Electronic Supplementary Information for Dalton Transactions

Butterfly and Rhombus Structures for Binuclear Cobalt Carbonyl Sulfur and Phosphinidene Complexes of the Type $Co_2(CO)_6E_2$ (E = S, PX): Comparison with their Iron Carbonyl Analogues

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Supporting Information

Table S1-S7: The vibrational frequencies for the structures of $Co_2(CO)_6E_2$ (E = S, PH, PCl, POH, POMe, PNH_2 or $PNMe_2$) at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

Table S8-S14: The Cartesian coordinates of the optimized $Co_2(CO)_6E_2$ (E = S, PH, PCl, POH, POMe, PNH_2 or $PNMe_2$) structures at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

Complete Gaussian 03 reference (Reference 42)

Table S1. The vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol, given in parentheses) of the $Co_2(CO)_6S_2$ structures at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

Isomers	B3LYP/6-311G(d)	BP86/6-311G(d)
Rhomb	23 (0), 34 (1), 45 (0), 68 (0), 70 (0), 81 (0), 83 (1), 86 (0), 89 (0), 100 (0), 105 (0), 120 (0), 168 (4), 172 (0), 285 (28), 313 (0), 319 (7), 339 (0), 342 (0), 360 (18), 360 (0), 379 (15), 414 (162), 420 (3), 429 (0), 446 (0), 452 (0), 453 (9), 474 (0), 475 (8), 498 (0), 498 (31), 528 (186), 530 (0), 545 (49), 547 (0), 2133 (0), 2133 (2324), 2134 (1192), 2137 (0), 2156 (1987), 2185 (0)	19 (0), 28 (0), 33 (0), 66 (0), 66 (0), 74 (0), 81 (0), 82 (0), 82 (0), 96 (0), 99 (0), 111 (0), 158 (0), 168 (1), 278 (15), 314 (0), 319 (4), 339 (0), 349 (0), 364 (0), 373 (5), 388 (13), 433 (0), 439 (0), 455 (0), 456 (90), 468 (6), 477 (0), 487 (8), 497 (0), 515 (37), 520 (0), 533 (153), 537 (0), 549 (0), 551 (65), 2032 (0), 2033 (1118), 2036 (1663), 2036 (0), 2067 (1668), 2091 (0)
Co-but-a	31 (0), 56 (0), 63 (0), 69 (0), 80 (0), 82 (0), 86 (0), 91 (0), 110 (0), 113 (1), 113 (0), 136 (0), 199 (6), 232 (0), 266 (0), 306 (0), 352 (11), 361 (0), 377 (7), 385 (11), 385 (10), 393 (0), 417 (0), 426 (3), 434 (32), 452 (1), 457 (0), 462 (1), 471 (2), 476 (15), 496 (0), 507 (51), 523 (24), 527 (34), 540 (118), 543 (30), 2130 (207), 2131 (0), 2148 (954), 2159 (1222), 2173 (1457), 2196 (103)	25 (0), 54 (0), 59 (0), 61 (0), 73 (0), 81 (0), 83 (0), 88 (0), 102 (0), 106 (0), 108 (1), 123 (0), 191 (3), 225 (0), 255 (0), 301 (0), 351 (8), 360 (0), 373 (2), 384 (6), 388 (0), 394 (4), 418 (1), 426 (7), 458 (0), 465 (4), 474 (6), 479 (4), 486 (0), 498 (1), 513 (0), 520 (42), 520 (55), 539 (63), 549 (11), 553 (83), 2031 (0), 2034 (26), 2049 (857), 2058 (1086), 2078 (1314), 2101 (106)
S-but-a	23 (0), 28 (0), 41 (0), 58 (1), 61 (0), 66 (0), 73 (0), 92 (0), 92 (0), 95 (0), 99 (0), 103 (1), 125 (0), 200 (17), 207 (2), 283 (0), 292 (1), 299 (1), 319 (13), 379 (0), 384 (0), 408 (2), 412 (4), 450 (4), 451 (5), 456 (16), 465 (16), 476 (13), 483 (38), 507 (4), 516 (32), 526 (4), 567 (69), 571 (30), 572 (38), 579 (21), 2083 (394), 2097 (1327), 2108 (192), 2110 (1151), 2147 (1552), 2169 (169)	23 (0), 27 (0), 44 (0), 61 (1), 64 (0), 65 (0), 73 (0), 88 (0), 89 (0), 92 (0), 95 (0), 98 (0), 126 (1), 196 (5), 206 (0), 272 (0), 293 (0), 297 (0), 318 (1), 375 (0), 376 (0), 421 (1), 429 (6), 456 (7), 460 (37), 471 (12), 481 (0), 495 (5), 507 (31), 527 (0), 537 (21), 541 (1), 568 (18), 572 (47), 588 (57), 592 (6), 1992 (324), 2003 (1212), 2011 (0), 2012 (1092), 2056 (1205), 2075 (129)
Co-but-b	48 (0), 61 (0), 71 (0), 84 (0), 88 (0), 90 (0), 100 (0), 105 (0), 119 (0), 120 (2), 127 (1), 143 (6), 184 (2), 244 (1), 254 (0), 304 (13), 332 (20), 336 (3), 364 (7), 372 (0), 380 (2), 394 (4), 415 (1), 432 (8), 434 (2), 445 (15), 463 (5), 477 (14), 485 (1), 491 (8), 498 (16), 526 (80), 535 (17), 551 (28), 557 (43), 619 (124), 1952 (451), 2141 (515), 2162 (1340), 2173 (498), 2174 (718), 2202 (376)	43 (0), 56 (1), 64 (0), 78 (0), 85 (0), 88 (0), 98 (0), 102 (0), 110 (0), 115 (3), 118 (0), 144 (2), 190 (1), 221 (0), 237 (0), 284 (6), 325 (8), 338 (2), 359 (4), 365 (3), 376 (0), 385 (4), 404 (1), 441 (14), 454 (1), 476 (5), 480 (1), 490 (1), 499 (15), 509 (10), 514 (5), 541 (100), 545 (42), 546 (22), 570 (33), 605 (93), 1903 (338), 2035 (475), 2055 (418), 2064 (1392), 2065 (489), 2100 (356)
S-but-b	16 (0), 34 (0), 53 (1), 55 (0), 73 (0), 76 (0), 79 (0), 88 (0), 94 (0), 95 (1), 98 (0), 110 (0), 136 (0), 209 (2), 234 (18), 253 (2), 284 (2), 290 (1), 319 (12), 371 (0), 376 (0), 408 (3), 417 (1), 439 (13), 439 (4), 450 (11), 460 (6), 485 (19), 488 (42), 510 (35), 514 (1), 529 (8), 557 (34), 563 (47), 568 (47), 576 (21), 2078 (168), 2100 (1497), 2106 (83), 2112 (1286), 2145 (1551), 2168 (182)	13 (0), 32 (0), 56 (0), 56 (1), 73 (0), 74 (0), 78 (0), 87 (0), 93 (0), 94 (0), 94 (0), 105 (0), 137 (1), 200 (1), 228 (11), 249 (0), 289 (0), 293 (0), 321 (0), 365 (1), 369 (0), 416 (4), 430 (4), 451 (28), 452 (14), 466 (7), 477 (2), 501 (14), 509 (28), 529 (15), 538 (1), 544 (9), 560 (18), 565 (48), 587 (45), 589 (14), 1987 (155), 2004 (1244), 2007 (106), 2015 (1088), 2054 (1213), 2074 (139)

Table S2. The vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol, given in parentheses) for the structures of $Co_2(CO)_6(PH)_2$ at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

isomer	B3LYP/6-311G(d)	BP86/6-311G(d)
Co-but	24 (0), 59 (0), 62 (0), 73 (0), 83 (0), 86 (0), 88 (0), 89 (0), 106 (0), 115 (0), 126 (0), 144 (1), 191 (1), 227 (0), 243 (0), 299 (6), 344 (0), 366 (0), 367 (1), 374 (1), 396 (6), 411 (0), 421 (6), 436 (2), 468 (57), 486 (7), 488 (0), 492 (1), 493 (0), 510 (0), 511 (9), 524 (78), 543 (35), 545 (1), 557 (40), 561 (169), 691 (0), 732 (6), 816 (2), 820 (23), 2105 (82), 2105 (0), 2124 (962), 2130 (1158), 2148 (1747), 2174 (237), 2299 (192), 2305 (33)	18 (0), 55 (0), 60 (0), 70 (0), 81 (0), 82 (0), 85 (0), 85 (0), 102 (0), 110 (0), 119 (0), 135 (0), 181 (0), 221 (0), 242 (0), 293 (8), 341 (0), 364 (0), 364 (1), 372 (0), 398 (6), 409 (0), 420 (8), 435 (7), 490 (0), 494 (23), 499 (4), 500 (0), 502 (0), 517 (0), 522 (0), 533 (59), 547 (46), 554 (73), 556 (4), 565 (113), 664 (0), 704 (8), 794 (22), 797 (2), 2014 (0), 2017 (5), 2033 (840), 2038 (1017), 2061 (1433), 2085 (175), 2209 (165), 2215 (26)
CoP-but	24 (1), 35 (1), 46 (1), 57 (0), 68 (0), 78 (0), 86 (0), 90 (0), 95 (0), 96 (1), 100 (0), 109 (0), 123 (4), 164 (1), 250 (1), 311 (3), 331 (0), 334 (1), 369 (1), 386 (15), 393 (2), 404 (13), 413 (1), 456 (13), 462 (48), 478 (8), 485 (16), 491 (6), 495 (18), 514 (22), 524 (12), 531 (22), 548 (54), 555 (40), 569 (71), 584 (43), 614 (15), 704 (26), 785 (61), 892 (30), 2076 (36), 2092 (504), 2096 (1364), 2109 (739), 2125 (1635), 2165 (569), 2347 (46), 2465 (35)	23 (0), 29 (0), 56 (0), 63 (0), 68 (0), 78 (0), 80 (0), 86 (0), 90 (1), 93 (0), 101 (0), 106 (0), 144 (3), 161 (1), 239 (2), 308 (2), 324 (1), 340 (1), 370 (2), 382 (17), 391 (1), 401 (6), 415 (7), 457 (19), 477 (13), 492 (2), 495 (4), 496 (5), 508 (20), 524 (9), 530 (52), 541 (17), 547 (61), 549 (22), 566 (47), 580 (21), 591 (29), 675 (14), 772 (62), 862 (25), 1990 (29), 2003 (840), 2008 (332), 2018 (981), 2041 (1337), 2072 (390), 2269 (34), 2375 (30)
P-but	20 (0), 36 (0), 48 (0), 48 (3), 61 (0), 72 (0), 79 (0), 85 (0), 88 (0), 96 (0), 97 (0), 101 (0), 151 (1), 159 (3), 229 (37), 237 (1), 318 (0), 321 (1), 363 (0), 384 (10), 388 (2), 390 (12), 416 (1), 446 (31), 447 (4), 461 (8), 463 (2), 480 (8), 487 (63), 502 (14), 515 (0), 518 (23), 566 (77), 571 (61), 574 (79), 580 (24), 642 (3), 711 (69), 723 (4), 815 (131), 2082 (223), 2094 (1635), 2100 (118), 2112 (1134), 2137 (1948), 2164 (197), 2340 (68), 2394 (42)	14 (0), 34 (0), 51 (0), 52 (2), 64 (0), 70 (0), 77 (0), 82 (0), 85 (0), 92 (0), 93 (0), 97 (0), 149 (1), 175 (1), 235 (15), 238 (2), 322 (0), 324 (0), 363 (2), 382 (3), 383 (8), 402 (11), 418 (5), 447 (51), 455 (2), 472 (6), 475 (8), 481 (0), 508 (32), 519 (6), 533 (6), 534 (28), 569 (29), 570 (23), 581 (103), 583 (41), 601 (4), 702 (4), 706 (44), 802 (113), 1995 (215), 2004 (1353), 2006 (43), 2019 (1005), 2051 (1513), 2071 (149), 2234 (74), 2295 (35)
Rhomb	22 (0), 35 (0), 54 (0), 67 (0), 70 (0), 78 (0), 82 (0), 87 (0), 95 (1), 104 (0), 110 (0), 111 (0), 169 (0), 206 (0), 261 (3), 289 (0), 332 (1), 334 (0), 340 (2), 372 (3), 380 (1), 409 (30), 411 (28), 433 (1), 443 (79), 447 (3), 473 (11), 489 (2), 494 (0), 501 (5), 506 (37), 516 (1), 533 (66), 536 (70), 542 (134), 545 (29), 566 (37), 702 (15), 757 (7), 787 (81), 2094 (118), 2111 (75), 2112 (1205), 2116 (1392), 2130 (2625), 2163 (63), 2295 (101), 2324 (76)	20 (0), 35 (0), 48 (0), 67 (0), 71 (0), 74 (0), 79 (0), 85 (0), 92 (0), 99 (0), 105 (0), 106 (0), 163 (0), 205 (0), 237 (3), 288 (2), 334 (0), 336 (1), 339 (1), 372 (1), 386 (2), 412 (0), 421 (25), 432 (3), 459 (0), 460 (41), 482 (8), 487 (8), 499 (2), 506 (0), 516 (8), 526 (68), 540 (111), 540 (32), 548 (13), 550 (39), 561 (57), 672 (19), 732 (7), 773 (73), 2005 (169), 2019 (2), 2020 (1188), 2023 (1092), 2046 (1951), 2073 (61), 2209 (78), 2245 (60)

