Supporting Information

Tuning the Electronic Properties of Hexanuclear Cobalt Sulfide Superatoms via Ligand Substitution

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Table S1. Total energies of the optimized ground state structure of anionic and neutral $Co_6S_8(PEt_3)_{6-x}(CO)_x$ (x = 0–3) clusters. The absolute values of the HOMO and LUMO along with HOMO-LUMO gap are given in eV. The ΔE in eV indicates the energy difference between the ground state and next isomers. The superscript shows the spin-multiplicity (2S+1) of the clusters.

	Energy (eV)	**ΔE (eV)**	**HOMO (eV)**	**LUMO (eV)**	**Gap (eV)**
Anionic clusters					
$^2Co_6S_8(PEt_3)_6^-$	-952.762276		-0.864	1.145	2.00
$^2Co_6S_8(PEt_3)_5(CO)^-$	-834.149686		-1.218	1.336	2.55
^{2}*cis*-$Co_6S_8(PEt_3)_4(CO)_2^-$	-715.340577		-1.420	1.144	2.56
^{2}*trans*-$Co_6S_8(PEt_3)_4(CO)_2^-$	-715.141098	0.20	-1.106	0.799	1.90
^{2}*mer*-$Co_6S_8(PEt_3)_3(CO)_3^-$	-596.489037		-1.634	0.650	2.28
^{2}*fac*-$Co_6S_8(PEt_3)_3(CO)_3^-$	-596.419529	0.07	-1.659	0.960	2.61
Neutral clusters					
$^1Co_6S_8(PEt_3)_6$	-951.696926		-4.876	-1.120	3.76
$^1Co_6S_8(PEt_3)_5(CO)$	-832.746714		-5.134	-1.414	3.72
^{1}*cis*-$Co_6S_8(PEt_3)_4(CO)_2$	-713.688205	0.07	-5.420	-1.684	3.74
^{1}*trans*-$Co_6S_8(PEt_3)_4(CO)_2$	-713.758306		-5.406	-1.746	3.66
^{1}*mer*-$Co_6S_8(PEt_3)_3(CO)_3$	-594.564298		-5.724	-2.056	3.67
^{1}*fac*-$Co_6S_8(PEt_3)_3(CO)_3$	-594.482414	0.08	-5.760	-1.986	3.77

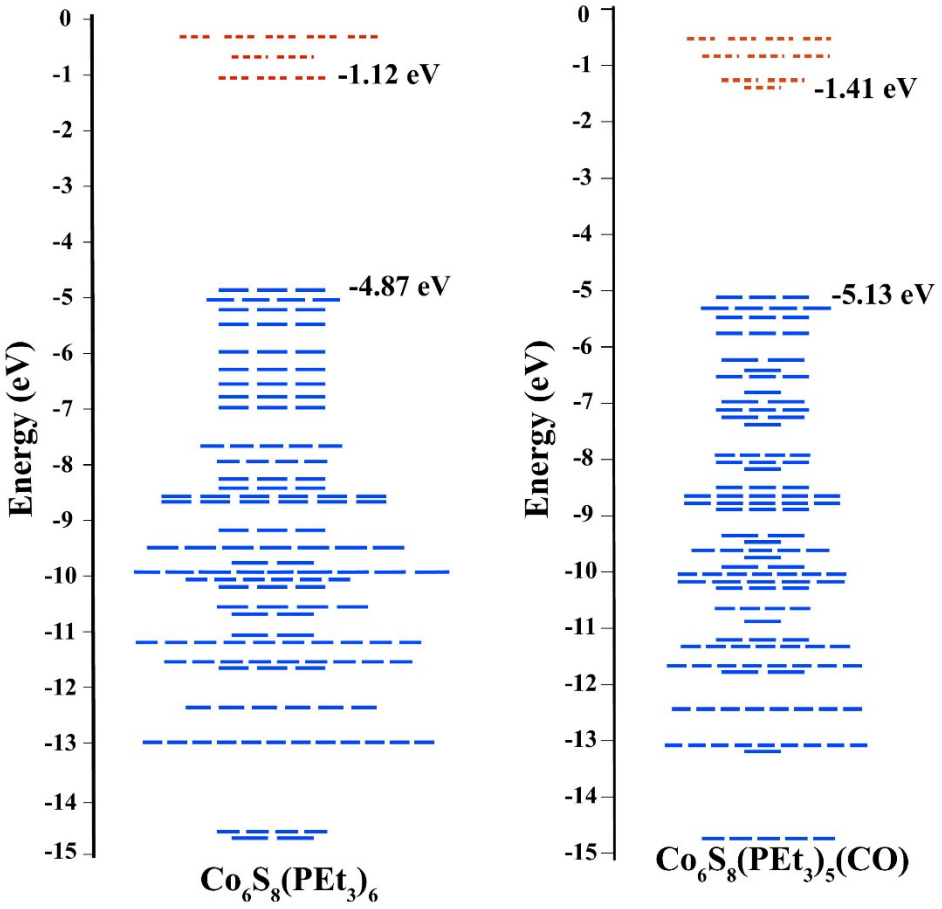

Figure S1. The one-electron energy levels of $Co_6S_8(PEt_3)_6$ and $Co_6S_8(PEt_3)_5(CO)$ clusters. Blue solid and red dashed lines show the occupied and unoccupied energy levels.

