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# Unusual Effects of the Bulky 1-Norbornyl Group in Cobalt Carbonyl Chemistry: Low-Energy Structures with Agostic Hydrogen Atoms

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## Supporting Information

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**Tables S1 to S10:** Optimized coordinates of the (nor)$Co(CO)_n$ structures ($n$ = 1 to 4) calucated at the B3PW91-D3/DZP level and B3PW91-D3/cc-pVTZ level.

**Tables S11 to S25:** Optimized coordinates of the $(nor)_2Co_2(CO)_n$ structures ($n$ = 5 to 7) calucated at the B3PW91-D3/DZP level and B3PW91-D3/cc-pVTZ level.

**Tables S26 to S40:** Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for $(nor)_2Co_2(CO)_n$ structures ($n$ = 5 to 7) caculated at the B3PW91-D3/DZP level.

Complete Gaussian09 reference (Reference 22).

**Table S1.**Optimized coordinates for the (nor)$Co(CO)_4$ structure **4S-1.**

| B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | -0.00404 | -2.89371 | 0.00000 | C | 0.001217 | -2.898293 | 0.000000 |
| Co | -0.00118 | -1.10046 | 0.00000 | Co | -0.000012 | -1.105536 | 0.000000 |
| C | 0.07011 | 0.99643 | 0.00000 | C | 0.072479 | 0.978465 | 0.000000 |
| C | 0.75602 | 1.61133 | 1.24427 | C | 0.754453 | 1.590353 | 1.240155 |
| C | 0.24383 | 3.08446 | 1.24888 | C | 0.241976 | 3.057574 | 1.245305 |
| C | -0.65506 | 3.14423 | 0.00000 | C | -0.653059 | 3.116578 | 0.000000 |
| C | -1.28262 | 1.73830 | 0.00000 | C | -1.276456 | 1.714899 | 0.000000 |
| C | 0.24383 | 3.08446 | -1.24888 | C | 0.241976 | 3.057574 | -1.245305 |
| C | 0.75602 | 1.61133 | -1.24427 | C | 0.754453 | 1.590353 | -1.240155 |
| C | -0.93232 | -0.95624 | -1.52532 | C | -0.936233 | -0.949084 | -1.523029 |
| H | 0.46584 | 1.10173 | 2.16889 | H | 0.463139 | 1.076418 | 2.155049 |
| H | 1.84833 | 1.54835 | 1.17501 | H | 1.840764 | 1.522727 | 1.171916 |
| H | -0.33512 | 3.29221 | 2.15705 | H | -0.336731 | 3.262362 | 2.147967 |
| H | 1.05956 | 3.81583 | 1.20357 | H | 1.052021 | 3.787471 | 1.203127 |
| H | 1.05956 | 3.81583 | -1.20357 | H | 1.052021 | 3.787471 | -1.203127 |
| H | -0.33512 | 3.29221 | -2.15705 | H | -0.336731 | 3.262362 | -2.147967 |
| H | 1.84833 | 1.54835 | -1.17501 | H | 1.840764 | 1.522727 | -1.171916 |
| H | 0.46584 | 1.10173 | -2.16889 | H | 0.463139 | 1.076418 | -2.155049 |
| H | -1.89048 | 1.54374 | -0.89183 | H | -1.878960 | 1.513846 | -0.887099 |
| H | -1.89048 | 1.54374 | 0.89183 | H | -1.878960 | 1.513846 | 0.887099 |
| H | -1.36188 | 3.98140 | 0.00000 | H | -1.355637 | 3.949788 | 0.000000 |
| C | -0.93232 | -0.95624 | 1.52532 | C | -0.936233 | -0.949084 | 1.523029 |
| O | -1.54201 | -0.87722 | 2.50147 | O | -1.539055 | -0.830222 | 2.482316 |
| O | -1.54201 | -0.87722 | -2.50147 | O | -1.539055 | -0.830222 | -2.482316 |
| O | -0.00106 | -4.04475 | 0.00000 | O | 0.007292 | -4.035178 | 0.000000 |
| C | 1.78409 | -0.97995 | 0.00000 | C | 1.783865 | -0.966402 | 0.000000 |
| O | 2.93661 | -0.92320 | 0.00000 | O | 2.918924 | -0.864821 | 0.000000 |

**Table S2.**Optimized coordinates for the (nor)$Co(CO)_4$ structure **4S-2.**

| B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | -0.571776 | -2.211691 | 1.256982 | C | -0.568550 | -2.167176 | 1.255237 |
| C | -0.342397 | -1.336815 | 0.000000 | C | -0.336623 | -1.302501 | 0.000000 |
| C | 1.206684 | -1.203973 | 0.000000 | C | 1.210102 | -1.179858 | 0.000000 |
| C | 1.442145 | -2.729862 | 0.000000 | C | 1.430394 | -2.703717 | 0.000000 |
| C | 0.657733 | -3.163732 | -1.252349 | C | 0.646280 | -3.128858 | -1.248710 |
| C | 0.657733 | -3.163732 | 1.252349 | C | 0.646280 | -3.128858 | 1.248710 |
| C | -0.571776 | -2.211691 | -1.256982 | C | -0.568550 | -2.167176 | -1.255237 |
| Co | 0.039770 | 1.252195 | 0.000000 | Co | 0.032436 | 1.260523 | 0.000000 |
| H | 1.613947 | -0.725565 | 0.900102 | H | 1.620553 | -0.707817 | 0.895311 |
| H | 1.613947 | -0.725565 | -0.900102 | H | 1.620553 | -0.707817 | -0.895311 |
| H | -0.593797 | -1.591923 | -2.161199 | H | -0.576871 | -1.539002 | -2.147650 |
| H | -1.532267 | -2.732539 | -1.194592 | H | -1.533218 | -2.669349 | -1.201323 |
| H | -1.532267 | -2.732539 | 1.194592 | H | -1.533218 | -2.669349 | 1.201323 |
| H | -0.593797 | -1.591923 | 2.161199 | H | -0.576871 | -1.539002 | 2.147650 |
| H | 0.367791 | -4.219668 | -1.204599 | H | 0.347370 | -4.176832 | -1.202186 |
| H | 1.261684 | -3.027921 | -2.157259 | H | 1.251062 | -3.000231 | -2.147726 |
| H | 2.491071 | -3.043863 | 0.000000 | H | 2.471130 | -3.024913 | 0.000000 |
| H | 1.261684 | -3.027921 | 2.157259 | H | 1.251062 | -3.000231 | 2.147726 |
| H | 0.367791 | -4.219668 | 1.204599 | H | 0.347370 | -4.176832 | 1.202186 |
| C | 1.592185 | 2.194844 | 0.000000 | C | 1.596969 | 2.180841 | 0.000000 |
| C | -1.268461 | -0.110407 | 0.000000 | C | -1.273550 | -0.091772 | 0.000000 |
| O | 2.560304 | 2.819200 | 0.000000 | O | 2.567545 | 2.774708 | 0.000000 |
| O | -2.468585 | -0.195802 | 0.000000 | O | -2.460551 | -0.195403 | 0.000000 |
| C | -0.571776 | 1.761763 | -1.574322 | C | -0.568550 | 1.730331 | -1.592084 |
| O | -1.030278 | 2.207740 | -2.537108 | O | -1.018410 | 2.119580 | -2.566368 |
| C | -0.571776 | 1.761763 | 1.574322 | C | -0.568550 | 1.730331 | 1.592084 |
| O | -1.030278 | 2.207740 | 2.537108 | O | -1.018410 | 2.119580 | 2.566368 |

**Table S3.**Optimized coordinates for the (nor)$Co(CO)_3$ structure **3S-1.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | -1.214674 | 1.664353 | -0.428036 | C | -1.187883 | 1.673389 | -0.431298 |
| Co | -1.027582 | -0.014054 | 0.077703 | Co | -1.050496 | -0.013220 | 0.071213 |
| C | 0.902383 | 0.083877 | -0.179877 | C | 0.883997 | 0.065299 | -0.151517 |
| C | 1.752157 | 1.258661 | -0.674689 | C | 1.711520 | 1.222583 | -0.707931 |
| C | 3.205553 | 0.779077 | -0.351796 | C | 3.173777 | 0.765688 | -0.427905 |
| C | 3.000513 | -0.653073 | 0.193360 | C | 2.995444 | -0.631951 | 0.191558 |
| C | 1.771310 | -1.114824 | -0.604605 | C | 1.751448 | -1.139219 | -0.542874 |
| C | 2.399749 | -0.587391 | 1.611328 | C | 2.442504 | -0.492730 | 1.617110 |
| C | 0.988276 | 0.045969 | 1.365846 | C | 1.005972 | 0.080190 | 1.388731 |
| C | -1.131506 | -1.441955 | -0.950533 | C | -1.095075 | -1.501404 | -0.871530 |
| H | 1.619499 | 1.413123 | -1.751973 | H | 1.530570 | 1.343778 | -1.776826 |
| H | 1.499791 | 2.200059 | -0.173106 | H | 1.467798 | 2.170979 | -0.227694 |
| H | 3.826171 | 0.763144 | -1.255494 | H | 3.752473 | 0.706414 | -1.351074 |
| H | 3.706927 | 1.426630 | 0.377924 | H | 3.701510 | 1.445213 | 0.243835 |
| H | 2.992185 | 0.024751 | 2.301701 | H | 3.040306 | 0.173357 | 2.241168 |
| H | 2.316243 | -1.592442 | 2.041515 | H | 2.403551 | -1.465143 | 2.110601 |
| H | 0.909674 | 1.045166 | 1.803817 | H | 0.897167 | 1.084625 | 1.794454 |
| H | 0.197760 | -0.586156 | 1.831553 | H | 0.260528 | -0.563781 | 1.889932 |
| H | 1.388433 | -2.084839 | -0.265831 | H | 1.384441 | -2.087577 | -0.147012 |
| H | 1.939134 | -1.154251 | -1.687620 | H | 1.881021 | -1.232475 | -1.622389 |
| H | 3.894324 | -1.283356 | 0.125287 | H | 3.886567 | -1.256679 | 0.129738 |
| O | -1.269181 | -2.278070 | -1.738656 | O | -1.167566 | -2.377749 | -1.600945 |
| O | -1.403667 | 2.705433 | -0.896686 | O | -1.322749 | 2.709530 | -0.892948 |
| C | -2.637679 | -0.180961 | 0.840317 | C | -2.690754 | -0.152191 | 0.767855 |
| O | -3.672391 | -0.291709 | 1.338636 | O | -3.733213 | -0.244243 | 1.218808 |

**Table S4.**Optimized coordinates for the (nor)$Co(CO)_3$ structure **3S-2.**

| B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | 0.274608 | 1.938260 | 1.258475 | C | 0.274709 | 1.896923 | 1.256019 |
| C | 0.113775 | 1.051797 | 0.000000 | C | 0.096083 | 1.021321 | 0.000000 |
| C | -1.423787 | 0.800479 | 0.000000 | C | -1.442297 | 0.803735 | 0.000000 |
| C | -1.769272 | 2.307688 | 0.000000 | C | -1.749701 | 2.315160 | 0.000000 |
| C | -1.021227 | 2.798644 | -1.253178 | C | -0.994243 | 2.786513 | -1.249301 |
| C | -1.021227 | 2.798644 | 1.253178 | C | -0.994243 | 2.786513 | 1.249301 |
| C | 0.274608 | 1.938260 | -1.258475 | C | 0.274709 | 1.896923 | -1.256019 |
| Co | -0.143544 | -1.358087 | 0.000000 | Co | -0.153791 | -1.380964 | 0.000000 |
| H | -1.798408 | 0.301005 | 0.904910 | H | -1.829703 | 0.318188 | 0.900475 |
| H | -1.798408 | 0.301005 | -0.904910 | H | -1.829703 | 0.318188 | -0.900475 |
| H | 0.341438 | 1.318686 | -2.159749 | H | 0.320037 | 1.268166 | -2.145974 |
| H | 1.193649 | 2.529639 | -1.196691 | H | 1.207505 | 2.456340 | -1.201159 |
| H | 1.193649 | 2.529639 | 1.196691 | H | 1.207505 | 2.456340 | 1.201159 |
| H | 0.341438 | 1.318686 | 2.159749 | H | 0.320037 | 1.268166 | 2.145974 |
| H | -0.811956 | 3.873380 | -1.206112 | H | -0.760061 | 3.850755 | -1.203616 |
| H | -1.613758 | 2.617704 | -2.157663 | H | -1.590373 | 2.621145 | -2.148034 |
| H | -2.839662 | 2.537511 | 0.000000 | H | -2.808795 | 2.569079 | 0.000000 |
| H | -1.613758 | 2.617704 | 2.157663 | H | -1.590373 | 2.621145 | 2.148034 |
| H | -0.811956 | 3.873380 | 1.206112 | H | -0.760061 | 3.850755 | 1.203616 |
| C | 1.126802 | -0.118630 | 0.000000 | C | 1.107547 | -0.143057 | 0.000000 |
| O | 2.321809 | -0.025095 | 0.000000 | O | 2.289581 | -0.037212 | 0.000000 |
| C | 0.274608 | -2.103605 | -1.539260 | C | 0.274709 | -2.077751 | -1.561532 |
| O | 0.681125 | -2.674801 | -2.463073 | O | 0.701114 | -2.579107 | -2.498722 |
| C | 0.274608 | -2.103605 | 1.539260 | C | 0.274709 | -2.077751 | 1.561532 |
| O | 0.681125 | -2.674801 | 2.463073 | O | 0.701114 | -2.579107 | 2.498722 |

**Table S5.**Optimized coordinates for the (nor)$Co(CO)_3$ structure **3T-3.**

| B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | -1.511762 | 0.205980 | 1.688597 | C | -1.449426 | 0.186125 | 1.705755 |
| Co | -1.073728 | -0.134990 | -0.082520 | Co | -1.090392 | -0.135313 | -0.087902 |
| C | 0.913116 | -0.052943 | 0.028265 | C | 0.889131 | -0.082055 | 0.016787 |
| C | 1.672886 | 1.118199 | 0.680829 | C | 1.642558 | 1.061222 | 0.708509 |
| C | 3.130124 | 0.973969 | 0.134754 | C | 3.094743 | 0.938573 | 0.158980 |
| C | 3.036085 | -0.266079 | -0.774012 | C | 3.000975 | -0.265062 | -0.789599 |
| C | 1.611969 | -0.120857 | -1.353264 | C | 1.581203 | -0.098656 | -1.360973 |
| C | 2.881901 | -1.513157 | 0.114770 | C | 2.846419 | -1.538787 | 0.051919 |
| C | 1.431683 | -1.363202 | 0.682076 | C | 1.398469 | -1.411433 | 0.617929 |
| C | -1.430309 | 1.540416 | -0.793058 | C | -1.359437 | 1.573718 | -0.760630 |
| H | 1.248241 | 2.085732 | 0.384965 | H | 1.211191 | 2.028863 | 0.444275 |
| H | 1.628940 | 1.071145 | 1.776233 | H | 1.591526 | 0.976422 | 1.795702 |
| H | 3.425568 | 1.859864 | -0.441474 | H | 3.387257 | 1.839574 | -0.384282 |
| H | 3.871563 | 0.840127 | 0.932065 | H | 3.833755 | 0.779549 | 0.946540 |
| H | 3.639906 | -1.550423 | 0.906847 | H | 3.599079 | -1.603798 | 0.839896 |
| H | 2.979285 | -2.431455 | -0.477892 | H | 2.946294 | -2.430689 | -0.570145 |
| H | 1.413568 | -1.300068 | 1.777136 | H | 1.368762 | -1.392047 | 1.708680 |
| H | 0.826508 | -2.237613 | 0.402537 | H | 0.790748 | -2.262936 | 0.298388 |
| H | 1.314826 | -0.985393 | -1.962820 | H | 1.275786 | -0.935097 | -1.994873 |
| H | 1.487974 | 0.792313 | -1.950040 | H | 1.449643 | 0.831660 | -1.918243 |
| H | 3.846066 | -0.342902 | -1.509021 | H | 3.808296 | -0.316077 | -1.521102 |
| O | -1.492041 | 2.598737 | -1.242972 | O | -1.328133 | 2.631355 | -1.177063 |
| O | -1.637791 | 0.424823 | 2.812064 | O | -1.491882 | 0.387603 | 2.823856 |
| C | -2.497721 | -1.173092 | -0.688178 | C | -2.562533 | -1.109593 | -0.688849 |
| O | -3.385122 | -1.805062 | -1.060990 | O | -3.469282 | -1.692244 | -1.050599 |

**Table S6.**Optimized coordinates for the (nor)$Co(CO)_2$ structure **2S-1.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| Co | 1.065690 | -0.150794 | -0.058589 | Co | 1.066714 | -0.155647 | -0.056958 |
| C | -0.763545 | 0.314978 | -0.084736 | C | -0.755737 | 0.303606 | -0.092356 |
| C | -1.731107 | 1.188969 | -0.871201 | C | -1.720185 | 1.178500 | -0.867261 |
| C | -3.114188 | 0.601799 | -0.411314 | C | -3.097149 | 0.592169 | -0.403236 |
| C | -2.739198 | -0.427635 | 0.686639 | C | -2.717882 | -0.435604 | 0.688242 |
| C | -1.470822 | 0.207822 | 1.282207 | C | -1.449784 | 0.195459 | 1.274788 |
| C | -2.130857 | -1.689827 | 0.039124 | C | -2.117307 | -1.692799 | 0.037241 |
| C | -0.837099 | -1.120216 | -0.626172 | C | -0.830002 | -1.124950 | -0.631998 |
| C | 1.584779 | 1.463305 | 0.104126 | C | 1.544880 | 1.470721 | 0.103097 |
| H | -1.638031 | 2.244224 | -0.589586 | H | -1.619615 | 2.226599 | -0.582222 |
| H | -1.581144 | 1.118928 | -1.954337 | H | -1.572300 | 1.111979 | -1.945287 |
| H | -3.756707 | 1.387167 | 0.003621 | H | -3.736259 | 1.371851 | 0.013359 |
| H | -3.663470 | 0.134837 | -1.238085 | H | -3.646414 | 0.127417 | -1.224216 |
| H | -2.782868 | -2.150841 | -0.711930 | H | -2.771899 | -2.148869 | -0.706538 |
| H | -1.906727 | -2.447978 | 0.799144 | H | -1.890313 | -2.448679 | 0.790959 |
| H | -0.866444 | -1.157342 | -1.719303 | H | -0.863577 | -1.163532 | -1.719714 |
| H | 0.061777 | -1.750930 | -0.325092 | H | 0.068497 | -1.752155 | -0.334404 |
| H | -0.964760 | -0.442671 | 2.007581 | H | -0.936870 | -0.453704 | 1.988431 |
| H | -1.636347 | 1.189507 | 1.740596 | H | -1.604459 | 1.172366 | 1.733997 |
| H | -3.556264 | -0.644052 | 1.384707 | H | -3.527682 | -0.651147 | 1.386092 |
| O | 1.916145 | 2.571420 | 0.202798 | O | 1.823911 | 2.578672 | 0.199372 |
| C | 2.639302 | -0.958301 | -0.028135 | C | 2.653449 | -0.939648 | -0.023285 |
| O | 3.695577 | -1.433267 | 0.002371 | O | 3.705829 | -1.387967 | 0.003879 |

