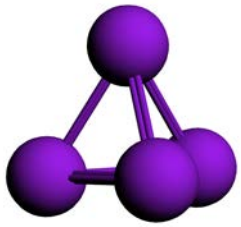
Electronic Supplementary Material (ESI) for Dalton Transactions


# Symmetrical $P_4$ Cleavage at Cobalt Half Sandwich Complexes [($\eta^5$-$C_5H_5$)Co(L)] (L = CO, NHC) – A Computational Case Study on the Mechanism of Symmetrical $P_4$ Degradation to $P_2$ Ligands

**Bartosz Zarzycki,[a] F. Matthias Bickelhaupt[a,b] and Udo Radius*[a]**

## Supporting Information

### $P_4$ Tetrahedron

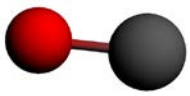


Cartesian coordinates:

P -0.792498 -0.792498 -0.792498
P -0.792498 0.792498 0.792498
P 0.792498 -0.792498 0.792498
P 0.792498 0.792498 -0.792498

NIMAG = 0
Total bonding energy: -1764.99 kJ/mol

### CO



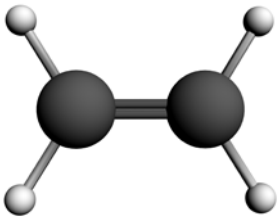
Cartesian coordinates:

C 0.0 0.0 -0.54727
O 0.0 0.0 0.589162

NIMAG = 0

Total bonding energy: -1392.62 kJ/mol

**Ethene**



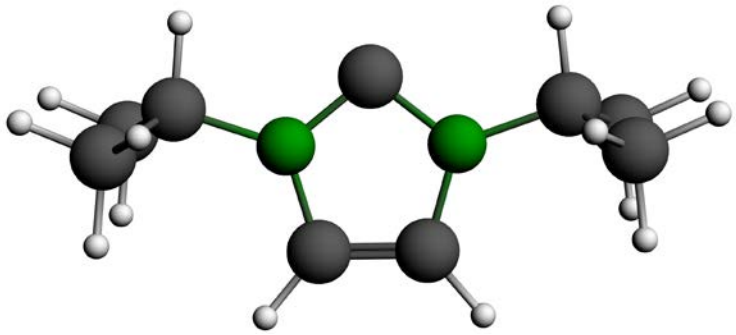
Cartesian coordinates:

C 0.0 0.666928 0.0
C 0.0 -0.666928 0.0
H -0.926207 -1.23981 0.0
H 0.926207 -1.23981 0.0
H -0.926207 1.23981 0.0
H 0.926207 1.23981 0.0

NIMAG = 0

Total bonding energy: -2963.80 kJ/mol

*i*$Pr_2$Im



Cartesian coordinates:

C 1.00668 -0.300717 0.0
N 0.236408 0.0867 -1.07251
N 0.236408 0.0867 1.07251
C -0.962411 0.692471 0.681083
C -0.962411 0.692471 -0.681083
C 0.675358 -0.114894 -2.47224
C -0.313963 -1.00453 -3.24952
C 0.934351 1.23264 -3.17522
C 0.675358 -0.114894 2.47224
C 0.934351 1.23264 3.17522
C -0.313963 -1.00453 3.24952
H -1.70493 1.06619 -1.37163
H -1.70493 1.06619 1.37163
H 1.62493 -0.647677 -2.36613
H 1.62493 -0.647677 2.36613
H -0.457699 -1.96288 -2.73812
H 0.0728219 -1.20241 -4.25678
H -1.2929 -0.519211 -3.35668
H 0.00566379 1.80565 -3.29696
H 1.35699 1.06149 -4.17293
H 1.64116 1.83845 -2.59751
H 0.00566379 1.80565 3.29696
H 1.64116 1.83845 2.59751
H 1.35699 1.06149 4.17293
H -0.457699 -1.96288 2.73812
H 0.0728219 -1.20241 4.25678
H -1.2929 -0.519211 3.35668

NIMAG = 0

Total bonding energy: -14273.95 kJ/mol

[CpCo(CO)]-Fragment

Cartesian Coordinates:

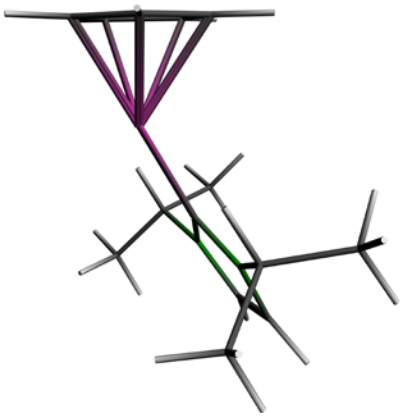
H 1.65176 2.00012 0.0
H -0.0256707 -1.80942 -1.35174
C -2.68054 0.239949 0.0
H 0.995453 0.540653 -2.19176
H 0.995453 0.540653 2.19176
Co -0.95955 0.733398 0.0
C 0.334371 -1.00932 -0.717311
C 0.863855 0.236416 -1.1604
C 1.18949 1.02038 0.0
C 0.863855 0.236416 1.1604
C 0.334371 -1.00932 0.717311
H -0.0256707 -1.80942 1.35174
O -3.76796 -0.169339 0.0

NIMAG = 0

Total bonding energy: -7727.98 kJ/mol

<S*S> = 2.02007

[CpCo(iPr$_2$Im)]-Fragment



Cartesian Coordinates:

C -0.210693 2.47451 0.680864
N 0.0740495 1.17142 1.08621
C 0.2312 0.327725 0.0
N 0.0740495 1.17142 -1.08621
C -0.210693 2.47451 -0.680864
Co 0.550574 -1.60499 0.0
C -1.1313 -2.94861 -0.716389
C 0.1375 -3.43475 -1.15998
C 0.928106 -3.74 0.0
C 0.1375 -3.43475 1.15998
C -1.1313 -2.94861 0.716389
C 0.177972 0.720536 -2.49567
C 1.35152 1.40999 -3.21833
C 0.177972 0.720536 2.49567
C 1.35152 1.40999 3.21833
C -1.16066 0.903925 -3.23565
C -1.16066 0.903925 3.23565
H -1.95125 -2.63439 -1.35121
H 0.439158 -3.58002 -2.19106
H 1.92226 -4.17128 0.0
H 0.439158 -3.58002 2.19106
H -1.95125 -2.63439 1.35121
H -0.384799 3.2844 -1.37331
H -0.384799 3.2844 1.37331
H 0.388535 -0.352249 -2.40736
H -1.08392 0.490716 -4.24888
H -1.96893 0.384204 -2.70971
H -1.42999 1.96466 -3.32646
H 1.46065 0.998256 -4.22912
H 2.29023 1.25028 -2.67629
H 1.18586 2.49136 -3.31353
H 0.388535 -0.352249 2.40736
H -1.08392 0.490716 4.24888
H -1.96893 0.384204 2.70971

H -1.42999 1.96466 3.32646
H 1.46065 0.998256 4.22912
H 2.29023 1.25028 2.67629
H 1.18586 2.49136 3.31353

NIMAG = 0

Total bonding energy: -20604.64 kJ/mol

<S*S> = 2.01966

[CpCo(CO)($\eta^2$-$C_2H_4$)]

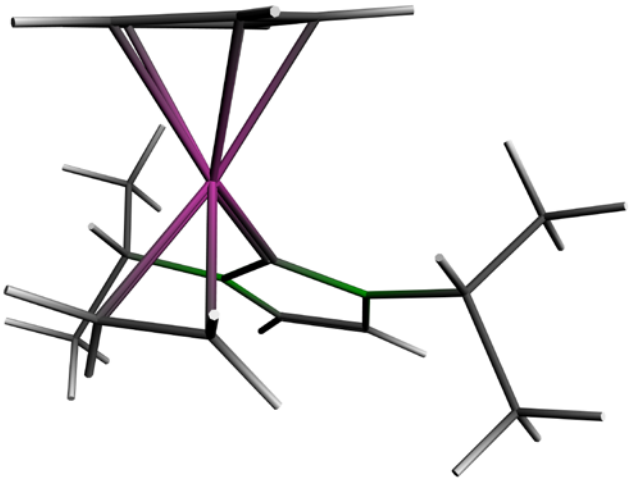
Cartesian coordinates:

H -1.21505 0.252233 2.43102
H -1.93093 -1.14 -1.96465
C -0.116522 1.11976 -0.000356203
H -1.80873 -2.97855 0.00612385
H 0.794807 -3.41165 0.580637
Co -0.00710236 -0.615596 0.194805
C 0.802999 -0.502938 2.10349
C -0.60686 -0.614635 2.18529
H 2.30496 -1.89756 -1.07856
H 0.60988 -0.442685 -2.60605
H -1.06849 -1.57183 2.42092
H 1.28948 0.452409 2.28387
C 0.423207 -2.73048 -0.175496
C -0.967379 -2.5071 -0.48587
C -1.03328 -1.54019 -1.51183
C 0.32806 -1.16177 -1.84683
C 1.2242 -1.93225 -1.04852
H 1.43507 -1.3711 2.27847
O -0.164615 2.27565 -0.139661

NIMAG = 0

Total bonding energy: -10785.85 kJ/mol

[CpCo(iPr$_2$Im)(η$^2$-C$_2$H$_4$)]



Cartesian coordinates:

C -0.674279 2.92185 -0.3515
N -1.08741 1.61207 -0.104001
C -0.00572957 0.760822 0.0453504
N 1.08607 1.60223 -0.103578
C 0.684983 2.91522 -0.352017
Co -0.00752698 -1.13307 0.318912
C 0.704616 -1.01384 2.22839
C -0.726072 -1.0446 2.22966
C 2.50169 1.15665 -0.0423303
C 3.27833 1.91352 1.05297
C -2.50596 1.18028 -0.0357024
C -3.25946 1.91933 1.08741
C 0.553843 -3.22113 -0.106555
C -0.861723 -3.08384 -0.304491
C -1.08171 -2.13995 -1.34143
C 0.216021 -1.66982 -1.76603
C 1.22779 -2.37116 -1.03565
C 3.18075 1.2721 -1.42182
C -3.1975 1.33809 -1.40422
H -2.03679 -1.84577 -1.75764
H -1.62814 -3.61095 0.251437
H 1.0267 -3.87256 0.618747
H 2.29856 -2.28554 -1.17254
H 0.391962 -0.94566 -2.55375
H 1.38235 3.72537 -0.502358
H -1.36388 3.7385 -0.502338
H 2.42529 0.0995981 0.231943
H 4.20044 0.870492 -1.36864
H 2.62689 0.706159 -2.17844
H 3.24904 2.31732 -1.75186
H 4.29023 1.49931 1.14007
H 2.78252 1.81683 2.02461

H 3.37611 2.98203 0.818662
H -2.43659 0.11586 0.211519
H -4.21803 0.938591 -1.35275
H -2.65204 0.792528 -2.18174
H -3.26502 2.39251 -1.70365
H -4.27584 1.51697 1.17687
H -2.75304 1.79125 2.04993
H -3.34393 2.99475 0.880846
H -1.28098 -0.138334 2.47048
H -1.24719 -1.96166 2.50588
H 1.21953 -0.0830215 2.46519
H 1.26734 -1.90582 2.50517

NIMAG = 0

Total bonding energy: -23643.05 kJ/mol

[CpCo(CO)($\eta^1$-$P_4$)] **1CO**

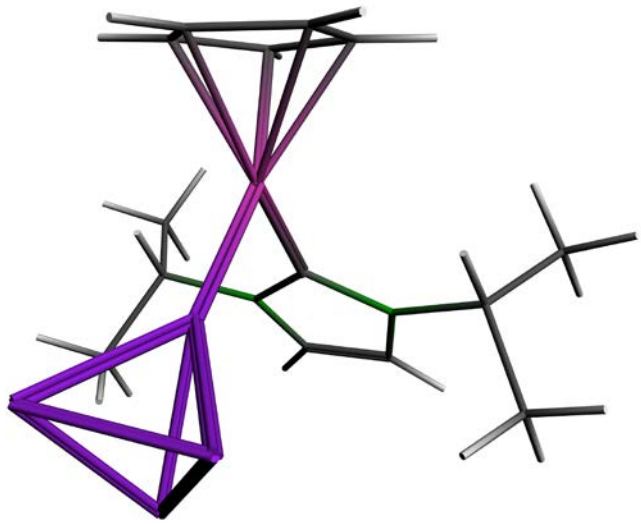
Cartesian coordinates:

P -1.55248 0.0770631 -3.23898
P -0.108984 -0.115456 -1.55711
C -0.405129 -3.15323 -0.0149066
C -0.724943 -2.78453 1.3099
C 0.513583 -2.40826 1.95035
C 1.60756 -2.64453 1.03052
C 1.03817 -3.07247 -0.185419
Co 0.246797 -1.07867 0.347174
H -1.10837 -3.45249 -0.782105
H -1.71006 -2.75513 1.75524
H 0.615584 -2.07073 2.97447
H 2.65799 -2.49011 1.2378
H 1.57316 -3.29929 -1.09912
P 0.696868 0.203691 -3.60609
P -0.372619 1.86732 -2.48983
C 0.321424 0.438611 1.22373
O 0.381077 1.44001 1.81642

NIMAG = 0

Total bonding energy: -9547.02 kJ/mol

[CpCo(iPr$_2$Im)($\eta^1$-P$_4$)] **1NHC**



Cartesian coordinates:

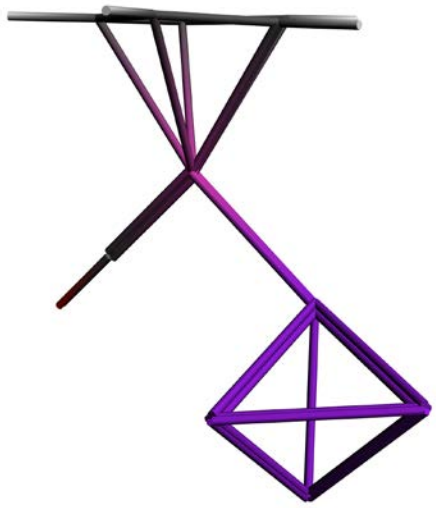
P 0.997339 -4.70828 0.768693
P 0.732209 -2.53266 0.389278
C -0.89375 -0.334114 3.12892
C -0.309549 0.875758 2.64051
C 1.1379 0.783544 2.75967
C 1.43238 -0.505858 3.25386
C 0.185557 -1.2084 3.45066
Co 0.337846 -0.680642 1.32817
H -1.94977 -0.548271 3.22961
H -0.851388 1.75278 2.30715
H 1.84488 1.57316 2.54021
H 2.41815 -0.912682 3.44213
H 0.0918458 -2.22445 3.81361
P 2.20306 -3.71031 -0.874959
P -0.0373102 -4.00419 -1.11886
C -0.0440677 0.221793 -0.330834
N 0.831011 0.903998 -1.15323
N -1.26727 0.374264 -0.955495
C 0.165572 1.46353 -2.24418
C -1.14766 1.1323 -2.12014
C 2.29254 1.014 -0.908922
C 2.69564 2.4735 -0.623376
C 3.09596 0.395536 -2.06832
C -2.54247 -0.19904 -0.451486
C -3.17825 -1.14355 -1.48896
C -3.51067 0.913846 -0.00474623
H 0.667592 2.03662 -3.0088
H -1.98585 1.36491 -2.75882
H 2.44576 0.414008 -0.00486533
H 3.7596 2.51927 -0.360916
H 2.11599 2.88388 0.210679

