

Cartesian xyz-coordinates

Numeric ligand IDs are adapted from the LKB-P (Ref. (9)). Alphabetic species IDs correspond to Figure 2B in the main manuscript.

15_A

P -0.000121 3.8e-05 -1.200975
 C 0.744967 1.575495 -0.458485
 C 1.267737 1.533444 0.98683
 C 1.834314 2.055559 -1.435632
 H -0.084215 2.298369 -0.499968
 C 1.691462 2.902963 1.538144
 H 2.119342 0.842395 1.045385
 H 0.496814 1.128438 1.486737
 H 2.681588 1.357369 -1.446822
 H 1.447658 2.120295 -2.456757
 H 1.965029 2.827605 2.596867
 H 0.871281 3.627328 1.457005
 C 0.991796 -1.432835 -0.458222
 C 0.694668 -1.86427 0.990204
 C 0.862398 -2.616538 -1.435016
 H 2.032448 -1.076326 -0.500242
 C 1.668993 -2.916144 1.53813
 H -0.3296 -2.256165 1.046553
 H 0.729924 -0.99414 1.649278
 H -0.165811 -3.001453 -1.445368
 H 1.110955 -2.314197 -2.456387
 H 1.467621 -3.115206 2.597015
 H 2.706429 -2.568268 1.456238
 C -1.736883 -0.142645 -0.457985
 C -1.961813 0.331459 0.990107
 C 2.697778 0.560081 -1.435144
 H -1.947997 -1.22225 -0.499098
 C -3.359636 0.013511 1.538705
 H -1.789444 1.414552 1.045503
 H -1.225515 -0.133269 1.649384
 H -2.517336 1.643031 -1.446568
 H -2.560426 0.192741 -2.456215
 H -3.431191 0.28841 2.597347
 H -3.57663 -1.059041 1.45789
 H -4.14788 0.553896 1.005311
 H -3.745147 0.403626 -1.155451
 H -2.222987 3.040683 -1.156079
 H -2.553798 3.315138 1.004906
 H -1.521597 -3.44551 -1.155819
 H -1.594186 -3.86908 1.005055

Zero-point correction = 0.372447

Thermal correction to Energy = 0.391065
 Thermal correction to Enthalpy = 0.39201
 Thermal correction to Gibbs Free Energy = 0.326395
 E(RB3LYP(GD3BJ)/6-31G(d) + SDD) = - 814.957361064
 CPCM(Toluene): E(RB3LYP(GD3BJ)/6-311++G(d,p) + SDD) = -815.130467999

15_B

Pd 2.447422 -0.000498 -0.000352
 P 0.207794 0.000104 -0.00017
 C -0.506391 -0.344023 1.71738
 C -1.968618 -0.826456 1.792077
 C 0.433207 -1.3112 2.457194
 H -0.4404315 0.636347 2.212195
 C -2.530142 -0.86269 3.219977
 H -2.039506 -1.828428 1.349088
 H -2.611199 -0.175954 1.196337
 H 0.418755 -2.302839 1.988668
 H 1.464851 -0.948993 2.426706
 H -3.595501 -1.119183 3.206928
 H -2.428991 0.116462 3.704411
 C -0.506712 -1.314878 -1.157205
 C -1.969669 -1.139704 -1.610316
 C 0.431647 -1.47004 -2.365967
 H -0.438971 -2.233942 -0.556254
 C -2.530771 -2.35854 -2.355404
 H -2.042491 -0.254866 -2.256059
 H -2.611261 -0.950231 -0.748211
 H 0.415691 -0.567749 -2.990151
 H -1.463771 -1.624029 -2.038254
 H -3.596612 -2.220193 -2.569377
 H -2.427636 -3.267807 -1.750205
 C -0.506293 1.659981 -0.56036
 C -1.969383 1.96478 -0.182247
 C 0.432047 2.784242 -0.09007
 H -0.438192 1.599589 -1.656734
 C -2.529741 3.220972 -0.863091
 H -2.042603 2.079662 0.907117
 H -2.611383 1.124292 -0.451032
 H 0.415533 2.873737 1.003392
 H 1.464284 2.57723 -0.386815
 H -3.595488 3.337392 -0.635962
 H -2.426786 3.153298 -1.953262
 H 0.131724 -2.317167 -2.991832
 H -2.023366 -2.532614 -3.308904
 H 0.133092 -1.429173 3.503765
 H -2.021504 -1.600161 3.847949
 H 0.132394 3.749786 -0.51102
 H -2.021679 4.132834 -0.535545