**Table S7.**Optimized coordinates for the (nor)$Co(CO)_2$ structure **2T-2.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| Co | -1.243889 | -0.142410 | 0.003488 | Co | -1.255566 | -0.149058 | 0.005805 |
| C | 0.735777 | -0.141221 | 0.044996 | C | 0.718043 | -0.171277 | 0.051282 |
| C | 1.377987 | 0.431301 | 1.336008 | C | 1.355865 | 0.465415 | 1.304781 |
| C | 2.878963 | 0.652801 | 0.954173 | C | 2.850564 | 0.670767 | 0.910571 |
| C | 2.936048 | 0.173326 | -0.506937 | C | 2.904580 | 0.122284 | -0.520803 |
| C | 1.552943 | 0.611711 | -1.030329 | C | 1.523294 | 0.530405 | -1.058409 |
| C | 2.800997 | -1.359186 | -0.520698 | C | 2.773417 | -1.404682 | -0.461358 |
| C | 1.301194 | -1.581621 | -0.132320 | C | 1.279139 | -1.610929 | -0.062080 |
| C | -1.653555 | 1.660503 | -0.191035 | C | -1.541951 | 1.679213 | -0.193199 |
| H | 0.918946 | 1.386041 | 1.627362 | H | 0.889674 | 1.426053 | 1.539303 |
| H | 1.263267 | -0.251711 | 2.188052 | H | 1.237999 | -0.168976 | 2.186083 |
| H | 3.152380 | 1.713016 | 1.030028 | H | 3.120417 | 1.728902 | 0.932525 |
| H | 3.566569 | 0.090016 | 1.597806 | H | 3.538137 | 0.145446 | 1.576442 |
| H | 3.493522 | -1.839841 | 0.181617 | H | 3.465358 | -1.848172 | 0.257492 |
| H | 3.012566 | -1.762942 | -1.519103 | H | 2.984165 | -1.852046 | -1.435269 |
| H | 1.192170 | -2.177551 | 0.783052 | H | 1.165772 | -2.162561 | 0.873448 |
| H | 0.785110 | -2.130107 | -0.932995 | H | 0.757522 | -2.184197 | -0.833282 |
| H | 1.358976 | 0.264016 | -2.054838 | H | 1.320843 | 0.134605 | -2.057602 |
| H | 1.414199 | 1.700919 | -0.998151 | H | 1.375021 | 1.613255 | -1.076403 |
| H | 3.803702 | 0.547253 | -1.063629 | H | 3.766066 | 0.468413 | -1.093341 |
| O | -1.712525 | 2.804422 | -0.319286 | O | -1.477765 | 2.808735 | -0.315557 |
| C | -2.876411 | -1.016935 | 0.095873 | C | -2.926679 | -0.950193 | 0.085903 |
| O | -3.874984 | -1.589189 | 0.165316 | O | -3.939524 | -1.466507 | 0.144774 |

**Table S8.**Optimized coordinates for the (nor)$Co(CO)_2$ structure **2T-3.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | -2.116257 | 1.355136 | -0.443452 | C | -2.123313 | 1.350777 | -0.439444 |
| C | -1.221849 | 0.138799 | -0.131192 | C | -1.214910 | 0.150274 | -0.135637 |
| C | -1.770161 | -0.313856 | 1.248045 | C | -1.747695 | -0.310718 | 1.241164 |
| C | -3.219578 | -0.451386 | 0.752091 | C | -3.191870 | -0.468697 | 0.751521 |
| C | -3.050988 | -1.440930 | -0.416143 | C | -3.013758 | -1.449689 | -0.415748 |
| C | -3.486727 | 0.954517 | 0.178268 | C | -3.481297 | 0.929794 | 0.184304 |
| C | -1.666835 | -1.050275 | -1.014865 | C | -1.641620 | -1.039532 | -1.016276 |
| Co | 2.085855 | -0.166036 | 0.024490 | Co | 2.068784 | -0.169122 | 0.021257 |
| H | -1.644436 | 0.449947 | 2.025391 | H | -1.626722 | 0.451487 | 2.013375 |
| H | -1.329343 | -1.257462 | 1.591133 | H | -1.288971 | -1.241824 | 1.578264 |
| H | -0.945842 | -1.873259 | -0.934320 | H | -0.907927 | -1.844415 | -0.935014 |
| H | -1.723967 | -0.762569 | -2.070994 | H | -1.701105 | -0.753113 | -2.067003 |
| H | -2.175274 | 1.543056 | -1.521347 | H | -2.185269 | 1.541992 | -1.511154 |
| H | -1.706026 | 2.258939 | 0.019781 | H | -1.721277 | 2.251702 | 0.024564 |
| H | -3.863365 | -1.353938 | -1.147240 | H | -3.826277 | -1.373740 | -1.139952 |
| H | -3.043515 | -2.476395 | -0.054809 | H | -2.991413 | -2.480746 | -0.058450 |
| H | -3.948448 | -0.771398 | 1.505042 | H | -3.910693 | -0.799676 | 1.501163 |
| H | -3.773005 | 1.650461 | 0.976364 | H | -3.773794 | 1.615640 | 0.981650 |
| H | -4.300492 | 0.948146 | -0.556688 | H | -4.294455 | 0.913593 | -0.543228 |
| C | 3.880825 | -0.188448 | 0.097642 | C | 3.868183 | -0.196358 | 0.099415 |
| C | 0.258568 | 0.348236 | -0.134033 | C | 0.254510 | 0.378466 | -0.138676 |
| O | 5.036110 | -0.223802 | 0.148904 | O | 5.008702 | -0.224213 | 0.151645 |
| O | 0.775595 | 1.475886 | -0.312868 | O | 0.756467 | 1.501650 | -0.301883 |

**Table S9.**Optimized coordinates for the (nor)Co(CO)$_2$ structure **2S-4.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | 1.593289 | 0.618701 | 1.258443 | C | 1.552740 | 0.635787 | 1.255030 |
| C | 0.777840 | 0.251000 | 0.000000 | C | 0.744917 | 0.270105 | 0.000000 |
| C | -0.295362 | 1.413021 | 0.000000 | C | -0.330460 | 1.424798 | 0.000000 |
| C | 0.773078 | 2.528142 | 0.000000 | C | 0.735769 | 2.537079 | 0.000000 |
| C | 1.593289 | 2.174602 | -1.254348 | C | 1.552740 | 2.186567 | -1.250257 |
| C | 1.593289 | 2.174602 | 1.254348 | C | 1.552740 | 2.186567 | 1.250257 |
| C | 1.593289 | 0.618701 | -1.258443 | C | 1.552740 | 0.635787 | -1.255030 |
| Co | -1.238645 | -0.578814 | 0.000000 | Co | -1.203801 | -0.605362 | 0.000000 |
| H | -0.925292 | 1.460841 | 0.909897 | H | -0.957408 | 1.474962 | 0.904983 |
| H | -0.925292 | 1.460841 | -0.909897 | H | -0.957408 | 1.474962 | -0.904983 |
| H | 1.116877 | 0.218566 | -2.160174 | H | 1.066957 | 0.236974 | -2.145775 |
| H | 2.595430 | 0.182293 | -1.196833 | H | 2.547530 | 0.195520 | -1.200137 |
| H | 2.595430 | 0.182293 | 1.196833 | H | 2.547530 | 0.195520 | 1.200137 |
| H | 1.116877 | 0.218566 | 2.160174 | H | 1.066957 | 0.236974 | 2.145775 |
| H | 2.603327 | 2.596407 | -1.204373 | H | 2.557467 | 2.607739 | -1.202461 |
| H | 1.115823 | 2.570573 | -2.158452 | H | 1.075648 | 2.581094 | -2.148822 |
| H | 0.371145 | 3.546741 | 0.000000 | H | 0.334901 | 3.550047 | 0.000000 |
| H | 1.115823 | 2.570573 | 2.158452 | H | 1.075648 | 2.581094 | 2.148822 |
| H | 2.603327 | 2.596407 | 1.204373 | H | 2.557467 | 2.607739 | 1.202461 |
| C | -2.236278 | -1.953063 | 0.000000 | C | -2.215681 | -1.974225 | 0.000000 |
| C | 0.334007 | -1.269902 | 0.000000 | C | 0.359580 | -1.286141 | 0.000000 |
| O | -2.850975 | -2.941182 | 0.000000 | O | -2.815630 | -2.954738 | 0.000000 |
| O | 1.063636 | -2.222686 | 0.000000 | O | 1.135234 | -2.182237 | 0.000000 |

**Table S10.**Optimized coordinates for the (nor)$Co(CO)_2$ structure **1T-1.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| Co | 0.465233 | 1.370164 | 0.000000 | Co | 0.461284 | 1.366957 | 0.000000 |
| C | -0.251957 | -0.453975 | 0.000000 | C | -0.253482 | -0.456652 | 0.000000 |
| C | -1.098465 | -0.843904 | 1.244669 | C | -1.092967 | -0.843285 | 1.241820 |
| C | -1.098465 | -2.407872 | 1.247743 | C | -1.092967 | -2.402230 | 1.244144 |
| C | -0.267237 | -2.752674 | 0.000000 | C | -0.264916 | -2.744958 | 0.000000 |
| C | 0.777596 | -1.617182 | 0.000000 | C | 0.775246 | -1.612059 | 0.000000 |
| C | -1.098465 | -2.407872 | -1.247743 | C | -1.092967 | -2.402230 | -1.244144 |
| C | -1.098465 | -0.843904 | -1.244669 | C | -1.092967 | -0.843285 | -1.241820 |
| H | -0.651046 | -0.467222 | 2.175944 | H | -0.638356 | -0.463326 | 2.161522 |
| H | -2.113564 | -0.428698 | 1.190963 | H | -2.100397 | -0.423918 | 1.192122 |
| H | -0.624296 | -2.801668 | 2.156053 | H | -0.619999 | -2.795335 | 2.147011 |
| H | -2.109544 | -2.831178 | 1.196581 | H | -2.098924 | -2.824202 | 1.194566 |
| H | -2.109544 | -2.831178 | -1.196581 | H | -2.098924 | -2.824202 | -1.194566 |
| H | -0.624296 | -2.801668 | -2.156053 | H | -0.619999 | -2.795335 | -2.147011 |
| H | -2.113564 | -0.428698 | -1.190963 | H | -2.100397 | -0.423918 | -1.192122 |
| H | -0.651046 | -0.467222 | -2.175944 | H | -0.638356 | -0.463326 | -2.161522 |
| H | 1.419262 | -1.636601 | -0.892389 | H | 1.414112 | -1.623360 | -0.887698 |
| H | 1.419262 | -1.636601 | 0.892389 | H | 1.414112 | -1.623360 | 0.887698 |
| H | 0.131216 | -3.774565 | 0.000000 | H | 0.130847 | -3.761634 | 0.000000 |
| C | 1.179765 | 3.044585 | 0.000000 | C | 1.176769 | 3.042863 | 0.000000 |
| O | 1.650003 | 4.100958 | 0.000000 | O | 1.641389 | 4.085639 | 0.000000 |

**Table S11.**Optimized coordinates for the $(nor)_2Co(CO)_7$ structure **7S-b1.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| Co | 2.022311 | -0.990391 | -0.141673 | Co | -0.731528 | -1.123535 | 0.334380 |
| C | 1.332112 | 1.861531 | -0.184247 | C | -3.393636 | 0.388005 | -0.121861 |
| C | 2.044175 | 2.613468 | -1.339911 | C | -4.122572 | -0.960781 | -0.192733 |
| C | 2.869567 | 3.697124 | -0.588267 | C | -5.326105 | -0.666564 | -1.127082 |
| C | 2.482693 | 3.479038 | 0.886554 | C | -5.160371 | 0.822935 | -1.456950 |
| C | 2.371102 | 1.946872 | 0.947030 | C | -3.637519 | 0.949767 | -1.547830 |
| C | 1.013763 | 3.906894 | 1.074314 | C | -5.468273 | 1.642763 | -0.196659 |
| C | 0.215600 | 2.784215 | 0.352679 | C | -4.251710 | 1.356033 | 0.723184 |
| H | 2.695070 | 1.944977 | -1.911292 | H | -3.475089 | -1.731322 | -0.609902 |
| H | 1.310504 | 3.028520 | -2.038583 | H | -4.428188 | -1.300935 | 0.796395 |
| H | 3.943940 | 3.535271 | -0.734719 | H | -5.268914 | -1.271397 | -2.033612 |
| H | 2.636982 | 4.712444 | -0.929368 | H | -6.286509 | -0.877158 | -0.654704 |
| H | 0.822248 | 4.899697 | 0.650652 | H | -6.416447 | 1.351368 | 0.257456 |
| H | 0.750714 | 3.943577 | 2.137545 | H | -5.532295 | 2.706484 | -0.431553 |
| H | -0.420558 | 3.147414 | -0.460704 | H | -4.530497 | 0.900522 | 1.673993 |
| H | -0.413490 | 2.242842 | 1.061232 | H | -3.690521 | 2.263741 | 0.938680 |
| H | 1.983226 | 1.563860 | 1.898708 | H | -3.277280 | 1.974015 | -1.647087 |
| H | 3.312600 | 1.435644 | 0.711896 | H | -3.192549 | 0.331704 | -2.328325 |
| H | 3.175660 | 3.936686 | 1.599501 | H | -5.711522 | 1.143353 | -2.340866 |
| C | 0.855184 | 0.500342 | -0.623120 | C | -1.932612 | 0.402637 | 0.229812 |
| C | 3.070390 | -2.078190 | 0.848840 | C | 0.589890 | -2.337799 | 0.407214 |
| O | -0.164477 | 0.370753 | -1.339673 | O | -1.416697 | 1.510915 | 0.425138 |
| O | 3.800765 | -2.742350 | 1.442226 | O | 1.437849 | -3.097490 | 0.441358 |
| C | -4.168584 | -0.547367 | 0.774128 | C | 3.802023 | -0.226761 | 0.829150 |
| C | -3.014895 | 0.344719 | 0.230092 | C | 3.334194 | 0.148667 | -0.579725 |
| C | -3.160548 | 0.168172 | -1.289018 | C | 4.366416 | 1.235749 | -0.968310 |
| C | -4.636071 | 0.596205 | -1.312851 | C | 5.570686 | 0.317949 | -0.733580 |
| C | -4.569678 | 1.985099 | -0.646302 | C | 5.246791 | -0.859982 | -1.663682 |
| C | -5.264274 | -0.397200 | -0.318408 | C | 5.346872 | -0.125939 | 0.720330 |
| C | -3.447784 | 1.818488 | 0.417165 | C | 3.702971 | -0.984352 | -1.559575 |
| H | -3.005628 | -0.860889 | -1.630655 | H | 4.333998 | 2.100695 | -0.303688 |
| H | -2.497123 | 0.828544 | -1.853378 | H | 4.248891 | 1.565386 | -2.001097 |
| H | -2.606873 | 2.488118 | 0.214785 | H | 3.217027 | -0.819766 | -2.520990 |
| H | -3.778586 | 2.006727 | 1.442850 | H | 3.375457 | -1.951282 | -1.179100 |
| H | -4.482125 | -0.200482 | 1.763930 | H | 3.454176 | -1.216989 | 1.120737 |
| H | -3.855127 | -1.591009 | 0.880871 | H | 3.407137 | 0.481553 | 1.556908 |
| H | -5.530425 | 2.274044 | -0.204068 | H | 5.761496 | -1.772610 | -1.360437 |
| H | -4.299473 | 2.753589 | -1.380030 | H | 5.548703 | -0.639027 | -2.688760 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -5.114977 | 0.598630 | -2.297389 | H | 6.546300 | 0.768752 | -0.913465 |
| H | -5.459684 | -1.359692 | -0.805518 | H | 5.737581 | 0.616094 | 1.418233 |
| H | -6.213700 | -0.031592 | 0.089748 | H | 5.845784 | -1.071145 | 0.937760 |
| C | 1.017774 | -2.196490 | -1.098718 | C | -1.727431 | -1.811381 | 1.642456 |
| C | -1.736699 | 0.007674 | 0.981469 | C | 1.936021 | 0.632738 | -0.713345 |
| O | 1.035749 | -3.052820 | -1.887007 | O | -2.370181 | -2.262684 | 2.470170 |
| O | -1.571331 | 0.407334 | 2.111173 | O | 1.361352 | 0.869310 | -1.755601 |
| C | 0.418536 | -1.460615 | 1.666597 | C | 0.688928 | 0.026043 | 1.713971 |
| O | 0.635078 | -1.793387 | 2.754007 | O | 1.068080 | -0.280087 | 2.764245 |
| O | 4.109404 | -0.275894 | -2.023212 | O | -1.150691 | -1.505521 | -2.522923 |
| C | 3.268204 | -0.493258 | -1.259714 | C | -0.985996 | -1.346069 | -1.404080 |
| C | -1.520432 | -2.357352 | -0.136511 | C | 1.308966 | 2.598049 | 0.870045 |
| O | -2.193108 | -3.285588 | -0.262285 | O | 1.900749 | 3.469759 | 1.310424 |
| Co | -0.348631 | -1.061369 | 0.109872 | Co | 0.522801 | 1.108872 | 0.333265 |

**Table S12.** Optimized coordinates for the $(nor)_2Co(CO)_7$ structure **7S-b2.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | -1.873861 | 2.096691 | -1.178428 | C | -1.921509 | 2.076195 | -1.182132 |
| C | -2.199987 | 1.063679 | -0.071523 | C | -2.218994 | 1.044983 | -0.072038 |
| C | -1.585245 | 1.740401 | 1.165042 | C | -1.611568 | 1.741885 | 1.151507 |
| C | -2.356843 | 3.057977 | 0.992579 | C | -2.414128 | 3.036561 | 0.979402 |
| C | -3.815834 | 2.567477 | 0.967707 | C | -3.855564 | 2.513060 | 0.971646 |
| C | -1.947509 | 3.462905 | -0.433841 | C | -2.031425 | 3.441084 | -0.448654 |
| C | -3.714472 | 1.200686 | 0.225494 | C | -3.730318 | 1.152061 | 0.232761 |
| Co | -1.571422 | -0.918406 | -0.412950 | Co | -1.564732 | -0.928505 | -0.412216 |
| H | -0.505540 | 1.871486 | 1.079547 | H | -0.540940 | 1.897853 | 1.055189 |
| H | -1.809707 | 1.231351 | 2.108893 | H | -1.813010 | 1.235777 | 2.095875 |
| H | -4.081468 | 0.388280 | 0.860457 | H | -4.076085 | 0.336740 | 0.866745 |
| H | -4.309824 | 1.178095 | -0.693903 | H | -4.325813 | 1.114261 | -0.679989 |
| H | -2.587713 | 2.035022 | -2.006927 | H | -2.627317 | 1.989300 | -2.008398 |
| H | -0.881797 | 1.943526 | -1.605884 | H | -0.928801 | 1.948636 | -1.603457 |
| H | -4.479938 | 3.276853 | 0.460028 | H | -4.540586 | 3.202039 | 0.474851 |
| H | -4.196113 | 2.429105 | 1.986989 | H | -4.219459 | 2.367757 | 1.990557 |
| H | -2.157484 | 3.825649 | 1.748245 | H | -2.227632 | 3.810158 | 1.724247 |
| H | -0.966809 | 3.954780 | -0.428285 | H | -1.072055 | 3.962219 | -0.457245 |
| H | -2.664174 | 4.155523 | -0.890388 | H | -2.769696 | 4.104646 | -0.901639 |
| C | -2.186079 | -1.220481 | 1.263198 | C | -2.147892 | -1.231509 | 1.276833 |
| C | -2.617298 | -0.653955 | -1.789586 | C | -2.613022 | -0.694026 | -1.795229 |
| O | -2.628887 | -1.412956 | 2.309239 | O | -2.561611 | -1.420314 | 2.320370 |
| O | -3.334754 | -0.508170 | -2.681412 | O | -3.318749 | -0.563949 | -2.680940 |
| C | 1.948335 | 2.008312 | -0.014404 | C | 1.946204 | 2.020570 | -0.014919 |
| C | 2.534372 | 0.579664 | -0.024997 | C | 2.535760 | 0.598063 | -0.022081 |
| C | 3.302136 | 0.586258 | -1.367202 | C | 3.307029 | 0.607487 | -1.357375 |
| C | 4.137718 | 1.830165 | -1.025125 | C | 4.132964 | 1.852551 | -1.015077 |
| C | 4.809234 | 1.399863 | 0.292777 | C | 4.798021 | 1.429806 | 0.302420 |
| C | 3.043125 | 2.864932 | -0.713926 | C | 3.036111 | 2.878633 | -0.711155 |
| C | 3.708769 | 0.534108 | 0.978157 | C | 3.703938 | 0.558348 | 0.981108 |
| Co | 1.117431 | -0.935335 | 0.411035 | Co | 1.131026 | -0.924904 | 0.414487 |
| H | 2.659167 | 0.725880 | -2.240114 | H | 2.669072 | 0.740431 | -2.228543 |
| H | 3.931106 | -0.296382 | -1.521806 | H | 3.936455 | -0.269321 | -1.506097 |
| H | 4.050186 | -0.496186 | 1.128746 | H | 4.049393 | -0.465630 | 1.128265 |
| H | 3.424676 | 0.924500 | 1.961272 | H | 3.415556 | 0.940477 | 1.960503 |
| H | 1.741924 | 2.352389 | 1.005478 | H | 1.735342 | 2.363075 | 0.998800 |
| H | 1.008457 | 2.051864 | -0.570794 | H | 1.011668 | 2.059918 | -0.570485 |
| H | 5.109464 | 2.259876 | 0.903165 | H | 5.088176 | 2.288046 | 0.911039 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 5.708835 | 0.804865 | 0.094376 | H | 5.699671 | 0.844951 | 0.111295 |
| H | 4.843455 | 2.150031 | -1.799490 | H | 4.837737 | 2.173849 | -1.781938 |
| H | 2.658180 | 3.311846 | -1.638454 | H | 2.653202 | 3.319735 | -1.633320 |
| H | 3.411388 | 3.679276 | -0.078740 | H | 3.395162 | 3.693873 | -0.080712 |
| C | 2.266247 | -1.925090 | -0.475621 | C | 2.244376 | -1.907687 | -0.527307 |
| C | 0.975763 | 0.004595 | 1.920989 | C | 0.959720 | 0.027347 | 1.914249 |
| O | 3.031102 | -2.611662 | -1.000853 | O | 2.974067 | -2.580764 | -1.088367 |
| O | 0.941835 | 0.532018 | 2.946030 | O | 0.908731 | 0.559466 | 2.920457 |
| C | 0.562293 | -2.385815 | 1.306834 | C | 0.634100 | -2.379200 | 1.334151 |
| O | 0.309771 | -3.320789 | 1.933464 | O | 0.415379 | -3.303416 | 1.964675 |
| O | -1.276114 | -3.758292 | -1.159627 | O | -1.208825 | -3.757156 | -1.114070 |
| C | -1.357203 | -2.654185 | -0.847819 | C | -1.317112 | -2.663727 | -0.823459 |
| C | 0.124765 | -0.360527 | -1.221774 | C | 0.112688 | -0.343809 | -1.229343 |
| O | 0.432160 | 0.018282 | -2.284577 | O | 0.423975 | 0.045033 | -2.271963 |