H 2.5395 3.11496 -1.5009
H 4.16597 0.419607 -1.82843
H 2.80448 -0.647674 -2.23207
H 2.95116 0.950966 -3.00453
H -2.23185 -0.781296 0.423371
H -4.06596 -1.62035 -1.05586
H -3.49786 -0.601979 -2.3893
H -2.47552 -1.92939 -1.78506
H -4.41406 0.467 0.428325
H -3.82068 1.54183 -0.850635
H -3.04839 1.5575 0.751475

NIMAG = 0

Total bonding energy: -22412.84 kJ/mol

**TS1CO**



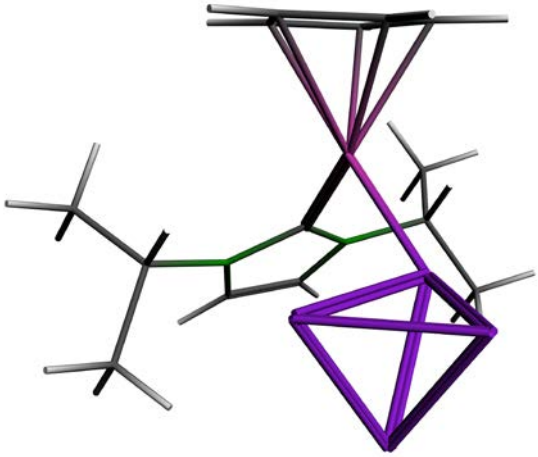
Cartesian coordinates:

P -1.86747 0.913167 -1.49892
P 0.253316 -0.138651 -1.93465
C 1.34841 -3.06599 -0.170474
C -0.0826098 -3.04006 -0.332372
C -0.695153 -2.62015 0.897393
C 0.353864 -2.2666 1.77794
C 1.62866 -2.54192 1.10938
Co 0.56259 -0.975371 0.0696352
H 2.06972 -3.37324 -0.91606
H -0.615876 -3.34921 -1.22399
H -1.75692 -2.54266 1.09039
H 0.246269 -1.8892 2.78693
H 2.60771 -2.4009 1.54903
P -1.43032 0.00386309 -3.46185
P -0.315302 1.86878 -2.76119
C 1.10367 0.535518 0.77468
O 1.45657 1.54217 1.24501

NIMAG = -124.19 $cm^{-1}$

Total bonding energy: -9518.06 kJ/mol

**TS1NHC**



Cartesian coordinates:

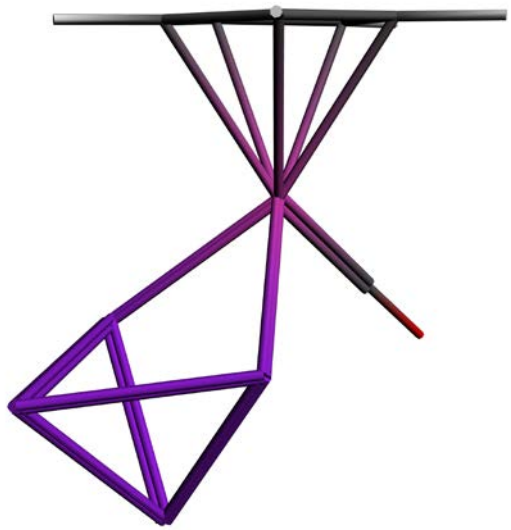
P -2.1775 0.404775 -1.64477
P 0.294886 0.208759 -1.91689
C 1.36 -2.87441 -0.385184
C -0.0642549 -2.87851 -0.554146
C -0.686267 -2.57593 0.707397
C 0.340637 -2.26002 1.61631
C 1.6234 -2.43653 0.936719
Co 0.593071 -0.812434 -0.0757451
H 2.09213 -3.1238 -1.14255
H -0.587195 -3.14185 -1.46581
H -1.75179 -2.53645 0.896751
H 0.219203 -1.97487 2.6541
H 2.59626 -2.3403 1.4022
P -1.24154 -0.110016 -3.5784
P -1.03688 1.96818 -2.69678
C 1.28669 0.737536 0.839495
N 2.58359 1.21526 0.842045
N 0.617916 1.60569 1.68043
C 2.70615 2.33923 1.65812
C 1.47636 2.5827 2.18386
H 5.32499 0.989457 1.47689
C 4.83758 0.151343 0.961415
H -1.23864 3.6683 2.15885
H 4.46823 -0.549595 1.7183
H 5.60049 -0.358721 0.36071
C 3.69513 0.632389 0.0473597
H 3.23578 -0.232039 -0.443373
C 4.17949 1.61988 -1.03087
H 3.35194 1.92223 -1.68199
H 4.94999 1.14355 -1.64952
H 4.61821 2.52155 -0.583194
C -0.828798 1.51559 2.00908
H -1.18339 0.675996 1.40191

C -1.03736 1.18586 3.49938
H -0.511631 0.265228 3.77522
H -2.10664 1.04691 3.70072
H -0.677187 1.99713 4.14599
C -1.57311 2.79489 1.58318
H -1.42192 2.99981 0.51784
H -2.64827 2.67075 1.76002
H 1.15176 3.35769 2.86127
H 3.63745 2.86704 1.79631

NIMAG = -135.79 $cm^{-1}$

Total bonding energy: -22380.09 kJ/mol

[CpCo(CO)($\eta^2$-$P_4$)] **3CO**



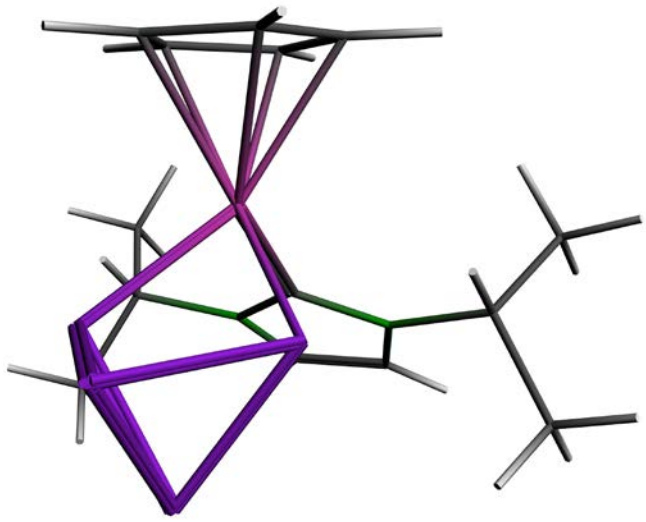
Cartesian coordinates:

P -1.08318 -3.33493 0.200701
P -2.46451 -1.58276 0.0101571
C -0.10433 1.02797 -0.216784
P -0.654646 -1.4287 1.36838
H 2.91794 0.373256 -2.08202
Co 0.881602 -0.412738 -0.0483357
C 2.84178 0.577453 0.163216
C 2.83982 -0.100751 -1.11254
C 2.69291 -1.48256 -0.858756
C 2.60561 -1.67011 0.568333
C 2.74296 -0.397024 1.19788
H 2.63464 -2.26791 -1.60208
H 2.49365 -2.62196 1.07256
H 2.72528 -0.200828 2.26154
H 2.93441 1.64709 0.305067
P -0.613678 -1.688 -1.29577
O -0.741204 1.99309 -0.319628

NIMAG = 0

Total bonding energy: -9599,30 kJ/mol

[CpCo(iPr$_2$Im)(η$^2$-P$_4$)] **3NHC**



Cartesian coordinates:

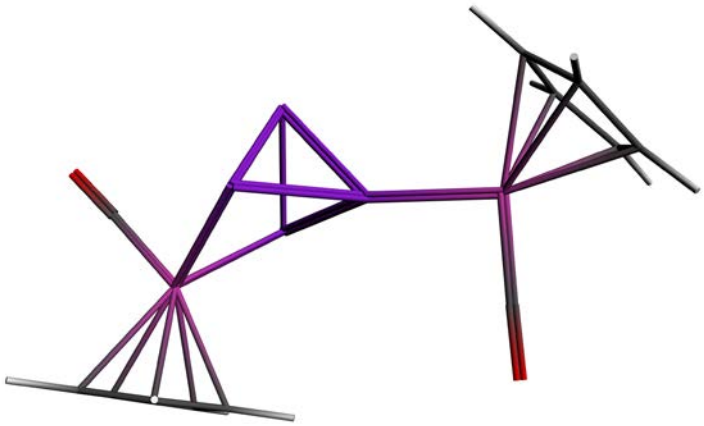
C -1.34019 2.1268 0.678461
N -0.741788 0.935537 1.08691
C -0.35608 0.170076 0.0
N -0.741788 0.935537 -1.08691
C -1.34019 2.1268 -0.678461
Co 0.643893 -1.50207 0.0
C 2.65154 -0.451794 0.0
C 2.60416 -1.28193 -1.16451
C 2.4584 -2.62459 -0.717768
C 2.4584 -2.62459 0.717768
C 2.60416 -1.28193 1.16451
C -0.529205 0.596118 -2.52062
C 0.45879 1.58062 -3.17735
C -0.529205 0.596118 2.52062
C 0.45879 1.58062 3.17735
P -0.785556 -2.68123 -1.33569
P -1.18352 -4.48455 0.0
P -2.62402 -2.77303 0.0
P -0.785556 -2.68123 1.33569
C -1.86985 0.519407 -3.27617
C -1.86985 0.519407 3.27617
H 2.66088 -0.948705 -2.19263
H 2.38252 -3.50318 -1.34656
H 2.38252 -3.50318 1.34656
H 2.66088 -0.948705 2.19263
H 2.74841 0.627409 0.0
H -1.71645 2.86191 -1.37318
H -1.71645 2.86191 1.37318
H -0.0765676 -0.396816 -2.50245
H -1.69276 0.175996 -4.30236

H -2.55124 -0.186878 -2.79089
H -2.36053 1.50005 -3.33198
H 0.658465 1.26667 -4.20925
H 1.40958 1.60569 -2.63395
H 0.0521005 2.59969 -3.21081
H -0.0765676 -0.396816 2.50245
H -1.69276 0.175996 4.30236
H -2.55124 -0.186878 2.79089
H -2.36053 1.50005 3.33198
H 0.658465 1.26667 4.20925
H 1.40958 1.60569 2.63395
H 0.0521005 2.59969 3.21081

NIMAG = 0

Total Bonding energy: -22474.69 kJ/mol

[{CpCo(CO)}$_2$(μ,η$^{2:1}$-P$_4$)] **4CO**



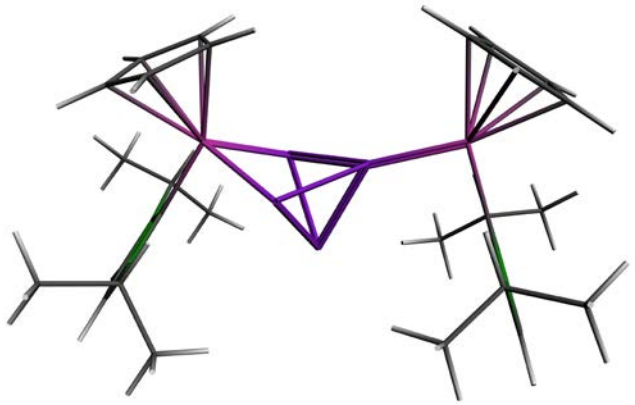
Cartesian coordinates:

| | | | |
|---|---|---|---|
| 1 C | 5.342526154000 | -0.371281292100 | -0.367259912300 |
| 2 C | 4.607875337000 | 0.833166320600 | -0.332967867700 |
| 3 C | 4.064531875000 | 0.968350235200 | 0.998627671300 |
| 4 C | 4.535150745000 | -0.112659669200 | 1.811149428000 |
| 5 C | 5.284784892000 | -0.970811489600 | 0.961560723100 |
| 6 Co | 3.299045101000 | -0.885078225600 | 0.161649186800 |
| 7 C | 3.048678356000 | -2.536148515000 | -0.369515483800 |
| 8 C | -1.684522620000 | -3.178848743000 | -0.519741702000 |
| 9 H | 3.433956809000 | 1.782451856000 | 1.335655846000 |
| 10 H | -4.561359877000 | -2.369983765000 | 1.005743772000 |
| 11 H | -2.113299662000 | -3.266224885000 | 1.688591097000 |
| 12 H | 5.764939883000 | -1.897304434000 | 1.250313469000 |
| 13 H | 4.325773454000 | -0.264749548100 | 2.860901899000 |
| 14 H | 4.448661598000 | 1.516373402000 | -1.156713061000 |
| 15 H | 5.864494520000 | -0.785797562800 | -1.220228177000 |
| 16 P | 0.090483270260 | 1.541284366000 | 0.021899228530 |
| 17 P | -0.706780540300 | -0.219994555900 | 1.258274819000 |
| 18 P | 1.187439454000 | -0.389411881300 | 0.016362652020 |
| 19 P | -0.469973836600 | -0.082464190200 | -1.494401067000 |
| 20 Co | -2.217473192000 | -1.055565749000 | -0.305069730700 |
| 21 C | -3.146296447000 | 0.438910097600 | -0.281225943200 |
| 22 C | -2.464087909000 | -3.061846537000 | 0.685111816600 |
| 23 C | -3.744719093000 | -2.586269419000 | 0.328904066900 |
| 24 C | -3.781089353000 | -2.439313607000 | -1.113040246000 |
| 25 C | -2.526408868000 | -2.837121825000 | -1.631825990000 |
| 26 H | -0.660791928900 | -3.527675270000 | -0.578547653800 |
| 27 H | -2.236955257000 | -2.839507061000 | -2.674464477000 |
| 28 H | -4.632051753000 | -2.097003390000 | -1.688345292000 |
| 29 O | 2.907644322000 | -3.639413130000 | -0.724342999900 |
| 30 O | -3.792327990000 | 1.402298881000 | -0.267453699600 |

NIMAG = 0

Total bonding energy: -17401.19 kJ/mol

[{CpCo(iPr$_2$Im)}$_2$(μ,η$^{2:1}$-P$_4$)] **4NHC**



Cartesian coordinates:

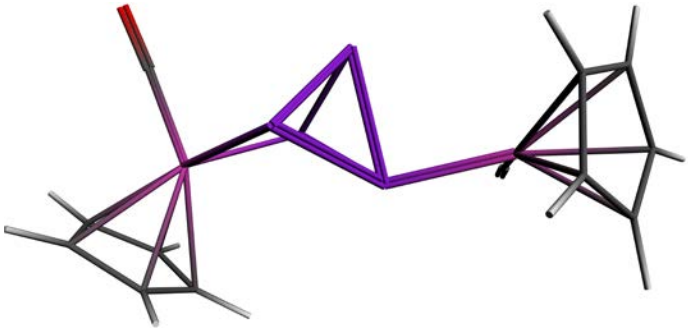
| | | | |
|---|---|---|---|
| 1 C | 4.939209162000 | -1.697428319000 | 1.399045772000 |
| 2 C | 3.788154006000 | -2.510611886000 | 1.519420514000 |
| 3 C | 3.360355985000 | -2.866165697000 | 0.189986341400 |
| 4 C | 4.288336575000 | -2.324103164000 | -0.756588683400 |
| 5 C | 5.236630809000 | -1.562432421000 | -0.018984185950 |
| 6 Co | 3.290764638000 | -0.690787595100 | 0.361164616100 |
| 7 H | 4.368197858000 | 4.153733817000 | 1.631380324000 |
| 8 C | -1.619757183000 | -3.053247795000 | -0.893718261600 |
| 9 H | 2.502697106000 | -3.482847199000 | -0.047932086860 |
| 10 H | -4.353430741000 | -2.650456728000 | 1.015208462000 |
| 11 H | -1.782413664000 | -3.417137623000 | 1.317599244000 |
| 12 H | 6.076207267000 | -1.015650400000 | -0.430889652400 |
| 13 H | 4.263265543000 | -2.460404026000 | -1.830125190000 |
| 14 H | 3.300538753000 | -2.804842043000 | 2.440230285000 |
| 15 H | 5.520064849000 | -1.275142529000 | 2.209314559000 |
| 16 P | -0.000963396054 | 1.581649199000 | 0.239885377400 |
| 17 P | -0.789104594900 | -0.265511164000 | 1.333013282000 |
| 18 P | 1.204156373000 | -0.298038841000 | 0.200108512800 |
| 19 P | -0.417013347300 | 0.026023109650 | -1.381471927000 |
| 20 Co | -2.183802512000 | -0.985720146100 | -0.335061698400 |
| 21 H | -5.477584875000 | 2.745532582000 | 1.026131525000 |
| 22 C | -2.257072527000 | -3.114890007000 | 0.392289959000 |
| 23 C | -3.602053946000 | -2.702175311000 | 0.238104646800 |
| 24 C | -3.803871462000 | -2.391471517000 | -1.156080920000 |
| 25 C | -2.599263807000 | -2.644679814000 | -1.856070176000 |
| 26 H | -0.592927219600 | -3.323063222000 | -1.105730940000 |
| 27 H | -2.433897616000 | -2.514763323000 | -2.918228920000 |
| 28 H | -4.732723195000 | -2.045171394000 | -1.593281897000 |
| 29 C | -3.347364166000 | 0.593134040600 | -0.323167649700 |
| 30 N | -4.066283488000 | 1.112426171000 | 0.740198704000 |
| 31 N | -3.732914863000 | 1.391697519000 | -1.388852485000 |
| 32 C | -4.641711500000 | 2.368450035000 | -0.986221982200 |
| 33 C | -4.850379359000 | 2.194012261000 | 0.343163327300 |
| 34 H | -2.149403056000 | 2.352799334000 | -4.285171053000 |

| | | | |
|---|---|---|---|
| 35 H | -5.055067036000 | 3.098909630000 | -1.664734791000 |
| 36 H | -1.708456350000 | 2.743655726000 | -2.610305350000 |
| 37 H | -3.212485108000 | 3.390704790000 | -3.316909071000 |
| 38 C | -3.292841382000 | 1.254937274000 | -2.804537004000 |
| 39 H | -2.591911713000 | 0.418361435800 | -2.794785829000 |
| 40 C | -4.482181135000 | 0.903142011000 | -3.720076609000 |
| 41 H | -4.987532835000 | -0.007440243377 | -3.380305584000 |
| 42 H | -4.119967586000 | 0.736032945200 | -4.741942040000 |
| 43 H | -5.220118570000 | 1.715018993000 | -3.757289662000 |
| 44 C | -2.546911824000 | 2.518108502000 | -3.276468622000 |
| 45 H | -6.205621214000 | 0.850246353900 | 2.559921686000 |
| 46 C | -4.064530377000 | 0.596432486000 | 2.135596378000 |
| 47 H | -3.349014295000 | -0.228044112100 | 2.118900621000 |
| 48 C | -3.563905265000 | 1.668266316000 | 3.122067315000 |
| 49 H | -2.569251736000 | 2.023901056000 | 2.834893210000 |
| 50 H | -3.497014427000 | 1.236064544000 | 4.127789537000 |
| 51 H | -4.248164655000 | 2.525744680000 | 3.170247102000 |
| 52 C | -5.454398556000 | 0.050718519310 | 2.518704813000 |
| 53 H | -5.793320691000 | -0.702938893400 | 1.799685820000 |
| 54 H | -5.406303534000 | -0.413509727600 | 3.511158240000 |
| 55 C | 3.743230523000 | 1.171623343000 | 0.324087022800 |
| 56 N | 3.859139249000 | 2.047984396000 | 1.387805153000 |
| 57 N | 4.048596282000 | 1.955700696000 | -0.774696097400 |
| 58 C | 4.345225900000 | 3.264776555000 | -0.395961964700 |
| 59 C | 4.227002623000 | 3.322482304000 | 0.957456918000 |
| 60 H | 2.652556560000 | 3.559864980000 | 3.437961768000 |
| 61 H | 5.807034727000 | 2.549272938000 | -2.894263026000 |
| 62 H | 4.605573491000 | 4.037893395000 | -1.102920815000 |
| 63 C | 4.033539996000 | 1.469512163000 | -2.176979982000 |
| 64 H | 3.712866271000 | 0.425492138100 | -2.079882110000 |
| 65 C | 2.997451380000 | 2.237223831000 | -3.020027753000 |
| 66 H | 1.997794322000 | 2.153668922000 | -2.579800329000 |
| 67 H | 2.963454144000 | 1.817059758000 | -4.032944392000 |
| 68 H | 3.255030952000 | 3.301470259000 | -3.108023444000 |
| 69 C | 5.443783802000 | 1.517205105000 | -2.796610260000 |
| 70 H | 6.160222019000 | 0.956642385200 | -2.186330437000 |
| 71 H | 5.423234459000 | 1.074184436000 | -3.800035527000 |
| 72 C | 3.598111429000 | 1.681034015000 | 2.802536293000 |
| 73 H | 3.312879813000 | 0.624151961700 | 2.741565881000 |
| 74 C | 4.874277423000 | 1.818612275000 | 3.654823341000 |
| 75 H | 5.694525721000 | 1.228661548000 | 3.231010416000 |
| 76 H | 4.679771732000 | 1.460382757000 | 4.673408705000 |
| 77 H | 5.202123796000 | 2.864569329000 | 3.725722983000 |
| 78 C | 2.419382690000 | 2.487894757000 | 3.379634256000 |
| 79 H | 1.522836768000 | 2.360629315000 | 2.763334621000 |
| 80 H | 2.196453927000 | 2.138084153000 | 4.395173064000 |

NIMAG = 0

Total bonding energy: -43124.33 kJ/mol

**TS2CO**



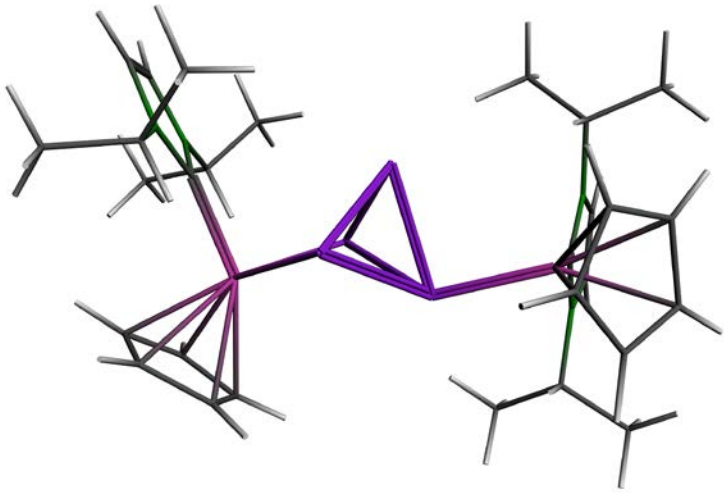
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 3.81214024 | 2.81429829 | 1.20308280 |
| C | 2.90092830 | 2.27656534 | 2.12893654 |
| C | 3.31272977 | 0.91435736 | 2.43744103 |
| C | 4.49776234 | 0.62931024 | 1.72065516 |
| C | 4.77598255 | 1.77714853 | 0.89765706 |
| Co | 2.89070513 | 1.00674377 | 0.25409555 |
| C | 3.23822797 | 0.79972911 | -1.44386214 |
| C | -1.40679221 | -3.08163174 | -0.57726513 |
| H | 2.81419669 | 0.25387435 | 3.13662066 |
| H | -4.20485164 | -2.67112516 | 1.23408782 |
| H | -1.58680454 | -3.16108293 | 1.66433218 |
| H | 5.61623553 | 1.87962316 | 0.22229465 |
| H | 5.06943830 | -0.28867305 | 1.75119239 |
| H | 2.03421435 | 2.77731039 | 2.54281398 |
| H | 3.78787323 | 3.80399726 | 0.76600571 |
| P | -0.24723794 | 1.76752015 | -0.09647112 |
| P | -0.97813169 | 0.11823459 | 1.23468209 |
| P | 1.02956030 | -0.19537752 | 0.09609752 |
| P | -0.60843526 | 0.08678771 | -1.53073928 |
| Co | -2.24457552 | -1.04446934 | -0.33034469 |
| C | -3.38004588 | 0.29253657 | -0.46349891 |
| C | -2.06720802 | -3.03898693 | 0.70182445 |
| C | -3.43731608 | -2.77695002 | 0.47843652 |
| C | -3.63658517 | -2.67091984 | -0.95042026 |
| C | -2.39335422 | -2.89693196 | -1.59624189 |
| H | -0.35231878 | -3.26545255 | -0.73999506 |
| H | -2.21576447 | -2.88240445 | -2.66360555 |
| H | -4.58127550 | -2.47498192 | -1.44228413 |
| O | 3.50056017 | 0.64848921 | -2.57225634 |
| O | -4.16736473 | 1.13852054 | -0.56175971 |

NIMAG = -138.83 $cm^{-1}$

Total bonding energy: -17366.15 kJ/mol

**TS2NHC**



Cartesian coordinates:

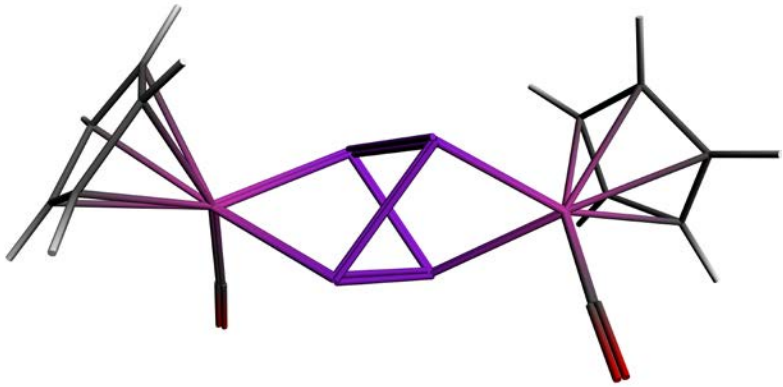
| | | | |
|---|---|---|---|
| C | 4.40325288 | 2.25864052 | 1.24455601 |
| C | 3.28744780 | 2.15396027 | 2.09793099 |
| C | 3.11544616 | 0.75890997 | 2.41714127 |
| C | 4.20022028 | 0.01475134 | 1.85233720 |
| C | 4.95829627 | 0.92085672 | 1.06689375 |
| Co | 2.93703512 | 0.90684993 | 0.20171706 |
| H | 3.79207172 | 2.71599674 | -4.52391587 |
| C | -1.77704269 | -3.02307352 | -0.83237459 |
| H | 2.33252054 | 0.35421270 | 3.04717172 |
| H | -3.81054318 | -2.53745870 | 1.80365448 |
| H | -1.21707636 | -3.15596579 | 1.33757372 |
| H | 5.85316721 | 0.68575016 | 0.50273528 |
| H | 4.37454131 | -1.04788412 | 1.96262937 |
| H | 2.64643269 | 2.96285103 | 2.42649712 |
| H | 4.81594390 | 3.17144898 | 0.83209624 |
| P | -0.23778313 | 1.80481127 | -0.04345127 |
| P | -0.89870113 | 0.09503970 | 1.24338123 |
| P | 1.07203312 | -0.17506876 | -0.01567423 |
| P | -0.70885563 | 0.16088098 | -1.50050421 |
| Co | -2.31901805 | -0.89748085 | -0.25148882 |
| H | -5.73728376 | 2.85845813 | 0.64246241 |
| C | -1.97453692 | -2.96463489 | 0.58746026 |
| C | -3.33640940 | -2.63642489 | 0.83564331 |
| C | -3.96905345 | -2.46237481 | -0.43705328 |
| C | -3.01874220 | -2.73758506 | -1.46699406 |
| H | -0.84500340 | -3.26189542 | -1.32931062 |
| H | -3.21078431 | -2.73014747 | -2.53274585 |
| H | -5.00968414 | -2.20166983 | -0.59106660 |
| H | -2.92329715 | 1.40257044 | -4.79722002 |
| C | -3.58815487 | 0.57200035 | -0.42198707 |
| N | -4.24792931 | 1.27267490 | 0.57207179 |

