.6195 1.0228

O -1.8737 3.4879 -0.8030

N -1.5312 0.0487 -0.2006

C -1.3599 -2.3960 -0.1745

C -2.1617 -1.1371 -0.4195

C -3.4941 -1.2057 -0.7950

H -3.9397 -2.1824 -0.9423

C -4.2055 -0.0175 -0.9681

H -5.2472 -0.0359 -1.2736

C -3.5552 1.1871 -0.7384

H -4.0564 2.1392 -0.8645

C -2.2145 1.2094 -0.3292

C -1.5707 2.5755 -0.0075

C 1.0273 0.2822 -1.7619

H 0.1463 0.3824 -2.3974

C 2.0753 -0.6409 -2.3627

H 2.5628 -0.1626 -3.2238

H 1.5413 -1.5125 -2.7560

C 3.1208 -1.1095 -1.3291

H 3.4772 -2.1084 -1.5963

H 3.9972 -0.4553 -1.3381

C 2.5437 -1.1622 0.0787

H 2.3389 -2.1533 0.4754

C 2.6041 -0.1107 0.9953

H 2.4744 -0.3580 2.0464

C 3.2192 1.2514 0.7234

H 2.9253 1.9123 1.5445

H 4.3136 1.1691 0.7658

C 2.7719 1.8862 -0.6092

H 3.4397 1.6104 -1.4300

H 2.8206 2.9748 -0.5200

C 1.3386 1.4877 -0.9848

H 0.7026 1.4077 0.3630

H 0.6776 2.3281 -1.1897

O 0.0072 -0.6183 2.4226

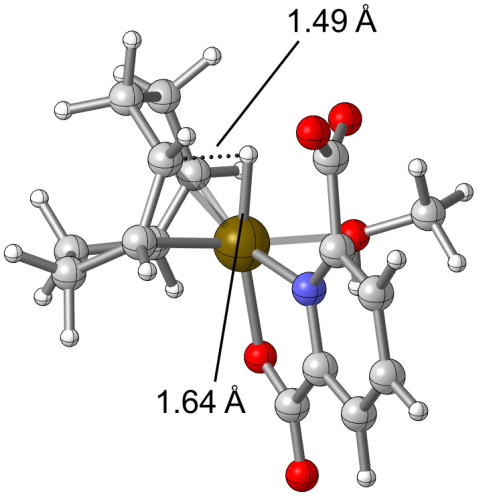
H -0.1836 -1.5708 2.4383

C -1.0436 0.0912 3.1209

H -0.8577 0.0406 4.1986

H -2.0237 -0.3415 2.8986

H -1.0119 1.1218 2.7672



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