**Table S13.** Optimized coordinates for the $(nor)_2Co(CO)_7$ structure **7S-b3.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | -3.038405 | -0.378617 | -1.951766 | C | -3.047781 | -0.368533 | -1.938665 |
| C | -2.768951 | -0.186191 | -0.432532 | C | -2.775043 | -0.187600 | -0.423243 |
| C | -2.886317 | 1.339685 | -0.278486 | C | -2.900249 | 1.332409 | -0.260575 |
| C | -4.270350 | 1.435354 | -0.939651 | C | -4.284816 | 1.424762 | -0.911860 |
| C | -5.094720 | 0.443319 | -0.094508 | C | -5.096404 | 0.428397 | -0.069881 |
| C | -3.993401 | 0.797233 | -2.308119 | C | -4.014424 | 0.796433 | -2.279951 |
| C | -4.059740 | -0.664693 | 0.275100 | C | -4.058496 | -0.676010 | 0.282074 |
| Co | -0.996897 | -0.999507 | 0.400624 | Co | -1.003595 | -1.007805 | 0.394591 |
| H | -2.108218 | 1.891032 | -0.820069 | H | -2.131568 | 1.887773 | -0.801146 |
| H | -2.895044 | 1.666582 | 0.766504 | H | -2.903062 | 1.653081 | 0.780812 |
| H | -3.945518 | -0.727444 | 1.360474 | H | -3.940301 | -0.750792 | 1.360922 |
| H | -4.358791 | -1.660919 | -0.069784 | H | -4.352124 | -1.665463 | -0.070714 |
| H | -3.505662 | -1.350227 | -2.142374 | H | -3.499746 | -1.340159 | -2.135993 |
| H | -2.130148 | -0.335301 | -2.552823 | H | -2.146492 | -0.308988 | -2.539194 |
| H | -5.954450 | 0.051545 | -0.650668 | H | -5.957189 | 0.040412 | -0.616843 |
| H | -5.479793 | 0.928609 | 0.810267 | H | -5.473393 | 0.903992 | 0.837362 |
| H | -4.702468 | 2.440719 | -0.991985 | H | -4.720932 | 2.422716 | -0.957158 |
| H | -3.497883 | 1.514535 | -2.973999 | H | -3.534240 | 1.516848 | -2.945418 |
| H | -4.910915 | 0.460551 | -2.804894 | H | -4.928359 | 0.455405 | -2.768957 |
| C | -1.632263 | -0.402200 | 1.983962 | C | -1.627450 | -0.404577 | 1.980694 |
| C | -1.568854 | -2.338059 | -0.561901 | C | -1.547240 | -2.343202 | -0.592658 |
| O | -2.044194 | -0.064791 | 3.006329 | O | -2.030347 | -0.068481 | 2.991564 |
| O | -1.961239 | -3.254792 | -1.144277 | O | -1.916966 | -3.243405 | -1.187931 |
| C | 3.038421 | 0.378101 | -1.951868 | C | 3.047769 | 0.367990 | -1.938768 |
| C | 2.768945 | 0.186057 | -0.432586 | C | 2.775036 | 0.187467 | -0.423295 |
| C | 2.886218 | -1.339788 | -0.278161 | C | 2.900202 | -1.332501 | -0.260225 |
| C | 4.270237 | -1.435709 | -0.939316 | C | 4.284763 | -1.425065 | -0.911491 |
| C | 5.094679 | -0.443509 | -0.094435 | C | 5.096382 | -0.428500 | -0.069780 |
| C | 3.993305 | -0.797922 | -2.307942 | C | 4.014383 | -0.797090 | -2.279748 |
| C | 4.059763 | 0.664642 | 0.274937 | C | 4.058507 | 0.676031 | 0.281884 |
| Co | 0.996927 | 0.999645 | 0.400380 | Co | 1.003608 | 1.007928 | 0.394325 |
| H | 2.108078 | -1.891227 | -0.819592 | H | 2.131501 | -1.887986 | -0.800644 |
| H | 2.894937 | -1.666414 | 0.766913 | H | 2.903013 | -1.652897 | 0.781247 |
| H | 3.945542 | 0.727627 | 1.360297 | H | 3.940318 | 0.751105 | 1.360713 |
| H | 4.358871 | 1.660778 | -0.070160 | H | 4.352161 | 1.665381 | -0.071170 |
| H | 3.505777 | 1.349621 | -2.142693 | H | 3.499755 | 1.339553 | -2.136359 |
| H | 2.130163 | 0.334742 | -2.552921 | H | 2.146475 | 0.308305 | -2.539274 |
| H | 5.954409 | -0.051908 | -0.650717 | H | 5.957177 | -0.040684 | -0.616847 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 5.479759 | -0.928598 | 0.810445 | H | 5.473360 | -0.903864 | 0.837589 |
| H | 4.702293 | -2.441113 | -0.991399 | H | 4.720851 | -2.423042 | -0.956527 |
| H | 3.497702 | -1.515358 | -2.973614 | H | 3.534180 | -1.517669 | -2.945023 |
| H | 4.910831 | -0.461449 | -2.804837 | H | 4.928326 | -0.456214 | -2.768845 |
| C | 1.568976 | 2.337915 | -0.562471 | C | 1.547320 | 2.343064 | -0.593238 |
| C | -0.181067 | 2.076426 | 1.223162 | C | -0.176463 | 2.079451 | 1.218144 |
| O | 1.961431 | 3.254486 | -1.145059 | O | 1.917084 | 3.243110 | -1.188726 |
| O | -0.815398 | 2.848008 | 1.795359 | O | -0.810312 | 2.835742 | 1.783844 |
| C | 1.632257 | 0.402799 | 1.983910 | C | 1.627456 | 0.405143 | 1.980601 |
| O | 2.044164 | 0.065699 | 3.006389 | O | 2.030351 | 0.069332 | 2.991567 |
| O | 0.815357 | -2.847424 | 1.796288 | O | 0.810277 | -2.835244 | 1.784665 |
| C | 0.181061 | -2.076030 | 1.223799 | C | 0.176453 | -2.079103 | 1.218736 |
| C | -0.000004 | -0.000101 | -0.974696 | C | -0.000002 | -0.000091 | -0.986086 |
| O | 0.000001 | -0.000233 | -2.143539 | O | -0.000023 | -0.000228 | -2.140643 |

**Table S14.**Optimized coordinates for the $(nor)_2Co(CO)_7$ structure **7T-b4.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| Co | 1.550314 | 1.005131 | -0.046710 | Co | 1.549032 | 1.012095 | -0.135717 |
| C | 3.526633 | -1.055383 | 0.195453 | C | 3.543249 | -1.038093 | 0.205417 |
| C | 4.409824 | -1.556406 | 1.358684 | C | 4.401420 | -1.592034 | 1.358069 |
| C | 5.850195 | -1.378241 | 0.798338 | C | 5.846185 | -1.436193 | 0.816991 |
| C | 5.615621 | -0.806252 | -0.614798 | C | 5.640914 | -0.825126 | -0.578396 |
| C | 4.383449 | 0.086270 | -0.385226 | C | 4.433716 | 0.090705 | -0.337946 |
| C | 5.025185 | -1.917145 | -1.506008 | C | 5.033154 | -1.894202 | -1.498711 |
| C | 3.580753 | -2.091336 | -0.953500 | C | 3.583932 | -2.044218 | -0.965709 |
| H | 4.246277 | -0.941379 | 2.251687 | H | 4.244437 | -1.000247 | 2.261441 |
| H | 4.162451 | -2.588530 | 1.624269 | H | 4.126652 | -2.618861 | 1.594125 |
| H | 6.424201 | -0.673039 | 1.411113 | H | 6.429605 | -0.764861 | 1.449541 |
| H | 6.409474 | -2.320731 | 0.768036 | H | 6.381337 | -2.386032 | 0.768912 |
| H | 5.611008 | -2.841934 | -1.447235 | H | 5.591540 | -2.830831 | -1.459462 |
| H | 5.005929 | -1.603530 | -2.556417 | H | 5.032647 | -1.557111 | -2.536677 |
| H | 3.368201 | -3.098083 | -0.580387 | H | 3.341562 | -3.049045 | -0.621629 |
| H | 2.829557 | -1.855624 | -1.716065 | H | 2.850471 | -1.772340 | -1.726199 |
| H | 3.974957 | 0.502946 | -1.315746 | H | 4.045666 | 0.540250 | -1.255808 |
| H | 4.557873 | 0.900479 | 0.329161 | H | 4.619501 | 0.878144 | 0.394873 |
| H | 6.492328 | -0.311043 | -1.044997 | H | 6.530282 | -0.345510 | -0.985666 |
| C | 2.097485 | -0.769921 | 0.603982 | C | 2.120036 | -0.727565 | 0.601894 |
| C | 1.584951 | 2.613047 | -0.890342 | C | 1.557003 | 2.590421 | -1.028533 |
| O | 1.431021 | -1.550175 | 1.245008 | O | 1.463295 | -1.468715 | 1.278800 |
| O | 1.605588 | 3.630277 | -1.433973 | O | 1.556374 | 3.579015 | -1.596251 |
| C | -4.532896 | -2.291164 | 0.394151 | C | -4.550294 | -2.306824 | 0.216804 |
| C | -3.918140 | -0.906952 | 0.111530 | C | -3.922343 | -0.911437 | 0.069749 |
| C | -4.654885 | -0.483634 | -1.186679 | C | -4.627373 | -0.372892 | -1.198867 |
| C | -6.050110 | -0.646844 | -0.560705 | C | -6.032836 | -0.581940 | -0.622836 |
| C | -5.951931 | 0.287265 | 0.660853 | C | -5.959478 | 0.237175 | 0.673790 |
| C | -6.006701 | -2.110196 | -0.076278 | C | -6.006758 | -2.077072 | -0.269212 |
| C | -4.471193 | 0.125010 | 1.113869 | C | -4.494947 | 0.028192 | 1.143700 |
| Co | -1.040711 | 0.327134 | -0.211264 | Co | -1.042298 | 0.328041 | -0.107527 |
| H | -4.460489 | -1.165093 | -2.023013 | H | -4.415418 | -0.976176 | -2.082778 |
| H | -4.422102 | 0.543466 | -1.489629 | H | -4.383218 | 0.670004 | -1.403424 |
| H | -3.914158 | 1.065272 | 1.026872 | H | -3.935367 | 0.964914 | 1.152727 |
| H | -4.367950 | -0.225877 | 2.146044 | H | -4.416260 | -0.411002 | 2.138185 |
| H | -4.446985 | -2.553773 | 1.453679 | H | -4.489902 | -2.659976 | 1.246174 |
| H | -4.011565 | -3.063394 | -0.181102 | H | -4.020574 | -3.026344 | -0.407440 |
| H | -6.662883 | 0.009013 | 1.446755 | H | -6.686749 | -0.102239 | 1.412134 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -6.161488 | 1.324996 | 0.377155 | H | -6.158319 | 1.292196 | 0.480276 |
| H | -6.890413 | -0.423336 | -1.226110 | H | -6.853507 | -0.297302 | -1.280370 |
| H | -6.239482 | -2.797290 | -0.898117 | H | -6.221921 | -2.685647 | -1.148939 |
| H | -6.730633 | -2.296597 | 0.724967 | H | -6.748064 | -2.328660 | 0.490232 |
| C | -1.737366 | 1.770459 | -1.019250 | C | -1.714329 | 1.846930 | -0.783198 |
| C | -2.444799 | -0.858135 | -0.043068 | C | -2.450156 | -0.862984 | -0.041083 |
| O | -2.235957 | 2.710198 | -1.468455 | O | -2.181078 | 2.822072 | -1.148082 |
| O | -1.652830 | -1.777374 | -0.203902 | O | -1.665433 | -1.767314 | -0.230006 |
| C | -0.992478 | 0.884935 | 1.527725 | C | -0.983482 | 0.703770 | 1.690456 |
| O | -1.113500 | 1.240443 | 2.619587 | O | -1.042882 | 0.948235 | 2.800829 |
| O | 2.013860 | 1.860540 | 2.727060 | O | 1.957865 | 2.011169 | 2.582403 |
| C | 1.814571 | 1.527909 | 1.638721 | C | 1.787395 | 1.619967 | 1.523005 |
| C | 0.757292 | 0.112048 | -1.362968 | C | 0.751310 | 0.082782 | -1.409599 |
| O | 0.471048 | -0.460169 | -2.353142 | O | 0.376341 | -0.486106 | -2.351112 |

**Table S15.**Optimized coordinates for the $(nor)_2Co(CO)_6$ structure **6T-b1.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| Co | -1.233899 | 1.566713 | -0.285243 | Co | -1.253169 | 1.559722 | -0.285622 |
| C | -2.532158 | -1.104012 | -0.209488 | C | -2.524360 | -1.120786 | -0.183949 |
| C | -3.699397 | -0.304925 | 0.402418 | C | -3.679028 | -0.344311 | 0.469466 |
| C | -4.642262 | -1.415581 | 0.950725 | C | -4.611954 | -1.469002 | 0.992966 |
| C | -3.916370 | -2.715084 | 0.551479 | C | -3.896047 | -2.750873 | 0.543284 |
| C | -2.446210 | -2.317783 | 0.746145 | C | -2.427060 | -2.363193 | 0.727355 |
| C | -3.994809 | -2.877235 | -0.980525 | C | -3.998229 | -2.862944 | -0.986215 |
| C | -3.023555 | -1.780132 | -1.509659 | C | -3.039322 | -1.751989 | -1.494090 |
| H | -3.334766 | 0.345915 | 1.209317 | H | -3.302330 | 0.276457 | 1.286952 |
| H | -4.192573 | 0.333765 | -0.338267 | H | -4.179791 | 0.316254 | -0.238379 |
| H | -4.737308 | -1.345290 | 2.040655 | H | -4.692245 | -1.433565 | 2.080649 |
| H | -5.651402 | -1.358634 | 0.526793 | H | -5.622667 | -1.397984 | 0.588622 |
| H | -5.017801 | -2.748923 | -1.353140 | H | -5.022061 | -2.725912 | -1.337728 |
| H | -3.655447 | -3.874529 | -1.283525 | H | -3.665320 | -3.844951 | -1.325624 |
| H | -3.507925 | -1.057973 | -2.176542 | H | -3.531828 | -1.011236 | -2.124992 |
| H | -2.174823 | -2.218652 | -2.045224 | H | -2.204311 | -2.169991 | -2.056756 |
| H | -1.722340 | -3.062595 | 0.399985 | H | -1.713165 | -3.093271 | 0.347685 |
| H | -2.198516 | -2.027861 | 1.775547 | H | -2.162864 | -2.108119 | 1.756135 |
| H | -4.249829 | -3.596423 | 1.109593 | H | -4.222038 | -3.644845 | 1.074390 |
| C | -1.224441 | -0.375299 | -0.358843 | C | -1.226317 | -0.385957 | -0.339667 |
| C | -1.221361 | 2.875569 | 0.994630 | C | -1.233285 | 2.898336 | 0.966216 |
| O | -0.199713 | -1.076223 | -0.665323 | O | -0.204552 | -1.075135 | -0.644411 |
| O | -1.204082 | 3.700945 | 1.799853 | O | -1.212781 | 3.732865 | 1.740971 |
| C | 3.706315 | 0.601678 | 0.224579 | C | 3.723341 | 0.608296 | 0.195669 |
| C | 3.215716 | -0.861076 | 0.177001 | C | 3.229049 | -0.848983 | 0.180842 |
| C | 2.975020 | -1.042110 | -1.342637 | C | 2.994498 | -1.063782 | -1.332201 |
| C | 4.410995 | -0.655453 | -1.726005 | C | 4.429271 | -0.692053 | -1.717355 |
| C | 5.237017 | -1.657935 | -0.894833 | C | 5.245507 | -1.675532 | -0.864456 |
| C | 4.533813 | 0.740668 | -1.086188 | C | 4.555210 | 0.712329 | -1.109935 |
| C | 4.414681 | -1.796487 | 0.420545 | C | 4.422793 | -1.779314 | 0.447660 |
| Co | 0.467697 | -0.014746 | 0.791984 | Co | 0.471380 | 0.005647 | 0.788910 |
| H | 2.209203 | -0.364232 | -1.734071 | H | 2.235831 | -0.395544 | -1.739597 |
| H | 2.702771 | -2.071380 | -1.601842 | H | 2.720544 | -2.093034 | -1.566769 |
| H | 4.063068 | -2.820927 | 0.579369 | H | 4.068434 | -2.793334 | 0.630779 |
| H | 4.976255 | -1.500748 | 1.313398 | H | 4.980026 | -1.465828 | 1.330992 |
| H | 4.288461 | 0.799629 | 1.131317 | H | 4.298090 | 0.825566 | 1.096526 |
| H | 2.858651 | 1.299035 | 0.224898 | H | 2.880768 | 1.303250 | 0.175629 |
| H | 6.258372 | -1.300033 | -0.719454 | H | 6.264063 | -1.321624 | -0.696854 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 5.309912 | -2.621781 | -1.412683 | H | 5.315747 | -2.646927 | -1.357204 |
| H | 4.636407 | -0.672603 | -2.797757 | H | 4.658233 | -0.733234 | -2.782089 |
| H | 4.099069 | 1.506894 | -1.738229 | H | 4.130843 | 1.463323 | -1.777928 |
| H | 5.577388 | 1.016706 | -0.896351 | H | 5.594188 | 0.987399 | -0.923004 |
| C | 0.287332 | 1.999511 | -1.205257 | C | 0.252733 | 1.991993 | -1.236388 |
| C | 1.986267 | -1.145557 | 1.006356 | C | 2.001507 | -1.112845 | 1.010277 |
| O | 1.248123 | 2.228209 | -1.802596 | O | 1.194176 | 2.212481 | -1.840421 |
| O | 1.830976 | -2.121023 | 1.710330 | O | 1.843086 | -2.067223 | 1.723558 |
| C | 0.941513 | 0.920909 | 2.202457 | C | 0.966968 | 0.976523 | 2.167875 |
| O | 1.266818 | 1.524175 | 3.132551 | O | 1.302246 | 1.598729 | 3.064370 |
| O | -3.120146 | 2.158080 | -2.483334 | O | -3.179963 | 2.123832 | -2.439554 |
| C | -2.412303 | 1.931037 | -1.600840 | C | -2.461531 | 1.907052 | -1.581745 |