Table S3. The vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol, given in parentheses) for the structures of $Co_2(CO)_6(PCl)_2$ at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

isomer	B3LYP/6-311G(d)	BP86/6-311G(d)
Co-but	17 (0), 49 (0), 54 (0), 73 (0), 76 (0), 82 (0), 83 (0), 89 (0), 94 (1), 98 (0), 109 (0), 115 (0), 116 (0), 116 (0), 149 (0), 185 (2), 188 (0), 216 (0), 225 (0), 300 (3), 319 (6), 360 (9), 361 (0), 363 (2), 400 (9), 404 (62), 406 (0), 415 (7), 438 (83), 446 (4), 454 (60), 475 (10), 484 (0), 488 (2), 490 (4), 507 (6), 519 (0), 523 (158), 536 (0), 537 (45), 548 (26), 552 (160), 2127 (2), 2130 (0), 2144 (893), 2146 (807), 2160 (1757), 2189 (382)	6 (0), 47 (0), 52 (0), 71 (0), 73 (0), 80 (0), 82 (0), 84 (0), 88 (0), 88 (0), 100 (0), 105 (0), 106 (0), 110 (0), 144 (0), 181 (1), 184 (0), 213 (0), 219 (0), 292 (2), 312 (11), 356 (9), 357 (0), 362 (0), 401 (68), 402 (11), 407 (0), 415 (14), 441 (1), 444 (122), 477 (26), 487 (5), 489 (0), 492 (0), 494 (0), 509 (1), 528 (0), 529 (117), 535 (33), 541 (59), 551 (17), 556 (114), 2032 (10), 2033 (0), 2047 (834), 2049 (712), 2070 (1387), 2095 (266)
CoP-but	21 (0), 28 (1), 42 (1), 55 (0), 64 (0), 69 (0), 80 (1), 82 (0), 84 (0), 85 (1), 97 (0), 98 (1), 103 (0), 109 (1), 124 (4), 141 (4), 167 (1), 203 (4), 233 (7), 299 (8), 328 (1), 333 (1), 337 (2), 371 (11), 383 (15), 397 (12), 409 (2), 437 (52), 445 (8), 461 (53), 473 (4), 478 (22), 481 (10), 489 (19), 502 (25), 510 (66), 522 (25), 536 (36), 547 (83), 553 (62), 567 (71), 579 (63), 2090 (72), 2111 (482), 2115 (759), 2122 (953), 2139 (1692), 2173 (594)	23 (0), 36 (0), 50 (0), 54 (0), 63 (0), 70 (0), 73 (0), 75 (0), 81 (0), 84 (0), 95 (0), 100 (1), 108 (3), 111 (0), 137 (2), 158 (1), 164 (1), 196 (2), 233 (9), 285 (6), 309 (9), 338 (1), 347 (6), 359 (3), 375 (23), 395 (0), 405 (17), 433 (71), 435 (18), 466 (12), 468 (27), 485 (2), 495 (31), 505 (51), 510 (16), 518 (3), 522 (3), 532 (95), 538 (69), 545 (45), 559 (79), 583 (33), 1999 (27), 2003 (223), 2026 (887), 2035 (667), 2052 (1458), 2079 (399)
P-but	17 (0), 29 (0), 48 (0), 49 (4), 57 (0), 63 (1), 71 (0), 75 (0), 81 (0), 87 (0), 89 (0), 95 (0), 97 (0), 115 (1), 144 (2), 151 (3), 153 (0), 186 (0), 232 (2), 244 (17), 315 (0), 321 (0), 364 (0), 373 (24), 379 (15), 386 (15), 406 (0), 409 (5), 427 (75), 436 (18), 453 (0), 459 (5), 471 (0), 485 (50), 492 (11), 499 (35), 506 (1), 527 (66), 554 (124), 564 (72), 567 (63), 571 (64), 2096 (63), 2117 (1369), 2121 (143), 2127 (1146), 2148 (2209), 2174 (202)	11 (0), 24 (0), 50 (0), 53 (2), 58 (0), 64 (0), 70 (0), 73 (0), 78 (0), 81 (0), 83 (0), 90 (0), 92 (0), 111 (0), 151 (1), 154 (0), 163 (0), 181 (0), 238 (2), 246 (3), 320 (0), 324 (0), 360 (29), 361 (1), 378 (6), 384 (8), 391 (87), 423 (19), 435 (6), 439 (38), 467 (2), 467 (1), 477 (6), 497 (32), 504 (14), 518 (33), 524 (29), 529 (44), 551 (92), 561 (73), 570 (81), 573 (59), 2009 (98), 2024 (91), 2026 (1174), 2030 (956), 2059 (1726), 2080 (187)
Rhomb	23 (0), 34 (0), 39 (0), 63 (0), 66 (0), 70 (0), 79 (0), 84 (0), 88 (0), 89 (0), 96 (0), 98 (0), 104 (0), 116 (1), 141 (1), 158 (0), 186 (0), 223 (0), 258 (5), 275 (0), 297 (13), 329 (1), 336 (1), 369 (1), 383 (59), 406 (22), 413 (5), 424 (16), 431 (12), 443 (55), 455 (0), 466 (24), 472 (3), 481 (3), 493 (19), 499 (11), 510 (0), 523 (91), 525 (208), 539 (82), 548 (170), 549 (25), 2120 (300), 2130 (0), 2131 (1170), 2139 (1033), 2148 (2328), 2179 (116)	23 (0), 32 (0), 38 (0), 65 (0), 65 (0), 66 (0), 75 (0), 82 (0), 83 (0), 85 (0), 89 (0), 93 (0), 98 (0), 112 (0), 140 (0), 155 (0), 181 (0), 220 (0), 244 (2), 266 (3), 295 (17), 330 (0), 335 (0), 370 (1), 384 (70), 411 (2), 418 (8), 425 (11), 442 (0), 458 (29), 468 (1), 473 (21), 484 (29), 484 (18), 500 (2), 506 (3), 512 (32), 529 (161), 532 (114), 537 (18), 546 (88), 551 (88), 2023 (274), 2032 (4), 2032 (1036), 2042 (906), 2059 (1769), 2084 (95)

Table S4. The vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol, given in parentheses) for the structures of $Co_2(CO)_6(POH)_2$ at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

isomer	B3LYP/6-311G(d)	BP86/6-311G(d)
Co-but	23 (0), 50 (0), 54 (0), 75 (0), 79 (0), 83 (0), 86 (0), 90 (0), 102 (0), 113 (0), 115 (0), 124 (0), 138 (0), 150 (0), 162 (0), 224 (0), 234 (0), 243 (10), 254 (2), 331 (5), 339 (16), 353 (0), 361 (121), 363 (1), 378 (0), 383 (4), 412 (3), 417 (0), 423 (7), 427 (0), 453 (63), 470 (14), 492 (0), 493 (3), 503 (1), 512 (1), 521 (60), 526 (0), 545 (6), 549 (59), 553 (14), 559 (166), 742 (354), 748 (0), 1056 (208), 1058 (37), 2107 (88), 2117 (0), 2118 (983), 2133 (1021), 2140 (1719), 2178 (484), 3799 (250), 3800 (49)	17 (0), 48 (0), 53 (0), 71 (0), 77 (0), 80 (0), 82 (0), 84 (0), 97 (0), 106 (0), 107 (0), 112 (0), 123 (1), 142 (0), 155 (0), 217 (0), 232 (0), 238 (7), 248 (1), 321 (9), 332 (23), 348 (0), 355 (128), 359 (1), 370 (0), 380 (0), 407 (0), 417 (0), 421 (12), 427 (0), 476 (31), 485 (6), 498 (11), 499 (0), 504 (1), 511 (1), 526 (39), 531 (0), 542 (53), 547 (43), 562 (30), 564 (100), 718 (327), 722 (1), 1024 (28), 1024 (201), 2017 (77), 2023 (0), 2028 (923), 2039 (891), 2055 (1359), 2086 (331), 3655 (220), 3656 (46)
CoP-but	25 (0), 27 (0), 51 (1), 59 (0), 69 (0), 75 (0), 80 (0), 84 (0), 89 (0), 93 (0), 96 (1), 103 (0), 110 (3), 128 (3), 158 (7), 180 (21), 213 (1), 251 (9), 260 (65), 273 (26), 281 (42), 327 (12), 331 (8), 344 (1), 363 (1), 384 (3), 396 (37), 416 (10), 418 (7), 456 (2), 472 (56), 486 (8), 490 (8), 499 (10), 508 (16), 518 (29), 522 (27), 542 (44), 550 (52), 559 (51), 572 (83), 580 (26), 772 (196), 815 (228), 1003 (100), 1037 (129), 2077 (277), 2091 (917), 2095 (137), 2108 (1275), 2127 (1693), 2163 (533), 3740 (10), 3786 (120)	21 (1), 28 (0), 56 (1), 61 (0), 70 (0), 73 (0), 76 (2), 81 (3), 85 (0), 88 (1), 94 (1), 97 (4), 103 (1), 131 (28), 146 (6), 163 (11), 203 (1), 234 (34), 249 (11), 268 (7), 318 (5), 323 (3), 342 (18), 352 (15), 359 (4), 379 (1), 398 (38), 411 (13), 427 (22), 460 (6), 478 (19), 491 (5), 499 (3), 506 (8), 513 (5), 528 (26), 533 (13), 537 (101), 541 (13), 561 (99), 562 (35), 578 (14), 758 (189), 784 (222), 974 (107), 998 (110), 1985 (444), 2005 (109), 2011 (363), 2021 (1144), 2039 (1390), 2072 (430), 3497 (15), 3646 (114)
P-but	26 (0), 35 (2), 44 (0), 48 (1), 49 (1), 73 (0), 74 (0), 90 (0), 93 (0), 95 (0), 98 (0), 99 (0), 124 (1), 148 (0), 172 (2), 189 (12), 207 (1), 245 (1), 265 (37), 298 (3), 329 (15), 336 (7), 339 (10), 345 (6), 390 (5), 391 (0), 397 (6), 400 (8), 426 (0), 457 (6), 459 (5), 475 (55), 491 (9), 494 (1), 500 (13), 509 (38), 515 (1), 565 (85), 571 (49), 579 (10), 584 (67), 593 (106), 705 (108), 801 (176), 1045 (78), 1175 (151), 2086 (170), 2096 (1728), 2104 (543), 2111 (656), 2136 (2354), 2166 (116), 3538 (51), 3811 (113)	25 (0), 37 (1), 42 (0), 49 (2), 52 (0), 70 (0), 72 (0), 84 (0), 88 (0), 89 (0), 93 (0), 93 (0), 115 (2), 146 (0), 176 (4), 189 (2), 202 (1), 245 (1), 268 (31), 298 (1), 329 (1), 332 (10), 336 (13), 351 (6), 382 (0), 383 (5), 388 (8), 398 (25), 426 (0), 459 (50), 471 (0), 493 (2), 494 (23), 506 (3), 509 (2), 521 (10), 525 (14), 564 (64), 572 (38), 585 (30), 591 (22), 618 (113), 670 (99), 778 (154), 1012 (78), 1159 (136), 2000 (210), 2007 (1405), 2010 (437), 2017 (600), 2050 (1736), 2073 (118), 3300 (44), 3664 (96)
Rhomb	23 (0), 35 (0), 46 (0), 62 (0), 66 (0), 76 (0), 79 (0), 83 (0), 84 (0), 93 (0), 97 (1), 103 (0), 108 (0), 168 (1), 171 (4), 208 (1), 235 (5), 243 (2), 273 (22), 287 (10), 307 (37), 334 (0), 341 (12), 343 (4), 372 (8), 418 (15), 420 (1), 435 (9), 447 (13), 460 (46), 466 (62), 469 (4), 485 (10), 494 (6), 502 (22), 513 (42), 524 (3), 526 (60), 538 (121), 548 (49), 555 (146), 563 (114), 726 (168), 816 (219), 1020 (128), 1054 (190), 2077 (997), 2095 (489), 2108 (629), 2118 (1305), 2135 (1702), 2164 (212), 3750 (48), 3769 (69)	21 (0), 33 (0), 41 (0), 60 (0), 65 (0), 73 (0), 76 (0), 78 (0), 82 (0), 88 (0), 92 (0), 96 (0), 99 (0), 152 (13), 169 (1), 199 (0), 230 (6), 239 (1), 264 (17), 270 (16), 303 (40), 332 (1), 338 (4), 340 (11), 371 (8), 419 (5), 420 (1), 437 (1), 446 (38), 464 (29), 477 (28), 479 (19), 487 (14), 501 (11), 509 (8), 513 (4), 524 (69), 529 (37), 541 (151), 545 (35), 557 (73), 561 (81), 711 (166), 785 (182), 978 (115), 1028 (178), 1988 (786), 2003 (415), 2015 (593), 2025 (1013), 2046 (1476), 2071 (155), 3602 (40), 3626 (57)

Diphosphine	15 (0), 19 (0), 30 (0), 42 (0), 66 (0), 76 (0), 80 (0), 88 (1), 92 (0), 97 (0), 103 (1), 112 (2), 115 (0), 132 (0), 164 (7), 185 (18), 198 (3), 212 (2), 260 (17), 260 (23), 304 (88), 317 (3), 322 (2), 334 (3), 369 (6), 396 (2), 399 (2), 403 (5), 429 (8), 433 (5), 474 (4), 477 (16), 481 (32), 490 (5), 494 (17), 508 (10), 521 (19), 534 (20), 557 (97), 573 (43), 600 (39), 606 (107), 713 (107), 756 (158), 1053 (92), 1067 (156), 2075 (890), 2084 (653), 2119 (1496), 2127 (345), 2142 (1491), 2199 (319), 3782 (81), 3794 (48)	17 (0), 23 (0), 32 (0), 46 (0), 66 (0), 73 (0), 73 (0), 80 (1), 85 (0), 93 (0), 95 (0), 98 (0), 102 (0), 127 (1), 157 (8), 182 (4), 196 (9), 208 (2), 249 (11), 280 (23), 310 (14), 323 (0), 331 (2), 342 (42), 373 (34), 385 (20), 391 (5), 393 (14), 430 (16), 465 (6), 468 (28), 482 (6), 488 (4), 502 (2), 510 (6), 515 (5), 525 (7), 532 (50), 557 (71), 572 (35), 587 (68), 598 (39), 702 (105), 736 (152), 1010 (84), 1030 (137), 1995 (724), 2002 (233), 2018 (1009), 2021 (922), 2042 (1270), 2084 (365), 3626 (69), 3636 (44)