| | | | |
|---|---|---|---|
| N | -4.12434209 | 1.09096814 | -1.59006163 |
| C | -5.06051055 | 2.08677011 | -1.31741471 |
| C | -5.13748255 | 2.20061730 | 0.03268304 |
| H | -3.35449720 | 0.27176901 | 2.12546990 |
| H | -3.94754504 | 2.59318000 | -3.97198721 |
| H | -5.58041023 | 2.63030337 | -2.09125013 |
| C | -4.10864775 | 1.05623718 | 2.03728516 |
| H | -3.42142754 | 2.11575685 | 3.80062799 |
| H | -5.27880092 | 0.29465645 | 3.69839413 |
| C | -3.58849672 | 2.32489245 | 2.73706170 |
| H | -2.63767428 | 2.64308882 | 2.29738000 |
| H | -4.30823964 | 3.15118679 | 2.66475122 |
| C | -5.43196068 | 0.54748780 | 2.64213736 |
| H | -6.22050034 | 1.30985965 | 2.59256192 |
| H | -5.78540660 | -0.34867275 | 2.11984686 |
| C | -3.81284775 | 0.64008799 | -2.97367641 |
| H | -3.04998747 | -0.12914782 | -2.84216794 |
| C | -5.05298036 | 0.00847742 | -3.63657988 |
| H | -5.43874632 | -0.82587523 | -3.04056229 |
| H | -4.78437954 | -0.37132418 | -4.62996457 |
| H | -5.85987771 | 0.74143972 | -3.76635583 |
| C | -3.21956178 | 1.78626255 | -3.81322029 |
| H | -2.33054300 | 2.19823812 | -3.32531096 |
| C | 3.33065036 | 1.08903030 | -1.66662193 |
| N | 3.32948776 | 2.23511648 | -2.44860773 |
| N | 3.75351164 | 0.10567404 | -2.54788931 |
| C | 3.99652251 | 0.62784442 | -3.81738491 |
| C | 3.73281287 | 1.96005387 | -3.75521294 |
| H | 1.91992371 | 4.24905805 | -3.80129793 |
| H | 5.73929145 | -1.71008696 | -3.36127596 |
| H | 4.32829704 | 0.02547142 | -4.64969970 |
| C | 3.92645945 | -1.32086759 | -2.18015878 |
| H | 3.64525309 | -1.34636229 | -1.12123602 |
| C | 2.96251818 | -2.22017833 | -2.97620111 |
| H | 1.92742480 | -1.88464241 | -2.84893717 |
| H | 3.03974048 | -3.25321216 | -2.61433968 |
| H | 3.20068867 | -2.22098533 | -4.04903594 |
| C | 5.39656930 | -1.75844529 | -2.31889052 |
| H | 6.05065615 | -1.12533820 | -1.70898839 |
| H | 5.50612698 | -2.79580831 | -1.97872112 |
| C | 2.93620484 | 3.58386430 | -1.97100043 |
| H | 2.66445171 | 3.42259331 | -0.92229344 |
| C | 4.12120672 | 4.56668450 | -2.04751628 |
| H | 4.98842656 | 4.18175253 | -1.50004012 |
| H | 3.83395186 | 5.53088189 | -1.60931733 |
| H | 4.42495073 | 4.75079901 | -3.08679069 |
| C | 1.70232340 | 4.10212353 | -2.73440682 |
| H | 0.86639010 | 3.40065045 | -2.63882154 |
| H | 1.39158842 | 5.07004209 | -2.32182058 |

NIMAG = -144.56 $cm^{-1}$

Total bonding energy: -43082.79 kJ/mol

$[\{CpCo(CO)\}_2(\mu,\eta^{2:2}\text{-}P_4)]$ **5CO**



Cartesian coordinates:

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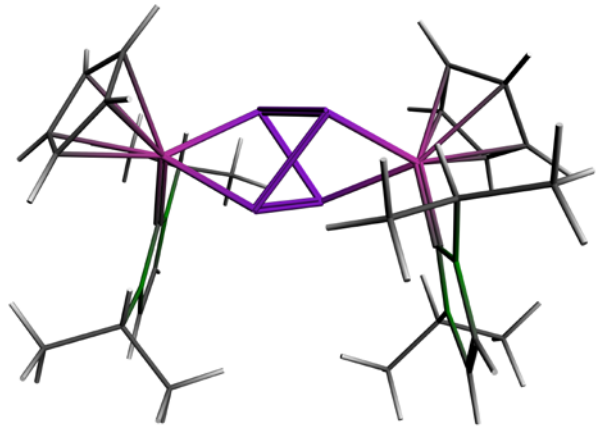
C 2.38707 2.52203 0.918054
C 3.49767 1.65403 1.18913
C 4.34787 1.68236 0.0590338
C 3.79569 2.62104 -0.901815
Co 2.36022 0.911355 -0.604808
C 2.88161 -0.216688 -1.84458
C -2.10109 -2.8051 1.18838
H 3.63205 1.04905 2.07609
H -4.88219 -0.946144 1.46548
H -2.58213 -1.32896 2.81906
H 4.22858 2.8673 -1.863
H 5.26448 1.12027 -0.0674073
H 1.5588 2.72217 1.5863
H 1.94816 3.86541 -0.834643
P 0.166481 1.00876 -1.40588
P -0.887603 0.582191 0.589914
P 1.03448 -0.67796 0.469769
P -0.341017 -1.22241 -1.29091
Co -2.37435 -1.0575 -0.153706
C -3.09881 0.0139929 -1.33991
C -2.88384 -1.8348 1.91102
C -4.08462 -1.62869 1.20089
C -4.06366 -2.49314 0.0368969
C -2.86179 -3.24426 0.0569649
H -1.12983 -3.18062 1.48617
H -2.55126 -3.97413 -0.679004
H -4.8489 -2.56582 -0.705187
O 3.27425 -0.941649 -2.6629
O -3.62875 0.697567 -2.11542

NIMAG = 0

Total bonding energy: -17430.83 kJ/mol

[{CpCo(iPr$_2$Im)}$_2$(μ,η$^{2:2}$-P$_4$)] **5NHC**



Cartesian coordinates:

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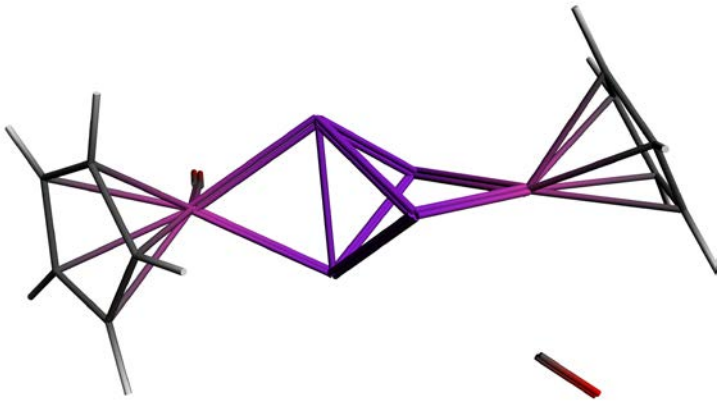
C 3.92254 1.0442 2.42671
C 4.38106 1.66691 1.22599
C 3.49544 2.74448 0.890861
Co 2.3884 0.777419 0.827819
C 3.03534 -0.250444 -0.662343
N 3.55361 -1.53483 -0.67934
C 4.01403 -1.88049 -1.94905
C 3.79832 -0.809905 -2.75586
N 3.20602 0.179378 -1.97238
C 2.8692 1.52682 -2.50336
C 4.14556 2.29823 -2.89768
C 3.66612 -2.44533 0.489856
C 2.88584 -3.75197 0.251142
P 0.338912 1.09798 -0.110587
P -0.925205 0.675406 1.74309
P 0.916509 -0.718507 1.73023
P -0.338658 -1.09466 -0.139484
Co -2.39297 -0.797519 0.796732
C -3.03224 0.266482 -0.671315
N -3.54989 1.55118 -0.659714
C -4.00292 1.92819 -1.92314
C -3.78323 0.877539 -2.75469
N -3.19586 -0.13104 -1.99238
C -3.66934 2.43251 0.530947
C -5.14934 2.6737 0.889222
C -2.8559 -1.46494 -2.55457
C -4.12994 -2.22595 -2.97566
C -3.93318 -1.10263 2.38197
C -4.38738 -1.69372 1.16388
C -3.50149 -2.76345 0.804789
C -2.45761 -2.78627 1.76918
C -2.71834 -1.76101 2.73953

C -2.88863 3.74505 0.328861
C -1.84256 -1.34519 -3.70845
C 5.14403 -2.6964 0.850024
C 1.86288 1.43571 -3.66596
H -3.60868 -3.4264 -0.0433809
H -5.27856 -1.4055 0.619266
H -4.41022 -0.295074 2.9212
H -2.10843 -1.54834 3.60821
H -1.61438 -3.46532 1.78403
H -4.43077 2.89779 -2.12651
H -3.98835 0.770812 -3.80889
H -3.19904 1.86594 1.33805
H -2.9021 4.32602 1.2593
H -1.84564 3.53584 0.0654269
H -3.33399 4.36573 -0.460794
H -5.21303 3.25655 1.81658
H -5.67644 1.72499 1.04118
H -5.67035 3.23652 0.103109
H -2.3795 -1.99504 -1.72782
H -1.55512 -2.34838 -4.04725
H -0.938423 -0.825727 -3.37546
H -2.26471 -0.808995 -4.56918
H -3.86345 -3.23889 -3.30295
H -4.83533 -2.30761 -2.14165
H -4.64053 -1.7285 -3.81108
H 4.44365 -2.84461 -2.17374
H 4.00934 -0.677273 -3.80597
H 3.19168 -1.89848 1.30812
H 5.20234 -3.30187 1.76311
H 5.671 -1.75213 1.02802
H 5.66894 -3.24024 0.053206
H 2.89424 -4.35601 1.16684
H 1.84434 -3.53562 -0.012405
H 3.33506 -4.35289 -0.551517
H 2.38776 2.03627 -1.6666
H 1.5773 2.44698 -3.98152
H 2.2903 0.921009 -4.53716
H 0.956839 0.90814 -3.35139
H 3.88075 3.31894 -3.20134
H 4.66141 1.82179 -3.74206
H 4.84584 2.35933 -2.0576
H 3.6051 3.42887 0.0601878
H 5.27476 1.39364 0.677806
H 4.39849 0.223735 2.94715
H 2.09253 1.45651 3.65663
H 1.60346 3.41894 1.88009

NIMAG = 0

Total bonding energy: -43288.11 kJ/mol

**TS3CO**



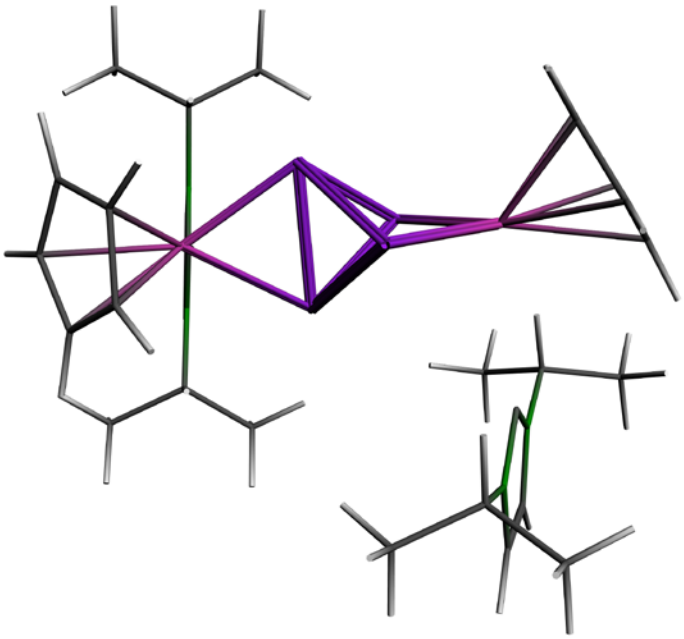
Cartesian coordinates:

C 2.88857 2.98956 -0.520804
C 2.89281 2.42273 0.809481
C 3.89933 1.3937 0.847813
C 4.43215 1.27201 -0.454006
C 3.8144 2.26586 -1.30245
Co 2.17044 0.91997 -0.481857
C 2.8768 -0.777907 -2.35149
C -2.12816 -2.69751 1.28196
H 4.15668 0.785967 1.70527
H -5.15552 -1.26817 1.05706
H -3.04821 -1.24469 2.73826
H 4.02439 2.41902 -2.35329
H 5.17969 0.555375 -0.770228
H 2.30867 2.77442 1.65088
H 2.2579 3.80194 -0.85795
P 0.151201 1.21383 -1.37493
P -0.927721 0.546515 0.555016
P 1.07743 -0.61206 0.694461
P -0.282705 -1.015 -1.11136
Co -2.44652 -1.10097 -0.179359
C -3.16745 -0.0769972 -1.4197
C -3.13833 -1.82681 1.8301
C -4.24124 -1.83764 0.949381
C -3.93177 -2.73796 -0.143154
C -2.64802 -3.29631 0.0876748
H -1.16356 -2.90441 1.72865
H -2.13791 -4.01226 -0.54334
H -4.58477 -2.96171 -0.977355
O 3.84427 -0.842482 -2.96605
O -3.70519 0.559188 -2.22839

NIMAG= -172.28 $cm^{-1}$

Total bonding energy: -17309.67 kJ/mol

**TS3NHC**



Cartesian coordinates:

| | | | |
|---|---|---|---|
| 1 C | 2.855070000000 | 2.779950000000 | 0.291566000000 |
| 2 C | 3.135560000000 | 1.815430000000 | 1.332070000000 |
| 3 C | 4.142980000000 | 0.925984000000 | 0.846828000000 |
| 4 C | 4.449700000000 | 1.315230000000 | -0.490127000000 |
| 5 C | 3.687890000000 | 2.477210000000 | -0.824506000000 |
| 6 Co | 2.223500000000 | 0.822423000000 | -0.317757000000 |
| 7 H | 3.447430000000 | -1.506340000000 | -6.011720000000 |
| 8 C | -2.814130000000 | -1.873890000000 | 1.629930000000 |
| 9 H | 4.564060000000 | 0.083529300000 | 1.379880000000 |
| 10 H | -5.333940000000 | -1.866380000000 | -0.566193000000 |
| 11 H | -4.639310000000 | -0.566496000000 | 1.694890000000 |
| 12 H | 3.715720000000 | 3.012230000000 | -1.764940000000 |
| 13 H | 5.129180000000 | 0.796189000000 | -1.154000000000 |
| 14 H | 2.688370000000 | 1.802180000000 | 2.318180000000 |
| 15 H | 2.158390000000 | 3.605450000000 | 0.367951000000 |
| 16 P | 0.291897000000 | 1.181460000000 | -1.368760000000 |
| 17 P | -0.975923000000 | 0.547072000000 | 0.448272000000 |
| 18 P | 0.979486000000 | -0.708941000000 | 0.689230000000 |
| 19 P | -0.325584000000 | -1.037070000000 | -1.181230000000 |
| 20 Co | -2.498800000000 | -0.992234000000 | -0.380009000000 |
| 21 H | -4.656610000000 | 2.438000000000 | -3.558480000000 |
| 22 C | -4.074220000000 | -1.352350000000 | 1.210680000000 |
| 23 C | -4.436230000000 | -2.041740000000 | 0.014932500000 |
| 24 C | -3.443730000000 | -3.043680000000 | -0.264511000000 |
| 25 C | -2.433540000000 | -2.924980000000 | 0.726626000000 |
| 26 H | -2.251740000000 | -1.562210000000 | 2.501150000000 |
| 27 H | -1.535680000000 | -3.525130000000 | 0.804114000000 |
| 28 H | -3.472380000000 | -3.763500000000 | -1.072340000000 |
| 29 H | 1.664710000000 | 2.109310000000 | -5.673640000000 |