**Table S16.**Optimized coordinates for the $(nor)_2Co(CO)_6$ structure **6S-b2.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| Co | -1.966758 | -0.982491 | -0.042459 | Co | -1.967559 | -1.009212 | -0.021272 |
| C | -1.532702 | 1.599757 | 0.317800 | C | -1.559158 | 1.599425 | 0.286482 |
| C | -2.204416 | 2.361858 | 1.482779 | C | -2.240940 | 2.362442 | 1.440879 |
| C | -3.096610 | 3.405014 | 0.753240 | C | -3.146999 | 3.379795 | 0.702110 |
| C | -2.810045 | 3.136145 | -0.736123 | C | -2.860938 | 3.099072 | -0.779534 |
| C | -2.658836 | 1.601220 | -0.747716 | C | -2.683697 | 1.571138 | -0.773319 |
| C | -1.374500 | 3.595307 | -1.054492 | C | -1.439602 | 3.577051 | -1.105716 |
| C | -0.492747 | 2.523378 | -0.357005 | C | -0.539562 | 2.536515 | -0.394242 |
| H | -2.804531 | 1.671036 | 2.086575 | H | -2.827435 | 1.672663 | 2.049879 |
| H | -1.452185 | 2.807033 | 2.141492 | H | -1.499084 | 2.823499 | 2.091826 |
| H | -4.156215 | 3.239328 | 0.980137 | H | -4.198659 | 3.202542 | 0.932774 |
| H | -2.854683 | 4.435853 | 1.035992 | H | -2.922596 | 4.412783 | 0.971443 |
| H | -1.180057 | 4.606958 | -0.680282 | H | -1.263325 | 4.593870 | -0.751908 |
| H | -1.196441 | 3.600365 | -2.135856 | H | -1.263636 | 3.568172 | -2.182268 |
| H | 0.207494 | 2.929129 | 0.380400 | H | 0.143597 | 2.964892 | 0.338242 |
| H | 0.079272 | 1.950667 | -1.092601 | H | 0.048658 | 1.972907 | -1.116331 |
| H | -2.337855 | 1.211610 | -1.721766 | H | -2.359045 | 1.174659 | -1.737324 |
| H | -3.579574 | 1.098017 | -0.426302 | H | -3.589434 | 1.056747 | -0.445098 |
| H | -3.568092 | 3.539380 | -1.414846 | H | -3.623448 | 3.480166 | -1.457236 |
| C | -0.889224 | 0.313816 | 0.799026 | C | -0.901416 | 0.329525 | 0.776205 |
| C | -3.135851 | -1.676845 | -1.209752 | C | -3.147494 | -1.779920 | -1.127666 |
| O | 0.042242 | 0.348752 | 1.647259 | O | 0.038110 | 0.386872 | 1.599680 |
| O | -3.926153 | -2.083611 | -1.943210 | O | -3.933535 | -2.232610 | -1.815723 |
| C | 4.064825 | -0.630540 | -0.744099 | C | 4.085852 | -0.603183 | -0.767515 |
| C | 2.869406 | 0.304859 | -0.413753 | C | 2.893860 | 0.313084 | -0.392545 |
| C | 3.091379 | 0.600013 | 1.077517 | C | 3.132207 | 0.554525 | 1.101606 |
| C | 4.521846 | 1.122020 | 0.874722 | C | 4.553758 | 1.089876 | 0.900758 |
| C | 4.304840 | 2.240007 | -0.164695 | C | 4.319423 | 2.240338 | -0.090167 |
| C | 5.191066 | -0.076111 | 0.175359 | C | 5.217470 | -0.074448 | 0.152145 |
| C | 3.163427 | 1.679897 | -1.059938 | C | 3.174452 | 1.709172 | -0.989325 |
| H | 3.038064 | -0.292317 | 1.709877 | H | 3.094693 | -0.356149 | 1.698658 |
| H | 2.389264 | 1.343892 | 1.466851 | H | 2.434112 | 1.275723 | 1.524643 |
| H | 2.277151 | 2.319904 | -1.019530 | H | 2.288115 | 2.337437 | -0.914796 |
| H | 3.440387 | 1.570493 | -2.112781 | H | 3.436140 | 1.640025 | -2.044140 |
| H | 4.305821 | -0.582553 | -1.810910 | H | 4.310174 | -0.522031 | -1.830667 |
| H | 3.837797 | -1.674266 | -0.506998 | H | 3.864376 | -1.649366 | -0.560845 |
| H | 5.217626 | 2.456026 | -0.732037 | H | 5.219998 | 2.482760 | -0.656438 |
| H | 3.993047 | 3.169296 | 0.326348 | H | 4.010761 | 3.145232 | 0.435791 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 5.040872 | 1.451815 | 1.780320 | H | 5.080488 | 1.387711 | 1.806345 |
| H | 5.496184 | -0.831060 | 0.909090 | H | 5.538118 | -0.848827 | 0.850606 |
| H | 6.082734 | 0.219301 | -0.389478 | H | 6.095483 | 0.244555 | -0.411287 |
| C | -2.773818 | -1.336232 | 1.472891 | C | -2.757796 | -1.291460 | 1.517560 |
| C | 1.566011 | -0.302946 | -0.900289 | C | 1.592428 | -0.275624 | -0.887724 |
| O | -3.261742 | -1.689936 | 2.461250 | O | -3.223271 | -1.586023 | 2.519787 |
| O | 1.176653 | -0.196636 | -2.036182 | O | 1.204121 | -0.148409 | -2.009819 |
| C | -0.617047 | -2.141338 | -0.847389 | C | -0.596828 | -2.122792 | -0.884783 |
| O | -0.571837 | -3.071614 | -1.565294 | O | -0.531797 | -3.015060 | -1.626806 |
| C | 1.625699 | -2.331292 | 0.740163 | C | 1.628685 | -2.314353 | 0.712603 |
| O | 2.347546 | -3.189615 | 1.021669 | O | 2.350502 | -3.161453 | 0.973418 |
| Co | 0.425796 | -1.132567 | 0.331085 | Co | 0.427065 | -1.116995 | 0.313752 |

**Table S17.**Optimized coordinates for the $(nor)_2Co(CO)_6$ structure **6S-b3.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| Co | 1.520392 | -1.435250 | -0.116817 | Co | 1.520938 | -1.435525 | -0.126841 |
| C | 1.822876 | 1.487721 | -0.431515 | C | 1.819275 | 1.496498 | -0.416879 |
| C | 3.254089 | 1.500975 | -1.013064 | C | 3.235777 | 1.539867 | -1.023096 |
| C | 3.991090 | 2.518582 | -0.092478 | C | 3.976215 | 2.543510 | -0.098233 |
| C | 2.917986 | 2.904630 | 0.945028 | C | 2.920828 | 2.901461 | 0.958802 |
| C | 2.125283 | 1.597941 | 1.080149 | C | 2.146965 | 1.587758 | 1.087213 |
| C | 1.880296 | 3.813129 | 0.258621 | C | 1.866566 | 3.806237 | 0.306076 |
| C | 1.171309 | 2.854956 | -0.739159 | C | 1.151149 | 2.859937 | -0.690336 |
| H | 3.711452 | 0.510232 | -0.929507 | H | 3.703899 | 0.558499 | -0.971538 |
| H | 3.260048 | 1.782510 | -2.071545 | H | 3.216098 | 1.842266 | -2.070280 |
| H | 4.855101 | 2.047847 | 0.390962 | H | 4.847293 | 2.073234 | 0.360862 |
| H | 4.357359 | 3.392535 | -0.643562 | H | 4.327975 | 3.425059 | -0.636315 |
| H | 2.349952 | 4.671036 | -0.236767 | H | 2.316198 | 4.673047 | -0.181028 |
| H | 1.163610 | 4.198258 | 0.992904 | H | 1.162439 | 4.173084 | 1.054347 |
| H | 1.321275 | 3.133013 | -1.787894 | H | 1.279057 | 3.153370 | -1.732534 |
| H | 0.095369 | 2.816205 | -0.557783 | H | 0.083901 | 2.809418 | -0.493705 |
| H | 1.211434 | 1.689203 | 1.676840 | H | 1.246267 | 1.658130 | 1.697466 |
| H | 2.717336 | 0.747413 | 1.446090 | H | 2.750970 | 0.742005 | 1.427212 |
| H | 3.323992 | 3.315568 | 1.875219 | H | 3.336589 | 3.301419 | 1.883012 |
| C | 0.966090 | 0.296358 | -0.797269 | C | 0.972805 | 0.306614 | -0.791520 |
| C | 2.154847 | -2.649278 | 1.061896 | C | 2.130055 | -2.661265 | 1.054668 |
| O | -0.086109 | 0.424913 | -1.484359 | O | -0.074347 | 0.441338 | -1.468723 |
| O | 2.631479 | -3.409827 | 1.785466 | O | 2.577257 | -3.422403 | 1.774310 |
| C | -4.023546 | 0.580615 | 1.202847 | C | -4.022718 | 0.551084 | 1.196926 |
| C | -2.896211 | 0.626885 | 0.148679 | C | -2.893233 | 0.619148 | 0.151648 |
| C | -3.073641 | -0.752981 | -0.555484 | C | -3.076978 | -0.737519 | -0.587279 |
| C | -4.549434 | -0.478564 | -0.918092 | C | -4.546425 | -0.445361 | -0.946037 |
| C | -4.432074 | 0.834745 | -1.714354 | C | -4.419719 | 0.882839 | -1.704187 |
| C | -5.161355 | -0.176342 | 0.462478 | C | -5.158470 | -0.176799 | 0.435109 |
| C | -3.286531 | 1.595997 | -0.989154 | C | -3.276815 | 1.617106 | -0.958144 |
| Co | -0.610717 | -0.466204 | 0.231551 | Co | -0.609110 | -0.472362 | 0.221717 |
| H | -2.969017 | -1.621298 | 0.108983 | H | -2.979120 | -1.618117 | 0.052578 |
| H | -2.458495 | -0.886010 | -1.454155 | H | -2.461244 | -0.851089 | -1.482019 |
| H | -2.427347 | 1.757251 | -1.649299 | H | -2.419285 | 1.791730 | -1.608487 |
| H | -3.586780 | 2.566176 | -0.581353 | H | -3.570720 | 2.573163 | -0.526871 |
| H | -4.294599 | 1.592486 | 1.519131 | H | -4.286650 | 1.550725 | 1.539254 |
| H | -3.690700 | 0.034932 | 2.093763 | H | -3.697128 | -0.017815 | 2.069533 |
| H | -5.373897 | 1.395207 | -1.712202 | H | -5.354219 | 1.445415 | -1.692537 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -4.166328 | 0.633386 | -2.758330 | H | -4.153001 | 0.708705 | -2.747482 |
| H | -5.051401 | -1.285555 | -1.460902 | H | -5.049102 | -1.230707 | -1.508425 |
| H | -5.418651 | -1.104878 | 0.985059 | H | -5.422833 | -1.112559 | 0.929899 |
| H | -6.075510 | 0.422176 | 0.379223 | H | -6.065281 | 0.425352 | 0.365988 |
| C | -0.047061 | -2.272308 | -0.642056 | C | -0.024424 | -2.277554 | -0.695960 |
| C | -1.559694 | 1.018368 | 0.767210 | C | -1.562621 | 0.994074 | 0.786212 |
| O | -0.513396 | -3.214066 | -1.147341 | O | -0.494768 | -3.188848 | -1.220190 |
| O | -1.346431 | 2.049642 | 1.353116 | O | -1.354438 | 2.001124 | 1.391707 |
| C | -0.359635 | -0.872512 | 1.889482 | C | -0.393242 | -0.926303 | 1.872334 |
| O | -0.198619 | -1.096123 | 3.014323 | O | -0.260749 | -1.180674 | 2.980179 |
| O | 3.398748 | -1.893568 | -2.266422 | O | 3.485567 | -1.857101 | -2.187839 |
| C | 2.688511 | -1.654947 | -1.383926 | C | 2.745072 | -1.632812 | -1.345006 |

**Table S18.**Optimized coordinates for the $(nor)_2Co(CO)_6$ structure **6T-b4.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| Co | 1.045952 | -1.188500 | 0.811304 | Co | 1.059739 | -1.186932 | 0.816903 |
| C | 2.147338 | 1.001308 | -0.576898 | C | 2.144867 | 1.009106 | -0.571771 |
| C | 3.570482 | 0.862277 | -1.166081 | C | 3.566132 | 0.907993 | -1.162842 |
| C | 4.353534 | 2.003310 | -0.455606 | C | 4.319539 | 2.063251 | -0.453960 |
| C | 3.293017 | 2.647907 | 0.459347 | C | 3.249291 | 2.679056 | 0.460388 |
| C | 2.458950 | 1.423096 | 0.875159 | C | 2.448685 | 1.437169 | 0.875973 |
| C | 2.284889 | 3.417854 | -0.415971 | C | 2.225409 | 3.422536 | -0.409532 |
| C | 1.507568 | 2.286987 | -1.146266 | C | 1.475281 | 2.278033 | -1.136059 |
| H | 3.986913 | -0.122094 | -0.921071 | H | 4.004838 | -0.061786 | -0.921322 |
| H | 3.554118 | 0.948855 | -2.256731 | H | 3.545263 | 0.994255 | -2.248248 |
| H | 5.182885 | 1.599127 | 0.136411 | H | 5.155859 | 1.680661 | 0.133213 |
| H | 4.774826 | 2.727101 | -1.162711 | H | 4.722065 | 2.794113 | -1.156804 |
| H | 2.785147 | 4.101624 | -1.111233 | H | 2.704931 | 4.115559 | -1.102188 |
| H | 1.609815 | 4.015773 | 0.208534 | H | 1.541348 | 4.002723 | 0.212730 |
| H | 1.596182 | 2.318958 | -2.236321 | H | 1.557327 | 2.312323 | -2.221385 |
| H | 0.440265 | 2.318109 | -0.903266 | H | 0.413455 | 2.282181 | -0.890434 |
| H | 1.567985 | 1.688392 | 1.457042 | H | 1.556236 | 1.677112 | 1.456662 |
| H | 3.046922 | 0.680785 | 1.432010 | H | 3.052698 | 0.712002 | 1.427383 |
| H | 3.712834 | 3.239832 | 1.278826 | H | 3.654468 | 3.277656 | 1.275038 |
| C | 1.311119 | -0.234481 | -0.814964 | C | 1.334973 | -0.238174 | -0.811696 |
| C | 0.123055 | -1.452997 | 2.368436 | C | 0.125040 | -1.469250 | 2.366149 |
| O | 1.044578 | -0.569424 | -2.001244 | O | 1.087761 | -0.579532 | -1.989976 |
| O | -0.417778 | -1.588025 | 3.376656 | O | -0.416507 | -1.616785 | 3.355995 |
| C | -3.881946 | 0.943801 | 1.021359 | C | -3.887364 | 0.894285 | 1.030785 |
| C | -2.463681 | 0.723954 | 0.457175 | C | -2.473463 | 0.699937 | 0.455436 |
| C | -2.488358 | 1.600529 | -0.810283 | C | -2.522512 | 1.584164 | -0.801819 |
| C | -2.885724 | 2.881149 | -0.060054 | C | -2.933757 | 2.848502 | -0.040836 |
| C | -1.761186 | 2.988040 | 0.988701 | C | -1.805787 | 2.965638 | 0.994716 |
| C | -4.176936 | 2.426859 | 0.652426 | C | -4.206779 | 2.370494 | 0.676864 |
| C | -1.465218 | 1.503323 | 1.339787 | C | -1.485421 | 1.488275 | 1.335003 |
| H | -3.237752 | 1.271435 | -1.540271 | H | -3.267956 | 1.248114 | -1.524895 |
| H | -1.514104 | 1.665280 | -1.312774 | H | -1.557724 | 1.667533 | -1.307674 |
| H | -0.442798 | 1.216847 | 1.068104 | H | -0.464664 | 1.220704 | 1.058717 |
| H | -1.602094 | 1.265905 | 2.399973 | H | -1.611777 | 1.243244 | 2.389499 |
| H | -3.916755 | 0.745747 | 2.096981 | H | -3.911675 | 0.686744 | 2.099755 |
| H | -4.587678 | 0.254955 | 0.544992 | H | -4.582287 | 0.201073 | 0.556427 |
| H | -2.071150 | 3.572779 | 1.862377 | H | -2.112940 | 3.539922 | 1.869895 |
| H | -0.875100 | 3.477600 | 0.565498 | H | -0.934942 | 3.467479 | 0.567977 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -3.007448 | 3.778964 | -0.675225 | H | -3.075011 | 3.744325 | -0.644909 |
| H | -5.036038 | 2.497987 | -0.025234 | H | -5.069468 | 2.434197 | 0.011337 |
| H | -4.397627 | 3.046421 | 1.529567 | H | -4.429297 | 2.977783 | 1.555767 |
| C | 2.644679 | -2.025952 | 0.880434 | C | 2.670032 | -1.999930 | 0.907947 |
| C | -2.074925 | -0.739758 | 0.283773 | C | -2.067611 | -0.752761 | 0.268154 |
| O | 3.647055 | -2.598340 | 0.864794 | O | 3.670284 | -2.547393 | 0.906966 |
| O | -2.656948 | -1.622546 | 0.879523 | O | -2.639333 | -1.640031 | 0.844350 |
| C | -0.446650 | -2.875349 | -0.609915 | C | -0.431826 | -2.881966 | -0.635459 |
| O | -0.406058 | -3.994836 | -0.345867 | O | -0.392181 | -3.988840 | -0.380489 |
| C | -1.934640 | -1.231801 | -2.293559 | C | -1.899418 | -1.211438 | -2.313822 |
| O | -2.757652 | -1.396493 | -3.083123 | O | -2.707575 | -1.360891 | -3.101420 |
| Co | -0.671401 | -1.072737 | -1.026985 | Co | -0.644266 | -1.069352 | -1.034743 |