Table S5. The vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol, given in parentheses) for the structures of $Co_2(CO)_6(POMe)_2$ at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

isomer	B3LYP/6-311G(d)	BP86/6-311G(d)
Co-but	21 (0), 45 (2), 47 (0), 49 (0), 49 (0), 73 (0), 74 (0), 77 (0), 78 (0), 83 (0), 83 (0), 86 (0), 94 (0), 104 (0), 108 (0), 116 (0), 126 (0), 151 (0), 165 (0), 181 (4), 204 (1), 214 (1), 238 (0), 257 (6), 280 (0), 329 (13), 361 (0), 362 (2), 401 (9), 409 (9), 410 (1), 414 (0), 426 (0), 443 (0), 453 (64), 475 (16), 491 (3), 492 (0), 503 (1), 512 (0), 520 (74), 524 (0), 544 (6), 548 (38), 552 (39), 557 (152), 692 (271), 697 (0), 1047 (650), 1053 (82), 1179 (0), 1179 (1), 1199 (0), 1199 (21), 1487 (10), 1487 (0), 1508 (28), 1508 (2), 1518 (20), 1518 (3), 2103 (67), 2112 (26), 2115 (910), 2128 (996), 2137 (1698), 2174 (504), 3019 (156), 3020 (39), 3084 (6), 3084 (59), 3129 (33), 3129 (12)	15 (0), 44 (0), 47 (0), 47 (3), 53 (0), 70 (0), 71 (0), 71 (0), 77 (0), 80 (0), 81 (0), 81 (0), 87 (0), 95 (0), 100 (0), 111 (0), 113 (0), 137 (0), 158 (0), 175 (3), 199 (1), 209 (0), 232 (0), 249 (9), 271 (0), 317 (20), 357 (0), 358 (2), 399 (10), 404 (2), 407 (5), 413 (0), 424 (1), 441 (8), 475 (33), 485 (7), 497 (13), 498 (0), 505 (2), 511 (1), 525 (44), 529 (0), 541 (53), 545 (46), 560 (32), 562 (89), 671 (252), 675 (0), 1000 (539), 1005 (80), 1133 (0), 1133 (1), 1155 (0), 1155 (11), 1432 (10), 1432 (1), 1454 (25), 1454 (3), 1467 (14), 1467 (6), 2014 (67), 2018 (5), 2025 (874), 2035 (850), 2051 (1348), 2082 (354), 2939 (145), 2940 (41), 3011 (7), 3011 (50), 3053 (30), 3053 (6)
CoP-but	21 (0), 28 (1), 43 (3), 47 (1), 53 (0), 61 (0), 69 (0), 74 (0), 78 (1), 83 (0), 86 (0), 94 (1), 99 (0), 101 (1), 109 (1), 116 (0), 116 (0), 125 (4), 151 (1), 178 (2), 199 (2), 229 (11), 260 (7), 272 (9), 307 (9), 334 (1), 340 (1), 344 (1), 380 (14), 386 (0), 404 (22), 410 (7), 424 (13), 462 (1), 474 (40), 490 (23), 493 (7), 500 (3), 504 (12), 514 (22), 522 (25), 545 (66), 550 (56), 559 (46), 578 (34), 588 (74), 685 (79), 758 (120), 1046 (376), 1056 (221), 1181 (2), 1181 (2), 1197 (9), 1202 (7), 1488 (3), 1492 (4), 1510 (7), 1513 (18), 1513 (12), 1519 (8), 2077 (47), 2083 (498), 2093 (1264), 2102 (732), 2120 (1741), 2158 (601), 3019 (77), 3032 (56), 3085 (24), 3101 (20), 3135 (17), 3150 (19)	18 (0), 24 (0), 42 (3), 48 (0), 58 (0), 64 (0), 66 (1), 74 (1), 75 (0), 77 (1), 83 (0), 85 (0), 90 (0), 102 (0), 105 (1), 110 (0), 119 (1), 142 (1), 160 (1), 164 (1), 199 (4), 225 (3), 250 (9), 258 (3), 314 (18), 320 (1), 330 (3), 347 (4), 367 (10), 376 (8), 394 (15), 409 (5), 431 (14), 458 (10), 482 (10), 498 (8), 502 (3), 507 (2), 516 (9), 526 (30), 528 (20), 536 (68), 545 (6), 559 (76), 566 (81), 577 (14), 662 (72), 733 (126), 995 (331), 1011 (170), 1135 (1), 1136 (1), 1151 (5), 1155 (3), 1434 (4), 1438 (5), 1457 (19), 1459 (10), 1461 (16), 1463 (7), 1990 (120), 1995 (60), 2006 (1134), 2009 (730), 2035 (1428), 2064 (419), 2936 (56), 2953 (59), 3005 (27), 3027 (18), 3062 (14), 3077 (13)

P-but	11 (0), 22 (0), 28 (0), 52 (1), 57 (1), 63 (1), 69 (1), 75 (0), 78 (1), 82 (0), 87 (3), 90 (0), 95 (0), 96 (0), 101 (0), 116 (1), 145 (4), 159 (4), 169 (6), 171 (3), 183 (2), 201 (2), 249 (4), 282 (3), 308 (3), 320 (0), 325 (1), 341 (2), 370 (3), 382 (11), 394 (2), 414 (2), 438 (3), 452 (11), 456 (17), 468 (10), 479 (6), 489 (22), 504 (23), 511 (14), 517 (32), 520 (41), 555 (143), 565 (27), 567 (85), 573 (47), 661 (98), 744 (116), 1049 (221), 1053 (307), 1177 (3), 1181 (0), 1198 (5), 1200 (5), 1483 (5), 1488 (2), 1507 (8), 1510 (22), 1519 (20), 1520 (6), 2078 (478), 2088 (513), 2104 (987), 2108 (956), 2125 (2208), 2159 (294), 3008 (85), 3054 (40), 3066 (30), 3124 (24), 3136 (15), 3153 (14)	14 (0), 22 (0), 26 (0), 51 (1), 59 (1), 61 (2), 64 (1), 73 (0), 75 (0), 80 (0), 83 (0), 88 (1), 90 (0), 94 (1), 95 (0), 111 (1), 140 (3), 152 (3), 163 (0), 179 (1), 180 (1), 196 (3), 249 (4), 278 (0), 310 (3), 321 (0), 322 (1), 331 (1), 364 (5), 377 (4), 390 (2), 407 (4), 445 (14), 456 (29), 467 (1), 477 (14), 485 (1), 498 (7), 516 (4), 522 (3), 530 (54), 533 (63), 555 (107), 564 (10), 569 (85), 574 (51), 631 (102), 718 (116), 995 (181), 999 (239), 1130 (2), 1136 (0), 1149 (4), 1151 (1), 1426 (5), 1433 (2), 1455 (8), 1457 (28), 1462 (12), 1466 (16), 1992 (609), 1998 (158), 2013 (791), 2015 (935), 2040 (1627), 2066 (291), 2931 (82), 2974 (33), 2995 (27), 3052 (18), 3060 (13), 3078 (11)
Rhomb	17 (0), 28 (1), 36 (0), 61 (0), 65 (0), 68 (0), 76 (0), 84 (0), 86 (0), 87 (0), 93 (0), 95 (0), 106 (1), 110 (1), 121 (1), 127 (1), 143 (4), 164 (2), 174 (1), 188 (0), 202 (1), 231 (2), 244 (2), 270 (1), 304 (2), 315 (8), 332 (1), 340 (1), 377 (1), 383 (1), 416 (6), 418 (3), 431 (0), 454 (23), 468 (38), 474 (1), 484 (9), 487 (4), 502 (9), 513 (14), 519 (61), 536 (38), 539 (104), 550 (63), 558 (39), 567 (173), 675 (130), 731 (153), 1043 (317), 1061 (250), 1175 (1), 1181 (2), 1194 (17), 1199 (9), 1487 (5), 1489 (3), 1510 (16), 1510 (31), 1515 (9), 1519 (13), 2088 (869), 2092 (329), 2101 (687), 2112 (1408), 2129 (1751), 2159 (209), 3009 (66), 3043 (44), 3067 (35), 3120 (23), 3129 (22), 3145 (17)	12 (0), 28 (1), 34 (0), 57 (1), 61 (0), 65 (0), 68 (0), 75 (0), 81 (0), 83 (0), 90 (0), 91 (1), 97 (0), 105 (0), 108 (1), 113 (3), 142 (1), 156 (2), 169 (2), 177 (0), 194 (2), 222 (3), 238 (2), 258 (1), 298 (1), 320 (12), 323 (1), 335 (1), 369 (1), 375 (2), 413 (5), 416 (1), 430 (8), 464 (6), 482 (4), 483 (4), 487 (12), 501 (18), 512 (24), 517 (22), 529 (26), 531 (39), 542 (10), 553 (53), 559 (94), 564 (159), 665 (109), 704 (123), 991 (232), 1006 (176), 1129 (1), 1133 (1), 1148 (5), 1153 (6), 1432 (3), 1433 (5), 1454 (21), 1458 (13), 1458 (8), 1463 (26), 1993 (582), 2002 (437), 2010 (939), 2016 (619), 2039 (1722), 2063 (93), 2938 (58), 2967 (34), 3003 (29), 3051 (17), 3060 (16), 3073 (11)
Diphosphine	17 (0), 19 (0), 29 (0), 42 (0), 58 (1), 65 (1), 71 (0), 75 (1), 80 (0), 83 (1), 88 (1), 92 (0), 100 (0), 108 (0), 115 (0), 116 (2), 140 (0), 143 (1), 152 (1), 168 (0), 202 (1), 220 (12), 246 (2), 256 (1), 306 (3), 321 (0), 333 (1), 372 (4), 382 (3), 396 (4), 400 (4), 415 (9), 432 (5), 435 (7), 469 (2), 476 (11), 480 (30), 488 (6), 493 (26), 504 (16), 520 (15), 530 (17), 557 (87), 575 (36), 597 (44), 603 (107), 666 (74), 693 (123), 1047 (309), 1057 (119), 1179 (3), 1184 (2), 1199 (3), 1200 (6), 1486 (3), 1490 (2), 1507 (13), 1510 (8), 1516 (5), 1519 (11), 2076 (831), 2081 (621), 2117 (1303), 2125 (449), 2132 (1606), 2191 (323), 2989 (58), 3013 (52), 3057 (58), 3079 (24), 3122 (24), 3132 (24)	22 (0), 27 (0), 36 (0), 47 (1), 63 (0), 66 (0), 72 (0), 77 (1), 82 (0), 84 (1), 86 (1), 92 (1), 94 (0), 97 (0), 102 (0), 131 (2), 138 (0), 151 (0), 158 (0), 193 (1), 202 (9), 222 (2), 249 (2), 278 (3), 305 (5), 328 (1), 332 (0), 366 (5), 378 (13), 386 (1), 391 (5), 408 (27), 441 (12), 457 (3), 470 (13), 480 (18), 491 (10), 507 (5), 511 (13), 513 (4), 520 (17), 526 (38), 558 (65), 571 (35), 573 (63), 593 (39), 650 (59), 673 (121), 1004 (202), 1012 (88), 1128 (6), 1136 (1), 1152 (2), 1155 (4), 1425 (8), 1432 (2), 1444 (2), 1446 (6), 1459 (10), 1461 (8), 1995 (662), 2000 (202), 2009 (1432), 2015 (379), 2040 (1373), 2074 (353), 2821 (46), 2941 (47), 2965 (70), 3012 (15), 3054 (19), 3064 (17)

Table S6. The vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol, given in parentheses) for the structures of $Co_2(CO)_6(PNH_2)_2$ at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