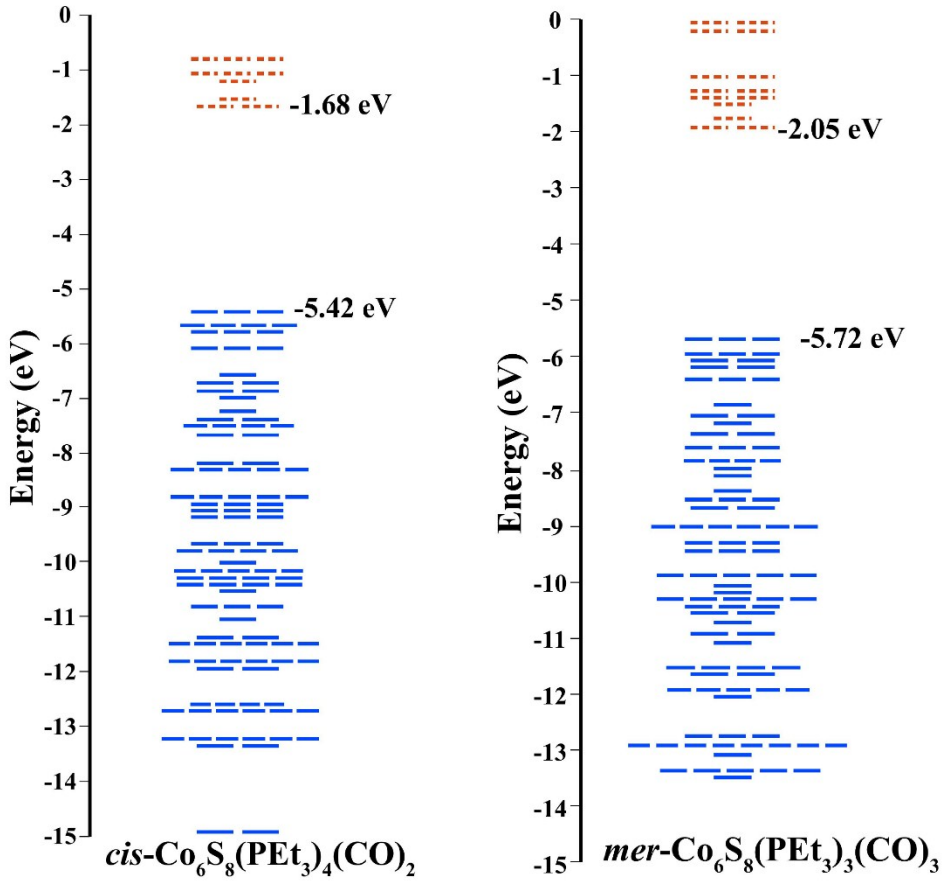

Figure S2. The one-electron energy levels of *cis*-$Co_6S_8(PEt_3)_4(CO)_2$ and *mer*-$Co_6S_8(PEt_3)_3(CO)_3$ clusters. Blue solid and red dashed lines show the occupied and unoccupied energy levels.

Cartesian coordinates of $Co_6S_8(PEt_3)_{6-x}(CO)_x^{-/0}$ (x = 0–3) clusters

$Co_6S_8(PEt_3)_6^-$

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XYZ

S -1.553319 1.649975 -1.570949

S 1.553539 -1.64981 1.570982

S 1.6238 1.546871 -1.597193

S -1.623577 -1.546732 1.597311
S -1.533585 1.645772 1.6249
S 1.533806 -1.645611 -1.624797
S -1.649535 -1.539319 -1.586106
S 1.649757 1.539465 1.586149
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Co -0.056784 -2.019541 -0.009442
Co -0.015451 0.003877 -2.018631
Co 0.015639 -0.00372 2.018705
Co -2.10559 0.067987 0.021054
Co 2.106185 -0.067861 -0.020989
P -4.388124 0.066544 0.02883
P 4.389034 -0.066414 -0.028632
P -0.075087 -0.018674 -4.187707
P 0.075682 0.018835 4.187763
P 0.074382 4.189233 -0.059246
P -0.073942 -4.18905 0.059344
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C -0.879109 -4.963747 1.544551
C -2.868147 0.230936 -4.65901
C 2.868851 -0.230557 4.658499
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C -0.189119 -4.648398 2.868196
C -0.120611 -1.711117 -4.946294
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C 0.3662 4.881926 2.675878
C -0.365885 -4.88181 -2.675773
C -5.246195 1.470184 -0.848299
C 5.247074 -1.470026 0.848618
C -1.51229 0.852902 -4.980476
C 1.513102 -0.852578 4.980307
C 2.684288 0.121551 -4.8327
C -2.683546 -0.121556 4.833286
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$Co_6S_8(PEt_3)_5(CO)^-$

126

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H -5.211489 2.898593 0.794172
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O -0.028554 0.031729 5.226861

***cis*-$Co_6S_8(PEt_3)_4(CO)_2^-$**

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XYZ

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S 1.523717 -1.615611 1.558953

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S -1.555829 1.589804 1.548295

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S 1.5743 1.503758 1.571721

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Co -0.033679 -0.021657 2.226634

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Co 1.984104 -0.04986 -0.048186

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H 5.241919 -3.52255 0.895229