**Table S19.**Optimized coordinates for the $(nor)_2Co(CO)_5$ structure **5T-b1.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| Co | -1.171931 | 1.774684 | 0.267605 | Co | -1.172866 | 1.765514 | 0.254738 |
| C | -2.706946 | -0.697804 | -0.306840 | C | -2.716146 | -0.702557 | -0.290040 |
| C | -3.771055 | -0.011627 | 0.568041 | C | -3.777141 | -0.007906 | 0.574499 |
| C | -4.801347 | -1.148383 | 0.832395 | C | -4.818330 | -1.130663 | 0.829733 |
| C | -4.217042 | -2.335824 | 0.041495 | C | -4.242804 | -2.320758 | 0.047344 |
| C | -2.710201 | -2.137248 | 0.261073 | C | -2.740101 | -2.139204 | 0.276493 |
| C | -4.352976 | -2.043778 | -1.467545 | C | -4.365104 | -2.029559 | -1.457296 |
| C | -3.294170 | -0.928105 | -1.716155 | C | -3.298460 | -0.926772 | -1.698869 |
| H | -3.319239 | 0.345586 | 1.505813 | H | -3.330343 | 0.342685 | 1.510740 |
| H | -4.216166 | 0.853901 | 0.065298 | H | -4.206717 | 0.858687 | 0.071562 |
| H | -4.858168 | -1.386213 | 1.901097 | H | -4.887412 | -1.365228 | 1.893191 |
| H | -5.811595 | -0.885929 | 0.498030 | H | -5.818582 | -0.858927 | 0.489710 |
| H | -5.368550 | -1.727127 | -1.732506 | H | -5.371306 | -1.707082 | -1.729594 |
| H | -4.121270 | -2.937777 | -2.058017 | H | -4.138786 | -2.921519 | -2.043442 |
| H | -3.723054 | -0.006381 | -2.124962 | H | -3.713819 | -0.004951 | -2.107473 |
| H | -2.505804 | -1.264746 | -2.397745 | H | -2.513197 | -1.268239 | -2.373488 |
| H | -2.071571 | -2.809588 | -0.321334 | H | -2.107423 | -2.814704 | -0.298761 |
| H | -2.405992 | -2.176466 | 1.314836 | H | -2.444169 | -2.180361 | 1.326969 |
| H | -4.619167 | -3.308654 | 0.343788 | H | -4.656401 | -3.283807 | 0.345752 |
| C | -1.346522 | -0.061573 | -0.292400 | C | -1.354346 | -0.080652 | -0.274080 |
| O | -0.386226 | -0.664899 | -0.881864 | O | -0.404474 | -0.691553 | -0.851745 |
| C | 3.797978 | 0.323301 | 0.577555 | C | 3.812765 | 0.319855 | 0.561626 |
| C | 3.104359 | -0.904457 | -0.052502 | C | 3.109506 | -0.904515 | -0.053714 |
| C | 2.855522 | -0.394743 | -1.492770 | C | 2.857100 | -0.403793 | -1.492836 |
| C | 4.335278 | -0.078507 | -1.753932 | C | 4.333207 | -0.099873 | -1.763508 |
| C | 5.000674 | -1.438885 | -1.460436 | C | 4.988946 | -1.457993 | -1.467140 |
| C | 4.649950 | 0.888252 | -0.596357 | C | 4.660331 | 0.867672 | -0.617230 |
| C | 4.155497 | -2.005882 | -0.281555 | C | 4.152414 | -2.009359 | -0.281702 |
| H | 2.200562 | 0.483228 | -1.525593 | H | 2.210657 | 0.474126 | -1.526838 |
| H | 2.438340 | -1.169720 | -2.145463 | H | 2.432552 | -1.176680 | -2.134540 |
| H | 3.661388 | -2.946651 | -0.545346 | H | 3.653743 | -2.945631 | -0.531724 |
| H | 4.744843 | -2.189987 | 0.623082 | H | 4.743636 | -2.189063 | 0.616484 |
| H | 4.394633 | 0.039587 | 1.451427 | H | 4.407558 | 0.040394 | 1.431685 |
| H | 3.055618 | 1.058288 | 0.910420 | H | 3.079338 | 1.057760 | 0.890507 |
| H | 6.061363 | -1.328097 | -1.205829 | H | 6.047824 | -1.354139 | -1.224390 |
| H | 4.938999 | -2.095748 | -2.336402 | H | 4.917364 | -2.117373 | -2.334059 |
| H | 4.567424 | 0.326119 | -2.744983 | H | 4.562076 | 0.295504 | -2.752988 |
| H | 4.335827 | 1.908511 | -0.845337 | H | 4.356520 | 1.884888 | -0.869303 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 5.720553 | 0.916073 | -0.362917 | H | 5.727303 | 0.889425 | -0.390602 |
| C | 0.480043 | 2.466355 | -0.069821 | C | 0.476048 | 2.482473 | -0.062543 |
| C | 1.845247 | -1.334803 | 0.658807 | C | 1.858856 | -1.325398 | 0.667757 |
| O | 1.524136 | 2.890779 | -0.333020 | O | 1.504096 | 2.918731 | -0.305691 |
| O | 1.613741 | -2.464449 | 1.041329 | O | 1.635809 | -2.440144 | 1.063760 |
| C | 0.862260 | 0.366284 | 2.406706 | C | 0.892861 | 0.392552 | 2.396005 |
| O | 1.182619 | 0.689542 | 3.471026 | O | 1.229452 | 0.728648 | 3.436015 |
| O | -2.869104 | 3.136821 | -1.692205 | O | -2.843161 | 3.115663 | -1.719697 |
| C | -2.262581 | 2.649040 | -0.835522 | C | -2.251548 | 2.636438 | -0.866946 |
| Co | 0.380668 | -0.123952 | 0.797917 | Co | 0.380551 | -0.123530 | 0.804304 |

**Table S20.**Optimized coordinates for the $(nor)_2Co(CO)_5$ structure **5S-b2.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | -3.205041 | -0.195553 | 1.606647 | C | -3.110418 | -0.298029 | 1.677056 |
| C | -2.476782 | -0.180256 | 0.247057 | C | -2.451624 | -0.254031 | 0.287217 |
| C | -2.187064 | -1.684739 | 0.054105 | C | -2.069357 | -1.735178 | 0.100513 |
| C | -3.652458 | -2.116792 | 0.203333 | C | -3.488490 | -2.263796 | 0.326905 |
| C | -4.332465 | -1.267035 | -0.889276 | C | -4.275226 | -1.484100 | -0.737975 |
| C | -4.002022 | -1.534033 | 1.584172 | C | -3.810582 | -1.684548 | 1.709705 |
| C | -3.532189 | 0.075151 | -0.855456 | C | -3.569582 | -0.095182 | -0.763602 |
| Co | -1.006635 | 1.146574 | -0.154321 | Co | -1.062582 | 1.159601 | -0.158674 |
| H | -1.524974 | -2.097555 | 0.823572 | H | -1.346094 | -2.086905 | 0.837583 |
| H | -1.772705 | -1.926950 | -0.930378 | H | -1.687867 | -1.959877 | -0.895711 |
| H | -3.072772 | 0.274747 | -1.831394 | H | -3.168485 | 0.115005 | -1.756919 |
| H | -4.163728 | 0.937664 | -0.613062 | H | -4.242768 | 0.724891 | -0.509783 |
| H | -3.863837 | 0.671034 | 1.727615 | H | -3.815953 | 0.520687 | 1.818623 |
| H | -2.482645 | -0.175987 | 2.429399 | H | -2.357890 | -0.216704 | 2.461255 |
| H | -5.400711 | -1.117950 | -0.691643 | H | -5.335290 | -1.405212 | -0.490793 |
| H | -4.239382 | -1.749962 | -1.869407 | H | -4.199929 | -1.974656 | -1.710133 |
| H | -3.846876 | -3.191043 | 0.110444 | H | -3.611757 | -3.344756 | 0.259273 |
| H | -3.667490 | -2.206577 | 2.383267 | H | -3.396064 | -2.315516 | 2.498150 |
| H | -5.081355 | -1.384347 | 1.707594 | H | -4.885395 | -1.607595 | 1.883178 |
| C | -2.066853 | 2.267154 | 0.663192 | C | -2.198737 | 2.229274 | 0.633309 |
| C | 0.057297 | 2.465235 | -0.751446 | C | -0.057010 | 2.526103 | -0.746054 |
| O | -2.704741 | 3.029524 | 1.250712 | O | -2.889839 | 2.947410 | 1.187332 |
| O | 0.683394 | 3.359965 | -1.122807 | O | 0.530782 | 3.436163 | -1.097533 |
| Co | 0.878987 | -0.436019 | -0.518876 | Co | 0.839389 | -0.353239 | -0.611334 |
| C | 2.645915 | -0.424761 | 0.298535 | C | 2.638728 | -0.361865 | 0.206434 |
| C | 2.958944 | 0.923763 | -0.386028 | C | 2.921247 | 1.151671 | 0.269960 |
| C | 4.522305 | 0.902115 | -0.474474 | C | 4.477725 | 1.216807 | 0.308421 |
| C | 4.898411 | -0.398926 | 0.261080 | C | 4.891333 | -0.261360 | 0.259679 |
| C | 3.778202 | -1.331184 | -0.219936 | C | 3.815736 | -0.847477 | -0.661142 |
| C | 4.554723 | -0.260394 | 1.760615 | C | 4.532824 | -0.923483 | 1.599389 |
| C | 2.993486 | -0.314807 | 1.784219 | C | 2.978826 | -0.994185 | 1.558348 |
| H | 2.526779 | 1.007239 | -1.401964 | H | 2.552152 | 1.672502 | -0.618827 |
| H | 2.588212 | 1.767855 | 0.201886 | H | 2.450546 | 1.613021 | 1.137712 |
| H | 4.856770 | 0.867546 | -1.517779 | H | 4.866519 | 1.759081 | -0.555042 |
| H | 4.959180 | 1.794092 | -0.010680 | H | 4.842979 | 1.719365 | 1.205554 |
| H | 4.945509 | 0.671803 | 2.185828 | H | 4.903083 | -0.349658 | 2.450761 |
| H | 4.986906 | -1.090017 | 2.332384 | H | 4.969559 | -1.921717 | 1.664268 |
| H | 2.546987 | 0.568709 | 2.249327 | H | 2.510169 | -0.467540 | 2.386770 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.625932 | -1.189408 | 2.331584 | H | 2.629231 | -2.027082 | 1.593959 |
| H | 3.789306 | -2.315963 | 0.261272 | H | 3.872294 | -1.933616 | -0.743243 |
| H | 3.760204 | -1.464027 | -1.308658 | H | 3.812627 | -0.414966 | -1.663982 |
| H | 5.925614 | -0.728295 | 0.070683 | H | 5.925624 | -0.417471 | -0.046650 |
| C | 0.062485 | 0.130948 | 1.086181 | C | 0.114736 | 0.233753 | 1.052303 |
| C | 1.107822 | -2.128872 | -0.704140 | C | 1.229248 | -1.977411 | -1.005267 |
| O | 0.003175 | -0.005754 | 2.248225 | O | 0.124136 | 0.159090 | 2.206415 |
| O | 1.196642 | -3.283191 | -0.742913 | O | 1.417072 | -3.094288 | -1.170587 |
| C | -0.198591 | -0.182114 | -1.928443 | C | -0.270220 | -0.081946 | -1.990014 |
| O | -0.741617 | -0.047667 | -2.946116 | O | -0.814154 | 0.048733 | -2.991489 |

**Table S21.**Optimized coordinates for the $(nor)_2Co(CO)_5$ structure **5S-b3.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| Co | -1.439670 | 1.711325 | 0.306250 | Co | -1.377232 | 1.663970 | 0.411693 |
| C | -2.104284 | -1.002380 | -0.479679 | C | -2.262943 | -0.861988 | -0.423303 |
| C | -3.505865 | -0.775079 | -1.092441 | C | -3.301342 | -0.730941 | -1.559395 |
| C | -4.380023 | -1.821655 | -0.339308 | C | -4.549245 | -1.433128 | -0.962062 |
| C | -3.386150 | -2.486441 | 0.633456 | C | -4.065974 | -1.911944 | 0.414332 |
| C | -2.460484 | -1.313698 | 0.987473 | C | -3.144540 | -0.757495 | 0.831229 |
| C | -2.432945 | -3.384884 | -0.178146 | C | -3.059030 | -3.053290 | 0.210584 |
| C | -1.584661 | -2.366454 | -0.990843 | C | -1.806534 | -2.334185 | -0.351615 |
| H | -3.858610 | 0.240271 | -0.892323 | H | -3.504838 | 0.315348 | -1.785111 |
| H | -3.495407 | -0.915738 | -2.178388 | H | -2.933606 | -1.197554 | -2.472718 |
| H | -5.191123 | -1.325886 | 0.206799 | H | -5.375390 | -0.727660 | -0.858067 |
| H | -4.836678 | -2.551893 | -1.017301 | H | -4.900091 | -2.259796 | -1.581326 |
| H | -2.978558 | -4.088850 | -0.817367 | H | -3.445368 | -3.816584 | -0.466723 |
| H | -1.790207 | -3.966850 | 0.492115 | H | -2.828939 | -3.542869 | 1.158046 |
| H | -1.720198 | -2.453760 | -2.073921 | H | -1.492133 | -2.693330 | -1.330621 |
| H | -0.520313 | -2.476953 | -0.777433 | H | -0.956084 | -2.431568 | 0.318551 |
| H | -1.578253 | -1.600271 | 1.570610 | H | -2.585014 | -0.948915 | 1.748868 |
| H | -2.971686 | -0.475184 | 1.482595 | H | -3.671394 | 0.196074 | 0.918492 |
| H | -3.861520 | -2.991557 | 1.480532 | H | -4.872463 | -2.147786 | 1.107275 |
| C | -1.116460 | 0.128355 | -0.646654 | C | -1.119250 | 0.101339 | -0.561007 |
| O | -0.130033 | 0.060216 | -1.427419 | O | -0.183251 | -0.047142 | -1.371419 |
| C | 3.909861 | -1.049139 | 0.981217 | C | 4.015060 | -1.043291 | 0.872943 |
| C | 2.740206 | -0.765947 | 0.014666 | C | 2.859945 | -0.791710 | -0.116135 |
| C | 3.040947 | 0.700856 | -0.415600 | C | 3.075277 | 0.703731 | -0.465035 |
| C | 4.459778 | 0.359650 | -0.919402 | C | 4.525622 | 0.485742 | -0.931657 |
| C | 4.162459 | -0.747326 | -1.948717 | C | 4.341458 | -0.585622 | -2.015726 |
| C | 5.092596 | -0.276758 | 0.332552 | C | 5.157548 | -0.162799 | 0.307225 |
| C | 2.971934 | -1.520398 | -1.313646 | C | 3.188287 | -1.461952 | -1.464230 |
| H | 3.058290 | 1.422555 | 0.412212 | H | 3.016145 | 1.381289 | 0.390145 |
| H | 2.407050 | 1.075261 | -1.229738 | H | 2.438290 | 1.068726 | -1.272700 |
| H | 2.073133 | -1.459434 | -1.937348 | H | 2.313718 | -1.431102 | -2.115060 |
| H | 3.180212 | -2.578024 | -1.124301 | H | 3.455492 | -2.507520 | -1.317479 |
| H | 4.079818 | -2.126092 | 1.074483 | H | 4.253989 | -2.104858 | 0.920393 |
| H | 3.678776 | -0.664638 | 1.981763 | H | 3.727347 | -0.728038 | 1.877638 |
| H | 5.035361 | -1.388147 | -2.118279 | H | 5.256924 | -1.155878 | -2.180224 |
| H | 3.875508 | -0.313269 | -2.913353 | H | 4.063146 | -0.129143 | -2.966739 |
| H | 5.025941 | 1.204238 | -1.324536 | H | 5.042626 | 1.380312 | -1.275848 |
| H | 5.474770 | 0.495918 | 1.009733 | H | 5.459351 | 0.597088 | 1.029827 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 5.929828 | -0.934924 | 0.073797 | H | 6.044869 | -0.744241 | 0.052913 |
| C | 0.137700 | 2.488165 | -0.165299 | C | 0.254629 | 2.340579 | 0.092706 |
| C | 1.388655 | -1.123128 | 0.620897 | C | 1.533941 | -1.294296 | 0.441908 |
| O | 0.696902 | 3.428030 | -0.583769 | O | 0.933142 | 3.240084 | -0.179153 |
| O | 1.094673 | -2.220922 | 1.029674 | O | 1.330602 | -2.445106 | 0.695378 |
| C | 0.349286 | 0.618491 | 2.114269 | C | 0.458680 | 0.200016 | 2.171136 |
| O | 0.154479 | 0.660604 | 3.257573 | O | 0.312212 | 0.102278 | 3.304064 |
| O | -3.617276 | 2.950855 | -1.134936 | O | -3.389822 | 3.022739 | -1.144251 |
| C | -2.797456 | 2.424221 | -0.503872 | C | -2.655378 | 2.467140 | -0.461471 |
| Co | 0.568683 | 0.522906 | 0.410236 | Co | 0.591791 | 0.313428 | 0.457972 |

**Table S22.**Optimized coordinates for the $(nor)_2Co(CO)_5$ structure **5S-b4.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | 3.485074 | -1.392021 | 1.038260 | C | 3.470289 | -1.432617 | 0.990813 |
| C | 3.044336 | -0.290896 | 0.048937 | C | 3.054741 | -0.290596 | 0.044004 |
| C | 4.149851 | 0.764874 | 0.283279 | C | 4.152618 | 0.747809 | 0.352952 |
| C | 5.310853 | -0.193186 | -0.024058 | C | 5.317724 | -0.194240 | 0.034244 |
| C | 4.941493 | -0.677860 | -1.438351 | C | 4.986064 | -0.613645 | -1.404046 |
| C | 5.043261 | -1.327945 | 0.983879 | C | 5.024856 | -1.369180 | 0.978481 |
| C | 3.384216 | -0.748537 | -1.388742 | C | 3.432362 | -0.684808 | -1.398448 |
| Co | 1.081443 | 0.147470 | 0.140150 | Co | 1.090560 | 0.155748 | 0.108775 |
| H | 4.181449 | 1.147373 | 1.310747 | H | 4.154251 | 1.083038 | 1.391802 |
| H | 4.095299 | 1.611616 | -0.412614 | H | 4.115520 | 1.621286 | -0.301591 |
| H | 2.930226 | -0.076655 | -2.125886 | H | 3.000521 | 0.015009 | -2.115244 |
| H | 3.007830 | -1.757942 | -1.593514 | H | 3.062052 | -1.678441 | -1.655946 |
| H | 3.098319 | -2.377254 | 0.752471 | H | 3.090816 | -2.398765 | 0.654830 |
| H | 3.113090 | -1.179154 | 2.047642 | H | 3.075901 | -1.265145 | 1.994519 |
| H | 5.396637 | -1.647339 | -1.673806 | H | 5.445808 | -1.566949 | -1.670642 |
| H | 5.278644 | 0.040039 | -2.195785 | H | 5.341278 | 0.132723 | -2.117010 |
| H | 6.316300 | 0.235317 | 0.049488 | H | 6.316490 | 0.225964 | 0.151940 |
| H | 5.462602 | -1.081514 | 1.966866 | H | 5.417852 | -1.170679 | 1.977384 |
| H | 5.489174 | -2.276729 | 0.662395 | H | 5.476757 | -2.298796 | 0.628086 |
| C | 1.611682 | 1.704615 | 0.836402 | C | 1.602186 | 1.691071 | 0.870243 |
| C | 0.778167 | -1.578185 | -0.260033 | C | 0.794204 | -1.552298 | -0.367857 |
| O | 1.915982 | 2.710183 | 1.303096 | O | 1.891069 | 2.667437 | 1.373463 |
| O | 0.540426 | -2.686278 | -0.462842 | O | 0.569059 | -2.637890 | -0.621239 |
| Co | -1.381170 | 0.653713 | -0.177394 | Co | -1.371054 | 0.656795 | -0.161253 |
| C | -3.078516 | -0.179944 | 0.208672 | C | -3.080479 | -0.185726 | 0.192240 |
| C | -2.667641 | -1.329058 | -0.740499 | C | -2.685430 | -1.375205 | -0.705552 |
| C | -4.053860 | -1.877946 | -1.219298 | C | -4.075054 | -1.934401 | -1.150093 |
| C | -5.058709 | -1.076490 | -0.368078 | C | -5.069892 | -1.069331 | -0.362183 |
| C | -4.402662 | 0.312016 | -0.397934 | C | -4.387283 | 0.298599 | -0.449992 |
| C | -4.900040 | -1.463525 | 1.120275 | C | -4.941755 | -1.382400 | 1.139534 |
| C | -3.551800 | -0.787867 | 1.530086 | C | -3.581495 | -0.730791 | 1.527369 |
| H | -2.074604 | -0.981100 | -1.612618 | H | -2.101594 | -1.072145 | -1.590950 |
| H | -2.081115 | -2.093251 | -0.224031 | H | -2.099222 | -2.113637 | -0.162343 |
| H | -4.209945 | -1.681405 | -2.286355 | H | -4.222239 | -1.808557 | -2.223813 |
| H | -4.127961 | -2.960205 | -1.061766 | H | -4.166780 | -2.997807 | -0.924114 |
| H | -4.881599 | -2.551157 | 1.259375 | H | -4.960688 | -2.455965 | 1.335617 |
| H | -5.734779 | -1.069962 | 1.711920 | H | -5.765889 | -0.934887 | 1.697359 |
| H | -2.827046 | -1.498700 | 1.941771 | H | -2.882489 | -1.441450 | 1.968691 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -3.706570 | -0.005697 | 2.281393 | H | -3.716404 | 0.079072 | 2.245123 |
| H | -4.906049 | 1.055702 | 0.230627 | H | -4.880995 | 1.077425 | 0.133214 |
| H | -4.295311 | 0.713092 | -1.412703 | H | -4.260655 | 0.648338 | -1.476031 |
| H | -6.089507 | -1.139436 | -0.733450 | H | -6.091274 | -1.128887 | -0.737944 |
| C | -0.807424 | 0.334718 | 1.455772 | C | -0.792984 | 0.251786 | 1.457231 |
| C | -2.165515 | 2.159558 | -0.569723 | C | -2.184579 | 2.146395 | -0.554603 |
| O | -0.654864 | 0.285559 | 2.612013 | O | -0.622253 | 0.145279 | 2.592191 |
| O | -2.662595 | 3.197853 | -0.692975 | O | -2.693383 | 3.162881 | -0.680404 |
| C | 0.102480 | 0.946675 | -1.307184 | C | 0.090769 | 1.005171 | -1.298358 |
| O | 0.569309 | 1.261238 | -2.337610 | O | 0.538403 | 1.356924 | -2.309253 |