isomer	B3LYP/6-311G(d)	BP86/6-311G(d)
Co-but	21 (0), 55 (0), 58 (0), 70 (0), 76 (0), 81 (0), 85 (0), 86 (0), 103 (0), 107 (0), 114 (0), 121 (1), 138 (0), 139 (0), 144 (0), 221 (0), 235 (0), 269 (2), 270 (3), 291 (154), 297 (0), 317 (5), 321 (77), 362 (0), 362 (1), 370 (0), 380 (0), 385 (3), 416 (9), 440 (0), 440 (0), 450 (0), 485 (7), 489 (140), 498 (23), 507 (0), 515 (17), 518 (5), 528 (72), 542 (0), 553 (32), 555 (2), 562 (168), 564 (55), 840 (241), 846 (10), 965 (5), 971 (22), 1653 (143), 1655 (10), 2074 (0), 2077 (54), 2094 (1110), 2103 (1382), 2124 (1719), 2151 (155), 3557 (53), 3558 (2), 3673 (71), 3673 (49)	16 (0), 53 (0), 57 (1), 66 (0), 70 (0), 79 (0), 81 (0), 83 (0), 97 (0), 100 (0), 107 (1), 112 (1), 129 (1), 132 (0), 136 (0), 216 (0), 231 (0), 263 (6), 264 (2), 282 (152), 287 (0), 309 (88), 310 (6), 358 (0), 358 (0), 362 (0), 376 (0), 387 (3), 414 (11), 437 (1), 440 (13), 451 (0), 497 (1), 499 (32), 500 (69), 511 (0), 518 (34), 519 (0), 537 (44), 545 (0), 550 (48), 557 (38), 561 (45), 564 (107), 825 (196), 830 (10), 931 (4), 935 (21), 1594 (142), 1596 (10), 1985 (0), 1992 (17), 2005 (936), 2014 (1185), 2039 (1412), 2063 (97), 3452 (43), 3452 (1), 3574 (76), 3575 (50)
CoP-but	26 (0), 31 (0), 55 (1), 59 (1), 68 (0), 78 (0), 82 (0), 84 (0), 90 (0), 93 (0), 97 (0), 104 (0), 115 (2), 137 (5), 147 (7), 179 (2), 213 (1), 251 (0), 270 (4), 290 (9), 303 (23), 319 (3), 339 (2), 343 (2), 363 (7), 391 (4), 394 (24), 406 (65), 417 (26), 428 (169), 441 (163), 463 (6), 475 (117), 488 (14), 492 (17), 503 (9), 513 (21), 521 (33), 529 (25), 537 (13), 551 (84), 562 (51), 564 (92), 579 (26), 828 (45), 869 (78), 981 (11), 989 (19), 1640 (15), 1643 (67), 2059 (231), 2074 (999), 2085 (199), 2092 (1230), 2117 (1645), 2152 (607), 3543 (11), 3551 (32), 3647 (28), 3657 (29)	20 (0), 24 (1), 59 (1), 62 (1), 68 (1), 72 (1), 78 (0), 83 (0), 85 (1), 86 (1), 90 (0), 103 (3), 106 (1), 141 (10), 154 (2), 163 (2), 200 (3), 247 (2), 260 (3), 282 (2), 296 (19), 317 (2), 334 (8), 345 (5), 358 (10), 379 (7), 383 (19), 403 (38), 411 (66), 422 (95), 463 (18), 468 (159), 482 (99), 492 (19), 503 (3), 507 (9), 514 (3), 527 (4), 532 (124), 539 (37), 544 (47), 559 (57), 563 (56), 577 (18), 809 (29), 848 (73), 943 (9), 952 (24), 1578 (16), 1582 (61), 1974 (162), 1987 (730), 1994 (439), 2010 (824), 2030 (1353), 2061 (453), 3413 (4), 3448 (35), 3525 (31), 3559 (31)
P-but	11 (0), 28 (1), 50 (1), 53 (2), 61 (0), 69 (0), 73 (0), 78 (0), 82 (2), 86 (0), 93 (0), 94 (0), 136 (3), 142 (0), 166 (3), 186 (3), 219 (1), 235 (4), 251 (20), 291 (15), 317 (1), 318 (3), 323 (3), 362 (10), 387 (14), 392 (11), 399 (3), 401 (55), 438 (16), 451 (1), 457 (11), 464 (4), 479 (6), 488 (7), 494 (56), 505 (49), 519 (9), 523 (33), 529 (68), 554 (125), 561 (101), 567 (20), 573 (59), 586 (266), 814 (35), 851 (62), 1016 (32), 1035 (1), 1642 (25), 1648 (133), 2063 (643), 2074 (1483), 2086 (75), 2104 (1208), 2119 (1923), 2152 (386), 3473 (3), 3547 (32), 3616 (25), 3649 (19)	24 (0), 34 (1), 39 (0), 51 (1), 55 (1), 70 (0), 72 (0), 78 (0), 85 (0), 88 (0), 88 (0), 91 (0), 126 (1), 153 (1), 162 (3), 177 (1), 217 (0), 236 (5), 260 (3), 301 (1), 320 (6), 330 (18), 335 (17), 360 (3), 378 (3), 388 (8), 404 (2), 409 (58), 428 (47), 440 (9), 467 (3), 474 (16), 490 (5), 500 (1), 505 (29), 512 (22), 528 (14), 537 (24), 545 (54), 559 (108), 567 (68), 571 (52), 585 (13), 601 (246), 803 (43), 818 (35), 980 (42), 991 (3), 1581 (32), 1592 (105), 1981 (821), 1987 (669), 1999 (735), 2010 (497), 2037 (1489), 2061 (288), 3334 (3), 3433 (27), 3519 (33), 3539 (19)
Rhomb	23 (0), 34 (0), 47 (2), 61 (1), 62 (0), 75 (1), 78 (0), 83 (0), 84 (0), 94 (0), 96 (0), 102 (1), 109 (0), 154 (15), 174 (0), 222 (4), 236 (1), 241 (1), 256 (6), 291 (1), 300 (5), 330 (1), 340 (0), 349 (1), 374 (1), 418 (19), 422 (8), 429 (18), 444 (38), 453 (122), 460 (24), 476 (5), 487 (17), 492 (26), 506 (17), 510 (48), 513 (50), 515 (153), 531 (50), 536 (134), 544 (130), 553 (27), 561 (113), 568 (74), 809 (57), 895 (117), 971 (61), 983 (11), 1640 (139), 1657 (52), 2061 (200), 2075 (631), 2080 (821), 2092 (1537), 2109 (2001), 2139 (88), 3529 (10), 3555 (44), 3624 (26), 3662 (22)	18 (0), 31 (0), 39 (1), 57 (1), 63 (0), 69 (1), 74 (0), 79 (0), 80 (0), 88 (1), 91 (0), 94 (0), 101 (1), 153 (15), 166 (0), 213 (6), 231 (0), 238 (1), 248 (2), 283 (1), 293 (7), 331 (3), 335 (1), 339 (3), 363 (5), 390 (143), 414 (3), 418 (10), 439 (1), 447 (17), 466 (18), 473 (14), 485 (19), 492 (41), 506 (15), 509 (77), 513 (13), 520 (160), 526 (84), 540 (140), 543 (22), 555 (60), 560 (47), 571 (65), 799 (49), 868 (86), 932 (39), 940 (35), 1573 (138), 1597 (47), 1977 (319), 1986 (566), 1992 (611), 2004 (1192), 2024 (1617), 2050 (96), 3432 (13), 3457 (41), 3533 (24), 3571 (22)

Table S7. The vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol, given in parentheses) for the structures of $Co_2(CO)_6(PNMe_2)_2$ at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

isomer	B3LYP/6-311G(d)	BP86/6-311G(d)
Co-but	21 (0), 25 (0), 37 (1), 50 (0), 61 (2), 69 (0), 70 (0), 78 (0), 80 (0), 91 (0), 95 (0), 99 (0), 101 (2), 109 (1), 111 (0), 132 (0), 136 (0), 151 (0), 164 (1), 175 (1), 188 (0), 198 (0), 205 (0), 219 (1), 234 (9), 245 (0), 267 (0), 293 (8), 331 (0), 342 (11), 352 (0), 354 (10), 385 (6), 387 (6), 392 (10), 415 (0), 421 (10), 422 (0), 431 (14), 452 (0), 478 (73), 493 (46), 493 (12), 508 (2), 512 (22), 515 (1), 527 (48), 527 (11), 552 (5), 553 (62), 562 (1), 567 (114), 658 (127), 666 (6), 982 (499), 987 (31), 1074 (5), 1074 (11), 1121 (0), 1121 (4), 1165 (0), 1165 (6), 1194 (0), 1195 (46), 1302 (87), 1302 (0), 1457 (3), 1457 (6), 1486 (13), 1486 (1), 1503 (1), 1503 (6), 1515 (9), 1515 (34), 1521 (0), 1521 (12), 1533 (5), 1533 (4), 2072 (8), 2073 (32), 2081 (1100), 2092 (1362), 2114 (1839), 2141 (226), 2998 (74), 2998 (53), 3005 (320), 3006 (0), 3046 (1), 3046 (127), 3051 (1), 3051 (19), 3133 (17), 3134 (3), 3203 (8), 3203 (6)	22 (0), 26 (0), 42 (1), 49 (0), 57 (3), 65 (0), 69 (0), 76 (0), 77 (0), 86 (0), 92 (0), 95 (2), 97 (0), 103 (1), 104 (0), 125 (0), 129 (0), 149 (0), 162 (2), 165 (0), 179 (0), 197 (0), 202 (0), 210 (1), 225 (11), 233 (1), 261 (1), 275 (6), 313 (1), 325 (15), 344 (0), 346 (11), 372 (11), 375 (1), 382 (7), 403 (0), 406 (20), 417 (0), 427 (1), 440 (2), 484 (22), 496 (4), 501 (47), 510 (0), 519 (31), 520 (4), 538 (19), 538 (1), 545 (43), 547 (58), 563 (9), 563 (83), 644 (109), 651 (5), 953 (401), 957 (28), 1037 (3), 1037 (6), 1077 (0), 1078 (4), 1119 (5), 1119 (0), 1160 (0), 1160 (39), 1254 (0), 1254 (46), 1401 (2), 1401 (11), 1428 (0), 1429 (10), 1448 (1), 1448 (5), 1459 (8), 1459 (35), 1465 (0), 1466 (18), 1480 (4), 1480 (5), 1984 (19), 1985 (50), 1992 (881), 2002 (1085), 2026 (1492), 2051 (193), 2921 (64), 2921 (53), 2927 (291), 2928 (0), 2974 (0), 2974 (119), 2979 (1), 2979 (4), 3051 (18), 3051 (2), 3116 (6), 3116 (5)
CoP-but	14 (0), 21 (0), 32 (0), 49 (1), 59 (1), 66 (1), 70 (0), 73 (0), 82 (0), 84 (0), 89 (1), 93 (0), 95 (1), 108 (0), 111 (0), 119 (1), 124 (1), 151 (2), 153 (2), 166 (0), 173 (0), 189 (0), 196 (1), 205 (1), 227 (1), 254 (3), 275 (7), 286 (0), 321 (2), 325 (4), 340 (4), 355 (0), 362 (3), 380 (2), 387 (16), 400 (24), 414 (12), 417 (1), 439 (2), 459 (6), 473 (47), 492 (12), 493 (13), 503 (4), 505 (24), 517 (35), 525 (14), 542 (65), 547 (59), 551 (39), 573 (21), 578 (69), 629 (23), 699 (57), 956 (151), 985 (216), 1072 (12), 1082 (12), 1121 (2), 1122 (3), 1166 (6), 1168 (3), 1189 (26), 1208 (45), 1270 (9), 1299 (43), 1458 (2), 1461 (3), 1487 (4), 1488 (1), 1498 (12), 1501 (3), 1511 (25), 1512 (5), 1514 (10), 1517 (10), 1533 (9), 1534 (13), 2055 (51), 2072 (1017), 2074 (248), 2086 (1022), 2105 (1682), 2143 (761), 2961 (83), 2968 (179), 2995 (27), 3000 (102), 3059 (27), 3064 (19), 3071 (43), 3076 (34), 3110 (22), 3139 (10), 3147 (11), 3152 (6)	15 (0), 22 (0), 31 (0), 38 (0), 52 (2), 61 (1), 68 (0), 69 (1), 78 (1), 80 (1), 84 (0), 86 (0), 89 (0), 103 (1), 108 (2), 110 (1), 114 (1), 141 (1), 154 (0), 163 (1), 168 (1), 182 (0), 186 (1), 193 (1), 209 (1), 237 (1), 251 (6), 274 (1), 301 (2), 327 (2), 338 (5), 345 (7), 350 (4), 365 (2), 372 (7), 381 (28), 404 (13), 414 (3), 425 (6), 459 (14), 481 (17), 498 (6), 503 (8), 509 (6), 519 (5), 526 (27), 532 (87), 537 (7), 544 (8), 557 (36), 561 (105), 573 (15), 609 (23), 684 (55), 935 (143), 955 (187), 1041 (7), 1046 (7), 1079 (2), 1081 (4), 1118 (2), 1119 (9), 1162 (23), 1171 (42), 1226 (7), 1254 (25), 1403 (5), 1404 (6), 1428 (2), 1430 (6), 1444 (10), 1445 (3), 1457 (5), 1457 (29), 1460 (11), 1463 (10), 1481 (8), 1481 (10), 1965 (20), 1982 (403), 1986 (627), 1996 (928), 2017 (1363), 2049 (554), 2888 (71), 2892 (211), 2925 (23), 2928 (102), 2981 (32), 2984 (6), 2994 (45), 3002 (18), 3032 (19), 3056 (9), 3061 (10), 3068 (4)