H 2.709842 -6.837128 0.122112

H 1.144255 -6.964811 -0.683819

H 1.22682 -6.858865 1.079176

H -3.541584 3.067055 -0.092973

H -4.98606 2.990298 0.921166

H -5.074791 3.743761 -0.678723

O -0.066663 -0.026418 5.245171

O 0.101313 4.882435 0.103196

***trans*-$Co_6S_8(PEt_3)_4(CO)_2^-$**

106

XYZ

S -1.533255 1.610015 -1.620344

S 1.537512 -1.609601 1.628061

S 1.640141 1.506611 -1.605136

S -1.636033 -1.506027 1.611992

S -1.540781 1.670014 1.5626

S 1.544979 -1.669771 -1.555487

S -1.627825 -1.5593 -1.556451

S 1.631814 1.559813 1.564402

Co 0.059729 2.01332 -0.031918

Co -0.055012 -2.01288 0.039387

Co 0.008828 -0.035651 -2.018114

Co -0.004441 0.035968 2.025575

Co -2.092237 0.069765 -0.000914

Co 2.090258 -0.068938 0.008197

P -4.373556 0.068759 0.044219

P 4.363351 -0.067503 -0.03876

C 0.007797 -0.068314 -3.764128

C -0.009011 0.068773 3.771564

P 0.078062 4.181941 -0.068051

P -0.078502 -4.181631 0.076067

C -1.604471 4.961197 -0.099879

C 1.602909 -4.963529 0.108061

C -5.214457 -1.395518 -0.742829

C 5.203751 1.397438 0.746417

C 0.927401 5.012547 1.358663

C -0.928697 -5.011339 -1.350607

C -5.109073 0.118324 1.752803

C 5.094304 -0.119032 -1.748575

C 0.959283 4.966481 -1.501669

C -0.960566 -4.964664 1.509936

C 0.317988 4.682967 -2.857386

C -0.318483 -4.681828 2.865422

C 0.261874 4.764608 2.709714

C -0.262525 -4.764355 -2.701512

C -5.255311 1.450014 -0.8415

C 5.243941 -1.448438 0.847592

C -4.977163 2.8213 -0.231256

C 4.967518 -2.820219 0.237882

C -4.884386 -2.723983 -0.065847

C 4.874203 2.725811 0.069184

C -1.659632 6.486325 -0.125308

C 1.655837 -6.488737 0.133689

C -6.629719 0.092142 1.875808

C 6.614791 -0.093307 -1.873698

H -2.104866 4.525757 -0.972071

H 2.103949 -4.528816 0.980241

H -2.125466 4.553986 0.773939

H 2.1246 -4.557311 -0.765803

H -6.298679 -1.22688 -0.781458

H 6.28781 1.227694 0.78379

H -4.847959 -1.405489 -1.77665

H 4.838223 1.407882 1.780531

H 1.944931 4.605056 1.361668

H -1.945666 -4.602478 -1.353932

H 1.002117 6.085578 1.13941

H -1.004811 -6.084235 -1.131199

H -4.647985 -0.723191 2.284134

H 4.632295 0.722097 -2.279634

H -4.68354 1.014513 2.22054

H 4.667524 -1.015665 -2.214242

H 1.036096 6.045077 -1.312458

H -1.038953 -6.043166 1.320853

H 1.974369 4.553872 -1.473378

H -1.975023 -4.550527 1.481927

H 0.925235 5.10594 -3.665358

H -0.925757 -5.104434 3.673563

H -0.684875 5.117104 -2.929414

H 0.684087 -5.116727 2.937076

H 0.229032 3.60541 -3.02216

H -0.229005 -3.604327 3.030268

H 0.849671 5.217187 3.516072

H -0.850288 -5.216959 -3.507876

H 0.178196 3.69182 2.90505

H -0.178602 -3.691653 -2.897223

H -0.74587 5.191622 2.74911

H 0.745027 -5.191898 -2.740432

H -4.871983 1.414514 -1.868649

H 4.860288 -1.412579 1.874552

H -6.332638 1.243385 -0.886757

H 6.320966 -1.240416 0.892707

H -3.80064 -2.865309 -0.012984

H 3.790573 2.868532 0.018205

H -5.31629 -3.563971 -0.622134

H 5.308228 3.565285 0.624543

H -5.27479 -2.764238 0.956929

H 5.262936 2.76511 -0.954239

H -7.09249 0.944548 1.366449

H 7.078253 -0.945177 -1.364098

H -6.940212 0.131263 2.926838

H 6.923323 -0.133864 -2.925197

H -7.054867 -0.819878 1.443177

H 7.040828 0.81923 -1.443075

H 5.39935 -2.909935 -0.764886

H 3.890296 -2.987624 0.151869

H 5.391716 -3.619088 0.856878

H 2.694795 -6.837354 0.152964

H 1.180311 -6.927513 -0.749732

H 1.157264 -6.898431 1.018388

H -1.161711 6.896888 -1.009981

H -1.184742 6.925711 0.75816

H -2.69911 6.833363 -0.144504

H -3.899671 2.987184 -0.144968

H -5.40887 2.911032 0.77159

H -5.400223 3.621265 -0.84967

O -0.011651 0.090214 4.918485

O 0.007682 -0.089739 -4.911088

***fac*-$Co_6S_8(PEt_3)_3(CO)_3^-$**

86

XYZ

S -1.522714 1.596911 -1.583262

S 1.580555 -1.620084 1.588097

S 1.646898 1.552804 -1.591415

S -1.619354 -1.545237 1.528312

S -1.553283 1.584734 1.544451

S 1.605736 -1.634982 -1.601049

S -1.593263 -1.558427 -1.587755

S 1.624002 1.537575 1.596184

Co 0.071344 1.991214 -0.002148

Co 0.001358 -2.011062 -0.008232

Co 0.039066 -0.012194 -2.006957

Co 0.010983 -0.013372 1.986976

Co -2.248278 0.041241 -0.030715

Co 2.036424 -0.039936 -0.000748

C -4.121472 0.08189 -0.038856

P 4.227393 -0.00836 -0.004267

P -0.088372 -0.023153 -4.177518

C -0.091314 -0.013117 3.734464

C 0.020803 3.740815 0.003557

P -0.064437 -4.184049 0.085989

C 1.607858 -4.988781 0.063207

C 5.028483 1.453963 0.813495

C 1.282127 0.862108 -5.066096

C -0.983975 -5.040036 -1.2806

C 4.99583 -0.044468 -1.69294

C -0.89066 -4.926615 1.572466

C -2.902563 0.145253 -4.590353

C -0.206197 -4.607224 2.898423

C -0.085809 -1.714769 -4.93756

C -0.321321 -4.894078 -2.646573

C 5.073859 -1.397551 0.893312