**Table S23.**Optimized coordinates for the $(nor)_2Co(CO)_5$ structure **5T-b5.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | -1.543573 | 1.617759 | -1.622840 | C | -1.585488 | 1.656006 | -1.600737 |
| C | -1.424121 | 1.046606 | -0.169071 | C | -1.469686 | 1.048568 | -0.167181 |
| C | -0.728132 | 2.232047 | 0.544101 | C | -0.782364 | 2.214287 | 0.575798 |
| C | -1.757748 | 3.297340 | 0.115958 | C | -1.814698 | 3.282634 | 0.175799 |
| C | -3.071288 | 2.697142 | 0.635819 | C | -3.120164 | 2.662834 | 0.676941 |
| C | -1.720374 | 3.157533 | -1.411550 | C | -1.776322 | 3.183701 | -1.349286 |
| C | -2.857929 | 1.166212 | 0.425149 | C | -2.899003 | 1.142604 | 0.428885 |
| Co | 0.324771 | -0.261332 | 1.058954 | Co | 0.353654 | -0.307055 | 1.052942 |
| H | 0.270350 | 2.450070 | 0.160208 | H | 0.211391 | 2.442874 | 0.200294 |
| H | -0.673199 | 2.136592 | 1.637719 | H | -0.727380 | 2.086007 | 1.660441 |
| H | -2.953438 | 0.633688 | 1.375256 | H | -2.988257 | 0.588952 | 1.361533 |
| H | -3.606067 | 0.734797 | -0.251252 | H | -3.640501 | 0.723158 | -0.253993 |
| H | -2.402458 | 1.185750 | -2.154443 | H | -2.429877 | 1.228390 | -2.147568 |
| H | -0.657857 | 1.421652 | -2.232871 | H | -0.695803 | 1.481981 | -2.203000 |
| H | -3.943508 | 3.082082 | 0.094430 | H | -3.991167 | 3.053692 | 0.148261 |
| H | -3.212877 | 2.929634 | 1.698493 | H | -3.264507 | 2.866422 | 1.739989 |
| H | -1.556207 | 4.313028 | 0.473904 | H | -1.621589 | 4.284924 | 0.558599 |
| H | -0.865968 | 3.703161 | -1.831275 | H | -0.932058 | 3.746092 | -1.753714 |
| H | -2.629095 | 3.544124 | -1.887325 | H | -2.684090 | 3.572216 | -1.813622 |
| C | -0.987542 | -0.630457 | 2.232765 | C | -0.971986 | -0.696458 | 2.201492 |
| O | -1.757509 | -0.915769 | 3.040905 | O | -1.752596 | -0.980740 | 2.979874 |
| Co | -1.188859 | -0.910238 | -0.803042 | Co | -1.191891 | -0.898717 | -0.796206 |
| C | 2.013242 | 0.269303 | -0.003950 | C | 2.025288 | 0.274972 | -0.002840 |
| C | 1.766898 | 0.536706 | -1.504652 | C | 1.772014 | 0.541924 | -1.497601 |
| C | 3.187928 | 0.485872 | -2.142969 | C | 3.190961 | 0.532944 | -2.134015 |
| C | 4.093685 | 0.168795 | -0.940599 | C | 4.101788 | 0.240389 | -0.936215 |
| C | 3.184585 | -0.736934 | -0.097244 | C | 3.222919 | -0.692644 | -0.097601 |
| C | 4.182572 | 1.420839 | -0.054221 | C | 4.152466 | 1.487863 | -0.050355 |
| C | 2.744591 | 1.531038 | 0.539413 | C | 2.717261 | 1.551969 | 0.545063 |
| H | 1.132337 | -0.241373 | -1.942586 | H | 1.162639 | -0.246544 | -1.938543 |
| H | 1.268488 | 1.496231 | -1.667958 | H | 1.247489 | 1.482452 | -1.654302 |
| H | 3.247647 | -0.307833 | -2.897569 | H | 3.272173 | -0.253207 | -2.887139 |
| H | 3.464614 | 1.427912 | -2.631809 | H | 3.439415 | 1.478302 | -2.620043 |
| H | 4.476521 | 2.312922 | -0.620545 | H | 4.417001 | 2.386160 | -0.611411 |
| H | 4.921415 | 1.276299 | 0.743689 | H | 4.893583 | 1.366507 | 0.742350 |
| H | 2.244753 | 2.452541 | 0.222239 | H | 2.189883 | 2.454187 | 0.236026 |
| H | 2.781414 | 1.559385 | 1.633100 | H | 2.755043 | 1.574572 | 1.633436 |
| H | 3.628527 | -0.994031 | 0.871350 | H | 3.669156 | -0.936986 | 0.867405 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.907552 | -1.665806 | -0.607790 | H | 2.974969 | -1.623894 | -0.607878 |
| H | 5.067281 | -0.251503 | -1.215666 | H | 5.082939 | -0.146884 | -1.211367 |
| C | 1.514909 | -0.441988 | 2.296050 | C | 1.531444 | -0.447153 | 2.307368 |
| O | 2.294145 | -0.617360 | 3.131982 | O | 2.300294 | -0.601082 | 3.138455 |
| C | -2.591106 | -1.976193 | -0.198255 | C | -2.564024 | -2.023770 | -0.207844 |
| O | -3.456396 | -2.593090 | 0.242017 | O | -3.397897 | -2.668501 | 0.215065 |
| C | -0.862971 | -1.729368 | -2.433374 | C | -0.847405 | -1.686444 | -2.447780 |
| O | -0.623302 | -2.263730 | -3.423977 | O | -0.602595 | -2.180510 | -3.440998 |
| C | 0.261168 | -1.912893 | 0.172026 | C | 0.313990 | -1.929655 | 0.135959 |
| O | 0.791986 | -2.955437 | 0.237293 | O | 0.841544 | -2.959286 | 0.143514 |

**Table S24.**Optimized coordinates for the $(nor)_2Co(CO)_5$ structure **5S-b6.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | -2.312362 | 0.955486 | 1.860680 | C | -2.295476 | 0.851203 | 1.893250 |
| C | -1.773625 | 0.162230 | 0.646046 | C | -1.772934 | 0.097150 | 0.650747 |
| C | -1.224688 | -1.075671 | 1.411094 | C | -1.216427 | -1.161772 | 1.369068 |
| C | -2.576585 | -1.459358 | 2.038194 | C | -2.555767 | -1.558930 | 2.007011 |
| C | -3.471987 | -1.599795 | 0.799905 | C | -3.468655 | -1.661186 | 0.785209 |
| C | -2.927245 | -0.148616 | 2.775861 | C | -2.889041 | -0.275649 | 2.786247 |
| C | -3.012623 | -0.409241 | -0.085186 | C | -3.020292 | -0.454124 | -0.074741 |
| Co | 0.324746 | -1.138627 | -0.581538 | Co | 0.343888 | -1.103725 | -0.628106 |
| H | -0.484178 | -0.819190 | 2.168874 | H | -0.466097 | -0.930485 | 2.117825 |
| H | -0.822919 | -1.928430 | 0.818119 | H | -0.831715 | -1.990050 | 0.743607 |
| H | -2.773923 | -0.723472 | -1.104836 | H | -2.800209 | -0.743571 | -1.100078 |
| H | -3.789430 | 0.357697 | -0.175555 | H | -3.792723 | 0.312856 | -0.136617 |
| H | -3.048190 | 1.708783 | 1.559317 | H | -3.035025 | 1.605629 | 1.624416 |
| H | -1.501211 | 1.485628 | 2.374015 | H | -1.482915 | 1.369269 | 2.405254 |
| H | -4.538392 | -1.561789 | 1.050175 | H | -4.525970 | -1.626373 | 1.051972 |
| H | -3.284222 | -2.558461 | 0.299066 | H | -3.295481 | -2.603131 | 0.258892 |
| H | -2.560781 | -2.344013 | 2.684151 | H | -2.531019 | -2.457940 | 2.622830 |
| H | -2.480243 | -0.132658 | 3.776946 | H | -2.422507 | -0.288492 | 3.772748 |
| H | -4.010846 | -0.033991 | 2.896359 | H | -3.964337 | -0.164209 | 2.935118 |
| C | -0.836203 | -2.117090 | -1.560704 | C | -0.810092 | -2.025099 | -1.668583 |
| O | -1.473140 | -2.827710 | -2.204919 | O | -1.438404 | -2.680346 | -2.353829 |
| Co | -0.474877 | 1.283287 | -0.456037 | Co | -0.513979 | 1.289797 | -0.433023 |
| C | 1.761125 | -0.305014 | 0.585767 | C | 1.774498 | -0.310242 | 0.576796 |
| C | 1.299946 | 0.911358 | 1.445505 | C | 1.299751 | 0.872130 | 1.464206 |
| C | 2.594682 | 1.735691 | 1.682212 | C | 2.585572 | 1.691500 | 1.741285 |
| C | 3.682793 | 0.796654 | 1.145081 | C | 3.679612 | 0.787725 | 1.171937 |
| C | 3.003376 | 0.266148 | -0.125904 | C | 3.007795 | 0.295414 | -0.113289 |
| C | 3.724558 | -0.461999 | 2.035669 | C | 3.737107 | -0.495516 | 2.014693 |
| C | 2.438596 | -1.244313 | 1.615286 | C | 2.458544 | -1.270891 | 1.577108 |
| H | 0.519882 | 1.598789 | 1.026863 | H | 0.531886 | 1.558950 | 1.038896 |
| H | 0.848337 | 0.580843 | 2.384435 | H | 0.832803 | 0.516686 | 2.379856 |
| H | 2.576369 | 2.668757 | 1.105222 | H | 2.561651 | 2.644397 | 1.208263 |
| H | 2.732222 | 1.997471 | 2.737886 | H | 2.717108 | 1.908583 | 2.802551 |
| H | 3.736427 | -0.205873 | 3.102090 | H | 3.755372 | -0.279137 | 3.084499 |
| H | 4.623112 | -1.055589 | 1.830738 | H | 4.634766 | -1.071848 | 1.784950 |
| H | 1.780113 | -1.470881 | 2.462266 | H | 1.804768 | -1.520469 | 2.414353 |
| H | 2.714853 | -2.203701 | 1.167471 | H | 2.737243 | -2.212745 | 1.107302 |
| H | 3.589505 | -0.506054 | -0.636843 | H | 3.597388 | -0.449277 | -0.649812 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.765330 | 1.052367 | -0.851235 | H | 2.760922 | 1.100733 | -0.806521 |
| H | 4.655763 | 1.280436 | 1.008540 | H | 4.642141 | 1.284600 | 1.052985 |
| C | 1.583453 | -2.266583 | -0.980569 | C | 1.593844 | -2.242050 | -1.032450 |
| O | 2.445087 | -2.942778 | -1.353491 | O | 2.442803 | -2.913320 | -1.399806 |
| C | -1.893202 | 2.232971 | -0.756248 | C | -1.953375 | 2.225307 | -0.687136 |
| O | -2.841575 | 2.824351 | -1.059389 | O | -2.900013 | 2.806462 | -0.961168 |
| C | 0.581349 | 2.569075 | -1.099802 | C | 0.503247 | 2.627113 | -1.019574 |
| O | 1.225873 | 3.453136 | -1.462752 | O | 1.127601 | 3.525997 | -1.335291 |
| C | 0.184209 | 0.198933 | -1.884478 | C | 0.246674 | 0.281621 | -1.878303 |
| O | 0.375326 | 0.300791 | -3.039448 | O | 0.485122 | 0.432437 | -3.005367 |

**Table S25.**Optimized coordinates for the $(nor)_2Co(CO)_5$ structure **5T-b7.**

| | B3PW91-D3/DZP | | | | B3PW91-D3/cc-pVTZ | | |
|---|---|---|---|---|---|---|---|
| | x | y | z | | x | y | z |
| C | 3.347111 | -0.263524 | -1.551545 | C | 3.330077 | -0.273894 | -1.547766 |
| C | 2.555480 | -0.169697 | -0.234411 | C | 2.567798 | -0.173955 | -0.216284 |
| C | 2.312448 | -1.660827 | 0.066223 | C | 2.306011 | -1.660198 | 0.075541 |
| C | 3.800918 | -2.036818 | 0.035281 | C | 3.781580 | -2.065190 | 0.007835 |
| C | 4.376942 | -1.075830 | 1.094968 | C | 4.400557 | -1.129144 | 1.056833 |
| C | 4.209105 | -1.548820 | -1.367612 | C | 4.166763 | -1.574147 | -1.394031 |
| C | 3.532879 | 0.225446 | 0.898846 | C | 3.579830 | 0.184569 | 0.893176 |
| Co | 1.063755 | 1.112697 | 0.040829 | Co | 1.062939 | 1.119129 | 0.037298 |
| H | 1.722087 | -2.160907 | -0.710254 | H | 1.692537 | -2.140212 | -0.688078 |
| H | 1.844024 | -1.838455 | 1.039766 | H | 1.858020 | -1.838435 | 1.052897 |
| H | 3.011957 | 0.487123 | 1.830367 | H | 3.084963 | 0.447501 | 1.831197 |
| H | 4.145363 | 1.089251 | 0.616755 | H | 4.198882 | 1.036256 | 0.608002 |
| H | 3.963850 | 0.624234 | -1.727863 | H | 3.956521 | 0.599490 | -1.728786 |
| H | 2.659736 | -0.359122 | -2.399966 | H | 2.629347 | -0.348059 | -2.380426 |
| H | 5.449425 | -0.896836 | 0.953954 | H | 5.468084 | -0.973143 | 0.892667 |
| H | 4.236286 | -1.482153 | 2.103520 | H | 4.278577 | -1.539899 | 2.060620 |
| H | 4.033157 | -3.090516 | 0.224901 | H | 3.994893 | -3.119940 | 0.181532 |
| H | 3.964047 | -2.301967 | -2.125961 | H | 3.891702 | -2.311122 | -2.150666 |
| H | 5.284799 | -1.347887 | -1.436986 | H | 5.239550 | -1.396148 | -1.486371 |
| C | 2.061197 | 2.221700 | -0.872327 | C | 2.136041 | 2.237932 | -0.774701 |
| C | -0.041095 | 2.443357 | 0.585265 | C | -0.071230 | 2.453339 | 0.499517 |
| O | 2.642733 | 2.959374 | -1.542728 | O | 2.773282 | 2.972933 | -1.369168 |
| O | -0.659528 | 3.351676 | 0.927514 | O | -0.705573 | 3.354891 | 0.777750 |
| Co | -0.907085 | -0.404900 | 0.595414 | Co | -0.914410 | -0.380007 | 0.588619 |
| C | -2.747119 | -0.260388 | -0.124820 | C | -2.771860 | -0.248381 | -0.107838 |
| C | -3.189297 | 1.220460 | -0.079503 | C | -3.242384 | 1.219985 | -0.077718 |
| C | -4.749427 | 1.134084 | -0.006149 | C | -4.796806 | 1.106697 | -0.008302 |
| C | -5.012408 | -0.384049 | 0.009524 | C | -5.032030 | -0.409809 | 0.015053 |
| C | -3.798498 | -0.904975 | 0.808931 | C | -3.816494 | -0.902665 | 0.820654 |
| C | -4.715661 | -0.945020 | -1.393455 | C | -4.720282 | -0.970723 | -1.378224 |
| C | -3.160852 | -0.839210 | -1.488260 | C | -3.171440 | -0.840746 | -1.466388 |
| H | -2.804070 | 1.732014 | 0.811881 | H | -2.869065 | 1.744515 | 0.804325 |
| H | -2.828145 | 1.776416 | -0.952991 | H | -2.891669 | 1.772456 | -0.951196 |
| H | -5.125394 | 1.607952 | 0.908961 | H | -5.181616 | 1.576857 | 0.898986 |
| H | -5.237415 | 1.624618 | -0.857001 | H | -5.289755 | 1.583418 | -0.857565 |
| H | -5.229316 | -0.376623 | -2.178275 | H | -5.237103 | -0.418873 | -2.165662 |
| H | -5.045889 | -1.988365 | -1.472559 | H | -5.031592 | -2.014804 | -1.454115 |
| H | -2.825452 | -0.200737 | -2.312535 | H | -2.844106 | -0.205237 | -2.289640 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -2.712661 | -1.826576 | -1.651182 | H | -2.709816 | -1.817392 | -1.622666 |
| H | -3.741764 | -2.000733 | 0.834237 | H | -3.740504 | -1.991849 | 0.854215 |
| H | -3.765962 | -0.523580 | 1.838548 | H | -3.794480 | -0.516478 | 1.842957 |
| H | -5.998630 | -0.658599 | 0.401491 | H | -6.010570 | -0.697881 | 0.401134 |
| C | -0.000925 | 0.098526 | -1.101281 | C | 0.011566 | 0.102376 | -1.120271 |
| C | -0.823304 | -2.222705 | 0.329440 | C | -0.824819 | -2.211296 | 0.363110 |
| O | -0.088929 | -0.101650 | -2.250638 | O | -0.075571 | -0.107203 | -2.252538 |
| O | -1.003180 | -3.341133 | 0.118245 | O | -0.988096 | -3.322685 | 0.184217 |
| C | 0.086800 | -0.087945 | 2.105778 | C | 0.116338 | -0.052939 | 2.076246 |
| O | 0.671920 | 0.049021 | 3.096765 | O | 0.696159 | 0.084790 | 3.053268 |