P-but	17 (0), 27 (0), 36 (0), 50 (1), 58 (0), 64 (0), 67 (0), 70 (0), 73 (0), 76 (0), 81 (0), 89 (0), 91 (0), 93 (1), 96 (0), 105 (1), 138 (0), 144 (0), 158 (3), 159 (0), 167 (0), 191 (1), 196 (2), 226 (2), 239 (0), 248 (0), 272 (0), 296 (6), 305 (2), 313 (6), 318 (3), 321 (2), 372 (3), 378 (1), 393 (1), 404 (2), 408 (2), 424 (8), 444 (15), 449 (8), 452 (19), 470 (4), 481 (3), 484 (17), 494 (12), 514 (85), 522 (35), 532 (32), 545 (48), 552 (66), 562 (130), 565 (18), 649 (51), 682 (56), 971 (143), 988 (230), 1071 (9), 1078 (8), 1121 (1), 1122 (2), 1165 (8), 1166 (2), 1200 (56), 1213 (23), 1287 (15), 1305 (38), 1451 (5), 1458 (2), 1477 (3), 1485 (4), 1500 (7), 1500 (2), 1510 (22), 1511 (11), 1515 (5), 1516 (11), 1531 (1), 1535 (13), 2067 (554), 2076 (234), 2081 (953), 2093 (1012), 2110 (1849), 2143 (607), 2967 (43), 2986 (75), 3009 (23), 3016 (138), 3054 (42), 3057 (61), 3058 (48), 3062 (4), 3112 (13), 3133 (14), 3159 (4), 3163 (5)	20 (0), 25 (0), 36 (1), 53 (0), 56 (0), 62 (0), 68 (0), 70 (0), 72 (0), 74 (0), 78 (1), 81 (1), 87 (0), 89 (0), 98 (1), 103 (1), 137 (0), 140 (0), 156 (2), 158 (2), 169 (0), 186 (3), 209 (2), 225 (0), 235 (1), 249 (0), 272 (2), 296 (16), 299 (3), 303 (2), 319 (1), 325 (1), 366 (2), 375 (0), 387 (2), 397 (0), 412 (0), 414 (10), 446 (17), 466 (7), 470 (8), 483 (21), 493 (11), 498 (4), 506 (11), 523 (70), 527 (72), 533 (31), 544 (47), 553 (26), 560 (81), 568 (67), 632 (47), 666 (52), 937 (117), 952 (177), 1030 (5), 1038 (4), 1076 (1), 1077 (1), 1119 (13), 1120 (1), 1163 (44), 1170 (23), 1238 (6), 1253 (14), 1392 (7), 1398 (4), 1418 (1), 1425 (5), 1445 (5), 1449 (1), 1453 (16), 1456 (13), 1459 (20), 1465 (7), 1476 (1), 1479 (14), 1975 (521), 1987 (195), 1990 (794), 2002 (854), 2023 (1375), 2050 (546), 2894 (39), 2916 (64), 2937 (18), 2943 (122), 2984 (70), 2986 (5), 2992 (38), 2996 (1), 3036 (11), 3053 (11), 3073 (2), 3074 (4)
Rhomb	22 (1), 31 (1), 38 (0), 49 (1), 60 (1), 63 (0), 69 (2), 77 (2), 82 (0), 86 (0), 93 (1), 97 (0), 101 (2), 104 (0), 109 (0), 116 (1), 123 (4), 132 (0), 153 (3), 167 (4), 182 (0), 195 (3), 211 (1), 218 (1), 229 (5), 236 (0), 257 (3), 289 (5), 305 (9), 312 (8), 339 (1), 346 (2), 373 (2), 385 (0), 387 (2), 410 (3), 418 (5), 425 (2), 442 (2), 473 (17), 474 (5), 480 (10), 487 (30), 506 (45), 510 (16), 514 (18), 526 (49), 536 (40), 547 (161), 554 (57), 564 (31), 571 (49), 646 (76), 689 (61), 968 (229), 995 (206), 1067 (11), 1074 (10), 1115 (1), 1118 (0), 1160 (3), 1164 (14), 1201 (49), 1203 (26), 1290 (29), 1303 (41), 1453 (4), 1455 (4), 1481 (5), 1481 (7), 1502 (10), 1507 (17), 1510 (14), 1513 (13), 1518 (15), 1520 (9), 1528 (6), 1532 (19), 2046 (473), 2065 (588), 2078 (843), 2085 (970), 2099 (1961), 2132 (314), 3003 (53), 3015 (88), 3020 (29), 3027 (120), 3058 (46), 3065 (31), 3073 (37), 3078 (10), 3113 (12), 3155 (10), 3159 (7), 3188 (4)	21 (1), 29 (0), 41 (0), 49 (1), 57 (2), 65 (0), 68 (1), 73 (2), 80 (0), 83 (0), 91 (1), 95 (1), 99 (1), 102 (0), 106 (0), 113 (2), 116 (2), 130 (0), 150 (3), 161 (4), 180 (1), 187 (2), 209 (1), 217 (0), 221 (5), 232 (1), 254 (3), 284 (5), 300 (1), 305 (14), 336 (0), 340 (2), 369 (1), 379 (1), 380 (1), 395 (5), 413 (1), 419 (5), 437 (2), 478 (11), 481 (9), 489 (29), 491 (14), 506 (10), 514 (54), 522 (2), 533 (30), 542 (118), 543 (30), 556 (89), 558 (11), 570 (41), 632 (64), 669 (53), 939 (176), 961 (159), 1033 (6), 1036 (6), 1070 (3), 1076 (0), 1116 (1), 1117 (12), 1162 (33), 1163 (27), 1245 (13), 1253 (19), 1397 (7), 1400 (6), 1424 (3), 1425 (6), 1447 (9), 1451 (16), 1454 (15), 1456 (13), 1462 (19), 1465 (10), 1476 (4), 1477 (20), 1961 (430), 1975 (547), 1990 (646), 1998 (793), 2012 (1526), 2043 (291), 2931 (35), 2938 (96), 2940 (27), 2946 (117), 2991 (49), 2994 (5), 2994 (33), 3001 (8), 3036 (11), 3076 (6), 3081 (7), 3107 (2)

Table S8. The Cartesian coordinates of the optimized $Co_2(CO)_6S_2$ structures at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

Rhomb (C_{2h}) B3LYP
0 1
Co,0,-0.0002587064,-0.0005292538,-0.0000652766
Co,0,0.0002587064,0.0005292538,3.3039173866
C,0,1.4887140474,0.0009338591,-1.0282767537
C,0,-0.9137571576,1.1752949599,-1.028276754
C,0,-0.775155437,-1.5857887458,-0.3123292867
C,0,-1.4887140474,-0.0009338591,4.3321288637
C,0,0.9137571576,-1.1752949599,4.332128864
C,0,0.775155437,1.5857887458,3.6161813967
S,0,-1.3301119056,0.650177067,1.6519260549
S,0,1.3301119056,-0.650177067,1.6519260551
O,0,2.4399963727,-0.0136908313,-1.6485119746
O,0,-1.5096553187,1.9169534564,-1.6485119749
O,0,-1.2676353913,-2.5932888311,-0.4874114191
O,0,-2.4399963727,0.0136908313,4.9523640846
O,0,1.5096553187,-1.9169534564,4.9523640849
O,0,1.2676353913,2.5932888311,3.7912635291

Rhomb (C_{2h}) BP86
0 1
Co,0,-0.0000535325,-0.0001068069,-0.000012623
Co,0,0.0000535326,0.0001068069,3.3787744929
C,0,1.4868563189,0.0018023345,-0.9936326596
C,0,-0.8883666382,1.1922875813,-0.9936326598
C,0,-0.7767846692,-1.5498191047,-0.3852371175
C,0,-1.4868563188,-0.0018023345,4.3723945295
C,0,0.8883666383,-1.1922875813,4.3723945297
C,0,0.7767846692,1.5498191047,3.7639989874
S,0,-1.2851394938,0.6441246296,1.6893809349
S,0,1.2851394938,-0.6441246296,1.689380935
O,0,2.4584581433,-0.0024431924,-1.6124554431
O,0,-1.4732240296,1.9681548132,-1.6124554433
O,0,-1.2819265573,-2.5576641096,-0.6187702748
O,0,-2.4584581433,0.0024431924,4.991217313
O,0,1.4732240296,-1.9681548131,4.9912173132
O,0,1.2819265574,2.5576641096,3.9975321447

Co-but-a (C_{2v}) B3LYP
0 1
Co,0,1.2027142831,0.,0.1017693201
Co,0,-1.2027142831,0.,0.1017693201
C,0,2.5730316109,0.,1.2727350424
C,0,1.5872078799,1.3620807574,-1.0258385139
C,0,1.5872078799,-1.3620807574,-1.0258385139
C,0,-2.5730316109,0.,1.2727350424
C,0,-1.5872078799,1.3620807574,-1.0258385139
C,0,-1.5872078799,-1.3620807574,-1.0258385139
S,0,0.,1.532676987,1.225263995
S,0,0.,-1.532676987,1.225263995
O,0,3.3995250512,0.,2.0472031423
O,0,1.8168764061,2.2271578036,-1.7243961478
O,0,1.8168764061,-2.2271578036,-1.7243961478
O,0,-3.3995250512,0.,2.0472031423
O,0,-1.8168764061,2.2271578036,-1.7243961478
O,0,-1.8168764061,-2.2271578036,-1.7243961478

Co-but-a (C_{2v}) BP86
0 1
Co,0,1.2095853856,0.,0.1032594691
Co,0,-1.2095853856,0.,0.1032594691
C,0,2.5797177931,0.,1.2408132774
C,0,1.5763904607,1.3523066439,-1.0048494391
C,0,1.5763904607,-1.3523066439,-1.0048494391
C,0,-2.5797177931,0.,1.2408132774
C,0,-1.5763904607,1.3523066439,-1.0048494391
C,0,-1.5763904607,-1.3523066439,-1.0048494391
S,0,0.,1.5262053039,1.2404495556
S,0,0.,-1.5262053039,1.2404495556
O,0,3.4370703077,0.,2.0054517731
O,0,1.8139657251,2.2248792621,-1.7176254594
O,0,1.8139657251,-2.2248792621,-1.7176254594
O,0,-3.4370703077,0.,2.0054517731
O,0,-1.8139657251,2.2248792621,-1.7176254594
O,0,-1.8139657251,-2.2248792621,-1.7176254594

S-but-a (C_2) B3LYP
0 1
Co,0,0.2572445336,1.7336872765,-0.0078032912
Co,0,-0.2572445336,-1.7336872765,-0.0078032912
C,0,-0.0806576676,3.0875754141,-1.1381288094
C,0,1.7507981118,2.4108151661,0.6385825291
C,0,-0.5452728913,1.5024080175,1.570798996
C,0,0.0806576676,-3.0875754141,-1.1381288094
C,0,0.5452728913,-1.5024080175,1.570798996
C,0,-1.7507981118,-2.4108151661,0.6385825291
S,0,1.0105526366,-0.2344059586,-1.1598817801
S,0,-1.0105526366,0.2344059586,-1.1598817801
O,0,-0.3807608667,3.9797293147,-1.7810358703
O,0,2.7407093975,2.80399427,1.0414068583
O,0,-1.1228077334,1.4812698732,2.55506237
O,0,0.3807608667,-3.9797293147,-1.7810358703
O,0,1.1228077334,-1.4812698732,2.55506237
O,0,-2.7407093975,-2.80399427,1.0414068583

S-but-a (C_2) BP86
0 1
Co,0,0.2517592454,1.7233346437,-0.0171988296
Co,0,-0.2517592454,-1.7233346437,-0.0171988296
C,0,-0.1401448862,3.0920891194,-1.0705064572
C,0,1.7605168916,2.378251915,0.5565173336
C,0,-0.490240183,1.4988324306,1.5773502062
C,0,0.1401448862,-3.0920891194,-1.0705064572
C,0,0.490240183,-1.4988324306,1.5773502062
C,0,-1.7605168916,-2.378251915,0.5565173336
S,0,1.0111445956,-0.2142004133,-1.1529493551
S,0,-1.0111445956,0.2142004133,-1.1529493551
O,0,-0.4609811286,4.0383102807,-1.6544944894
O,0,2.7836231028,2.7704400182,0.9244331986
O,0,-1.0157674417,1.5318513816,2.6081053927
O,0,0.4609811286,-4.0383102807,-1.6544944894
O,0,1.0157674417,-1.5318513816,2.6081053927
O,0,-2.7836231028,-2.7704400182,0.9244331986

Co-but-b (C_s) B3LYP
0 1
Co,0,1.1079766668,0.,0.0075050292
Co,0,-1.2805210336,0.,1.0787194155
C,0,2.5466602388,0.,1.1996800004
C,0,1.5683104456,1.4168241406,-1.0326509005
C,0,1.5683104456,-1.4168241406,-1.0326509005
C,0,-0.7215093487,0.,-0.7193654175
C,0,-2.42282585,1.3739262376,0.9748181259
C,0,-2.42282585,-1.3739262376,0.9748181259
S,0,0.2582134447,1.6024311582,1.4763637277
S,0,0.2582134447,-1.6024311582,1.4763637277
O,0,3.3866453881,0.,1.9574019839
O,0,1.8578526325,2.3013622007,-1.675732982
O,0,1.8578526325,-2.3013622007,-1.675732982
O,0,-1.2734124473,0.,-1.7410534856
O,0,-3.1495433345,2.2452099065,0.9358535965
O,0,-3.1495433345,-2.2452099065,0.9358535965

Co-but-b (C_s) BP86
0 1
Co,0,1.0844033976,0.,-0.0115739589
Co,0,-1.2383145782,0.,1.0377265895
C,0,2.4161456961,0.,1.2377012573
C,0,1.5580172587,1.3830926076,-1.0333027886
C,0,1.5580172587,-1.3830926076,-1.0333027886
C,0,-0.7756147935,0.,-0.7712093222
C,0,-2.3589285009,1.357981052,0.98639283
C,0,-2.3589285009,-1.357981052,0.98639283
S,0,0.2870853962,1.6009138577,1.5023941288
S,0,0.2870853962,-1.6009138577,1.5023941288
O,0,3.2863295609,0.,1.9893676121
O,0,1.8889422249,2.2607779729,-1.6954876293
O,0,1.8889422249,-2.2607779729,-1.6954876293
O,0,-1.3073209578,0.,-1.8146169696
O,0,-3.1099634465,2.2326867756,0.9788043801
O,0,-3.1099634465,-2.2326867756,0.9788043801

S-but-b (C_s) B3LYP
0 1
Co,0,0.1116203429,1.7701656753,0.014659054
Co,0,0.1116203429,-1.7701656753,0.014659054
C,0,-0.0871735874,1.5611017128,1.7803773108
C,0,1.2369407728,3.0157880945,-0.6329789318
C,0,-1.3611631252,2.7042281207,-0.2257428753
C,0,-0.0871735874,-1.5611017128,1.7803773108
C,0,1.2369407728,-3.0157880945,-0.6329789318
C,0,-1.3611631252,-2.7042281207,-0.2257428753
S,0,1.4711124316,0.,-0.4814178967
S,0,-0.3304901515,0.,-1.4959708213
O,0,-0.1406088833,1.6145120002,2.9192128781
O,0,1.9705150652,3.8340350168,-0.9361029719
O,0,-2.3354417255,3.2621094833,-0.4170541051
O,0,-0.1406088833,-1.6145120002,2.9192128781
O,0,1.9705150652,-3.8340350168,-0.9361029719
O,0,-2.3354417255,-3.2621094833,-0.4170541051

S-but-b (C_s) BP86
0 1
Co,0,0.1206431864,1.7641282549,-0.0028411849
Co,0,0.1206431864,-1.7641282549,-0.0028411849
C,0,-0.0693384398,1.535491284,1.7494218321
C,0,1.2285486716,3.0087630128,-0.6034280899
C,0,-1.3289973161,2.698940649,-0.2426943177
C,0,-0.0693384398,-1.535491284,1.7494218321
C,0,1.2285486716,-3.0087630128,-0.6034280899
C,0,-1.3289973161,-2.698940649,-0.2426943177
S,0,1.4366423667,0.,-0.565101063
S,0,-0.4173505378,0.,-1.4674619708
O,0,-0.1364172379,1.6377876323,2.9004471254
O,0,1.9506078724,3.870630822,-0.8783021521
O,0,-2.3136926513,3.2731109845,-0.4340156963
O,0,-0.1364172379,-1.6377876323,2.9004471254
O,0,1.9506078724,-3.870630822,-0.8783021521
O,0,-2.3136926513,-3.2731109845,-0.4340156963

Table S9. The Cartesian coordinates of the optimized $Co_2(CO)_6(PH)_2$ structures at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