C -1.568483 0.802373 -4.932438

C 2.647403 0.20115 -4.903645

C 4.877983 -2.760781 0.237166

C 4.737667 2.790253 0.135954

C 1.643245 -6.513185 0.12961

C -0.166185 -1.78802 -6.459924

C 6.520616 -0.028403 -1.761132

H 2.152855 -4.539412 0.900858

H 2.096196 -4.612581 -0.842967

H 6.108076 1.266117 0.876683

H 4.635058 1.458552 1.83656

H 1.010043 0.959327 -6.124874

H 1.296072 1.86947 -4.634736

H -1.975388 -4.57346 -1.291058

H -1.114854 -6.095492 -1.009839

H 4.562271 0.811614 -2.222295

H 4.579062 -0.933988 -2.179385

H -0.967751 -6.009995 1.413722

H -1.90757 -4.518357 1.568028

H -3.732065 0.722603 -5.013328

H -3.041469 0.089968 -3.506883

H -2.966272 -0.873658 -4.987071

H -0.776927 -5.026777 3.73425

H 0.806909 -5.021109 2.94306

H -0.133246 -3.525857 3.042808

H 0.819604 -2.201017 -4.556844

H -0.924161 -2.238456 -4.464678

H -0.960119 -5.308714 -3.43424

H -0.141625 -3.839158 -2.869105

H 0.641166 -5.41556 -2.687293

H 4.634235 -1.395853 1.89731

H 6.13902 -1.154807 0.997981

H -1.546577 1.828988 -4.549429

H -1.413854 0.850116 -6.018132

H 3.435164 0.824074 -5.341756

H 2.683271 -0.777403 -5.394532

H 2.875596 0.051676 -3.845005

H 3.660115 2.959905 0.059358

H 5.174736 3.614595 0.710199

H 5.153773 2.829979 -0.87638

H 0.674352 -1.274218 -6.938532

H -1.089726 -1.3389 -6.839137

H -0.147012 -2.830656 -6.797401

H 6.960543 -0.889372 -1.246731

H 6.86159 -0.06039 -2.802397

H 6.937638 0.8771 -1.308555

H 5.3768 -2.8157 -0.736471

H 3.814757 -2.958742 0.077779

H 5.286863 -3.558124 0.867707

H 2.676709 -6.876829 0.096015

H 1.108409 -6.970562 -0.709518

H 1.194335 -6.889416 1.054489

O -0.155857 -0.014684 4.878839

O -0.011239 4.886452 0.004624

O -5.270071 0.102685 -0.042123

***mer*-$Co_6S_8(PEt_3)_3(CO)_3^-$**

86

XYZ

S -1.577174 1.608302 3.608299

S 1.57805 -1.562851 0.429571

S -1.560772 1.634856 0.428574

S 1.566484 -1.595886 3.58194

S 1.598422 1.581805 3.623773

S -1.604305 -1.538758 0.416019

S -1.616269 -1.547738 3.570345

S 1.60732 1.58673 0.44312

Co 0.022212 2.033578 2.030384

Co -0.024328 -2.003006 1.996724

Co -2.150607 0.047454 2.000296

Co 2.15029 -0.002035 2.025418

Co -0.003092 -0.002854 4.015773

Co -0.000121 0.024828 0.011792

P 0.079559 -0.124895 6.182841

P -0.082532 0.022177 -2.155028

C -3.984391 0.069296 1.990259

C 3.985038 -0.020147 2.030787

P 0.053258 4.203336 2.07786

C -0.045335 -3.752808 1.981117

C 0.043738 4.935151 3.781241

C -0.702012 -1.620512 6.954454

C 0.766125 1.444249 -2.993593

C 1.50519 5.013611 1.252813

C 1.801494 -0.099532 6.869094

C -1.801801 0.044759 -2.847471

C -1.356631 5.054182 1.221255

C -2.719646 4.789583 1.85526

C 2.848072 4.701699 1.907904

C -0.798826 1.224906 7.106014

C 0.732637 -1.414264 -2.999823

C -0.173767 2.603771 6.921782

C 0.08685 -2.764612 -2.701449

C -0.053318 -2.948178 6.574556

C 0.147799 2.805934 -2.689858

C 0.077086 6.45815 3.877903

C 1.939213 -0.191456 8.386188

C -1.928951 0.054612 -4.368447

H -0.847232 4.520293 4.265605

H 0.89878 4.480033 4.293543

H -0.706518 -1.476788 8.042711

H 0.789467 1.248702 -4.073362

H -1.744353 -1.601582 6.615917

H 1.799216 1.41099 -2.628971

H 1.494744 4.63869 0.222954

H 1.320264 6.094873 1.213017

H 2.323561 -0.920478 6.364779

H -2.283533 0.917958 -2.393095

H 2.25461 0.816759 6.474179

H -2.301779 -0.824106 -2.404705

H -1.13709 6.128765 1.177209

H -1.33984 4.67137 0.194408
H -3.515492 5.253357 1.262025
H -2.779143 5.195901 2.870571
H -2.916363 3.715213 1.911967
H 3.667363 5.151966 1.336689
H 3.013455 3.621479 1.951509
H 2.89965 5.090519 2.930499
H -1.821306 1.218122 6.711434
H 1.76776 -1.405149 -2.639481
H -0.850867 0.947923 8.166731
H 0.756623 -1.21243 -4.078509
H -0.056931 -3.083333 5.489687
H 0.11001 2.97261 -1.609297
H -0.599684 -3.783081 7.027138
H 0.740011 3.607722 -3.14502
H 0.986436 -3.003898 6.91365
H -0.874123 2.882204 -3.076168
H 1.427444 0.633358 8.893521
H -1.473698 -0.832621 -4.820806
H 2.994261 -0.151678 8.679662
H -2.983477 0.068748 -4.666133
H 1.526996 -1.128074 8.775543
H -1.452476 0.935397 -4.811786
H -0.940912 -2.814263 -3.076159
H 0.059046 -2.948451 -1.623903
H 0.655432 -3.573582 -3.173091
H -0.78639 6.916697 3.384793
H 0.981206 6.874961 3.42225
H 0.062338 6.777532 4.926227
H -0.083275 2.838745 5.858354
H 0.826792 2.656819 7.363971
H -0.791057 3.375626 7.394843
O 5.13307 -0.027318 2.031293
O -5.132275 0.085667 1.984731
O -0.058847 -4.899021 1.970116

Neutral

$Co_6S_8(PEt_3)_6$

146

XYZ

S -1.536915 1.634142 -1.575365
S 1.537424 -1.633993 1.575473
S 1.630416 1.54019 -1.576368
S -1.629911 -1.540032 1.576484
S -1.549398 1.632968 1.597244
S 1.549922 -1.632814 -1.597132