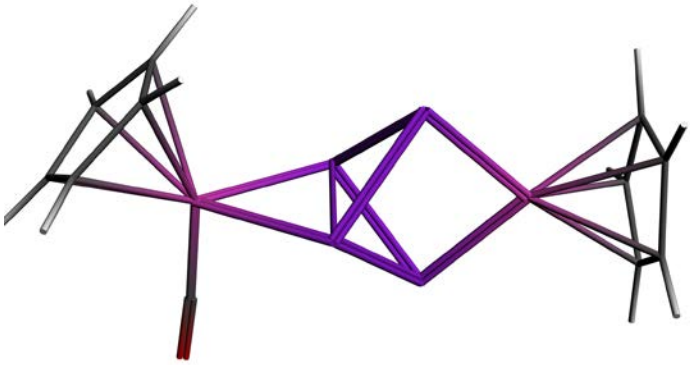
| | | | |
|---|---|---|---|
| 30 C | 3.055690000000 | -0.971057000000 | -2.752960000000 |
| 31 N | 3.120100000000 | -0.557660000000 | -4.062120000000 |
| 32 N | 3.261550000000 | -2.324380000000 | -2.848650000000 |
| 33 C | 3.450030000000 | -2.740080000000 | -4.170990000000 |
| 34 C | 3.361360000000 | -1.619730000000 | -4.940600000000 |
| 35 H | 2.009030000000 | 0.535244000000 | -6.414080000000 |
| 36 H | 4.938640000000 | -4.506630000000 | -2.268830000000 |
| 37 H | 3.623540000000 | -3.766730000000 | -4.459690000000 |
| 38 C | 3.268650000000 | -3.217010000000 | -1.663980000000 |
| 39 H | 3.040080000000 | -2.544510000000 | -0.832036000000 |
| 40 C | 2.159340000000 | -4.280710000000 | -1.761060000000 |
| 41 H | 1.183160000000 | -3.802890000000 | -1.899740000000 |
| 42 H | 2.128140000000 | -4.869650000000 | -0.836202000000 |
| 43 H | 2.335980000000 | -4.973360000000 | -2.595170000000 |
| 44 C | 4.662020000000 | -3.836020000000 | -1.444280000000 |
| 45 H | 5.426090000000 | -3.054450000000 | -1.364250000000 |
| 46 H | 4.667920000000 | -4.423050000000 | -0.517578000000 |
| 47 C | 2.966190000000 | 0.861282000000 | -4.463970000000 |
| 48 H | 2.707720000000 | 1.366720000000 | -3.529690000000 |
| 49 C | 4.293560000000 | 1.433310000000 | -4.998970000000 |
| 50 H | 5.095120000000 | 1.310400000000 | -4.262100000000 |
| 51 H | 4.181660000000 | 2.503370000000 | -5.214400000000 |
| 52 H | 4.599960000000 | 0.933953000000 | -5.927830000000 |
| 53 C | 1.807020000000 | 1.042540000000 | -5.461110000000 |
| 54 H | 0.874066000000 | 0.649416000000 | -5.044270000000 |
| 55 C | -3.162480000000 | -0.033411000000 | -1.936250000000 |
| 56 N | -3.745490000000 | 1.217600000000 | -2.002180000000 |
| 57 N | -3.265030000000 | -0.506334000000 | -3.234090000000 |
| 58 C | -3.883550000000 | 0.427177000000 | -4.064030000000 |
| 59 C | -4.182600000000 | 1.505230000000 | -3.294170000000 |
| 60 H | -5.921380000000 | 2.884520000000 | -1.381360000000 |
| 61 H | -4.052820000000 | 0.255301000000 | -5.116010000000 |
| 62 H | -2.134870000000 | -1.228690000000 | -5.708090000000 |
| 63 C | -2.806060000000 | -1.838940000000 | -3.707140000000 |
| 64 H | -2.352570000000 | -2.292950000000 | -2.823150000000 |
| 65 C | -3.999490000000 | -2.702660000000 | -4.160940000000 |
| 66 H | -4.745550000000 | -2.795220000000 | -3.364070000000 |
| 67 H | -3.648330000000 | -3.708120000000 | -4.424330000000 |
| 68 H | -4.491460000000 | -2.278760000000 | -5.046360000000 |
| 69 C | -1.732520000000 | -1.701160000000 | -4.802010000000 |
| 70 H | -0.885975000000 | -1.108870000000 | -4.440470000000 |
| 71 H | -1.361730000000 | -2.695420000000 | -5.079720000000 |
| 72 C | -3.917180000000 | 2.151970000000 | -0.858403000000 |
| 73 H | -3.457100000000 | 1.628650000000 | -0.016056500000 |
| 74 C | -3.157860000000 | 3.468680000000 | -1.105540000000 |
| 75 H | -2.105460000000 | 3.267100000000 | -1.335590000000 |
| 76 H | -3.205930000000 | 4.094440000000 | -0.205941000000 |
| 77 H | -3.598020000000 | 4.039350000000 | -1.934640000000 |
| 78 C | -5.410890000000 | 2.375430000000 | -0.553096000000 |
| 79 H | -5.921060000000 | 1.423730000000 | -0.365753000000 |

80 H -5.513850000000 3.004750000000 0.339441000000

NIMAG = -89.42 $cm^{-1}$

Total bonding energy: -43058.23 kJ/mol

[{CpCo(CO)}(μ,η$^{2:2}$-P$_4$){CpCo}] **6CO**



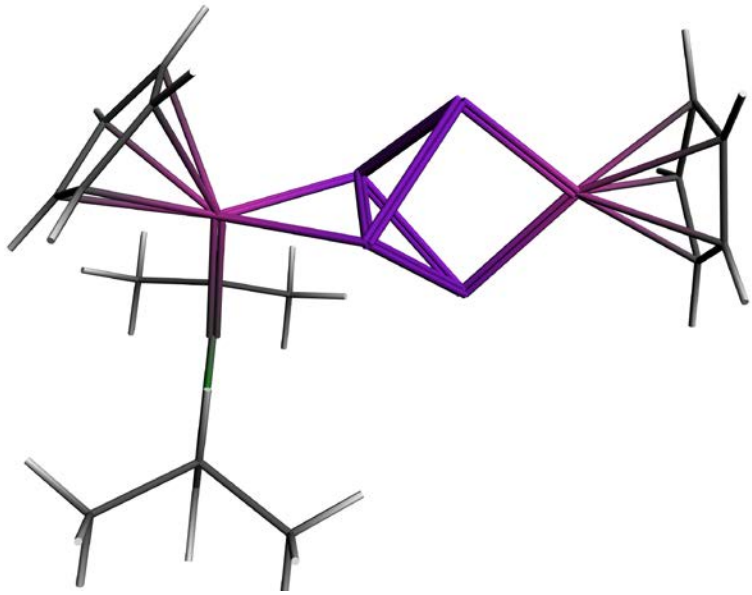
Cartesian coordinates:

Co -4.08954 -0.239282 0.00364934
P -2.17219 0.833696 -0.0106534
P -1.20189 -0.912868 1.14282
P -2.87922 -2.06272 0.0221768
P -1.21731 -0.93476 -1.14504
Co 0.799231 -1.43278 -0.00904807
C 1.37228 0.235167 -0.030154
H 0.172763 -3.96931 -1.37578
H 2.39955 -2.65953 -2.18465
H 3.70328 -1.82134 0.0288251
H -6.31399 -1.58432 -1.37736
C 2.05947 -2.83793 1.16943
C 0.898526 -3.51768 0.706201
C -5.58125 1.39651 0.00742576
C -5.7523 0.584901 -1.1534
C 0.918892 -3.51519 -0.73555
C -6.10941 -0.744424 -0.726059
H -6.33346 -1.61073 1.32406
H -5.67792 0.86961 2.18473
C 2.09039 -2.83188 -1.1623
C 2.78093 -2.38858 0.0151034
H 2.34038 -2.67163 2.201
H 0.134771 -3.97473 1.32296
C -6.11937 -0.758165 0.692865
C -5.76545 0.561241 1.15061
H -5.30633 2.44272 0.0199682
H -5.6513 0.912411 -2.18032
O 1.82301 1.30501 -0.0449848

NIMAG = 0

Total bonding energy: -15941.82 kJ/mol

[{CpCo(iPr$_2$Im)}{CpCo}(μ,η$^{2:2}$-P$_4$)] **6NHC**



Cartesian coordinates:

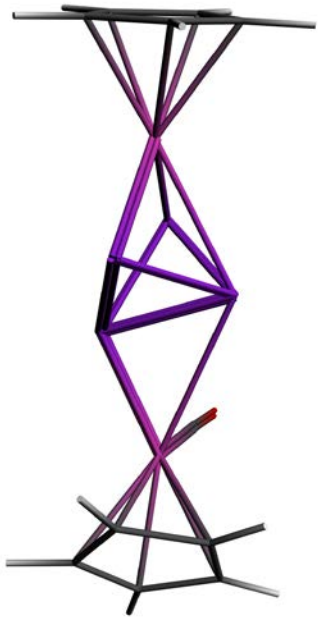
Co -6.41367 -1.6658 -2.64342
P -4.49868 -0.601673 -2.63509
P -3.44951 -2.41016 -1.6328
P -5.18583 -3.4677 -2.77535
P -3.52063 -2.28314 -3.89676
Co -1.51593 -2.82765 -2.8524
C -0.818707 -1.00234 -2.77532
N -0.499689 -0.165564 -3.82764
C 0.0643205 1.0245 -3.37068
C 0.112721 0.946285 -2.01561
N -0.42209 -0.290779 -1.65963
C -0.148514 -4.27146 -1.81912
C -1.33634 -4.93353 -2.24965
C -7.91859 -0.0403312 -2.51643
C -8.12181 -0.798019 -3.70961
C -1.39984 -4.85818 -3.68216
C -8.45494 -2.1467 -3.33403
H 0.375138 1.81837 -4.03222
H 0.473102 1.66056 -1.2914
C -0.250809 -4.14943 -4.14384
C 0.500441 -3.76061 -2.98903
H 0.203879 -4.17899 -0.800065
H -2.05835 -5.42962 -1.61366
C -8.422 -2.22612 -1.91491
C -8.06801 -0.926998 -1.4071
H -7.64516 1.00566 -2.46414
H -8.0567 -0.420426 -4.72247
H -2.17739 -5.28839 -4.30057
H 0.0108558 -3.94954 -5.17483

H 1.42251 -3.19201 -2.99999
H -8.6721 -2.95868 -4.01587
H -8.60976 -3.10977 -1.31871
H -7.95424 -0.66455 -0.362666
C -0.526626 -0.759774 -0.251393
C 0.870898 -0.905856 0.382533
C -1.45402 0.154847 0.571174
H -0.984247 -1.74852 -0.334531
H 1.37673 0.0641461 0.474296
H 1.50686 -1.57101 -0.212281
H 0.775789 -1.32816 1.39041
H -1.03227 1.16237 0.683446
H -1.58618 -0.265779 1.57546
H -2.43754 0.238141 0.0974984
C -0.704726 -0.469159 -5.26996
C -1.68551 0.529392 -5.91404
C 0.64383 -0.532102 -6.01415
H -1.15747 -1.46353 -5.27059
H -2.63323 0.552124 -5.36643
H -1.88906 0.226949 -6.94851
H -1.26991 1.5454 -5.93847
H 1.14252 0.445756 -6.03043
H 1.32034 -1.25625 -5.54654
H 0.476395 -0.837045 -7.05449

NIMAG = 0

Total bonding energy: -28819.65 kJ/mol

**TS4CO**



Cartesian coordinates:

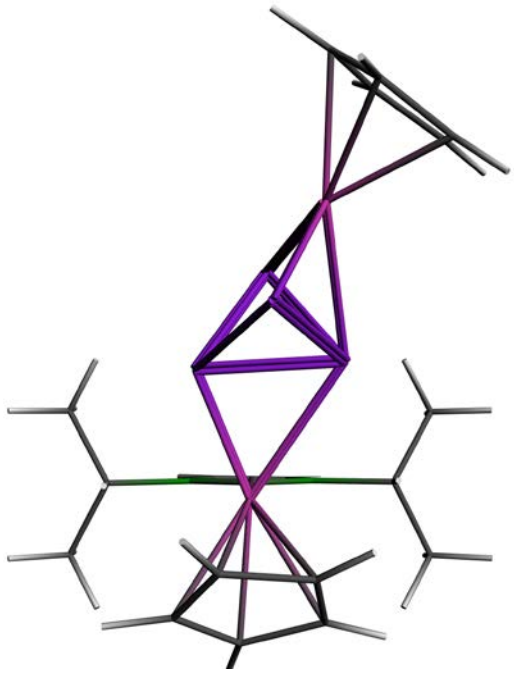
C 3.6444 -1.80528 -0.159817
C 3.11826 -1.92011 1.18642
C 1.96166 -2.74096 1.14315
C 1.73129 -3.08196 -0.232136
C 2.80511 -2.54176 -1.02765
Co 1.61802 -0.914625 -0.0707052
C 1.93899 0.800366 0.160397
H -5.56296 -2.19258 0.356227
H 3.55224 -1.47092 2.07069
H 1.347 -3.03193 1.98491
H 0.92159 -3.6998 -0.600996
P -0.299372 -0.603476 -1.14841
P -2.09193 -1.95426 -0.591364
P -1.16714 -0.588338 0.975734
P -1.72638 1.06849 -0.475797
Co -3.46821 -0.265467 -0.417952
C -5.437 -1.18301 -0.0123118
C -5.29377 -0.00559438 0.791478
C -5.16031 1.12057 -0.0794458
C -5.18116 0.638377 -1.42346
C -5.35655 -0.788977 -1.38115
H 2.92531 -2.65407 -2.09732
H 4.52701 -1.24627 -0.44373
H -5.29519 0.0269028 1.87399
H -5.03485 2.15064 0.227408
H -5.09096 1.23906 -2.3195
H -5.41874 -1.44491 -2.23995

O 2.2058 1.92273 0.31267

NIMAG = -136.33 $cm^{-1}$

Total bonding energy: -15920.64 kJ/mol

**TS4NHC**



Cartesian coordinates:

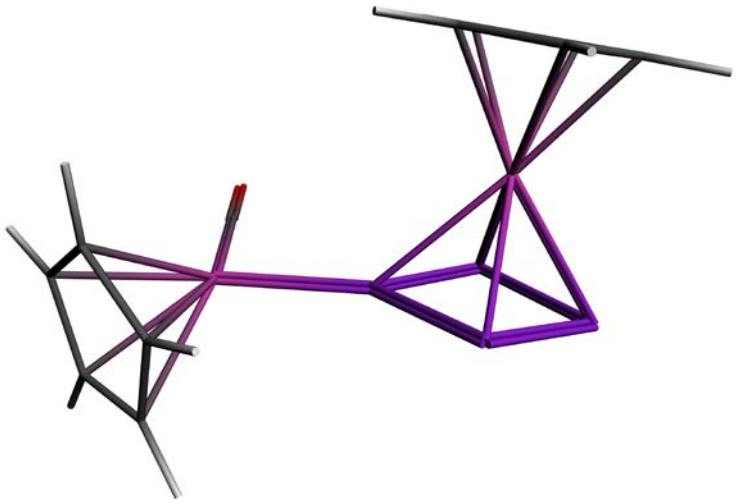
| | | | |
|---|---|---|---|
| Co | 3.23170000 | 0.02267360 | 0.29847800 |
| P | 1.40356000 | 0.65844800 | 1.30357000 |
| P | 1.04959000 | 0.08447460 | -0.86973400 |
| P | 2.24776000 | -1.78664000 | -0.41896600 |
| P | 0.31721600 | -1.32315000 | 0.79742500 |
| Co | -1.34929000 | -0.97092400 | -0.63059600 |
| C | -2.14758000 | 0.56109100 | 0.28068900 |
| N | -2.86156000 | 0.54036600 | 1.46889000 |
| C | -3.40471000 | 1.79515000 | 1.75210000 |
| C | -3.06183000 | 2.61875000 | 0.72494100 |
| N | -2.27664000 | 1.86805000 | -0.15296200 |
| C | -3.05039000 | -0.65207500 | 2.34272000 |
| C | -4.53945000 | -1.03759000 | 2.43735000 |
| C | -1.69341000 | 2.41429000 | -1.40920000 |
| C | -0.72721700 | 3.57729000 | -1.11452000 |
| C | -2.41200000 | -0.43447900 | 3.72786000 |
| C | -2.80299000 | 2.81013000 | -2.40392000 |
| C | 4.84537000 | 0.54286600 | -1.08636000 |
| C | 4.41087000 | 1.73047000 | -0.40471800 |
| C | 4.70008000 | 1.56897000 | 0.98650700 |
| C | 5.30586000 | 0.28776600 | 1.16995000 |
| C | 5.39581000 | -0.34551500 | -0.10896900 |
| C | -2.33839000 | -1.11866000 | -2.63055000 |
| C | -1.17502000 | -1.93710000 | -2.61205000 |
| C | -1.35386000 | -2.93569000 | -1.59414000 |
| C | -2.66177000 | -2.77125000 | -1.02275000 |
| C | -3.25286000 | -1.63473000 | -1.63429000 |
| H | -3.99097000 | 1.99714000 | 2.63695000 |

| | | | |
|---|---|---|---|
| H | -3.29163000 | 3.66240000 | 0.56536000 |
| H | -2.51117000 | -1.44772000 | 1.81927000 |
| H | -4.64570000 | -1.96495000 | 3.01525000 |
| H | -4.96814000 | -1.20067000 | 1.44140000 |
| H | -5.12914000 | -0.26118900 | 2.94418000 |
| H | -1.12588000 | 1.57484000 | -1.82175000 |
| H | -0.23714200 | 3.89004000 | -2.04573000 |
| H | -1.25515000 | 4.45012000 | -0.70548500 |
| H | 0.04526110 | 3.26962000 | -0.40100400 |
| H | -2.50119000 | -1.35171000 | 4.32490000 |
| H | -1.34947000 | -0.18421300 | 3.63267000 |
| H | -2.91158000 | 0.37400400 | 4.27965000 |
| H | -2.35221000 | 3.13092000 | -3.35237000 |
| H | -3.40799000 | 3.64467000 | -2.02333000 |
| H | -3.47182000 | 1.96536000 | -2.60681000 |
| H | 4.77318000 | 0.35435000 | -2.15145000 |
| H | 3.95268000 | 2.60062000 | -0.86151900 |
| H | 4.46599000 | 2.28675000 | 1.76470000 |
| H | 5.60619000 | -0.14498400 | 2.11755000 |
| H | 5.79201000 | -1.33529000 | -0.30378500 |
| H | -2.52524000 | -0.28456400 | -3.29724000 |
| H | -0.29894100 | -1.81602000 | -3.23916000 |
| H | -0.64098000 | -3.71342000 | -1.34271000 |
| H | -3.10575000 | -3.38902000 | -0.24994200 |
| H | -4.22755000 | -1.22050000 | -1.39929000 |

NIMAG = -107.9 $cm^{-1}$

Total bonding energy: -28776.33 kJ/mol

[{CpCo(CO)}($\eta^{1:4}$-$P_4$){CpCo}] **7CO**



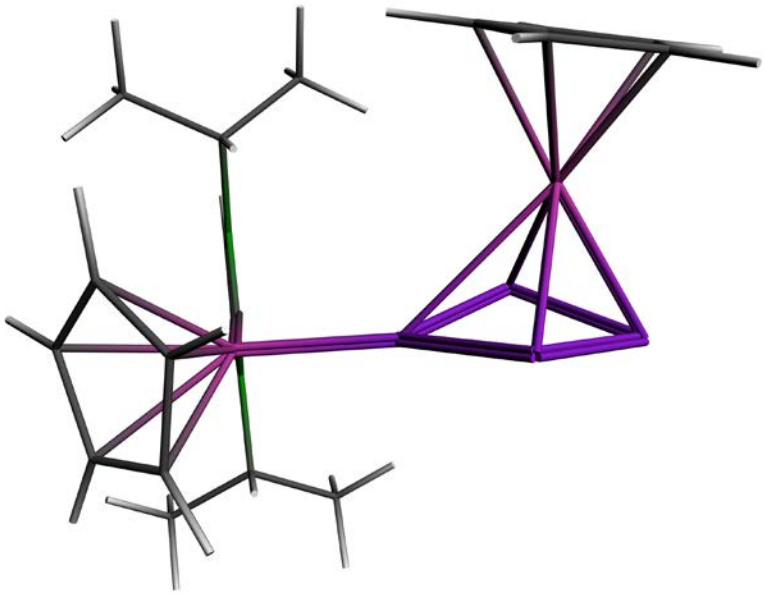
Cartesian coordinates:

Co 2.87574 0.198855 0.00563939
P 1.8405 2.10792 -0.962833
P 3.58063 1.19772 -1.99706
P 2.57298 -0.775885 -2.14297
P 0.809558 0.19141 -1.26957
Co -1.18778 -0.518355 -0.970142
C -1.61878 0.838538 0.0526423
H -0.0757389 -2.98983 -2.04849
H -1.54704 -3.19487 0.21585
H 4.3282 -2.21771 0.700002
H -3.7218 -1.61444 -0.0934841
H -3.65096 -0.534397 -2.57495
H -1.39314 -1.38858 -3.78472
H 5.67403 0.12056 0.846899
H 4.04188 1.95219 1.98184
H 1.86852 -1.84666 1.7771
H 1.68927 0.736604 2.56268
C 4.66695 -0.0568728 1.20177
C 3.801 0.913452 1.79552
C 2.54904 0.267707 2.1021
C 2.64527 -1.09835 1.68908
C 3.9498 -1.29373 1.11756
C -2.90784 -1.20033 -2.15578
C -1.72769 -1.64773 -2.78855
C -1.0178 -2.49319 -1.85165
C -1.79396 -2.60888 -0.659199
C -2.94075 -1.77498 -0.82577
O -1.90545 1.74091 0.733357

NIMAG = 0

Total bonding energy: -15987.78 kJ/mol

[{CpCo(iPr$_2$Im)}($\eta^{1:4}$-P$_4$){CpCo}] **7NHC**



Cartesian coordinates:

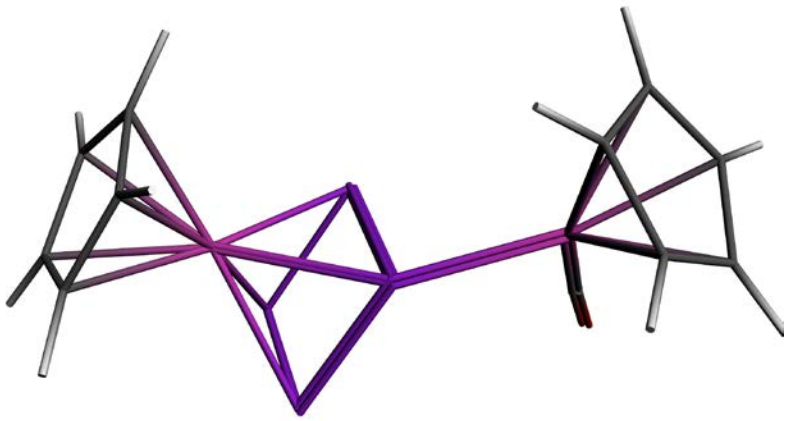
Co 4.14212 -3.0677 1.8924
P 3.11386 -1.08611 1.14048
P 4.8701 -1.91414 0.0423849
P 3.74879 -3.81058 -0.302617
P 1.91323 -2.73798 0.298251
Co -0.0939503 -3.33561 0.339969
C -0.70619 -1.70779 1.18738
N -0.841549 -1.44632 2.5359
C -1.40811 -0.189686 2.74921
C -1.6281 0.35841 1.52515
N -1.19597 -0.570895 0.57993
H -2.28035 -3.57597 -1.67394
H 0.106071 -4.73914 -2.20605
H 6.55084 -4.60357 2.32818
H 6.35865 -2.19276 3.54976
H 2.52576 -4.26895 4.02848
H 3.86904 -1.97548 4.57094
C 5.68178 -4.21484 2.84313
C 5.58075 -2.94302 3.49015
C 4.25566 -2.82846 4.02891
C 3.54369 -4.03956 3.74272
C 4.41713 -4.88568 2.99084
C -1.67313 -4.14639 -0.983256
C -0.428194 -4.77062 -1.2653
C 0.00799533 -5.45341 -0.0754408
C -0.988211 -5.27935 0.937321
C -2.00514 -4.44558 0.387413
H -1.60003 0.209002 3.73346
H -2.04331 1.31822 1.25879

H -0.971875 -5.70143 1.93383
H 4.17511 -5.86842 2.60648
H -2.8943 -4.10547 0.904569
H 0.918294 -6.03139 0.0189981
H -2.23832 -2.17091 4.86143
H -0.700849 1.77129 -0.906481
C -1.24021 -0.356879 -0.890709
H -0.828529 -1.28642 -1.29691
C -2.69222 -0.1865 -1.37736
H -3.31066 -1.04012 -1.07788
H -2.70978 -0.113568 -2.47159
H -3.14909 0.727525 -0.975438
C -0.333222 0.816403 -1.30503
H 0.690643 0.660039 -0.948189
H -0.310772 0.896212 -2.39855
C -0.43975 -2.38019 3.62029
H 0.0750268 -3.18619 3.08663
C 0.543658 -1.70325 4.59334
H 1.40533 -1.29581 4.05496
H 0.904437 -2.43954 5.32149
H 0.0645539 -0.891257 5.15579
C -1.67315 -2.95661 4.34283
H -2.34446 -3.45732 3.63698
H -1.35289 -3.68931 5.09403

NIMAG = 0

Total bonding energy: -28856.04 kJ/mol

**TS5CO**



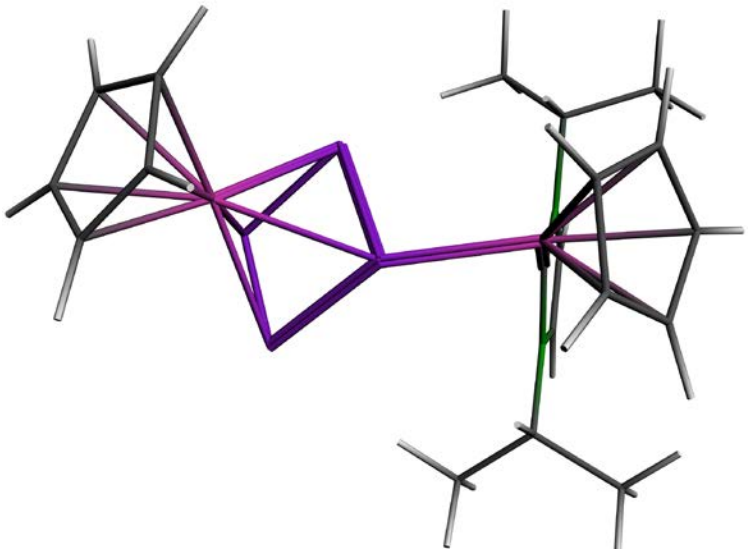
Cartesian coordinates:

Co 3.04035 0.418588 0.0477965
P 1.59946 2.15909 -0.782354
P 2.95972 1.15053 -2.20382
P 2.05618 -0.81707 -1.69477
P 0.661355 0.215736 -0.241285
Co -1.15593 -0.935533 -0.996314
C -1.15516 -0.277035 -2.62692
H -2.74135 -0.112584 1.42029
H -4.0168 -0.454838 -0.935948
H 3.84488 -2.0179 1.36388
H -3.09943 -2.74832 -2.06608
H -1.24639 -3.81961 -0.410851
H -0.967994 -2.13141 1.68397
H 5.63955 -0.785812 -0.246866
H 5.5291 1.87031 0.265406
H 2.64836 -0.124629 2.88622
H 3.68665 2.27359 2.20389
C 5.00026 -0.303038 0.48095
C 4.94327 1.10304 0.754725
C 3.96659 1.31583 1.78503
C 3.42037 0.0472695 2.14779
C 4.04699 -0.955059 1.33363
C -1.79754 -2.90181 -0.253636
C -1.65737 -2.00343 0.858624
C -2.60706 -0.933354 0.728343
C -3.25695 -1.10009 -0.513562
C -2.75963 -2.33329 -1.12564
O -1.22937 0.154206 -3.70579

NIMAG = -144.41 $cm^{-1}$

Total bonding energy: -15898.60 kJ/mol

**TS5NHC**



Cartesian coordinates:

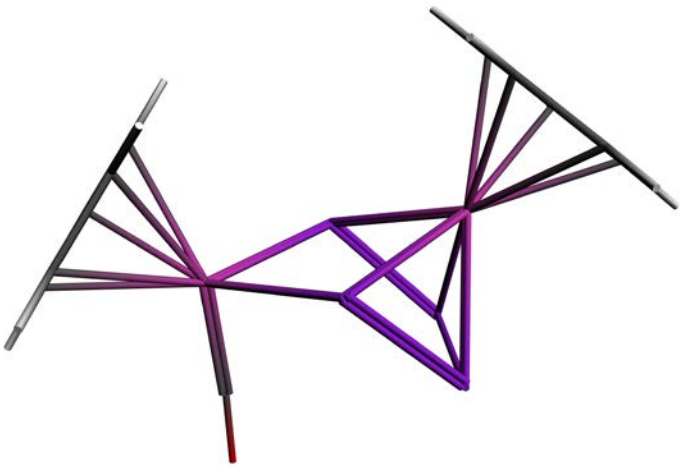
Co 3.13266 0.255509 -0.0939926
P 1.81925 2.12588 -0.778009
P 3.08337 1.10961 -2.28486
P 2.02118 -0.799211 -1.85028
P 0.668706 0.254313 -0.368435
Co -1.26364 -0.703923 -1.06102
H -2.1151 2.17006 -5.23543
H -2.08558 -0.072467 1.76306
H -3.87781 0.392543 -0.200005
H 3.71094 -2.32114 1.06864
H -3.81949 -1.72756 -1.89295
H -2.06656 -3.54775 -0.913425
H -0.936538 -2.46255 1.2923
H 5.64044 -1.1467 -0.425313
H 5.75214 1.46634 0.268406
H 2.65645 -0.441817 2.70692
H 3.90526 1.89835 2.19496
C 5.0328 -0.658765 0.325911
C 5.09494 0.72041 0.696421
C 4.1117 0.948946 1.71799
C 3.45661 -0.289721 1.99481
C 4.00442 -1.28039 1.11671
C -2.28548 -2.57358 -0.495354
C -1.70198 -2.00254 0.679928
C -2.32757 -0.736728 0.943292
C -3.23259 -0.471315 -0.106397
C -3.19906 -1.61107 -1.01267
C -1.38053 -0.0257851 -2.86807
N -1.77908 1.22341 -3.30242
N -1.19176 -0.73369 -4.04096