$Co_2(CO)_6(PH)_2$ Co-but (C_{2v}) B3LYP

0 1
Co,0,1.236135419,0.,0.1952236121
Co,0,-1.236135419,0.,0.1952236121
C,0,2.6138164707,0.,1.3162562449
C,0,1.5704043494,1.349408579,-0.9328534385
C,0,1.5704043494,-1.349408579,-0.9328534385
C,0,-2.6138164707,0.,1.3162562449
C,0,-1.5704043494,1.349408579,-0.9328534385
C,0,-1.5704043494,-1.349408579,-0.9328534385
P,0,0.,1.4339433479,1.4945918204
P,0,0.,-1.4339433479,1.4945918204
O,0,3.503706932,0.,2.0241023329
O,0,1.7911932423,2.2036692478,-1.6527499774
O,0,1.7911932423,-2.2036692478,-1.6527499774
O,0,-3.503706932,0.,2.0241023329
O,0,-1.7911932423,2.2036692478,-1.6527499774
O,0,-1.7911932423,-2.2036692478,-1.6527499774
H,0,0.,2.6429145913,0.7257104965
H,0,0.,-2.6429145913,0.7257104965

$Co_2(CO)_6(PH)_2$ Co-but (C_{2v}) BP86

0 1
Co,0,1.240683539,0.,0.192028878
Co,0,-1.240683539,0.,0.192028878
C,0,2.6136690236,0.,1.2987525156
C,0,1.5648341519,1.3447187206,-0.922759788
C,0,1.5648341519,-1.3447187206,-0.922759788
C,0,-2.6136690236,0.,1.2987525156
C,0,-1.5648341519,1.3447187206,-0.922759788
C,0,-1.5648341519,-1.3447187206,-0.922759788
P,0,0.,1.4239096595,1.5056686632
P,0,0.,-1.4239096595,1.5056686632
O,0,3.5199915295,0.,2.0107941736
O,0,1.7934934216,2.2085323173,-1.6534583324
O,0,1.7934934216,-2.2085323173,-1.6534583324
O,0,-3.5199915295,0.,2.0107941736
O,0,-1.7934934216,2.2085323173,-1.6534583324
O,0,-1.7934934216,-2.2085323173,-1.6534583324
H,0,0.,2.6489236662,0.7327187672
H,0,0.,-2.6489236662,0.7327187672

$Co_2(CO)_6(PH)_2$ CoP-but (C_1) B3LYP

0 1
Co,0,1.2269529232,0.7174056736,0.0484461312
Co,0,-1.1770566559,-0.8972961128,-0.041716867
C,0,1.7231482833,-0.9737045503,-0.0833364439
C,0,2.6349835127,1.3437225878,0.9681499701
C,0,1.2721194953,1.2473510111,-1.6601124625
C,0,-1.0249186198,-1.8886915224,-1.5161060123
C,0,-2.5286576834,0.0954992549,-0.608590155
C,0,-1.2580419488,-2.2221528131,1.1448988065
P,0,-0.12180863,2.5813751184,0.7436007268
P,0,-0.499451718,0.5709187095,1.3677931332
O,0,2.156671534,-2.0305107324,-0.1462959471
O,0,3.5454683408,1.7543007659,1.517310074
O,0,1.3358103156,1.619289561,-2.7375545739
O,0,-0.9059096364,-2.505532952,-2.465342799
O,0,-3.482632262,0.6499225075,-0.9015764989
O,0,-1.4257065157,-3.0467224887,1.9158472356
H,0,-1.0786682628,2.5532187801,-0.310933011
H,0,-0.4083024721,0.441607202,2.7655186932

$Co_2(CO)_6(PH)_2$ CoP-but (C_1) BP86

0 1
Co,0,1.1805238517,0.6890325618,0.01350239
Co,0,-1.1139181371,-0.8574366946,0.0009432802
C,0,1.6065627733,-1.0234663188,-0.0572981958
C,0,2.5894248245,1.2682604482,0.9261820927
C,0,1.3412699818,1.2296634342,-1.6784047422
C,0,-0.8949678946,-1.7130236975,-1.5295843534
C,0,-2.5777891946,-0.010048333,-0.471569182
C,0,-1.2396315511,-2.2132967379,1.1375341022
P,0,-0.134977777,2.6337764033,0.6241599785
P,0,-0.4979619316,0.6577040224,1.3763521941
O,0,2.0703297455,-2.0856092179,-0.076965548
O,0,3.5268370417,1.6312328343,1.4948093329
O,0,1.4735384846,1.6103543236,-2.7610616675
O,0,-0.7647034879,-2.2619409941,-2.5380782574
O,0,-3.6119085716,0.4475118778,-0.7239188615
O,0,-1.4575480801,-3.0860976504,1.8657375134
H,0,-1.1483292389,2.5163881892,-0.3907115626
H,0,-0.3627508385,0.5769955494,2.7883714865

$Co_2(CO)_6(PH)_2$ P-but (C_s) B3LYP

0 1
Co,0,0.013808156,1.9062910811,-0.0274530158
Co,0,0.013808156,-1.9062910811,-0.0274530158
C,0,-0.1074004928,1.7328605607,1.7494515412
C,0,1.2105503963,2.9754028552,-0.7939388437
C,0,-1.3858186986,2.9637301422,-0.2444509379
C,0,-0.1074004928,-1.7328605607,1.7494515412
C,0,1.2105503963,-2.9754028552,-0.7939388437
C,0,-1.3858186986,-2.9637301422,-0.2444509379
P,0,1.0980249996,0.,-0.4254231076
P,0,-0.9688384504,0.,-1.1393142675
O,0,-0.1056168774,1.7271362225,2.8902635867
O,0,2.0167474923,3.6638599204,-1.2190979251
O,0,-2.3131108998,3.6053457073,-0.405193533
O,0,-0.1056168774,-1.7271362225,2.8902635867
O,0,2.0167474923,-3.6638599204,-1.2190979251
O,0,-2.3131108998,-3.6053457073,-0.405193533
H,0,1.9597972966,0.,-1.5488935332
H,0,-0.6733020074,0.,-2.5321848304

$Co_2(CO)_6(PH)_2$ P-but (C_s) BP86

0 1
Co,0,0.0207216402,1.8845624137,-0.0410804684
Co,0,0.0207216402,-1.8845624137,-0.0410804684
C,0,-0.0870386761,1.7158853853,1.724440739
C,0,1.2450546515,2.9386293525,-0.7391187562
C,0,-1.3524195775,2.9509314349,-0.281088533
C,0,-0.0870386761,-1.7158853853,1.724440739
C,0,1.2450546515,-2.9386293525,-0.7391187562
C,0,-1.3524195775,-2.9509314349,-0.281088533
P,0,1.0284510101,0.,-0.5313774187
P,0,-1.0884830636,0.,-1.0767370065
O,0,-0.0749165401,1.7483641423,2.8802981505
O,0,2.0831711422,3.6421068052,-1.1198546505
O,0,-2.2826888553,3.6130107573,-0.4584116374
O,0,-0.0749165401,-1.7483641423,2.8802981505
O,0,2.0831711422,-3.6421068052,-1.1198546505
O,0,-2.2826888553,-3.6130107573,-0.4584116374
H,0,1.8845711891,0.,-1.6775032778
H,0,-0.8423067034,0.,-2.4971859857

$Co_2(CO)_6(PH)_2$ Rhomb (C_s) B3LYP	$Co_2(CO)_6(PH)_2$ Rhomb (C_s) BP86
0 1	0 1
Co,0,0.0176952166,-0.0144482145,0.0134832205	Co,0,0.,0.,0.
Co,0,0.0176952163,-0.0144482143,3.5331586106	Co,0,-0.0000000002,0.0000000002,3.5466418311
C,0,1.7950166685,-0.0131361713,0.0283601173	C,0,1.763878537,0.,0.0139980486
C,0,-0.5015420395,1.2951448914,-1.1247020661	C,0,-0.4864161031,1.2992416857,-1.1440719687
C,0,-0.3603638962,-1.4529260211,-0.9681344713	C,0,-0.3595694908,-1.453702982,-0.9435120607
C,0,-0.5015420399,1.2951448917,4.6713438969	C,0,-0.4864161034,1.2992416861,4.6907137996
C,0,-0.3603638965,-1.4529260208,4.5147763025	C,0,-0.3595694912,-1.4537029817,4.4901538919
C,0,1.7950166683,-0.0131361711,3.518281714	C,0,1.7638785368,0.0000000002,3.5326437827
P,0,0.032864461,1.5941391063,1.7733209155	P,0,0.0262873873,1.5690841653,1.7733209155
P,0,-0.6689899694,-0.9812458,1.7733209156	P,0,-0.7250331509,-0.9561937149,1.7733209156
O,0,2.9347874912,-0.0397677011,0.0310776145	O,0,2.9189083913,-0.0364807948,0.0015530792
O,0,-0.8172149266,2.1435387614,-1.8144885254	O,0,-0.787176189,2.1540172955,-1.8580889493
O,0,-0.5811696893,-2.4091136553,-1.5475361769	O,0,-0.5668196088,-2.4385999854,-1.5108480987
O,0,-0.817214927,2.1435387619,5.3611303561	O,0,-0.7871761894,2.1540172959,5.4047307801
O,0,-0.5811696897,-2.4091136549,5.0941780082	O,0,-0.5668196092,-2.438599985,5.05748993
O,0,2.934787491,-0.0397677009,3.515564217	O,0,2.9189083911,-0.0364807945,3.5450887522
H,0,1.4064778631,1.9981760176,1.7733209155	H,0,1.4141725993,1.9785806725,1.7733209155
H,0,-0.9322372831,-2.3832219046,1.7733209156	H,0,-0.8695124375,-2.3882020213,1.7733209156

Table S10. The Cartesian coordinates of the optimized $Co_2(CO)_6(PCl)_2$ isomers at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

$Co_2(CO)_6(PCl)_2$ Co-but (C_{2v}) B3LYP
0 1
Co,0,1.2340990934,0.,0.2269604399
Co,0,-1.2340990934,0.,0.2269604399
C,0,2.6499705384,0.,1.3040348844
C,0,1.5840933173,1.3396359423,-0.9275405639
C,0,1.5840933173,-1.3396359423,-0.9275405639
C,0,-2.6499705384,0.,1.3040348844
C,0,-1.5840933173,1.3396359423,-0.9275405639
C,0,-1.5840933173,-1.3396359423,-0.9275405639
P,0,0.,1.3385658754,1.6023791254
P,0,0.,-1.3385658754,1.6023791254
O,0,3.5605487184,0.,1.9827285321
O,0,1.8214924364,2.1620281957,-1.673217061
O,0,1.8214924364,-2.1620281957,-1.673217061
O,0,-3.5605487184,0.,1.9827285321
O,0,-1.8214924364,2.1620281957,-1.673217061
O,0,-1.8214924364,-2.1620281957,-1.673217061
Cl,0,0.,3.3807043956,0.9628854261
Cl,0,0.,-3.3807043956,0.9628854261

$Co_2(CO)_6(PCl)_2$ Co-but (C_{2v}) BP86
0 1
Co,0,1.240712986,0.,0.2096260054
Co,0,-1.240712986,0.,0.2096260054
C,0,2.6578660327,0.,1.2608578885
C,0,1.5690021823,1.3430394626,-0.9254944779
C,0,1.5690021823,-1.3430394626,-0.9254944779
C,0,-2.6578660327,0.,1.2608578885
C,0,-1.5690021823,1.3430394626,-0.9254944779
C,0,-1.5690021823,-1.3430394626,-0.9254944779
P,0,0.,1.3094494774,1.6154641377
P,0,0.,-1.3094494774,1.6154641377
O,0,3.5903280928,0.,1.9364714395
O,0,1.8023709112,2.1866405775,-1.6729981779
O,0,1.8023709112,-2.1866405775,-1.6729981779
O,0,-3.5903280928,0.,1.9364714395
O,0,-1.8023709112,2.1866405775,-1.6729981779
O,0,-1.8023709112,-2.1866405775,-1.6729981779
Cl,0,0.,3.3716997364,1.0521251875
Cl,0,0.,-3.3716997364,1.0521251875

$Co_2(CO)_6(PCl)_2$ CoP-but (C_1) B3LYP
0 1
Co,0,-0.0120646596,-0.0016002898,0.0048677692
Co,0,-0.0198658606,0.0234560192,2.9270852939
C,0,1.6722850744,0.049529839,0.5695804713
C,0,0.1888785792,0.877433852,-1.5457026145
C,0,-0.2003905886,-1.7575654998,-0.3337855411
C,0,0.9583550506,-1.4144306974,3.3324540595
C,0,-1.5029901727,-0.587176304,3.6828902481
C,0,1.021743834,1.281243324,3.6742676631
P,0,-2.3152339841,0.511790488,-0.0268166208
P,0,-0.9631774143,1.2562893511,1.4724107675
O,0,2.7858429104,0.1078755967,0.8160999364
O,0,0.3235853496,1.4074269206,-2.5434520447
O,0,-0.3418573845,-2.8596705398,-0.5798072798
O,0,1.5828643574,-2.3378438329,3.5579417317
O,0,-2.3815340746,-0.8939555382,4.3397157489
O,0,1.5981380814,2.0734208534,4.2534873891
Cl,0,-0.8123683353,3.3397544553,1.3813555105
Cl,0,-3.3595641287,-1.0766207904,0.9444395626

$Co_2(CO)_6(PCl)_2$ CoP-but (C_1) BP86
0 1
Co,0,0.081073748,-0.0613182093,0.1625897057
Co,0,-0.0424683398,0.1550227929,2.8275153157
C,0,1.7097641797,0.2003305957,0.8274975409
C,0,0.2557001173,0.9295852622,-1.2901112131
C,0,0.1705835048,-1.7645395433,-0.4045733384
C,0,0.2761498205,-1.5743863875,2.785780668
C,0,-1.2892376304,0.0201113358,4.0417318063
C,0,1.2345690994,1.1727589462,3.6119724977
P,0,-2.3018276626,0.0075609123,-0.0665351589
P,0,-1.2136195827,1.1783853962,1.3985901997
O,0,2.8385145182,0.3542523709,1.0322500239
O,0,0.4037054755,1.5560252181,-2.2464484635
O,0,0.2055035828,-2.8341842311,-0.8295357504
O,0,0.490488227,-2.7116823607,2.8136458208
O,0,-2.0946607023,-0.0514513986,4.8665644054
O,0,2.0130690596,1.7513317572,4.2362979422
Cl,0,-1.416154713,3.2355946082,1.026012497
Cl,0,-3.0985060681,-1.5640398582,1.133787552