S -1.623291 -1.532376 -1.589734

S 1.623802 1.532522 1.589849

Co 0.053012 2.016329 0.007487

Co -0.052502 -2.016167 -0.007376

Co 0.001971 0.002928 -2.014035

Co -0.00147 -0.002778 2.01415

Co -2.019538 0.057239 0.002811

Co 2.020057 -0.057079 -0.002699

P -4.206336 0.047805 0.028838

P 4.206857 -0.047584 -0.028705

P -0.069047 -0.010923 -4.198192

P 0.069508 0.011056 4.198308

P 0.090858 4.200781 -0.053889

P -0.090326 -4.200611 0.053943

C -1.583861 4.99231 -0.031141

C 1.584365 -4.992197 0.031108

C -5.017402 -1.41361 -0.776637

C 5.0177 1.413897 0.776865

C 1.326503 0.849654 -5.066288

C -1.326102 -0.849479 5.066349

C 1.00387 5.042704 1.324312

C -1.003353 -5.042399 -1.32433

C -4.948921 0.09621 1.725044

C 4.949491 -0.095831 -1.724896

C 0.923858 4.955419 -1.530391

C -0.923275 -4.955454 1.530377

C -2.874205 0.191228 -4.647539

C 2.87464 -0.191212 4.647932

C 0.240244 4.6579 -2.861572

C -0.239598 -4.658231 2.861592

C -0.087506 -1.703278 -4.951145

C 0.088018 1.703363 4.951366

C 0.342503 4.883973 2.689372

C -0.342007 -4.883502 -2.689384

C -5.038485 1.44287 -0.867371

C 5.039212 -1.442555 0.867465

C -1.52949 0.837221 -4.966869

C 1.529864 -0.837174 4.967066

C 2.675295 0.157193 -4.899968

C -2.674865 -0.156966 4.900007

C -4.829962 2.805221 -0.214204

C 4.831036 -2.804899 0.214184

C -4.726536 -2.749596 -0.100007

C 4.726567 2.749865 0.100313

C -1.622065 6.517468 -0.080996

C 1.622512 -6.517356 0.080951

C -0.143306 -1.774276 -6.475079

C 0.14376 1.774244 6.475309

C -6.473345 0.089432 1.806

C 6.473918 -0.088941 -1.805803

H -2.123122 4.550359 -0.876358

H 2.12367 -4.550283 0.876318

H -2.075108 4.606064 0.869129

H 2.075589 -4.605954 -0.869177

H -6.09624 -1.219496 -0.82219

H 6.096571 1.219957 0.822394

H -4.641841 -1.421411 -1.806027

H 4.642147 1.421574 1.80626

H 1.061842 0.954513 -6.12574

H -1.061473 -0.954361 6.125808

H 1.361472 1.856242 -4.634981

H -1.361096 -1.856064 4.635032

H 2.001798 4.590275 1.331611

H -2.001283 -4.589973 -1.331565

H 1.124556 6.10112 1.062179

H -1.124029 -6.100844 -1.062305

H -4.515608 -0.760123 2.253583

H 4.516127 0.760499 -2.253397

H -4.523606 0.986429 2.202079

H 4.524256 -0.986057 -2.201989

H 1.002968 6.036247 -1.359447

H -1.002421 -6.036252 1.359255

H 1.941134 4.548077 -1.528929

H -1.940543 -4.548089 1.529025

H -3.693274 0.782817 -5.070449

H 3.693639 -0.78287 5.070887

H -3.018659 0.121541 -3.565625

H 3.019218 -0.121445 3.566039

H -2.945689 -0.820354 -5.060306

H 2.946122 0.820334 5.06079

H 0.823248 5.070492 -3.691975

H -0.822586 -5.070975 3.691933

H -0.762541 5.094792 -2.908651

H 0.763174 -5.09517 2.908542

H 0.1418 3.578647 -3.009053

H -0.141112 -3.579012 3.009289

H 0.802594 -2.206321 -4.556549

H -0.802042 2.206475 4.556771

H -0.943473 -2.212873 -4.494905

H 0.944032 2.212944 4.4952

H 0.978218 5.301682 3.477223

H -0.977736 -5.301111 -3.477274

H 0.168883 3.828037 2.910745
H -0.168382 -3.827538 -2.91064
H -0.622714 5.398969 2.732849
H 0.623206 -5.3985 -2.732939
H -4.610699 1.436288 -1.876065
H 4.611365 -1.436129 1.876137
H -6.105522 1.20559 -0.960532
H 6.106198 -1.205073 0.960706
H -1.503213 1.863745 -4.584311
H 1.503588 -1.863678 4.584448
H -1.361544 0.886069 -6.049924
H 1.361811 -0.886082 6.050102
H 3.477303 0.764985 -5.332021
H -3.476902 -0.764731 5.332044
H 2.692434 -0.818186 -5.397087
H -2.691976 0.818411 5.39713
H 2.896295 -0.002405 -3.841701
H -2.895844 0.002647 3.841736
H -3.648089 -2.920152 -0.036661
H 3.648084 2.920223 0.036997
H -5.176215 -3.571855 -0.66698
H 5.176101 3.572177 0.667323
H -5.131133 -2.785158 0.916732
H 5.131135 2.78556 -0.916431
H 0.715727 -1.279382 -6.939342
H -0.715328 1.279376 6.939501
H -1.05072 -1.308143 -6.871678
H 1.051124 1.308015 6.871913
H -0.139185 -2.817198 -6.810037
H 0.139701 2.817141 6.810346
H -6.913944 0.948567 1.290081
H 6.91456 -0.948068 -1.289908
H -6.80156 0.132739 2.850192
H 6.802173 -0.13218 -2.849985
H -6.900651 -0.8178 1.367521
H 6.901146 0.818301 -1.367269
H 5.320612 -2.862999 -0.763376
H 3.765884 -3.000989 0.067726
H 5.245166 -3.60131 0.841509
H 2.65733 -6.875413 0.05199
H 1.09797 -6.967645 -0.767889
H 1.168462 -6.906586 0.997623
H -1.167969 6.906719 -0.997634
H -1.097603 6.967775 0.767883
H -2.656901 6.875477 -0.052106
H -3.764755 3.001082 -0.067817