**Table S26**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_5$ structure **5T-1**

| B3PW91 | | |
|---|---|---|
| -9(0) | 763(35) | 1301(1) |
| 16(1) | 773(3) | 1305(5) |
| 27(1) | 776(9) | 1310(6) |
| 29(1) | 801(3) | 1327(8) |
| 44(0) | 806(3) | 1328(9) |
| 48(0) | 823(14) | 1337(1) |
| 57(1) | 824(24) | 1338(0) |
| 68(0) | 833(1) | 1343(0) |
| 73(0) | 834(3) | 1348(3) |
| 78(0) | 879(22) | 1466(103) |
| 84(0) | 883(19) | 1471(3) |
| 100(2) | 940(1) | 1473(0) |
| 109(1) | 942(2) | 1488(8) |
| 123(1) | 947(4) | 1489(2) |
| 142(1) | 951(10) | 1489(2) |
| 149(4) | 955(0) | 1490(7) |
| 161(1) | 955(2) | 1495(9) |
| 175(0) | 975(2) | 1495(6) |
| 200(1) | 977(4) | 1523(1) |
| 222(0) | 986(5) | 1523(1) |
| 238(3) | 989(15) | 1766(543) |
| 268(4) | 1017(2) | 2042(754) |
| 288(23) | 1023(7) | 2077(1645) |
| 299(4) | 1033(4) | 2107(532) |
| 343(2) | 1034(4) | 3035(35) |
| 349(0) | 1061(7) | 3071(54) |
| 356(1) | 1062(1) | 3072(14) |
| 398(20) | 1099(10) | 3074(34) |
| 402(4) | 1109(41) | 3076(28) |
| 407(0) | 1137(1) | 3078(32) |
| 421(31) | 1139(1) | 3081(38) |
| 437(7) | 1162(49) | 3086(25) |
| 444(1) | 1175(49) | 3086(27) |
| 453(3) | 1184(0) | 3090(25) |
| 460(19) | 1186(15) | 3112(6) |
| 472(4) | 1215(13) | 3119(11) |
| 475(1) | 1216(2) | 3120(23) |
| 496(43) | 1247(1) | 3121(32) |

| | | |
|---|---|---|
| 503(5) | 1248(6) | 3124(26) |
| 532(23) | 1250(7) | 3125(21) |
| 546(5) | 1253(2) | 3134(24) |
| 550(2) | 1262(9) | 3138(27) |
| 553(3) | 1267(7) | 3145(21) |
| 596(73) | 1271(1) | 3147(41) |
| 661(3) | 1275(5) | 3149(12) |
| 761(79) | 1300(4) | 3149(41) |

**Table S27**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_5$ structure **5S-2**

| B3PW91 | | |
|---|---|---|
| 18(0) | 606(48) | 1289(24) |
| 33(1) | 756(1) | 1300(1) |
| 43(1) | 762(0) | 1303(7) |
| 53(0) | 768(24) | 1317(19) |
| 66(0) | 769(23) | 1320(9) |
| 71(0) | 804(0) | 1326(3) |
| 75(1) | 808(3) | 1334(5) |
| 81(0) | 817(1) | 1341(1) |
| 93(1) | 829(1) | 1342(0) |
| 97(0) | 847(2) | 1462(1) |
| 107(0) | 853(3) | 1473(1) |
| 114(1) | 909(3) | 1481(5) |
| 117(7) | 912(2) | 1484(5) |
| 119(1) | 927(8) | 1488(3) |
| 132(0) | 937(6) | 1490(2) |
| 167(1) | 946(2) | 1491(5) |
| 182(0) | 954(0) | 1495(13) |
| 197(1) | 957(4) | 1520(2) |
| 206(2) | 958(3) | 1520(1) |
| 213(17) | 968(5) | 1959(463) |
| 229(1) | 976(1) | 2037(456) |
| 256(1) | 996(18) | 2084(859) |
| 265(3) | 1002(18) | 2089(1360) |
| 279(1) | 1011(19) | 2129(417) |
| 356(1) | 1012(2) | 2968(27) |
| 359(1) | 1024(18) | 3065(26) |
| 362(9) | 1032(0) | 3068(39) |
| 404(2) | 1061(2) | 3071(51) |
| 405(11) | 1062(3) | 3072(15) |
| 417(11) | 1114(7) | 3075(38) |
| 423(26) | 1116(1) | 3076(49) |
| 427(6) | 1135(3) | 3082(24) |
| 437(5) | 1144(0) | 3087(23) |
| 457(1) | 1177(27) | 3091(20) |
| 462(3) | 1178(3) | 3111(7) |
| 470(2) | 1204(1) | 3115(48) |
| 484(39) | 1207(1) | 3118(60) |
| 490(11) | 1226(25) | 3119(19) |

| | | |
|---|---|---|
| 494(9) | 1241(11) | 3122(12) |
| 497(13) | 1245(6) | 3126(18) |
| 522(55) | 1251(10) | 3133(25) |
| 541(6) | 1252(5) | 3135(14) |
| 547(9) | 1265(9) | 3142(21) |
| 564(141) | 1268(6) | 3142(29) |
| 582(52) | 1280(1) | 3145(30) |
| 597(24) | 1282(25) | 3152(33) |

**Table S28**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_5$ structure **5S-3**

| B3PW91 | | |
|---|---|---|
| 9(0) | 762(59) | 1298(1) |
| 13(0) | 768(5) | 1299(1) |
| 28(2) | 769(1) | 1300(4) |
| 37(1) | 804(12) | 1325(10) |
| 50(0) | 805(2) | 1328(6) |
| 60(0) | 806(17) | 1337(0) |
| 77(1) | 825(18) | 1342(2) |
| 83(0) | 831(2) | 1342(1) |
| 84(1) | 837(3) | 1345(0) |
| 93(1) | 878(20) | 1472(1) |
| 105(4) | 881(17) | 1473(1) |
| 115(0) | 941(0) | 1484(2) |
| 130(7) | 942(1) | 1488(3) |
| 137(0) | 955(15) | 1490(9) |
| 153(3) | 956(2) | 1492(2) |
| 158(2) | 957(0) | 1494(17) |
| 176(0) | 959(0) | 1495(11) |
| 196(1) | 976(4) | 1519(26) |
| 198(2) | 976(2) | 1524(2) |
| 238(3) | 987(52) | 1530(100) |
| 277(1) | 993(16) | 1812(587) |
| 282(2) | 1018(5) | 1975(1011) |
| 306(7) | 1022(0) | 2060(1550) |
| 321(1) | 1037(11) | 2090(632) |
| 353(2) | 1042(3) | 3049(24) |
| 355(0) | 1058(2) | 3055(14) |
| 382(1) | 1058(1) | 3074(29) |
| 407(0) | 1086(15) | 3075(47) |
| 409(3) | 1106(8) | 3076(23) |
| 421(1) | 1140(31) | 3077(27) |
| 436(4) | 1140(34) | 3085(41) |
| 451(4) | 1153(3) | 3089(22) |
| 455(0) | 1158(43) | 3096(25) |
| 459(1) | 1184(3) | 3101(26) |
| 471(2) | 1186(1) | 3122(2) |
| 494(6) | 1210(0) | 3124(20) |
| 519(6) | 1212(4) | 3125(9) |
| 526(4) | 1239(2) | 3127(23) |

| | | |
|---|---|---|
| 541(19) | 1243(2) | 3127(31) |
| 546(0) | 1248(3) | 3130(11) |
| 547(0) | 1252(3) | 3134(20) |
| 554(37) | 1265(18) | 3134(34) |
| 557(8) | 1270(8) | 3147(10) |
| 624(94) | 1274(6) | 3153(34) |
| 667(8) | 1276(1) | 3157(25) |
| 738(97) | 1297(2) | 3182(7) |

**Table S29**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_5$ structure **5S-4**

| B3PW91 | | |
|---|---|---|
| -19(0) | 638(203) | 1284(12) |
| 20(0) | 752(1) | 1299(1) |
| 27(0) | 762(1) | 1302(5) |
| 41(0) | 767(13) | 1316(15) |
| 50(0) | 772(12) | 1320(10) |
| 62(1) | 801(1) | 1325(3) |
| 66(1) | 807(5) | 1331(2) |
| 75(0) | 814(1) | 1339(1) |
| 83(1) | 828(2) | 1343(0) |
| 93(0) | 844(3) | 1456(1) |
| 98(2) | 856(1) | 1472(0) |
| 105(1) | 904(3) | 1480(4) |
| 108(0) | 916(3) | 1487(2) |
| 125(2) | 926(6) | 1487(4) |
| 140(0) | 935(1) | 1490(4) |
| 156(0) | 945(2) | 1492(5) |
| 179(2) | 952(0) | 1493(6) |
| 190(0) | 953(5) | 1520(1) |
| 192(1) | 963(6) | 1520(1) |
| 205(0) | 964(1) | 1950(421) |
| 225(7) | 978(1) | 2008(582) |
| 232(0) | 993(13) | 2089(538) |
| 279(14) | 1002(22) | 2091(1491) |
| 312(2) | 1012(13) | 2154(158) |
| 353(2) | 1014(0) | 2937(23) |
| 357(1) | 1029(21) | 3063(26) |
| 366(34) | 1029(8) | 3065(30) |
| 369(0) | 1058(0) | 3066(28) |
| 399(11) | 1061(3) | 3071(36) |
| 408(1) | 1115(3) | 3074(25) |
| 411(6) | 1115(3) | 3075(55) |
| 425(7) | 1132(6) | 3076(24) |
| 432(9) | 1146(0) | 3077(33) |
| 447(24) | 1176(29) | 3083(29) |
| 466(0) | 1178(7) | 3110(3) |
| 466(2) | 1204(0) | 3114(12) |
| 482(0) | 1206(1) | 3117(50) |
| 491(3) | 1223(20) | 3119(61) |

| | | |
|---|---|---|
| 512(14) | 1241(6) | 3121(27) |
| 525(1) | 1248(9) | 3127(1) |
| 537(6) | 1251(14) | 3128(10) |
| 539(61) | 1252(4) | 3132(41) |
| 549(5) | 1256(9) | 3136(43) |
| 556(136) | 1268(12) | 3136(13) |
| 583(40) | 1276(1) | 3142(38) |
| 586(141) | 1283(28) | 3146(36) |

**Table S30**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_5$ structure **5T-5**

| B3PW91 | | |
|---|---|---|
| 31(0) | 598(55) | 1281(13) |
| 39(1) | 755(13) | 1292(0) |
| 44(0) | 759(8) | 1296(2) |
| 56(1) | 760(4) | 1310(12) |
| 60(0) | 770(7) | 1316(9) |
| 65(0) | 797(1) | 1330(3) |
| 67(0) | 802(2) | 1333(1) |
| 70(0) | 831(1) | 1341(0) |
| 74(0) | 834(1) | 1348(0) |
| 80(1) | 840(3) | 1464(1) |
| 94(2) | 854(2) | 1472(0) |
| 96(0) | 898(1) | 1480(4) |
| 101(0) | 915(4) | 1485(5) |
| 115(1) | 925(2) | 1489(1) |
| 121(0) | 936(2) | 1491(8) |
| 131(2) | 938(1) | 1494(6) |
| 156(0) | 949(0) | 1495(3) |
| 171(4) | 952(0) | 1519(1) |
| 187(1) | 958(4) | 1521(1) |
| 208(1) | 960(3) | 1952(590) |
| 218(2) | 963(1) | 2080(358) |
| 223(4) | 993(5) | 2094(829) |
| 241(1) | 1001(13) | 2107(1592) |
| 243(2) | 1007(0) | 2145(721) |
| 316(2) | 1013(2) | 3056(12) |
| 333(7) | 1015(2) | 3058(13) |
| 343(4) | 1027(0) | 3063(54) |
| 352(3) | 1044(0) | 3065(38) |
| 362(1) | 1049(1) | 3066(34) |
| 390(20) | 1101(2) | 3069(41) |
| 401(12) | 1115(1) | 3074(38) |
| 415(26) | 1145(0) | 3076(36) |
| 420(0) | 1152(1) | 3083(24) |
| 428(0) | 1164(6) | 3086(22) |
| 432(1) | 1174(9) | 3112(3) |
| 444(2) | 1192(0) | 3114(40) |
| 450(5) | 1203(0) | 3117(17) |
| 456(2) | 1235(3) | 3118(49) |

| | | |
|---|---|---|
| 466(4) | 1238(9) | 3119(34) |
| 479(6) | 1239(6) | 3121(22) |
| 486(16) | 1247(4) | 3135(11) |
| 496(23) | 1251(2) | 3139(25) |
| 547(0) | 1261(5) | 3143(40) |
| 548(1) | 1270(4) | 3144(17) |
| 563(4) | 1276(1) | 3146(36) |
| 579(50) | 1280(18) | 3167(13) |

**Table S31**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_5$ structure **5S-6**

| B3PW91 | | |
|---|---|---|
| 20(0) | 614(54) | 1292(1) |
| 52(0) | 751(1) | 1299(0) |
| 55(0) | 756(1) | 1313(2) |
| 72(0) | 756(11) | 1318(9) |
| 77(0) | 761(11) | 1320(4) |
| 83(0) | 802(3) | 1336(0) |
| 87(0) | 805(1) | 1339(8) |
| 94(0) | 824(0) | 1347(1) |
| 97(0) | 827(1) | 1356(0) |
| 105(0) | 854(4) | 1456(2) |
| 108(0) | 858(2) | 1476(0) |
| 119(1) | 912(6) | 1477(1) |
| 123(0) | 916(3) | 1490(6) |
| 139(0) | 936(3) | 1491(3) |
| 148(1) | 938(2) | 1493(13) |
| 160(0) | 941(2) | 1496(14) |
| 172(1) | 944(0) | 1514(4) |
| 191(1) | 953(1) | 1519(5) |
| 216(2) | 957(3) | 1571(10) |
| 222(0) | 964(2) | 1941(387) |
| 243(0) | 971(5) | 2074(511) |
| 254(0) | 991(6) | 2079(989) |
| 284(4) | 998(3) | 2113(1485) |
| 317(4) | 1006(8) | 2138(453) |
| 362(0) | 1018(3) | 2850(117) |
| 373(8) | 1026(1) | 2882(42) |
| 379(2) | 1038(1) | 3065(41) |
| 416(3) | 1054(2) | 3067(14) |
| 424(6) | 1056(0) | 3068(33) |
| 430(3) | 1107(6) | 3069(31) |
| 432(15) | 1113(0) | 3078(44) |
| 442(2) | 1147(0) | 3080(50) |
| 444(12) | 1153(0) | 3083(7) |
| 463(3) | 1168(8) | 3090(20) |
| 473(3) | 1172(4) | 3115(20) |
| 488(42) | 1195(1) | 3116(1) |
| 495(19) | 1203(2) | 3118(34) |
| 503(17) | 1230(5) | 3119(29) |

| | | |
|---|---|---|
| 517(33) | 1238(11) | 3120(8) |
| 539(3) | 1241(11) | 3123(40) |
| 547(5) | 1244(2) | 3134(3) |
| 556(34) | 1259(11) | 3135(25) |
| 559(8) | 1270(3) | 3139(26) |
| 572(37) | 1279(4) | 3141(52) |
| 587(48) | 1284(7) | 3143(46) |
| 599(23) | 1291(3) | 3178(19) |

**Table S32**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_5$ structure **5T-7**

| B3PW91 | | |
|---|---|---|
| 26(1) | 576(42) | 1287(24) |
| 28(0) | 761(2) | 1294(2) |
| 41(0) | 763(12) | 1299(3) |
| 53(0) | 769(26) | 1309(6) |
| 56(0) | 773(10) | 1319(10) |
| 66(0) | 799(0) | 1329(1) |
| 67(0) | 805(1) | 1331(6) |
| 73(0) | 828(1) | 1339(0) |
| 76(0) | 829(4) | 1339(0) |
| 83(0) | 850(1) | 1471(1) |
| 89(0) | 853(3) | 1471(0) |
| 98(0) | 911(2) | 1485(6) |
| 99(2) | 911(1) | 1487(1) |
| 113(1) | 929(4) | 1488(9) |
| 126(3) | 936(6) | 1489(4) |
| 138(1) | 948(1) | 1492(6) |
| 145(3) | 952(0) | 1494(11) |
| 162(1) | 953(1) | 1518(3) |
| 187(6) | 960(5) | 1521(1) |
| 191(9) | 963(1) | 1968(397) |
| 205(2) | 973(1) | 2044(746) |
| 242(1) | 990(6) | 2091(914) |
| 252(1) | 1003(17) | 2098(869) |
| 262(11) | 1005(1) | 2137(505) |
| 327(1) | 1008(5) | 3052(16) |
| 348(2) | 1018(4) | 3054(32) |
| 354(1) | 1031(0) | 3056(23) |
| 364(19) | 1049(1) | 3063(38) |
| 384(7) | 1061(3) | 3069(33) |
| 396(17) | 1109(16) | 3070(47) |
| 406(1) | 1114(7) | 3074(51) |
| 410(17) | 1138(0) | 3079(26) |
| 415(6) | 1139(0) | 3079(43) |
| 418(1) | 1168(13) | 3082(19) |
| 435(1) | 1177(7) | 3105(6) |
| 447(30) | 1196(1) | 3108(8) |
| 454(1) | 1203(3) | 3110(69) |
| 461(9) | 1224(7) | 3113(15) |

| | | |
|---|---|---|
| 467(13) | 1235(12) | 3116(22) |
| 475(4) | 1238(3) | 3116(37) |
| 480(29) | 1249(9) | 3120(26) |
| 499(68) | 1256(9) | 3128(34) |
| 513(25) | 1260(7) | 3132(16) |
| 543(11) | 1265(4) | 3136(51) |
| 547(1) | 1274(1) | 3140(47) |
| 555(79) | 1283(26) | 3146(19) |

**Table S33**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_6$ structure **6T-1**

| B3PW91 | | |
|---|---|---|
| 11(1) | 625(47) | 1300(2) |
| 15(0) | 664(1) | 1301(3) |
| 24(0) | 760(94) | 1304(4) |
| 29(1) | 762(31) | 1309(7) |
| 43(0) | 774(5) | 1326(8) |
| 47(0) | 777(10) | 1328(7) |
| 60(0) | 804(2) | 1337(1) |
| 67(1) | 806(5) | 1338(0) |
| 70(0) | 822(24) | 1346(0) |
| 74(0) | 824(21) | 1351(3) |
| 77(0) | 834(2) | 1465(108) |
| 82(0) | 835(2) | 1473(3) |
| 90(0) | 879(21) | 1474(0) |
| 101(2) | 883(22) | 1488(2) |
| 125(1) | 941(2) | 1490(7) |
| 127(1) | 942(3) | 1490(5) |
| 142(1) | 949(5) | 1491(6) |
| 152(1) | 950(11) | 1496(12) |
| 161(1) | 953(0) | 1496(2) |
| 175(0) | 958(0) | 1524(2) |
| 198(1) | 977(3) | 1524(1) |
| 219(1) | 977(3) | 1777(534) |
| 248(2) | 986(8) | 2073(669) |
| 274(6) | 989(12) | 2078(222) |
| 291(25) | 1018(2) | 2099(1525) |
| 317(1) | 1025(10) | 2139(771) |
| 349(1) | 1033(2) | 3050(32) |
| 350(0) | 1035(2) | 3063(36) |
| 359(1) | 1061(2) | 3072(39) |
| 379(10) | 1063(4) | 3074(35) |
| 400(5) | 1094(19) | 3075(19) |
| 406(0) | 1111(35) | 3078(38) |
| 410(11) | 1138(2) | 3079(33) |
| 432(9) | 1139(0) | 3086(30) |
| 439(3) | 1162(50) | 3089(40) |
| 450(11) | 1175(54) | 3091(11) |
| 456(6) | 1182(1) | 3114(6) |

| | | |
|---|---|---|
| 461(1) | 1187(24) | 3117(9) |
| 467(25) | 1214(10) | 3120(23) |
| 478(9) | 1215(6) | 3122(28) |
| 484(19) | 1249(7) | 3124(33) |
| 487(30) | 1249(1) | 3125(23) |
| 500(42) | 1252(4) | 3135(25) |
| 511(27) | 1254(1) | 3137(36) |
| 533(26) | 1263(8) | 3145(26) |
| 545(13) | 1268(7) | 3148(35) |
| 550(1) | 1275(0) | 3150(21) |
| 554(3) | 1275(5) | 3154(22) |