Zero-point correction = 0.373821

Thermal correction to Energy = 0.394353

Thermal correction to Enthalpy = 0.395297

Thermal correction to Gibbs Free Energy = 0.324029
 E(RB3LYP(GD3BJ)/6-31G(d) + SDD) = - 942.923815002
 CPCM(Toluene): E(RB3LYP(GD3BJ)/6-311++G(d,p) + SDD) = -943.096857026

15_C

Pd 0.000304 2.1e-05 -0.001044
 P 2.318699 0.000205 -0.000149
 P -2.318207 -0.000222 -0.000551
 C 3.032057 1.675296 0.503663
 C 4.492249 1.978703 0.118278
 C 2.078137 2.770088 -0.006316
 H 2.962456 1.6544 1.601791
 C 5.040517 3.266037 0.748393
 H 4.567482 2.050255 -0.974838
 H 5.13959 1.153177 0.42105
 H 2.102056 2.827022 -1.102203
 H 1.046779 2.550209 0.285969
 H 6.104731 3.386523 0.515656
 H 4.939005 3.240103 1.840598
 C 3.031831 -1.273336 1.199184
 C 4.491725 -1.090796 1.655441
 C 2.077352 -1.379224 2.401837
 H 2.962827 -2.213991 0.632105
 C 5.040262 2.280536 0.2454505
 H 4.566091 -0.180403 2.264811
 H 5.139433 -0.939057 0.789621
 H 2.101143 -0.458767 2.999316
 H 1.046121 -1.522256 2.064832
 H 6.104201 -2.138661 2.676183
 H 4.93988 -3.212958 1.884942
 C 3.03308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 H 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 H 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H 1.047865 -0.267123 -2.352091
 H 6.106067 -1.248548 -3.188382
 H 4.941557 -0.027001 -3.724632
 C -3.01844 -1.727394 -0.276189
 H 4.93988 -3.212958 1.884942
 H -1.796116 3.059381 -1.960319
 C 5.030308 -0.40146 -1.702245
 C 4.493014 -0.887698 -1.771378
 C 2.079149 -1.390038 -2.396048
 C 2.964419 0.560006 -2.233331
 C 5.042055 -0.985958 -3.200995
 H 4.567379 -1.870221 -1.286839
 C 5.140423 -0.213139 -1.207448
 H 2.102644 -2.367742 -1.8977
 H