$Co_2(CO)_6(PCl)_2$ P-but (C_s) B3LYP
0 1
Co,0,-0.0242960382,1.8900398106,0.3851391523
Co,0,-0.0242960382,-1.8900398106,0.3851391523
C,0,0.0171096746,1.7262725949,2.1637827196
C,0,1.4232971001,2.9072356289,0.2238470091
C,0,-1.1668628902,3.0327347645,-0.3900860722
C,0,0.0171096746,-1.7262725949,2.1637827196
C,0,1.4232971001,-2.9072356289,0.2238470091
C,0,-1.1668628902,-3.0327347645,-0.3900860722
P,0,1.0689323211,0.,-0.5919045301
P,0,-1.0716174834,0.,-0.0332078606
O,0,-0.01133067,1.7124493153,3.3029647896
O,0,2.3746077951,3.5183816479,0.1045543249
O,0,-1.9271120793,3.7604856295,-0.8229104272
O,0,-0.01133067,-1.7124493153,3.3029647896
O,0,2.3746077951,-3.5183816479,0.1045543249
O,0,-1.9271120793,-3.7604856295,-0.8229104272
Cl,0,1.0459982424,0.,-2.7289695931

$Co_2(CO)_6(PCl)_2$ P-but (C_s) BP86
0 1
Co,0,-0.0357137827,1.8668440768,0.3676810478
Co,0,-0.0357137827,-1.8668440768,0.3676810478
C,0,0.0023392982,1.7097384745,2.1348515792
C,0,1.3919101134,2.8885378916,0.1695004923
C,0,-1.2146904199,3.0072146121,-0.3090134392
C,0,0.0023392982,-1.7097384745,2.1348515792
C,0,1.3919101134,-2.8885378916,0.1695004923
C,0,-1.2146904199,-3.0072146121,-0.3090134392
P,0,1.1946335149,0.,-0.5181344787
P,0,-0.9934668917,0.,-0.1332316841
O,0,-0.0277434771,1.7176160304,3.2892136857
O,0,2.3486007691,3.5174981238,0.0310729147
O,0,-2.0106741773,3.7507248079,-0.6900164229
O,0,-0.0277434771,-1.7176160304,3.2892136857
O,0,2.3486007691,-3.5174981238,0.0310729147
O,0,-2.0106741773,-3.7507248079,-0.6900164229
Cl,0,1.2574532575,0.,-2.6752324342

Cl,0,-2.4101388616,0.,-1.6368490101

$Co_2(CO)_6(PCl)_2$ Rhomb (C_s) B3LYP
0 1
Co,0,0.,0.,0.
Co,0,0.0000000007,-0.0000000023,3.5603361012
C,0,1.7930856468,0.,0.0202439248
C,0,-0.3811083399,1.3624221489,-1.1065935955
C,0,-0.5180047653,-1.3438905553,-1.1016273616
C,0,-0.5180047643,-1.343890559,4.6619634613
C,0,1.7930856474,-0.0000000023,3.5400921758
C,0,-0.3811083388,1.3624221452,4.6669296986
P,0,-0.539584378,0.9663008025,1.7801680513
P,0,-0.2768001064,-1.564293677,1.7801680496
O,0,2.928552513,0.0368473369,0.0228848877
O,0,-0.6096315913,2.2516643404,-1.7757103353
O,0,-0.833740002,-2.2092069293,-1.7672265971
O,0,-0.8337400007,-2.2092069339,5.3275626958
O,0,2.9285525137,0.0368473347,3.5374512125
O,0,-0.60963159,2.2516643358,5.3360464397
Cl,0,-1.0718028509,3.0011648888,1.7801680527
Cl,0,1.523223411,-2.7655593284,1.7801680485

Cl,0,-2.3626765236,0.,-1.716329119

$Co_2(CO)_6(PCl)_2$ Rhomb (C_s) BP86
0 1
Co,0,-0.0109461164,0.0012528167,-0.0131390247
Co,0,-0.0109461158,0.0012528143,3.5734751259
C,0,1.7642689899,0.016783842,0.0230298691
C,0,-0.3940195356,1.3503636527,-1.1175311549
C,0,-0.4868708845,-1.3535751315,-1.0969100661
C,0,-0.4868708834,-1.3535751353,4.6572461657
C,0,1.7642689906,0.0167838397,3.5373062315
C,0,-0.3940195345,1.3503636489,4.677867258
P,0,-0.5587294819,0.9736697818,1.7801680513
P,0,-0.3060351406,-1.5400693755,1.7801680497
O,0,2.915449622,0.0598516546,0.0286360443
O,0,-0.6261977848,2.244840524,-1.8051748971
O,0,-0.7786276402,-2.2402197864,-1.772781528
O,0,-0.7786276389,-2.240219791,5.3331176266
O,0,2.9154496226,0.0598516524,3.5317000559
O,0,-0.6261977835,2.2448405194,5.3655110014
Cl,0,-0.9517871222,3.0403044535,1.7801680527
Cl,0,1.4437814425,-2.799214635,1.7801680485

Table S11. The Cartesian coordinates of the optimized $Co_2(CO)_6(POH)_2$ structures at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

$Co_2(CO)_6(POH)_2$ Co-but (C_{2v}) B3LYP

0 1
Co,0,1.2426181879,0.,0.3232459645
Co,0,-1.2426181879,0.,0.3232459645
C,0,2.5683362715,0.,1.4892853071
C,0,1.6127237047,1.3418185775,-0.8190021391
C,0,1.6127237047,-1.3418185775,-0.8190021391
C,0,-2.5683362715,0.,1.4892853071
C,0,-1.6127237047,1.3418185775,-0.8190021391
C,0,-1.6127237047,-1.3418185775,-0.8190021391
P,0,0.,1.4096308723,1.6032039313
P,0,0.,-1.4096308723,1.6032039313
O,0,3.4308130639,0.,2.2346658507
O,0,1.862956228,2.1784184449,-1.547162292
O,0,1.862956228,-2.1784184449,-1.547162292
O,0,-3.4308130639,0.,2.2346658507
O,0,-1.862956228,2.1784184449,-1.547162292
O,0,-1.862956228,-2.1784184449,-1.547162292
O,0,0.,2.9180639836,0.8457866623
O,0,0.,-2.9180639836,0.8457866623
H,0,0.,3.6312172292,1.494158606
H,0,0.,-3.6312172292,1.494158606

$Co_2(CO)_6(POH)_2$ Co-but (C_{2v}) BP86

0 1
Co,0,1.2472563985,0.,0.3035413517
Co,0,-1.2472563985,0.,0.3035413517
C,0,2.5723644992,0.,1.4563108055
C,0,1.6052464663,1.3388695947,-0.8249552275
C,0,1.6052464663,-1.3388695947,-0.8249552275
C,0,-2.5723644992,0.,1.4563108055
C,0,-1.6052464663,1.3388695947,-0.8249552275
C,0,-1.6052464663,-1.3388695947,-0.8249552275
P,0,0.,1.3969050433,1.6066689442
P,0,0.,-1.3969050433,1.6066689442
O,0,3.4507473505,0.,2.2067442225
O,0,1.8589622629,2.1890179484,-1.5607742543
O,0,1.8589622629,-2.1890179484,-1.5607742543
O,0,-3.4507473505,0.,2.2067442225
O,0,-1.8589622629,2.1890179484,-1.5607742543
O,0,-1.8589622629,-2.1890179484,-1.5607742543
O,0,0.,2.933928908,0.8830814983
O,0,0.,-2.933928908,0.8830814983
H,0,0.,3.6229052457,1.5732446162
H,0,0.,-3.6229052457,1.5732446162

$Co_2(CO)_6(POH)_2$ CoP-but (C_1) B3LYP

0 1
Co,0,-1.2764123803,-0.3238396514,0.4000072738
Co,0,1.4930714358,0.0265222604,-0.0444875752
C,0,-0.4786717287,-1.8224552312,0.9304643719
C,0,-2.8291618102,-1.0085706672,-0.1397734313
C,0,-1.5195483954,0.533400025,1.9551572265
C,0,2.1301002998,-0.1383467816,1.6158179883
C,0,2.0379338555,1.6783814862,-0.3040959624
C,0,2.3390444684,-1.330503422,-0.8474894056
P,0,-1.7154384748,1.5708390033,-0.9585360858
P,0,-0.1477540503,0.1404534638,-1.3800323553
O,0,-0.071424408,-2.8327031223,1.2752085164
O,0,-3.8329183559,-1.4374917614,-0.4663542333
O,0,-1.7115051529,1.0885653473,2.9338067249
O,0,2.5150415503,-0.2392149488,2.6833960265
O,0,2.5441042305,2.6762688587,-0.5451597412
O,0,2.9569500067,-2.1121459863,-1.4011248061
O,0,-0.9518753454,2.8877098125,-0.2934801853
O,0,-0.357701723,-0.7969289936,-2.7221230015
H,0,-0.2767646882,2.7344962451,0.3810738264
H,0,-0.3375084532,-0.2946568616,-3.545746821

$Co_2(CO)_6(POH)_2$ CoP-but (C_1) BP86

0 1
Co,0,-1.2135411174,-0.3562583449,0.4249344962
Co,0,1.4364987378,0.0383968586,-0.0714123528
C,0,-0.4027745343,-1.8762738566,0.8585221843
C,0,-2.758006115,-1.0136005497,-0.1117240806
C,0,-1.5065528667,0.4215225467,2.0108702213
C,0,1.8595796431,0.0256903797,1.6466186002
C,0,2.1233346459,1.6002373002,-0.4474842184
C,0,2.3656209023,-1.3154711513,-0.7668633343
P,0,-1.7225215276,1.6150936587,-0.8376835054
P,0,-0.1948974069,0.1725531384,-1.404867293
O,0,0.0078976462,-2.9187979864,1.1444289936
O,0,-3.7740999476,-1.4479481009,-0.4476737394
O,0,-1.741564475,0.924425852,3.0232327915
O,0,2.1323841769,0.0307050285,2.7708278959
O,0,2.7226509467,2.5480196401,-0.7509771312
O,0,3.0672500543,-2.1056840097,-1.2345985776
O,0,-0.8748556597,2.8906797277,-0.1842315404
O,0,-0.4266962855,-0.7335542464,-2.77921384
H,0,-0.0207549312,2.6814534889,0.2551117789
H,0,-0.5693910057,-0.181410299,-3.571288998

$Co_2(CO)_6(POH)_2$ P-but (C_1) B3LYP

0 1
Co,0,0.0488394536,1.8904576288,0.1746357951
Co,0,0.0265471736,-1.9193121863,0.2221284581
C,0,0.6761103784,1.7002086298,1.8260433836
C,0,0.7483013014,2.8686314274,-1.131026039
C,0,-1.2908608477,2.998368904,0.569094409
C,0,-0.6892160567,-1.7120928321,1.8347667582
C,0,1.3467970211,-3.0128960095,0.7122454779
C,0,-0.5535385682,-2.913954058,-1.1296576035
P,0,1.2093859292,0.0427356187,-0.4333209331
P,0,-1.043874135,-0.0877078485,-0.4752870379
O,0,1.1463092432,1.6465016807,2.8650619719
O,0,1.2591093168,3.522585119,-1.9141051567
O,0,-2.1885445259,3.6594205224,0.8041585672

$Co_2(CO)_6(POH)_2$ P-but (C_1) BP86

0 1
Co,0,0.02949499,1.8665881972,0.1677785249
Co,0,0.0327836191,-1.8949442752,0.2119942014
C,0,0.6437336292,1.6640304162,1.8105892678
C,0,0.7722749363,2.8654208421,-1.0807461436
C,0,-1.3177936731,2.950380816,0.5433796545
C,0,-0.6521237868,-1.6723987236,1.8227029803
C,0,1.3610986799,-2.9680656834,0.6719757636
C,0,-0.6148478016,-2.9174072418,-1.0664269242
P,0,1.2384711311,0.0269769249,-0.4440069554
P,0,-1.0298807251,-0.0737704123,-0.4903087647
O,0,1.109659047,1.6195734915,2.8686773291
O,0,1.3202900205,3.5559359285,-1.8299237628
O,0,-2.2408153633,3.6084645303,0.7686969404

O,0,-1.2189479841,-1.6480275635,2.8441912976
O,0,2.2290186013,-3.6658124807,1.0128079897
O,0,-0.99798785,-3.5692621253,-1.9500164642
O,0,1.5437538452,0.0467100906,-2.0518904352
O,0,-1.1425390554,-0.1992603619,-2.1786301301
H,0,0.7395437125,0.0580478553,-2.6090910732
H,0,-1.9402069533,0.214657989,-2.5262492355

$Co_2(CO)_6(POH)_2$ Rhomb (C_1) B3LYP
0 1
Co,0,1.769053391,-0.0445190562,-0.0817988713
Co,0,-1.8037152262,0.1016225744,-0.0953053879
C,0,2.8284736111,-1.3234665417,-0.7933238414
C,0,1.7409917544,-0.2634992564,1.6974199031
C,0,2.8207072956,1.3599810368,-0.3081313247
C,0,-2.7915885893,1.5884286791,-0.2179451984
C,0,-2.8801955111,-1.0316992192,-0.9892952191
C,0,-1.844008941,-0.2553267379,1.6484793379
P,0,0.0098084343,1.0270436588,-0.4764270862
P,0,-0.0314108309,-1.5474092911,-0.4528790168
O,0,3.469906832,-2.1494077967,-1.2448805863
O,0,1.7295769654,-0.3562781955,2.8306314725
O,0,3.3982961041,2.338989346,-0.4458034149
O,0,-3.3888340092,2.55556825,-0.2776500605
O,0,-3.5369947129,-1.7734696753,-1.5553439958
O,0,-1.8559730943,-0.4734191319,2.7674418832
O,0,0.0257316278,2.6628353666,-0.6725943889
O,0,0.0830199885,-2.4149419593,0.9956088026
H,0,0.9005447139,3.0690681907,-0.7417766665
H,0,-0.6133898032,-3.0761002412,1.0966636595