H -5.31947 2.863512 0.763377

H -5.243941 3.60168 -0.841566

$Co_6S_8(PEt_3)_5(CO)$

126

XYZ

S -1.532112 1.634179 -1.611063

S 1.535833 -1.611751 1.567551

S 1.628562 1.536614 -1.606322

S -1.633421 -1.523752 1.551178

S -1.549749 1.640799 1.547614

S 1.54829 -1.638635 -1.605778

S -1.621316 -1.541509 -1.604552

S 1.619549 1.534652 1.55602

Co 0.054534 2.021034 -0.023857

Co -0.051598 -2.015091 -0.01364

Co 0.001988 -0.004818 -2.037871

Co -0.011423 0.011369 1.984723

Co -2.013976 0.061751 -0.028387

Co 2.013667 -0.053376 -0.02429

P -4.195081 0.055675 0.064967

P 4.199567 -0.033422 -0.027059

P -0.070535 -0.034033 -4.22056

C -0.017448 0.018203 3.741024

P 0.098529 4.204927 -0.003501

P -0.088687 -4.199867 0.084686

C -1.574451 4.99887 -0.02103

C 1.587931 -4.985821 0.081125

C -5.032462 -1.409015 -0.704808

C 4.99273 1.440375 0.771055

C 1.323296 0.826973 -5.088601

C 0.954186 4.97961 1.447039

C -0.99428 -5.05632 -1.288394

C -4.863992 0.120958 1.790272

C 4.955637 -0.098359 -1.716187

C 0.99348 5.000701 -1.419578

C -0.92766 -4.926962 1.569828

C -2.878313 0.167079 -4.658395

C 0.348598 4.759698 -2.781452

C -0.253499 -4.608388 2.901216

C -0.082565 -1.733003 -4.957109

C 0.281002 4.712826 2.790737

C -0.329195 -4.910206 -2.653067

C -5.05304 1.443181 -0.81651

C 5.022149 -1.413747 0.897178

C -1.533431 0.805311 -4.991833

C 2.676005 0.145342 -4.910005
C -4.808672 2.816084 -0.199471
C 4.830181 -2.785574 0.25896
C -4.718841 -2.746039 -0.040869
C 4.700594 2.770464 0.083279
C -1.607032 6.52503 0.00087
C 1.627304 -6.51009 0.154881
C -0.139956 -1.817601 -6.480361
C -6.383768 0.106765 1.932947
C 6.480756 -0.084589 -1.782808
H -2.076514 4.599453 -0.909275
H 2.122015 -4.532094 0.923279
H -2.106208 4.575567 0.838427
H 2.083148 -4.613164 -0.822643
H -6.112119 -1.214112 -0.708137
H 6.07229 1.252721 0.824123
H -4.698902 -1.417352 -1.748729
H 4.612902 1.452427 1.798767
H 1.062203 0.91999 -6.150078
H 1.34825 1.838079 -4.66703
H 1.969168 4.56646 1.443964
H -1.994196 -4.608537 -1.302798
H 1.039916 6.056028 1.252697
H -1.112246 -6.112117 -1.014717
H -4.401117 -0.722365 2.314937
H 4.523679 0.749702 -2.259107
H -4.424215 1.018626 2.239266
H 4.539519 -0.996246 -2.187077
H 1.082706 6.073374 -1.207175
H -1.002107 -6.010416 1.413364
H 2.004491 4.578459 -1.399331
H -1.94735 -4.525735 1.556119
H -3.696326 0.748997 -5.096372
H -3.024815 0.123617 -3.575424
H -2.949967 -0.853812 -5.047389
H 0.964911 5.189449 -3.578135
H -0.832353 -5.028162 3.730473
H -0.644288 5.21637 -2.845671
H 0.756559 -5.027032 2.954712
H 0.238255 3.687813 -2.970137
H -0.17633 -3.528269 3.051676
H 0.810175 -2.228668 -4.559269
H -0.936013 -2.241869 -4.495435
H 0.86781 5.151379 3.604365
H -0.959878 -5.34185 -3.43731
H 0.191768 3.638899 2.975468

H -0.161148 -3.856159 -2.887667
H -0.723564 5.145574 2.834154
H 0.639091 -5.42009 -2.686816
H -4.672895 1.415211 -1.843996
H 4.581299 -1.39406 1.900111
H -6.124542 1.211419 -0.857125
H 6.086697 -1.170686 1.001882
H -1.502667 1.837212 -4.624415
H -1.369305 0.837984 -6.07609
H 3.474362 0.752123 -5.349895
H 2.700022 -0.836865 -5.393087
H 2.897126 0.002669 -3.8493
H -3.641041 -2.931029 -0.041254
H 3.622201 2.938605 0.011477
H -5.210656 -3.563838 -0.578294
H 5.143763 3.597697 0.647899
H -5.063862 -2.774086 0.997636
H 5.110949 2.801264 -0.931311
H 0.71512 -1.321306 -6.950298
H -1.051247 -1.361574 -6.879613
H -0.129194 -2.863354 -6.805794
H -6.850818 0.956887 1.425279
H 6.920879 -0.934225 -1.251114
H -6.667752 0.161936 2.989188
H 6.818607 -0.140252 -2.823187
H -6.82398 -0.808384 1.524582
H 6.899092 0.83075 -1.352832
H 5.337373 -2.8555 -0.708874
H 3.768968 -2.989716 0.095561
H 5.235991 -3.571021 0.904953
H 2.662788 -6.866591 0.137783
H 1.108659 -6.974452 -0.689948
H 1.168867 -6.884813 1.075215
H -1.097734 6.957353 -0.866269
H -1.13564 6.929893 0.901735
H -2.641349 6.884935 -0.015581
H -3.737465 3.01871 -0.127797
H -5.23379 2.888967 0.806632
H -5.266149 3.600263 -0.811844
O -0.021184 0.023257 4.883985

***cis*-$Co_6S_8(PEt_3)_4(CO)_2$**

106

XYZ

S -1.537692 1.605671 -1.598397
S 1.536497 -1.620063 1.57427

S 1.608867 1.537068 -1.589551
S -1.640904 -1.555617 1.549214
S -1.561479 1.605472 1.562653
S 1.558049 -1.633421 -1.592007
S -1.617052 -1.558799 -1.598658
S 1.588402 1.525347 1.583472
Co 0.036763 2.001245 -0.007493
Co -0.046643 -2.029564 -0.008565
Co -1.4E-05 -0.015022 -2.027699
Co -0.025729 -0.01552 1.997087
Co -2.018741 0.041846 -0.019048
Co 2.005914 -0.045085 -0.005267
P -4.198524 0.118486 0.064233
P 4.194131 0.008846 0.000897
P -0.075471 -0.024484 -4.212406
C -0.041569 -0.021325 3.755071
C 0.081234 3.759258 -0.00667
P -0.069974 -4.21488 0.078022
C 1.612404 -4.986908 0.066088
C -5.076964 -1.273594 -0.787728
C 4.959736 1.488749 0.810966
C 1.307679 0.864078 -5.066795
C -0.974983 -5.063669 -1.299102
C -4.873916 0.116064 1.787454
C 4.951135 -0.035961 -1.687765
C -0.903009 -4.953181 1.559847
C -2.888888 0.154706 -4.637834
C -0.232974 -4.634794 2.893346
C -0.069499 -1.71736 -4.961282
C -0.315637 -4.903662 -2.665027
C -4.981271 1.58954 -0.745579
C 5.025028 -1.370168 0.918066
C -1.549642 0.806709 -4.968338
C 2.6691 0.196674 -4.899927
C -4.636541 2.928504 -0.099398
C 4.84661 -2.740657 0.272867
C -4.828875 -2.647841 -0.172511
C 4.655967 2.821046 0.131718
C 1.66167 -6.511443 0.129568
C -0.131545 -1.787511 -6.485138
C -6.393512 0.179393 1.920121
C 6.47609 0.003329 -1.749253
H 2.144996 -4.535389 0.910383
H 2.103624 -4.60469 -0.835839
H -6.147866 -1.036229 -0.806273
H 6.041018 1.31189 0.86661

H -4.720689 -1.251505 -1.824043
H 4.578531 1.489516 1.838342
H 1.044708 0.968398 -6.126538
H 1.31881 1.869853 -4.632121
H -1.977626 -4.621356 -1.305579
H -1.086196 -6.122084 -1.033135
H -4.463933 -0.782171 2.262591
H 4.508598 0.80888 -2.227018
H -4.39085 0.959888 2.292851
H 4.551169 -0.937935 -2.164612
H -0.967341 -6.036461 1.398431
H -1.926519 -4.56166 1.546066
H -3.711516 0.734711 -5.069025
H -3.035408 0.099156 -3.555246
H -2.953694 -0.863122 -5.035925
H -0.807624 -5.06587 3.719508
H 0.781533 -5.042718 2.945038
H -0.167988 -3.554892 3.050704
H 0.830567 -2.206139 -4.571557
H -0.915431 -2.240678 -4.501988
H -0.946951 -5.332964 -3.449838
H -0.154226 -3.847083 -2.892917
H 0.655113 -5.408083 -2.706245
H -4.635709 1.570083 -1.785567
H 4.584462 -1.358991 1.921308
H -6.065903 1.424993 -0.760258
H 6.087085 -1.117659 1.024894
H -1.525329 1.83676 -4.595481
H -1.389148 0.848762 -6.052641
H 3.459065 0.823302 -5.326309
H 2.707081 -0.774914 -5.403042
H 2.893206 0.03455 -3.8425
H -3.758396 -2.871514 -0.149255
H 3.578299 2.994707 0.071304
H -5.330284 -3.424768 -0.758863
H 5.102223 3.645143 0.697468
H -5.208343 -2.707156 0.852518
H 5.058156 2.859013 -0.88573
H 0.714271 -1.274045 -6.953268
H -1.050977 -1.341021 -6.876168
H -0.106698 -2.829721 -6.820535
H -6.803546 1.094697 1.482136
H 6.928922 -0.841563 -1.220759
H -6.683397 0.164999 2.975905
H 6.817186 -0.04114 -2.788966
H -6.88287 -0.671794 1.435988