C 6.451174 0.98663 -3.447926
 H 6.697218 1.843481 -4.069779
 C 7.116645 -0.206272 -3.596211
 C 6.765204 -1.307657 -2.780894
 H 7.903217 -0.309339 -4.338143
 C 5.77532 -1.195313 -1.831494
 H 7.280506 -2.255523 -2.90656
 H 5.523087 -2.05721 -1.228575
 Zero-point correction = 1.038375
 Thermal correction to Energy = 1.099975
 Thermal correction to Enthalpy = 1.10092
 Thermal correction to Gibbs Free Energy = 0.944316
 E(RB3LYP(GD3BJ)/6-31G(d) + SDD) = -3005.26925098
 CPCM(Toluene): E(RB3LYP(GD3BJ)/6-311++G(d,p) + SDD) = -3005.9077653
 187_G
 Pd 1.643491 0.63531 -0.395389
 P 3.749217 0.807972 -1.479414
 Pd -2.056456 -1.25607 -0.604433
 P -3.920644 -1.426649 0.821275
 I 0.208103 -0.927879 -2.1265
 I -0.672351 0.395347 1.032453
 I 2.184754 2.419049 1.583347
 I -2.726119 -3.083089 -2.484951
 C 5.113996 0.09958 -0.45064
 C 6.435908 0.491485 -0.822589
 C 4.946337 -0.844251 0.567874
 C 7.55054 -0.030243 -0.223981
 H 6.566388 1.225678 -1.604129
 C 6.11652 -1.452906 -1.157913
 C 3.633915 -1.286761 1.139965
 C 7.426591 -1.029782 0.770305
 H 8.54105 0.304463 -0.520711
 C 3.296475 -0.918105 2.486878
 C 2.821534 -2.178832 0.464893
 C 1.653389 -2.716961 1.053538
 H 3.098745 -2.502472 -0.52664
 C 1.306364 -2.363309 2.332583
 H 1.031294 -3.392587 0.474726
 H 0.407814 -2.761681 2.793581
 C -4.577908 0.258835 1.230579
 C -5.294621 0.362352 0.460819
 C -4.546928 1.367376 0.368887
 C -5.992023 1.485902 2.81512
 H -5.295537 -0.477813 3.139396
 C -5.37467 2.509768 0.681656
 C -3.661915 1.518443 -0.830924
 C -6.085503 2.578078 1.920525
 H -6.507596 1.533997 3.770582
 C -2.63041 2.522763 -0.807239
 C -3.837493 0.770989 -1.980755
 C -1.800372 2.688374 -1.96301
 C -3.028418 0.95479 -3.125559
 H -4.626911 0.040844 -2.027213
 C -2.02906 1.893654 -3.115487
 H -3.189459 0.31917 -3.990028
 H -1.383296 2.027455 -3.979086
 C 4.169359 2.666949 -1.851273
 C 5.050237 2.970484 -3.079987
 C 2.804321 3.341438 -2.102634
 C 4.878509 3.313623 -0.644156
 H 6.062051 2.567864 -2.998096
 H 4.613989 2.637911 -4.022433
 H 5.1495 4.061424 -3.138759
 H 2.147483 3.277992 -1.236416
 H 2.969907 4.401602 -2.333844
 H 2.284425 2.888733 -2.953161
 H 4.803153 4.403419 -0.746828
 H 4.433732 3.042651 0.309623
 H 5.939382 3.054471 -0.615326
 C 3.965348 -0.189254 -3.124315
 C 3.694987 -1.675311 -2.832958
 C 2.969072 0.345346 -4.170379
 C 5.387372 -0.162089 -3.72517
 H 4.444635 -2.078015 -2.145267
 H 2.70449 -1.861061 -2.426692
 H 3.774196 -2.232978 -3.774014
 H 3.277488 1.313764 -4.570588
 H 2.92264 -0.357358 -5.011282
 H 1.958226 0.4525 -3.775201
 H 5.367402 -0.780654 -4.631161
 H 5.72929 0.826311 -4.019795
 H 6.122056 -0.601876 -3.047654
 C -3.339456 -2.330176 2.442499
 C -4.430388 -3.002534 3.303038
 C -2.373334 -3.431092 1.951411
 C -2.564941 -1.383291 3.381304
 H -5.097274 -2.285215 3.787601
 H -5.036212 -3.725757 2.761855
 H -3.918862 -3.548252 4.105113
 H -1.54411 -3.00442 1.380913
 H -1.96403 -3.957613 2.823306
 H -2.86892 -4.167275 1.313425
 H -2.392004 -1.909382 4.32853
 H -1.592033 -1.114457 2.979463
 H -3.106166 -0.461856 3.608527
 C -5.549566 -2.308551 0.237406
 C -5.981327 -1.722427 -1.116415
 C -5.322715 -3.822773 0.069884
 C -6.740121 -2.066743 1.190714