C -1.4684 0.0550757 -5.15634
C -1.83635 1.27891 -4.69442
H -3.96616 2.97998 -3.46812
H 0.180093 -2.12784 -6.08828
H -1.3691 -0.303428 -6.16931
C -2.14304 2.36016 -2.41632
H -1.87526 2.00931 -1.41489
C -1.32061 3.61696 -2.75381
H -0.246794 3.40739 -2.7116
H -1.54569 4.40623 -2.02632
H -1.56579 4.00555 -3.7513
C -3.66004 2.63162 -2.47269
H -4.23257 1.72894 -2.23402
H -3.92453 3.41217 -1.74864
C -0.785798 -2.16214 -4.11583
H -0.494426 -2.40988 -3.08982
C -1.9754 -3.05008 -4.53246
H -2.8192 -2.92617 -3.84571
H -1.67296 -4.10462 -4.52183
H -2.31679 -2.80795 -5.54765
C 0.42903 -2.35026 -5.04219
H 1.26052 -1.7094 -4.73199
H 0.763419 -3.39363 -4.99555

NIMAG = -119.52 $cm^{-1}$

Total bonding energy: -28759.73 kJ/mol

[CpCo(μ,$\eta^{4:2}$-$P_4$)Co(CO)Cp] **8CO**



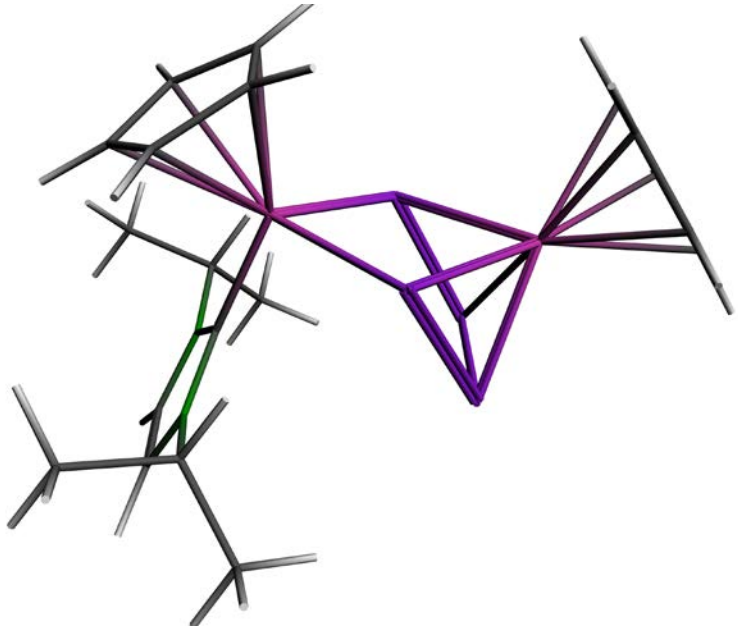
Cartesian coordinates:

H 2.1713 -1.99548 -1.35537
H 3.74384 0.0413002 -2.18578
H 4.71497 1.29451 0.0
C -2.09382 2.33934 0.0
H -4.80306 0.779185 0.0
Co -1.84768 0.598739 0.0
P -0.00444271 0.716539 -1.40066
Co 1.87416 0.554899 0.0
P 1.21456 2.53615 -1.09945
P 1.21456 2.53615 1.09945
P -0.00444271 0.716539 1.40066
H -3.64773 -0.294422 2.18999
H -1.73703 -2.01582 1.35164
H -1.73703 -2.01582 -1.35164
H -3.64773 -0.294422 -2.18999
C 2.70619 -1.30496 -0.716892
C 2.70619 -1.30496 0.716892
C 3.55031 -0.234417 1.15727
C 4.06667 0.427296 0.0
C 3.55031 -0.234417 -1.15727
C -3.39864 -0.525619 1.16279
C -4.01062 0.0411132 0.0
C -3.39864 -0.525619 -1.16279
C -2.38769 -1.42763 -0.717968
C -2.38769 -1.42763 0.717968
H 3.74384 0.0413002 2.18578
H 2.1713 -1.99548 1.35537
O -2.33273 3.47344 0.0

NIMAG = 0

Total bonding energy: -15998.78 kJ/mol

[CpCo(μ,$\eta^{4:2}$-$P_4$)Co(*i*$Pr_2$Im)Cp] **8NHC**



Cartesian coordinates:

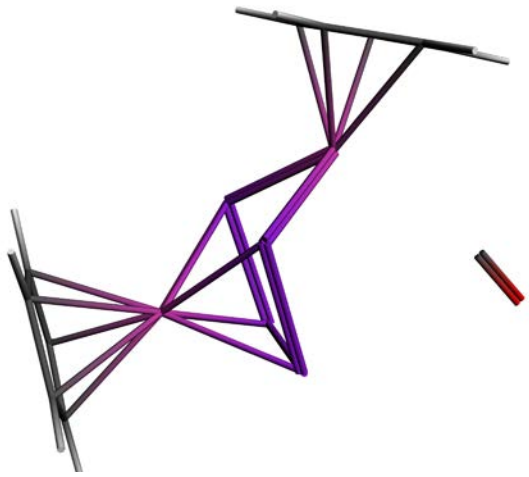
C 1.4519 -3.99357 1.21786
C 2.19212 -3.87893 0.0829089
N 1.5596 -2.93035 -0.719416
C 0.423996 -2.44476 -0.107882
N 0.377408 -3.11337 1.09511
Co -0.837432 -1.16595 -0.838991
P -1.57578 2.56928 1.87839
Co 0.118508 2.67489 0.263355
P 0.309632 2.52726 2.67298
P 1.73052 1.13937 1.21526
P 0.241888 0.464216 -0.0706425
C 2.05668 -2.48623 -2.04843
C 3.45351 -1.84931 -1.92976
C -0.657121 -2.90801 2.14576
C -1.49596 -4.18545 2.34263
C -0.888253 3.89019 -1.22802
C 0.202152 3.22193 -1.87027
C 1.41407 3.70143 -1.28923
C 1.08282 4.69775 -0.317637
C -0.328341 4.81776 -0.280523
C -1.82883 -1.3642 -2.80622
C -2.06342 -2.53607 -2.03703
C -2.78718 -2.16247 -0.840153
C -2.98098 -0.755934 -0.873299
C -2.36426 -0.255564 -2.07016
C -0.0231178 -2.41477 3.45926
C 2.01494 -3.64063 -3.06687
H 2.41168 3.35734 -1.52961
H 0.123049 2.47402 -2.64816

H -1.93959 3.77385 -1.45606
H -0.893978 5.45554 0.38601
H 1.78591 5.2321 0.30875
H -1.76815 -3.54358 -2.30321
H -1.32963 -1.31529 -3.76556
H -2.33661 0.782416 -2.37439
H -3.47588 -0.157512 -0.119268
H -3.14479 -2.84305 -0.0786334
H 3.10119 -4.38233 -0.208441
H 1.60494 -4.61361 2.08772
H -1.29034 -2.11484 1.73803
H -0.814477 -2.19684 4.18649
H 0.55367 -1.49872 3.29474
H 0.635602 -3.17524 3.89965
H -2.30845 -3.98838 3.05239
H -1.93564 -4.52142 1.3968
H -0.889445 -5.00554 2.74934
H 1.33906 -1.71529 -2.34787
H 3.76146 -1.45435 -2.90565
H 4.20694 -2.58285 -1.61343
H 3.44381 -1.02409 -1.20961
H 2.31536 -3.27188 -4.05528
H 2.703 -4.4499 -2.78894
H 1.0051 -4.0587 -3.14639

NIMAG = 0

Total bonding energy: -28876.41 kJ/mol

**TS6CO**



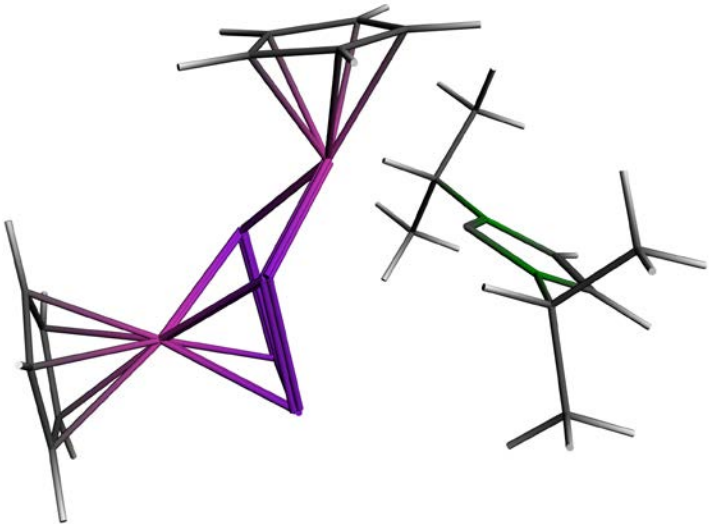
Cartesian coordinates:

H 2.6805 -1.95065 -1.35403
H 3.88021 0.32388 -2.18658
H 4.63191 1.72297 0.0
C -2.43281 3.34719 0.0
H -4.68578 1.20118 0.0
Co -1.66678 0.400654 0.0
P 0.0600646 0.287891 -1.42454
Co 1.94194 0.516142 0.0
P 0.899032 2.29076 -1.12153
P 0.899032 2.29076 1.12153
P 0.0600646 0.287891 1.42454
H -3.71786 -0.0248509 2.18954
H -2.07289 -2.01285 1.35909
H -2.07289 -2.01285 -1.35909
H -3.71786 -0.0248509 -2.18954
C 3.08887 -1.178 -0.716188
C 3.08887 -1.178 0.716188
C 3.73381 0.0230111 1.1572
C 4.13079 0.763647 0.0
C 3.73381 0.0230111 -1.1572
C -3.49733 -0.286422 1.163
C -4.02091 0.345833 0.0
C -3.49733 -0.286422 -1.163
C -2.60475 -1.31452 -0.725765
C -2.60475 -1.31452 0.725765
H 3.88021 0.32388 2.18658
H 2.6805 -1.95065 1.35403
O -2.47095 4.48498 0.0

NIMAG = -115.27 $cm^{-1}$

Total bonding energy: -15843.77 kJ/mol

**TS6NHC**



Cartesian coordinates:

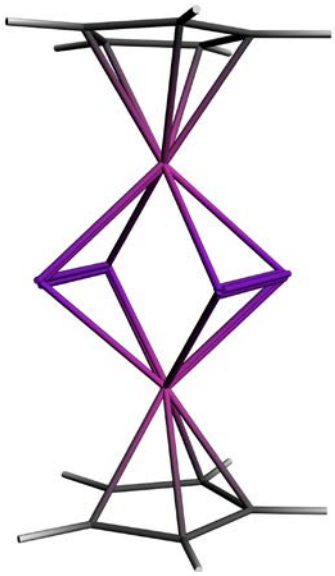
C 1.82132 -3.97062 2.21303
C 2.62414 -3.98128 1.11296
N 1.91816 -3.31644 0.105374
C 0.685162 -2.88473 0.530576
N 0.652525 -3.29944 1.83996
Co -1.27633 -0.281066 -0.984572
P -1.62836 1.32347 0.536603
Co 0.152537 2.84366 0.131667
P 0.242995 1.05859 1.64511
P 1.63502 1.04229 -0.103259
P 0.1392 1.30566 -1.68185
C 2.40601 -3.10486 -1.27866
C 3.75916 -2.37061 -1.29355
C -0.516283 -3.06951 2.72313
C -1.26135 -4.3886 3.00813
C -0.976477 4.68857 0.0233816
C 0.00435447 4.68116 -1.0204
C 1.29875 4.63746 -0.41009
C 1.11988 4.61775 1.00842
C -0.284518 4.64973 1.27796
C -1.61445 -1.72988 -2.68307
C -2.09273 -2.38183 -1.50619
C -3.10708 -1.5853 -0.906547
C -3.23345 -0.390658 -1.68643
C -2.30597 -0.487385 -2.79802
C -0.112646 -2.33286 4.01336
C 2.44912 -4.43386 -2.0586
H 2.24655 4.60866 -0.932007
H -0.195986 4.70495 -2.08331
H -2.04954 4.72456 -0.109828
H -0.744951 4.63408 2.25739

H 1.90867 4.57237 1.74836
H -1.6891 -3.29725 -1.09485
H -0.844755 -2.09734 -3.34905
H -2.19712 0.23748 -3.59472
H -3.94126 0.411793 -1.52136
H -3.65721 -1.82003 -0.0046464
H 3.6153 -4.391 0.982688
H 1.99571 -4.37044 3.20141
H -1.16286 -2.41589 2.13072
H -1.00884 -2.09897 4.60096
H 0.401048 -1.3938 3.78071
H 0.545856 -2.94824 4.64055
H -2.16746 -4.18972 3.59395
H -1.55306 -4.87986 2.07282
H -0.635097 -5.08456 3.5818
H 1.64671 -2.45502 -1.72295
H 4.04682 -2.14655 -2.32808
H 4.55579 -2.98343 -0.851316
H 3.69543 -1.42673 -0.74131
H 2.73489 -4.24887 -3.10166
H 3.18306 -5.12666 -1.62618
H 1.46797 -4.9223 -2.04825

NIMAG = -75.77 $cm^{-1}$

Total bonding energy: -28734.04 kJ/mol

[{CpCo(μ,η$^{2:2}$-$P_2$)}$_2$] **9**



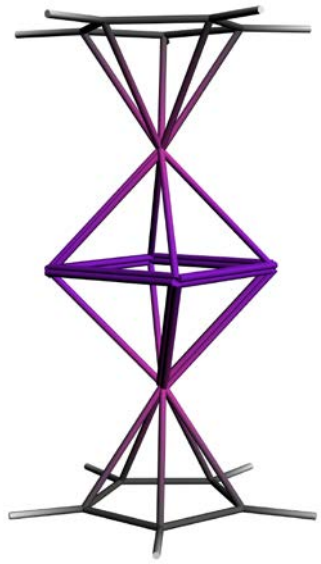
Cartesian coordinates:

C 3.44483 0.713688 -0.964438
C 3.37708 1.1564 0.396299
C 3.33605 0.0 1.24167
C 3.37708 -1.1564 0.396299
C 3.44483 -0.713688 -0.964438
Co 1.595 0.0 -0.0213763
P 0.0 1.34966 -1.17226
Co -1.595 0.0 -0.0213763
C -3.44483 0.713688 -0.964438
C -3.44483 -0.713688 -0.964438
C -3.37708 -1.1564 0.396299
C -3.33605 0.0 1.24167
C -3.37708 1.1564 0.396299
P 0.0 1.46244 0.927213
P 0.0 -1.46244 0.927213
P 0.0 -1.34966 -1.17226
H -3.47801 -1.35061 -1.83896
H -3.35202 -2.1867 0.72797
H -3.29137 0.0 2.32283
H -3.35202 2.1867 0.72797
H -3.47801 1.35061 -1.83896
H 3.35202 2.1867 0.72797
H 3.29137 0.0 2.32283
H 3.35202 -2.1867 0.72797
H 3.47801 -1.35061 -1.83896
H 3.47801 1.35061 -1.83896

NIMAG = 0

Total bonding energy: -14544.35 kJ/mol

$[\{CpCo(\mu,\eta^{4:4}\text{-}P_2)\}_2]^{2+}$ **$9^{2+}$**



Cartesian coordinates:

| | | | |
|---|---|---|---|
| 1 C | -0.984370000000 | -3.495400000000 | -0.716410000000 |
| 2 C | 0.378060000000 | -3.477260000000 | -1.160660000000 |
| 3 C | 1.222440000000 | -3.467450000000 | 0.00000000000 |
| 4 C | 0.378060000000 | -3.477260000000 | 1.160660000000 |
| 5 C | -0.984370000000 | -3.495400000000 | 0.716410000000 |
| 6 Co | 0.003290000000 | -1.725220000000 | 0.000000000000 |
| 7 P | -1.158120000000 | -0.000840000000 | -1.158330000000 |
| 8 Co | -0.003290000000 | 1.725220000000 | 0.000000000000 |
| 9 C | -1.222440000000 | 3.467450000000 | 0.000000000000 |
| 10 C | -0.378060000000 | 3.477260000000 | 1.160660000000 |
| 11 C | 0.984370000000 | 3.495400000000 | 0.716410000000 |
| 12 C | 0.984370000000 | 3.495400000000 | -0.716410000000 |
| 13 C | -0.378060000000 | 3.477260000000 | -1.160660000000 |
| 14 P | 1.158120000000 | 0.000840000000 | -1.158330000000 |
| 15 P | 1.158120000000 | 0.000840000000 | 1.158330000000 |
| 16 P | -1.158120000000 | -0.000840000000 | 1.158330000000 |
| 17 H | -0.711540000000 | 3.477410000000 | 2.191900000000 |
| 18 H | 1.861610000000 | 3.503680000000 | 1.353200000000 |
| 19 H | 1.861610000000 | 3.503680000000 | -1.353200000000 |
| 20 H | -0.711540000000 | 3.477410000000 | -2.191900000000 |
| 21 H | -2.306390000000 | 3.462680000000 | 0.000000000000 |
| 22 H | 0.711540000000 | -3.477410000000 | -2.191900000000 |
| 23 H | 2.306390000000 | -3.462680000000 | 0.000000000000 |
| 24 H | 0.711540000000 | -3.477410000000 | 2.191900000000 |
| 25 H | -1.861610000000 | -3.503680000000 | 1.353200000000 |
| 26 H | -1.861610000000 | -3.503680000000 | -1.353200000000 |

NIMAG = 0

Total bonding energy: -12993.71 kJ/mol

[$CpCo(CO)_2$]

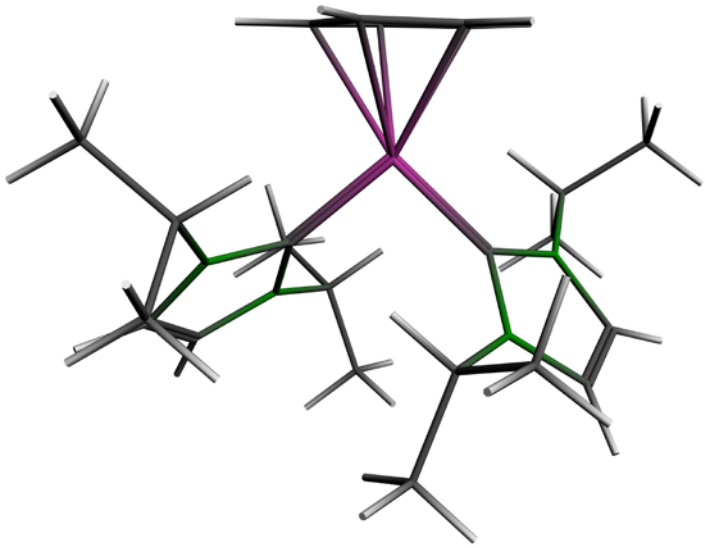
Cartesian coordinates:

| | | | |
|---|---|---|---|
| H | 1.62046116 | 2.03620661 | 0.23396157 |
| H | 0.20492258 | -1.77985140 | -1.38167944 |
| C | -2.59805785 | 0.23328942 | 0.01615797 |
| H | 1.44045293 | 0.53602326 | -2.01421614 |
| H | 0.52485366 | 0.64476497 | 2.27590161 |
| Co | -0.92536229 | 0.71258865 | -0.28148502 |
| C | 0.43679066 | -0.96632906 | -0.70711444 |
| C | 1.08034398 | 0.24443025 | -1.03593954 |
| C | 1.17229910 | 1.05242948 | 0.17237671 |
| C | 0.60266730 | 0.32395861 | 1.24587262 |
| C | 0.09215822 | -0.90142588 | 0.69590913 |
| H | -0.42103187 | -1.67605174 | 1.25255548 |
| O | -3.69935057 | -0.07880286 | 0.21141718 |
| C | -1.39570265 | 2.21884669 | -1.07956657 |
| O | -1.70352852 | 3.21119405 | -1.59767356 |

NIMAG = 0

Total bonding energy: -9284.70 kJ/mol

[$CpCo(iPr_2Im)_2$]



Cartesian coordinates:

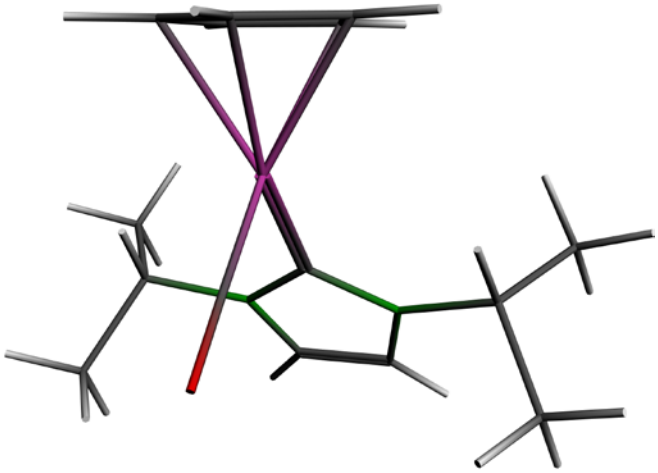
| | | | |
|---|---|---|---|
| C | -0.84290397 | 2.59651414 | 0.20241499 |
| N | -0.13047535 | 1.50426370 | 0.69545042 |
| C | -0.06461825 | 0.45478464 | -0.23178552 |
| N | -0.77617890 | 0.99000742 | -1.32008089 |
| C | -1.24685361 | 2.27590949 | -1.05242051 |
| Co | 0.73555802 | -1.27357580 | -0.00194498 |
| C | -0.75235943 | -2.65995685 | -0.91825386 |
| C | 0.54776928 | -3.15353860 | -1.20632606 |
| C | 1.17749597 | -3.42378761 | 0.05354882 |
| C | 0.23320566 | -3.17574361 | 1.11222530 |
| C | -0.94558671 | -2.67055034 | 0.51334699 |
| C | -1.00359499 | 0.31270698 | -2.61558436 |
| C | -0.46042526 | 1.14432619 | -3.79735629 |
| C | 0.34666435 | 1.42397789 | 2.09301791 |
| C | 1.31172955 | 2.57965744 | 2.42052497 |
| C | -2.49704733 | -0.02530068 | -2.80869509 |
| C | -0.83575289 | 1.35075877 | 3.08175846 |
| H | -1.50714516 | -2.39000805 | -1.64446528 |
| H | 0.97586364 | -3.32345589 | -2.18639100 |
| H | 2.17728784 | -3.82255769 | 0.17576354 |
| H | 0.38053122 | -3.37437933 | 2.16636009 |
| H | -1.85312974 | -2.37984697 | 1.02915901 |
| H | -1.81575569 | 2.85448575 | -1.76465953 |
| H | -1.00530857 | 3.49959428 | 0.77145913 |
| H | -0.42522337 | -0.61266698 | -2.53536196 |
| H | -2.63654756 | -0.61924507 | -3.72083018 |
| H | -2.88388460 | -0.59654863 | -1.95914540 |
| H | -3.09924640 | 0.88778637 | -2.90875061 |
| H | -0.55905458 | 0.57128205 | -4.72795129 |
| H | 0.59665365 | 1.39162523 | -3.65622111 |
| H | -1.01726778 | 2.08174480 | -3.92494298 |

| | | | |
|---|---|---|---|
| H | 0.88314905 | 0.47279406 | 2.12232196 |
| H | -0.46033888 | 1.21397297 | 4.10413550 |
| H | -1.48722159 | 0.50466738 | 2.83639232 |
| H | -1.43599706 | 2.27022497 | 3.06422668 |
| H | 1.69107615 | 2.47388234 | 3.44450806 |
| H | 2.16659534 | 2.58310926 | 1.73547917 |
| H | 0.81274676 | 3.55607541 | 2.35703780 |
| C | 4.58024049 | -0.27850993 | 1.33965601 |
| N | 3.31816710 | -0.85090589 | 1.50246381 |
| C | 3.01353628 | 0.49818568 | -1.84256288 |
| C | 3.85587354 | -0.30273316 | -2.85709751 |
| C | 2.91229141 | -1.56669736 | 2.73293075 |
| C | 3.65243995 | -2.91261681 | 2.87281288 |
| C | 3.14609582 | 2.01995708 | -2.04343475 |
| C | 3.10267466 | -0.69281055 | 3.99162510 |
| C | 2.49941619 | -0.63532606 | 0.38050537 |
| H | 5.38299940 | 0.87104912 | -0.36890785 |
| H | 5.35338523 | -0.33500495 | 2.09129931 |
| H | 1.96657769 | 0.19848080 | -1.94505671 |
| H | 2.85881044 | 2.28997277 | -3.06735128 |
| H | 2.49756997 | 2.56490555 | -1.34875996 |
| H | 4.17950173 | 2.36071124 | -1.89294647 |
| H | 3.54144439 | -0.05797507 | -3.87986077 |
| H | 3.71998513 | -1.37882321 | -2.70170436 |
| N | 3.34138658 | 0.10967567 | -0.45301706 |
| H | 4.92569024 | -0.06996638 | -2.77003268 |
| H | 1.84465456 | -1.75626287 | 2.58380349 |
| H | 2.68743731 | -1.21022829 | 4.86550678 |
| H | 2.59415116 | 0.27087889 | 3.88922985 |
| H | 4.16393153 | -0.49923552 | 4.19612194 |
| H | 3.28352753 | -3.45456721 | 3.75293350 |
| H | 3.49661822 | -3.54062286 | 1.99110098 |
| H | 4.73247148 | -2.75936474 | 3.00186096 |
| C | 4.59399601 | 0.32149302 | 0.12240563 |

NIMAG = 0

Total bonding energy: -34952.62 kJ/mol

[CpCo(CO)(iPr$_2$Im)]



Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -0.32119814 | 2.39277279 | 0.68971377 |
| N | 0.02434481 | 1.10130992 | 1.08882240 |
| C | 0.22357531 | 0.28096996 | -0.00172543 |
| N | -0.00300347 | 1.10534245 | -1.08299754 |
| C | -0.34024860 | 2.39414839 | -0.67053429 |
| Co | 0.74391137 | -1.57803119 | -0.01192655 |
| C | -1.01380938 | -2.67222591 | -0.83347522 |
| C | 0.16454007 | -3.38988695 | -1.14152338 |
| C | 0.80546448 | -3.72741901 | 0.10531827 |
| C | -0.02623301 | -3.27754212 | 1.18744379 |
| C | -1.12501009 | -2.59151409 | 0.61301625 |
| C | 0.15062927 | 0.68213498 | -2.49880825 |
| C | 1.29269927 | 1.45778467 | -3.18282626 |
| C | 0.21398659 | 0.66826172 | 2.49778160 |
| C | 1.38262587 | 1.42685270 | 3.15598910 |
| C | -1.18236255 | 0.79849062 | -3.26085028 |
| C | -1.09692822 | 0.79141456 | 3.29650442 |
| H | -1.72782530 | -2.27092572 | -1.54211581 |
| H | 0.53441067 | -3.63146706 | -2.13017322 |
| H | 1.73287075 | -4.27748500 | 0.20699319 |
| H | 0.16558196 | -3.42222933 | 2.24308834 |
| H | -1.93546157 | -2.11638217 | 1.15237847 |
| H | -0.56202919 | 3.19410872 | -1.36049980 |
| H | -0.52504094 | 3.19126689 | 1.38686570 |
| H | 0.43393136 | -0.37322018 | -2.41728659 |
| H | -1.06166713 | 0.40472390 | -4.27742167 |
| H | -1.97213635 | 0.22709318 | -2.76058528 |
| H | -1.51174828 | 1.84269248 | -3.34519200 |
| H | 1.44381409 | 1.07261054 | -4.19862580 |
| H | 2.22951719 | 1.34166968 | -2.62719124 |
| H | 1.06330019 | 2.52894216 | -3.26175833 |
| H | 0.48525903 | -0.38917609 | 2.40136896 |

| | | | |
|---|---|---|---|
| H | -0.95211229 | 0.38998636 | 4.30696809 |
| H | -1.90514744 | 0.23003649 | 2.81459285 |
| H | -1.41445531 | 1.83796835 | 3.39640375 |
| H | 1.56151456 | 1.02809175 | 4.16185465 |
| H | 2.30134669 | 1.31034401 | 2.57101626 |
| H | 1.16433698 | 2.49864139 | 3.25496261 |
| C | 2.41863691 | -1.13144692 | -0.01381692 |
| O | 3.54927186 | -0.80694931 | -0.01092489 |

NIMAG = 0

Total bonding energy: -22166.11 kJ/mol