H 6.876922 0.923648 -1.313691

H 5.35288 -2.800042 -0.696055

H 3.78747 -2.956219 0.110306

H 5.262514 -3.524518 0.914151

H 2.69946 -6.860436 0.106759

H 1.143583 -6.973533 -0.716782

H 1.208884 -6.895312 1.048856

H -3.555785 3.09325 -0.094632

H -4.989513 2.982842 0.935253

H -5.103169 3.749164 -0.653748

O -0.052674 -0.026743 4.896749

O 0.109298 4.900702 -0.006839

***trans*-$Co_6S_8(PEt_3)_4(CO)_2$**

106

XYZ

S -1.52655 1.597544 -1.618186

S 1.525538 -1.597105 1.62518

S 1.637085 1.507645 -1.583161

S -1.638081 -1.507099 1.590015

S -1.55598 1.658641 1.539885

S 1.554936 -1.658216 -1.533032

S -1.611053 -1.553754 -1.560946

S 1.610054 1.554292 1.56795

Co 0.051984 2.017815 -0.030062

Co -0.05287 -2.017362 0.037

Co 0.019239 -0.034277 -2.003119

Co -0.020102 0.034751 2.010038

Co -2.015737 0.057562 -0.011159

Co 2.014379 -0.057059 0.018084

P -4.199986 0.04089 0.0592

P 4.198761 -0.04043 -0.051978

C 0.033791 -0.066139 -3.758886

C -0.03533 0.066527 3.765784

P 0.095869 4.204463 -0.059826

P -0.096974 -4.203965 0.066725

C -1.57914 4.990924 -0.10906

C 1.578022 -4.990466 0.115827

C -5.015845 -1.443507 -0.693352

C 5.014595 1.443799 0.700857

C 0.938068 5.005211 1.383599

C -0.9393 -5.004674 -1.376651

C -4.881696 0.137489 1.777601

C 4.880668 -0.136774 -1.770281

C 1.002417 4.965875 -1.485632

C -1.003484 -4.965299 1.492603

C 0.367463 4.702307 -2.848382

C -0.368506 -4.701611 2.855316

C 0.253348 4.765892 2.726679

C -0.254594 -4.765454 -2.719754

C -5.047184 1.406265 -0.863827

C 5.045804 -1.405987 0.870854

C -4.817642 2.793209 -0.273294

C 4.816413 -2.792841 0.279992

C -4.694158 -2.769656 -0.011996

C 4.693311 2.770018 0.019396

C -1.613429 6.517188 -0.125126

C 1.612295 -6.516731 0.132035

C -6.40216 0.106021 1.907998

C 6.401152 -0.105382 -1.900516

H -2.072691 4.570625 -0.99238

H 2.071707 -4.570084 0.999032

H -2.11751 4.58766 0.755845

H 2.11629 -4.587304 -0.749191

H -6.09698 -1.257774 -0.701917

H 6.095707 1.25799 0.709831

H -4.680161 -1.459145 -1.736389

H 4.678547 1.459544 1.74378

H 1.953787 4.594058 1.396993

H -1.954986 -4.593435 -1.390032

H 1.024434 6.077381 1.167745

H -1.02575 -6.07683 -1.160761

H -4.412058 -0.687437 2.324886

H 4.411149 0.68825 -2.317529

H -4.457506 1.051533 2.208009

H 4.456491 -1.050715 -2.20094

H 1.091323 6.041883 -1.290878

H -1.092379 -6.041318 1.297917

H 2.013677 4.545189 -1.449796

H -2.014753 -4.544631 1.456769

H 0.986862 5.126415 -3.645112

H -0.987827 -5.125752 3.652088

H -0.627289 5.152537 -2.925301

H 0.626299 -5.151723 2.932217

H 0.265627 3.629079 -3.031375

H -0.266774 -3.628365 3.038261

H 0.831196 5.225216 3.535095

H -0.83252 -5.224717 -3.528151

H 0.166401 3.696249 2.935566

H -0.167518 -3.695824 -2.928659

H -0.752958 5.196008 2.750995

H 0.751659 -5.195697 -2.744094

H -4.651766 1.354353 -1.884474
H 4.650219 -1.354359 1.891456
H -6.116956 1.169173 -0.914432
H 6.11557 -1.168945 0.92175
H -3.615583 -2.950461 -0.009879
H 3.614749 2.950893 0.016759
H -5.181799 -3.596429 -0.538968
H 5.180737 3.596738 0.546646
H -5.038318 -2.786428 1.027018
H 5.037983 2.786826 -1.01945
H -6.876404 0.93521 1.373226
H 6.875286 -0.934678 -1.36581
H -6.695775 0.186057 2.959849
H 6.694879 -0.18527 -2.952343
H -6.825677 -0.826284 1.521638
H 6.824683 0.826829 -1.513945
H 5.26209 -2.887533 -0.715306
H 3.747516 -3.001653 0.190841
H 5.263014 -3.56117 0.919448
H 2.647 -6.873944 0.164264
H 1.147253 -6.945029 -0.761237
H 1.098379 -6.927169 1.00684
H -1.099373 6.927723 -0.999805
H -1.148548 6.945407 0.768266
H -2.648134 6.874391 -0.157498
H -3.748718 3.002038 -0.184546
H -5.262993 2.888077 0.722132
H -5.264462 3.561417 -0.912745
O -0.044521 0.087122 4.907748
O 0.042546 -0.086821 -4.900976