**Table S34**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_6$ structure **6S-2**

| B3PW91 | | |
|---|---|---|
| 7(0) | 651(75) | 1295(2) |
| 27(1) | 672(38) | 1299(3) |
| 34(0) | 748(82) | 1299(0) |
| 45(0) | 759(67) | 1300(2) |
| 50(0) | 765(7) | 1326(7) |
| 64(0) | 771(5) | 1330(9) |
| 69(0) | 799(2) | 1341(0) |
| 73(0) | 812(1) | 1342(6) |
| 80(0) | 816(20) | 1345(0) |
| 81(1) | 823(28) | 1347(2) |
| 96(1) | 833(2) | 1471(0) |
| 104(0) | 837(1) | 1477(0) |
| 109(0) | 878(21) | 1488(6) |
| 114(0) | 885(18) | 1490(4) |
| 130(1) | 941(1) | 1492(6) |
| 133(2) | 947(0) | 1493(5) |
| 152(1) | 955(2) | 1495(7) |
| 191(0) | 956(26) | 1500(15) |
| 193(0) | 957(6) | 1523(8) |
| 208(1) | 963(0) | 1528(3) |
| 219(1) | 967(2) | 1540(267) |
| 242(3) | 977(3) | 1792(287) |
| 257(0) | 989(25) | 1941(489) |
| 258(3) | 996(32) | 2078(814) |
| 317(9) | 1014(2) | 2092(1405) |
| 347(0) | 1023(1) | 2131(1003) |
| 348(1) | 1040(9) | 3063(16) |
| 357(2) | 1043(4) | 3073(26) |
| 364(2) | 1056(3) | 3074(41) |
| 403(8) | 1059(0) | 3076(36) |
| 413(0) | 1102(11) | 3077(29) |
| 417(1) | 1121(1) | 3084(35) |
| 421(14) | 1137(37) | 3095(16) |
| 436(4) | 1143(4) | 3096(26) |
| 445(6) | 1152(22) | 3100(25) |
| 461(0) | 1154(34) | 3101(18) |
| 466(11) | 1191(2) | 3123(11) |
| 468(6) | 1193(1) | 3124(4) |

| | | |
|---|---|---|
| 479(4) | 1209(1) | 3127(6) |
| 491(12) | 1210(3) | 3127(28) |
| 510(6) | 1236(1) | 3128(21) |
| 513(4) | 1238(2) | 3131(35) |
| 538(36) | 1246(5) | 3133(34) |
| 543(20) | 1253(3) | 3147(23) |
| 547(28) | 1264(4) | 3154(3) |
| 550(1) | 1271(7) | 3159(28) |
| 566(100) | 1281(5) | 3159(25) |
| 607(55) | 1282(6) | 3163(13) |

**Table S35**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_6$ structure **6S-3**

| B3PW91 | | |
|---|---|---|
| 29(1) | 655(76) | 1298(2) |
| 34(1) | 667(11) | 1299(0) |
| 42(0) | 738(108) | 1299(2) |
| 45(1) | 758(70) | 1303(7) |
| 49(0) | 769(6) | 1324(12) |
| 58(0) | 770(2) | 1327(7) |
| 65(0) | 803(7) | 1339(0) |
| 74(0) | 805(26) | 1342(1) |
| 83(1) | 807(3) | 1343(2) |
| 89(0) | 824(19) | 1348(0) |
| 90(2) | 829(3) | 1472(0) |
| 101(1) | 837(3) | 1472(1) |
| 109(4) | 877(21) | 1487(5) |
| 119(1) | 881(19) | 1487(2) |
| 134(5) | 943(0) | 1488(2) |
| 139(1) | 944(1) | 1492(7) |
| 154(0) | 956(15) | 1493(19) |
| 163(2) | 957(2) | 1496(9) |
| 176(0) | 959(1) | 1514(82) |
| 196(1) | 959(1) | 1522(2) |
| 201(2) | 979(2) | 1525(42) |
| 236(2) | 981(3) | 1825(622) |
| 277(7) | 986(57) | 1997(918) |
| 279(1) | 991(18) | 2074(124) |
| 316(4) | 1021(4) | 2083(1464) |
| 321(2) | 1025(0) | 2134(1134) |
| 350(1) | 1036(12) | 3057(19) |
| 353(2) | 1040(2) | 3058(14) |
| 380(3) | 1061(1) | 3073(39) |
| 391(3) | 1061(2) | 3075(24) |
| 401(5) | 1084(15) | 3075(30) |
| 407(1) | 1103(12) | 3077(31) |
| 419(1) | 1139(37) | 3086(39) |
| 426(7) | 1139(27) | 3087(30) |
| 434(6) | 1156(2) | 3092(22) |
| 452(4) | 1161(51) | 3097(25) |
| 461(1) | 1183(4) | 3121(10) |
| 471(6) | 1185(0) | 3125(3) |

| | | |
|---|---|---|
| 472(13) | 1211(0) | 3126(42) |
| 496(12) | 1214(6) | 3127(8) |
| 513(7) | 1240(2) | 3128(21) |
| 528(20) | 1245(3) | 3130(15) |
| 534(26) | 1249(4) | 3135(32) |
| 541(42) | 1250(2) | 3140(7) |
| 549(1) | 1263(16) | 3147(36) |
| 549(0) | 1272(5) | 3149(14) |
| 562(15) | 1273(5) | 3155(28) |
| 571(27) | 1274(7) | 3174(11) |

**Table S36**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_6$ structure **6T-4**

| B3PW91 | | |
|---|---|---|
| 25(0) | 645(4) | 1297(4) |
| 33(0) | 696(28) | 1298(1) |
| 48(0) | 743(77) | 1301(2) |
| 50(0) | 767(13) | 1303(3) |
| 54(0) | 772(9) | 1327(10) |
| 56(0) | 777(7) | 1328(2) |
| 60(0) | 802(1) | 1338(0) |
| 61(0) | 806(4) | 1341(0) |
| 69(0) | 815(11) | 1342(1) |
| 73(0) | 829(8) | 1346(1) |
| 76(0) | 833(6) | 1472(0) |
| 85(1) | 836(3) | 1476(1) |
| 89(0) | 878(11) | 1487(4) |
| 98(0) | 886(17) | 1489(3) |
| 126(2) | 941(0) | 1490(4) |
| 135(1) | 943(0) | 1493(7) |
| 146(0) | 954(6) | 1494(6) |
| 152(2) | 955(0) | 1500(2) |
| 161(0) | 959(1) | 1521(2) |
| 199(1) | 962(6) | 1528(0) |
| 211(4) | 967(5) | 1552(178) |
| 217(0) | 974(5) | 1756(319) |
| 234(0) | 991(16) | 2083(972) |
| 262(0) | 999(31) | 2088(341) |
| 306(8) | 1017(1) | 2106(1656) |
| 311(1) | 1019(2) | 2141(534) |
| 342(2) | 1038(4) | 3059(22) |
| 350(1) | 1040(6) | 3063(26) |
| 354(1) | 1053(1) | 3068(35) |
| 365(14) | 1060(4) | 3071(29) |
| 382(13) | 1107(5) | 3072(40) |
| 387(5) | 1112(3) | 3074(21) |
| 402(8) | 1140(0) | 3081(16) |
| 413(0) | 1144(23) | 3085(39) |
| 416(1) | 1147(7) | 3093(29) |
| 441(10) | 1165(71) | 3094(24) |
| 443(11) | 1190(0) | 3117(6) |
| 450(43) | 1196(5) | 3121(26) |

| | | |
|---|---|---|
| 454(8) | 1208(1) | 3122(6) |
| 462(25) | 1213(4) | 3124(6) |
| 472(23) | 1237(1) | 3124(33) |
| 483(20) | 1243(1) | 3125(20) |
| 489(7) | 1250(4) | 3126(37) |
| 501(30) | 1250(3) | 3131(36) |
| 510(18) | 1259(12) | 3140(30) |
| 547(1) | 1262(4) | 3147(13) |
| 551(0) | 1278(4) | 3151(28) |
| 606(120) | 1280(4) | 3152(43) |

**Table S37**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_7$ structure **7S-1**

| B3PW91 | | |
|---|---|---|
| 18(1) | 554(24) | 1285(8) |
| 26(1) | 562(15) | 1294(2) |
| 33(0) | 572(27) | 1297(2) |
| 46(0) | 647(58) | 1301(1) |
| 55(0) | 669(47) | 1304(2) |
| 63(0) | 738(138) | 1331(8) |
| 70(0) | 757(80) | 1331(6) |
| 75(1) | 766(12) | 1339(0) |
| 83(0) | 769(8) | 1341(0) |
| 91(1) | 803(4) | 1346(6) |
| 95(0) | 811(5) | 1349(2) |
| 97(1) | 816(31) | 1475(0) |
| 105(2) | 824(19) | 1478(1) |
| 113(2) | 833(2) | 1489(5) |
| 123(1) | 839(2) | 1492(2) |
| 132(3) | 880(27) | 1493(6) |
| 138(2) | 885(20) | 1496(8) |
| 148(3) | 941(2) | 1497(12) |
| 151(2) | 943(2) | 1502(14) |
| 160(2) | 957(20) | 1526(1) |
| 196(2) | 957(10) | 1529(1) |
| 201(0) | 959(17) | 1560(123) |
| 204(1) | 961(1) | 1774(352) |
| 226(2) | 968(4) | 2010(572) |
| 268(7) | 969(4) | 2066(324) |
| 274(3) | 986(31) | 2086(1080) |
| 293(9) | 995(29) | 2105(1387) |
| 327(0) | 1013(1) | 2145(967) |
| 337(9) | 1015(4) | 3072(27) |
| 347(1) | 1041(12) | 3073(49) |
| 359(1) | 1044(6) | 3074(34) |
| 383(3) | 1056(1) | 3076(35) |
| 393(4) | 1057(4) | 3077(26) |
| 413(2) | 1122(2) | 3096(30) |
| 415(1) | 1126(0) | 3098(23) |
| 424(1) | 1139(44) | 3099(18) |
| 436(7) | 1143(1) | 3103(25) |
| 448(10) | 1145(27) | 3104(18) |

| | | |
|---|---|---|
| 454(2) | 1162(67) | 3122(12) |
| 459(18) | 1197(4) | 3124(27) |
| 461(2) | 1198(0) | 3127(2) |
| 469(2) | 1209(1) | 3128(35) |
| 488(14) | 1210(4) | 3129(36) |
| 490(19) | 1236(1) | 3132(19) |
| 511(37) | 1237(3) | 3133(26) |
| 519(28) | 1251(5) | 3150(19) |
| 529(70) | 1251(2) | 3156(20) |
| 545(10) | 1266(5) | 3161(21) |
| 548(13) | 1267(12) | 3168(16) |
| 549(11) | 1285(2) | 3182(7) |

**Table S38**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_7$ structure **7S-2**

| B3PW91 | | |
|---|---|---|
| 23(0) | 549(1) | 1279(2) |
| 34(0) | 557(30) | 1283(13) |
| 52(0) | 567(31) | 1289(16) |
| 58(0) | 574(32) | 1301(0) |
| 60(0) | 583(94) | 1303(1) |
| 72(0) | 587(45) | 1323(8) |
| 79(0) | 602(117) | 1323(9) |
| 82(0) | 757(2) | 1333(6) |
| 86(0) | 760(14) | 1335(4) |
| 87(0) | 761(5) | 1342(1) |
| 100(0) | 766(25) | 1346(0) |
| 101(0) | 799(1) | 1472(0) |
| 103(0) | 805(1) | 1474(0) |
| 110(0) | 832(2) | 1487(1) |
| 113(1) | 834(2) | 1490(3) |
| 116(0) | 846(6) | 1492(4) |
| 122(0) | 847(1) | 1495(8) |
| 124(0) | 913(4) | 1495(7) |
| 135(0) | 914(11) | 1501(10) |
| 148(1) | 942(1) | 1522(2) |
| 152(0) | 943(1) | 1526(1) |
| 187(2) | 952(1) | 1960(393) |
| 201(0) | 956(3) | 2077(71) |
| 220(3) | 957(2) | 2086(497) |
| 224(2) | 960(9) | 2099(968) |
| 226(1) | 970(2) | 2108(769) |
| 234(8) | 972(2) | 2123(824) |
| 267(14) | 998(9) | 2164(721) |
| 353(9) | 1006(12) | 3067(30) |
| 356(6) | 1012(1) | 3067(21) |
| 361(35) | 1020(1) | 3068(58) |
| 364(33) | 1033(0) | 3069(35) |
| 385(23) | 1038(0) | 3080(40) |
| 396(1) | 1060(1) | 3084(31) |
| 404(15) | 1061(1) | 3086(34) |
| 408(7) | 1117(5) | 3096(23) |
| 416(3) | 1118(7) | 3098(10) |
| 428(8) | 1140(0) | 3101(9) |

| | | |
|---|---|---|
| 435(100) | 1149(1) | 3115(10) |
| 445(5) | 1178(3) | 3117(21) |
| 447(35) | 1181(8) | 3118(37) |
| 459(4) | 1205(1) | 3119(33) |
| 463(2) | 1212(1) | 3122(34) |
| 474(12) | 1243(9) | 3123(25) |
| 478(4) | 1251(14) | 3137(32) |
| 484(11) | 1253(4) | 3141(37) |
| 499(48) | 1254(3) | 3150(22) |
| 533(13) | 1259(7) | 3170(13) |
| 542(0) | 1262(4) | 3176(15) |
| 546(6) | 1275(0) | 3183(15) |

**Table S39**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_7$ structure **7S-3**

| B3PW91 | | |
|---|---|---|
| -10(0) | 545(0) | 1280(1) |
| 26(0) | 547(0) | 1289(21) |
| 39(0) | 561(52) | 1290(10) |
| 50(0) | 580(53) | 1298(0) |
| 56(0) | 587(35) | 1298(1) |
| 68(0) | 590(161) | 1323(13) |
| 76(0) | 595(36) | 1323(3) |
| 81(0) | 756(0) | 1333(6) |
| 85(0) | 756(1) | 1333(0) |
| 92(0) | 759(8) | 1346(2) |
| 94(0) | 760(39) | 1346(1) |
| 97(0) | 804(0) | 1475(0) |
| 100(0) | 804(6) | 1475(0) |
| 103(0) | 834(0) | 1491(5) |
| 113(0) | 834(2) | 1491(2) |
| 117(0) | 842(2) | 1497(16) |
| 124(1) | 843(5) | 1497(5) |
| 125(0) | 911(2) | 1498(15) |
| 126(0) | 912(14) | 1498(1) |
| 145(0) | 942(2) | 1526(1) |
| 164(1) | 942(0) | 1526(1) |
| 198(0) | 952(0) | 1965(381) |
| 198(1) | 952(4) | 2075(150) |
| 221(12) | 963(0) | 2089(379) |
| 221(1) | 963(6) | 2097(639) |
| 223(4) | 968(0) | 2106(732) |
| 250(0) | 968(1) | 2125(1458) |
| 290(8) | 1004(1) | 2162(288) |
| 351(126) | 1004(20) | 3069(39) |
| 359(0) | 1017(0) | 3069(58) |
| 360(3) | 1017(2) | 3071(63) |
| 367(0) | 1037(0) | 3071(7) |
| 387(2) | 1037(0) | 3078(0) |
| 389(1) | 1060(0) | 3078(45) |
| 399(0) | 1060(2) | 3089(44) |
| 406(11) | 1117(14) | 3089(17) |
| 435(0) | 1117(0) | 3099(25) |
| 435(49) | 1143(0) | 3099(12) |

| | | |
|---|---|---|
| 438(45) | 1143(0) | 3117(99) |
| 445(0) | 1177(8) | 3117(8) |
| 445(13) | 1177(1) | 3121(16) |
| 462(18) | 1204(2) | 3121(0) |
| 463(14) | 1204(1) | 3125(4) |
| 480(4) | 1238(7) | 3125(61) |
| 481(1) | 1239(6) | 3145(2) |
| 488(0) | 1253(27) | 3145(20) |
| 501(76) | 1253(0) | 3148(5) |
| 530(1) | 1262(14) | 3148(66) |
| 534(24) | 1262(4) | 3180(12) |
| 544(8) | 1280(14) | 3181(5) |

**Table S40**. Harmonic vibrational frequencies (in $cm^{-1}$) and infrared intensities (in parentheses, in km/mol) for the $(nor)_2Co_2(CO)_7$ structure **7T-4**

| B3PW91 | | |
|---|---|---|
| 1(0) | 547(26) | 1282(8) |
| 12(1) | 555(3) | 1296(2) |
| 19(1) | 564(74) | 1302(1) |
| 26(0) | 606(14) | 1304(3) |
| 31(0) | 638(6) | 1312(19) |
| 37(0) | 741(101) | 1327(8) |
| 42(0) | 767(31) | 1329(6) |
| 53(0) | 768(39) | 1340(0) |
| 56(0) | 775(24) | 1341(0) |
| 66(0) | 804(2) | 1347(3) |
| 74(1) | 804(1) | 1349(4) |
| 76(0) | 810(14) | 1474(0) |
| 81(2) | 829(28) | 1474(0) |
| 88(0) | 832(2) | 1490(2) |
| 90(0) | 841(35) | 1490(4) |
| 103(0) | 878(17) | 1491(7) |
| 106(3) | 887(56) | 1492(7) |
| 120(4) | 941(1) | 1496(12) |
| 131(19) | 941(2) | 1496(9) |
| 140(1) | 953(18) | 1523(2) |
| 142(1) | 957(8) | 1525(3) |
| 155(7) | 957(0) | 1728(121) |
| 185(1) | 958(6) | 1779(395) |
| 194(0) | 974(3) | 1936(728) |
| 201(0) | 981(2) | 2057(266) |
| 258(24) | 989(32) | 2074(813) |
| 272(79) | 990(21) | 2089(1460) |
| 294(8) | 1016(1) | 2136(841) |
| 329(0) | 1026(18) | 3059(37) |
| 339(2) | 1032(2) | 3070(39) |
| 344(0) | 1041(14) | 3073(30) |
| 369(6) | 1057(4) | 3076(35) |
| 390(53) | 1066(13) | 3077(27) |
| 398(26) | 1099(48) | 3083(26) |
| 404(0) | 1114(2) | 3084(38) |
| 407(1) | 1139(0) | 3086(22) |
| 414(50) | 1145(1) | 3088(21) |
| 424(41) | 1154(86) | 3092(26) |

| | | |
|---|---|---|
| 430(2) | 1180(104) | 3120(1) |
| 446(26) | 1183(27) | 3121(24) |
| 460(1) | 1194(0) | 3123(33) |
| 463(30) | 1209(2) | 3125(5) |
| 465(13) | 1218(34) | 3127(29) |
| 475(1) | 1239(2) | 3128(40) |
| 484(33) | 1250(6) | 3130(26) |
| 495(1) | 1251(7) | 3144(10) |
| 511(67) | 1255(8) | 3146(9) |
| 530(7) | 1264(17) | 3150(28) |
| 535(42) | 1266(7) | 3151(44) |
| 546(37) | 1271(6) | 3152(36) |

**Complete Gaussian 09 reference (Reference 22)**

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