***fac*-$Co_6S_8(PEt_3)_3(CO)_3$**

86

XYZ

S -1.540587 1.606668 -1.591226
S 1.535843 -1.613891 1.577632
S 1.599481 1.538565 -1.586299
S -1.634852 -1.554152 1.550057
S -1.568283 1.599126 1.562216
S 1.554791 -1.627818 -1.588766
S -1.611056 -1.566952 -1.591634
S 1.583026 1.528515 1.586701
Co 0.029581 1.999175 -0.000752
Co -0.044309 -2.030349 -0.00276
Co -0.007813 -0.014315 -2.026739
Co -0.028854 -0.012323 1.99937

Co -2.019106 0.035134 -0.0227	C 1.640777 -6.519436 0.137705
Co 2.004857 -0.040834 -0.002192	C -0.142508 -1.782277 -6.484488
C -3.779145 0.072245 -0.03488	C 6.470863 0.006209 -1.751859
P 4.19383 0.012382 0.001119	H 2.136477 -4.545844 0.917255
P -0.091605 -0.020987 -4.214623	H 2.092639 -4.615965 -0.82954
C -0.046053 -0.01845 3.760404	H 6.037801 1.315777 0.867205
C 0.064033 3.759966 0.000335	H 4.576448 1.491955 1.84025
P -0.079046 -4.217927 0.086904	H 1.029757 0.971893 -6.124023
C 1.600625 -4.994522 0.073507	H 1.303303 1.874713 -4.63133
C 4.956433 1.492175 0.812438	H -1.989563 -4.605166 -1.296605
C 1.293187 0.868219 -5.064354	H -1.111293 -6.112467 -1.023697
C -0.990685 -5.055507 -1.290854	H 4.504323 0.816101 -2.226349
C 4.945749 -0.030561 -1.68909	H 4.544075 -0.931173 -2.167049
C -0.915758 -4.944624 1.57072	H -0.987057 -6.027515 1.410044
C -2.906694 0.14959 -4.638243	H -1.93707 -4.547763 1.556211
C -0.242029 -4.631306 2.903548	H -3.728227 0.725234 -5.07631
C -0.084332 -1.714622 -4.960178	H -3.068432 0.095532 -3.558367
C -0.328895 -4.905102 -2.656781	H -2.964117 -0.868517 -5.036365
C 5.020732 -1.369671 0.915835	H -0.821875 -5.055058 3.729594
C -1.569168 0.808997 -4.961687	H 0.767899 -5.050261 2.956297
C 2.654751 0.201151 -4.89814	H -0.164909 -3.552301 3.061919
C 4.83839 -2.739541 0.270385	H 0.814353 -2.204686 -4.568918
C 4.651765 2.824203 0.133152	H -0.932975 -2.237515 -4.505478

H -0.965712 -5.32829 -3.440228
H -0.154069 -3.851421 -2.888725
H 0.635658 -5.421321 -2.69748
H 4.583568 -1.357479 1.920528
H 6.083526 -1.119225 1.01979
H -1.549834 1.838088 -4.585722
H -1.405398 0.857197 -6.045356
H 3.44337 0.826333 -5.328965
H 2.691516 -0.772073 -5.398105
H 2.88205 0.042648 -3.840835
H 3.574139 2.998354 0.073225
H 5.097917 3.648273 0.698891
H 5.05389 2.862531 -0.884238
H 0.706935 -1.272291 -6.949674
H -1.059162 -1.331881 -6.877099
H -0.121298 -2.824367 -6.820169
H 6.922742 -0.841218 -1.226756
H 6.809949 -0.035953 -2.792196
H 6.874043 0.924557 -1.314474
H 5.340248 -2.798694 -0.700747
H 3.778563 -2.955515 0.112782
H 5.257289 -3.523484 0.909416
H 2.676454 -6.874174 0.113088
H 1.118401 -6.978704 -0.707433
H 1.187537 -6.900023 1.058027
O -0.056951 -0.024486 4.900652
O 0.086723 4.900116 -0.000768
O -4.919256 0.094384 -0.044143

***mer*-$Co_6S_8(PEt_3)_3(CO)_3$**

86

XYZ

S -1.561646 1.598308 3.610276
S 1.565967 -1.563448 0.427867
S -1.551106 1.625983 0.439066
S 1.558662 -1.597244 3.576247
S 1.589722 1.568091 3.618158
S -1.598842 -1.534054 0.42064
S -1.605048 -1.551791 3.571514
S 1.593781 1.581378 0.446516
Co 0.022861 2.03334 2.033703
Co -0.025389 -1.996593 1.995091
Co -2.010984 0.043112 2.007839
Co 2.009113 -0.004422 2.020367
Co -0.000428 -0.010831 4.023999
Co -0.002115 0.022787 0.00584

P	0.076887	-0.123079	6.207979
P	-0.075889	0.02646	-2.178163
C	-3.769224	0.072738	2.003902
C	3.767434	-0.02099	2.020912
P	0.050723	4.219697	2.072412
C	-0.049145	-3.757154	1.977071
C	0.043687	4.941023	3.776388
C	-0.703338	-1.624258	6.960297
C	0.777404	1.454194	-2.993054
C	1.504181	5.009842	1.239434
C	1.80063	-0.090857	6.879615
C	-1.796433	0.049388	-2.85779
C	-1.36736	5.046474	1.21426
C	-2.728789	4.791039	1.855217
C	2.849013	4.711214	1.896569
C	-0.8099	1.231099	7.10774
C	0.744487	-1.413168	-3.003501
C	-0.185224	2.611412	6.934093
C	0.095373	-2.764791	-2.718643
C	-0.046999	-2.950505	6.588892
C	0.159682	2.817042	-2.694023
C	0.076956	6.465043	3.866456
C	1.935452	-0.184476	8.397443
C	-1.919044	0.063052	-4.379695
H	-0.847895	4.531344	4.263896
H	0.900744	4.491234	4.289895
H	-0.7078	-1.478704	8.047706
H	0.79872	1.259627	-4.072403
H	-1.747667	-1.60883	6.628171
H	1.812876	1.417425	-2.635955
H	1.492798	4.636415	0.209155
H	1.315531	6.08966	1.195352
H	2.327708	-0.910388	6.378448
H	-2.281163	0.921899	-2.405525
H	2.251029	0.828879	6.489905
H	-2.296976	-0.822559	-2.421926
H	-1.147469	6.120169	1.165641
H	-1.352477	4.665711	0.186753
H	-3.520925	5.262909	1.265149
H	-2.781969	5.19936	2.869429
H	-2.940064	3.7198	1.912452
H	3.661202	5.172783	1.326049
H	3.032867	3.634325	1.939334
H	2.896623	5.10167	2.918109
H	-1.833206	1.220787	6.715814
H	1.780576	-1.404254	-2.6463

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