$Co_2(CO)_6(POH)_2$ Diphosphine (C_1) B3LYP
0 1
Co,0,0.0120207325,0.0216450487,-0.0255053381
Co,0,-0.0384945782,0.0249609119,4.0743581596
C,0,0.6469198348,0.0892724044,-1.6739595175
C,0,1.6790428224,0.1041608913,0.6709723905
C,0,-1.6741715911,0.2403851852,-0.6022279079
C,0,-0.4057194256,1.7546644316,4.1399932719
C,0,-0.9654933198,-0.6023783522,5.45798902
C,0,1.7214572602,0.0807323925,4.3078006477
P,0,-0.8029585429,-0.3192216798,2.0333554671
P,0,-0.0195017861,-2.0542382313,3.1084066877
O,0,1.0451662651,0.0676250396,-2.7413651
O,0,2.7371495389,0.2816654749,1.0332867844
O,0,-2.7139556315,0.4339887087,-1.0092722654
O,0,-0.6518662509,2.8716336838,4.1481567537
O,0,-1.5034962063,-0.9979940274,6.3877293052
O,0,2.8480871714,0.1059114644,4.4957773589
O,0,-2.4772712347,-0.4486225404,1.925490526
O,0,1.556553215,-2.1737283101,2.4724659214
H,0,1.724779414,-3.062370486,2.1370014504
H,0,-2.9238323011,-0.1360575616,2.7205790716

O,0,-1.1724931046,-1.6194743306,2.8548236671
O,0,2.269152918,-3.6213870218,0.9568757327
O,0,-1.1127951739,-3.6141159298,-1.84339866
O,0,1.5553180312,0.0268157609,-2.0735152667
O,0,-1.1105838664,-0.1964880799,-2.2101578541
H,0,0.7186059142,0.0439674039,-2.6119886457
H,0,-1.8915494217,0.269897387,-2.5611610845

$Co_2(CO)_6(POH)_2$ Rhomb (C_1) BP86
0 1
Co,0,1.7909169053,-0.0437767868,-0.1018639621
Co,0,-1.8229652172,0.0955878645,-0.106441611
C,0,2.8371257863,-1.3535649976,-0.7458480124
C,0,1.7614200777,-0.214305128,1.6647293623
C,0,2.8333703474,1.3522965479,-0.3760093821
C,0,-2.8073302239,1.5737598,-0.223717279
C,0,-2.8871025284,-1.0488606277,-0.9800119139
C,0,-1.8553590559,-0.2628650782,1.6233127707
P,0,0.0081430194,1.0262643144,-0.4790352864
P,0,-0.0216883579,-1.5274318303,-0.4948597496
O,0,3.4929688771,-2.210836147,-1.1558210831
O,0,1.756302003,-0.2807481913,2.8158094201
O,0,3.4241354248,2.338393503,-0.5374693467
O,0,-3.4236857025,2.5477235699,-0.2759450328
O,0,-3.5579432289,-1.8084686137,-1.5378805656
O,0,-1.8750943022,-0.4849449812,2.7578066228
O,0,0.0263758215,2.6862886813,-0.5597932416
O,0,0.1060125836,-2.4527282799,0.9201876535
H,0,0.9238230212,3.0736894169,-0.6029942072
H,0,-0.6794252505,-3.0114730364,1.0789348442

$Co_2(CO)_6(POH)_2$ Diphosphine (C_1) BP86
0 1
Co,0,-0.0043496343,-0.0568944341,-0.0031672457
Co,0,-0.0743071678,-0.0309499076,4.0336458767
C,0,0.5242919323,-0.3357212719,-1.6650923017
C,0,1.6391477542,0.1624817406,0.6259258062
C,0,-1.5053002541,0.74256965,-0.459633513
C,0,-0.5702614733,1.6593365012,4.0511874412
C,0,-0.9536887153,-0.698966547,5.4217433541
C,0,1.6643297484,0.1524025454,4.3130745669
P,0,-0.7935705582,-0.4025482406,2.0055010177
P,0,0.1029842857,-2.1115157075,3.097294189
O,0,0.8330345733,-0.6238294232,-2.7405404301
O,0,2.696950698,0.4901408729,0.9463706043
O,0,-2.412381994,1.3859752047,-0.7681454096
O,0,-0.9043323752,2.7690027326,4.0317619293
O,0,-1.4815030408,-1.1155366318,6.3660341435
O,0,2.7917829293,0.2735107142,4.5402991049
O,0,-2.4673827175,-0.578588686,1.8961733119
O,0,1.7139695705,-2.1482423981,2.5438343997
H,0,1.9118161517,-3.0111933738,2.1311872989
H,0,-2.9168143274,-0.2393988919,2.6935785428

Table S12. The Cartesian coordinates of the optimized $Co_2(CO)_6(POMe)_2$ structures at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

$Co_2(CO)_6(POMe)_2$ Co-but (C_2) B3LYP	$Co_2(CO)_6(POMe)_2$ Co-but (C_2) BP86
0 1	0 1
Co,0,-1.2445436221,-0.0188757457,0.1393648428	Co,0,-1.2491082954,-0.0127407347,0.1940909418
Co,0,1.2445436221,0.0188757457,0.1393648428	Co,0,1.2491082954,0.0127407347,0.1940909418
C,0,-2.5787546296,-0.0730603372,-1.0165022438	C,0,-2.5834054118,-0.1054658881,-0.9449802961
C,0,-1.6597208831,1.319787921,1.2704991055	C,0,-1.6830938043,1.3348572788,1.2859080781
C,0,-1.5568996635,-1.3632477079,1.2931571259	C,0,-1.5126385452,-1.3410973419,1.3584749822
C,0,2.5787546296,0.0730603372,-1.0165022438	C,0,2.5834054118,0.1054658881,-0.9449802961
C,0,1.5568996635,1.3632477079,1.2931571259	C,0,1.5126385452,1.3410973419,1.3584749822
C,0,1.6597208831,-1.319787921,1.2704991055	C,0,1.6830938043,-1.3348572788,1.2859080781
P,0,-0.0352447773,1.411836901,-1.1460589322	P,0,-0.0353714962,1.3956859831,-1.1189663907
P,0,0.0352447773,-1.411836901,-1.1460589322	P,0,0.0353714962,-1.3956859831,-1.1189663907
O,0,-3.4513097915,-0.1057613438,-1.7496674197	O,0,-3.473049611,-0.1633258541,-1.6802716504
O,0,-1.9452884121,2.1516561492,1.9915767307	O,0,-2.0009401767,2.1874007259,1.9942226159
O,0,-1.7684821644,-2.203583658,2.0303435299	O,0,-1.6954423327,-2.1859413585,2.1221114312
O,0,3.4513097915,0.1057613438,-1.7496674197	O,0,3.473049611,0.1633258541,-1.6802716504
O,0,1.7684821644,2.203583658,2.0303435299	O,0,1.6954423327,2.1859413585,2.1221114312
O,0,1.9452884121,-2.1516561492,1.9915767307	O,0,2.0009401767,-2.1874007259,1.9942226159
O,0,-0.0864929004,2.9076509705,-0.3874603296	O,0,-0.0850768481,2.9256446356,-0.4046449235
O,0,0.0864929004,-2.9076509705,-0.3874603296	O,0,0.0850768481,-2.9256446356,-0.4046449235
C,0,0.0973095941,4.0738318919,-1.1958299748	C,0,0.1350201487,4.051721185,-1.2792367191
C,0,-0.0973095941,-4.0738318919,-1.1958299748	C,0,-0.1350201487,-4.051721185,-1.2792367191
H,0,-0.2766369615,4.9181044292,-0.6171036274	H,0,-0.3859521688,4.9072990475,-0.8277771189
H,0,1.15811672,4.2275200859,-1.4146339431	H,0,1.2129367493,4.2725595632,-1.3471416033
H,0,-0.4561321429,4.0005866404,-2.1367618634	H,0,-0.2639072222,3.8646278502,-2.2908663468
H,0,0.2766369615,-4.9181044292,-0.6171036274	H,0,0.3859521688,-4.9072990475,-0.8277771189
H,0,-1.15811672,-4.2275200859,-1.4146339431	H,0,-1.2129367493,-4.2725595632,-1.3471416033
H,0,0.4561321429,-4.0005866404,-2.1367618634	H,0,0.2639072222,-3.8646278502,-2.2908663468

$Co_2(CO)_6(POMe)_2$ CoP-but (C_1) B3LYP	$Co_2(CO)_6(POMe)_2$ CoP-but (C_1) BP86
0 1	0 1
Co,0,0.1519119561,-0.0521965573,0.1161386517	Co,0,0.1416444719,-0.0355162755,0.1672359771
Co,0,0.285021164,0.2387205114,2.9911537504	Co,0,0.2214814639,0.2435026664,2.8934766041
C,0,1.8693735322,0.1755788136,0.5065559476	C,0,1.8398287415,0.1740667823,0.642332437
C,0,0.0993359876,0.697390787,-1.4976950585	C,0,0.1562374485,0.7888959885,-1.3912265424
C,0,0.0743533897,-1.8323737112,-0.0676984773	C,0,0.0626269642,-1.780952797,-0.212403022
C,0,1.3594854146,-1.1109737711,3.4416251318	C,0,1.0227880716,-1.3130641883,3.1207810887
C,0,-1.1632139402,-0.4112999471,3.7837213881	C,0,-1.1969391599,-0.1588630373,3.8443138248
C,0,1.2623890895,1.5919156999,3.6102470908	C,0,1.3459695882,1.4132943981,3.6294098852
P,0,-2.2163498869,0.3860318264,0.2836745504	P,0,-2.2670104566,0.359234267,0.243331634
P,0,-0.7278969528,1.3470712996,1.4951115828	P,0,-0.8041169084,1.4067893024,1.4563956224
O,0,2.9893281605,0.3480101377,0.6569951943	O,0,2.9773219179,0.3320600513,0.7890938172
O,0,0.0670817972,1.1520621307,-2.5432160221	O,0,0.1806162622,1.3166746546,-2.418902952
O,0,0.0630479182,-2.9620477747,-0.2435948762	O,0,0.05814379,-2.8905395189,-0.540780045
O,0,2.0463934356,-1.9841493131,3.6956078826	O,0,1.529860519,-2.3440048305,3.2638925699
O,0,-2.0165037451,-0.7635346408,4.4553109442	O,0,-2.0452018357,-0.3789309235,4.6028158454
O,0,1.8134090793,2.462244055,4.1030744948	O,0,2.0110101568,2.1403890877,4.2367624045
O,0,-2.8533632404,-0.6457919876,1.4413076055	O,0,-2.9379392363,-0.5998283206,1.4551290379
O,0,-0.5655025505,2.9526527493,1.2052224775	O,0,-0.6216032186,3.0174098474,1.1370619958
C,0,-1.5257662125,3.8666865522,1.7561462494	C,0,-1.6069698097,3.9391707152,1.6649702793
H,0,-1.1823652403,4.8657892023,1.495176469	H,0,-1.2633291525,4.9406324667,1.3782324993
H,0,-2.5145782944,3.6917278407,1.3255237125	H,0,-2.597863394,3.7433517712,1.2250998738
H,0,-1.5754266087,3.7689138366,2.843787966	H,0,-1.6617375557,3.8657413385,2.7628081152
C,0,-3.3163550536,-1.9354429854,1.038874671	C,0,-3.0795892359,-2.0137719214,1.2298623873
H,0,-3.8490322358,-2.3537392173,1.8919549674	H,0,-3.7555929889,-2.383605422,2.0120015384
H,0,-3.9989945371,-1.8692587775,0.1849153828	H,0,-3.5102227481,-2.2301324314,0.2366402842
H,0,-2.4791464758,-2.5897488221,0.7809470675	H,0,-2.1027777449,-2.517765734,1.3225335838

$Co_2(CO)_6(POMe)_2$ P-but (C_1) B3LYP
0 1
Co,0,0.5212545722,-0.2569377329,2.0014449781
Co,0,0.2569332717,-0.5217872191,-1.7214300826
C,0,1.9400737127,-1.3199432139,1.8613015368
C,0,1.3359157709,1.0679321234,2.857350325
C,0,-0.7493050498,-0.587987354,3.2170168553
C,0,1.709552725,-1.5356676304,-1.5371089814
C,0,0.9437100609,0.7290139681,-2.7770987921
C,0,-0.9719153076,-1.1390086201,-2.8512799454
P,0,0.1944089903,1.1297586088,0.033646539
P,0,-0.5772229494,-0.9271584654,0.2503114155
O,0,2.8248094177,-2.0413993514,1.8577169477
O,0,1.8570091667,1.9499199221,3.3570995546
O,0,-1.5300553837,-0.8530162369,4.003857111
O,0,2.6121353612,-2.2332657385,-1.5035476215
O,0,1.4001371229,1.5510430251,-3.4230535769
O,0,-1.6927292839,-1.5840751665,-3.6195481443
O,0,-1.3192334306,1.8984904463,0.0830437209
O,0,-2.1803236037,-1.0762318301,0.5426848793
C,0,-1.2788021699,3.3184243489,-0.0636144813
C,0,-3.2004762484,-0.7934819448,-0.4281469615
H,0,-2.3031163253,3.6750545547,0.0439806009
H,0,-0.6555978656,3.7821301237,0.7084723545
H,0,-0.8980202022,3.6069719435,-1.04931954
H,0,-4.1481215186,-0.9277904822,0.0906883454
H,0,-3.1103250483,0.2330360769,-0.7814050714
H,0,-3.1431597853,-1.4925541555,-1.2640619655

$Co_2(CO)_6(POMe)_2$ Rhomb (C_1) B3LYP
0 1
Co,0,0.0385992179,0.0265635966,-0.0329852704
Co,0,-0.0258458298,-0.0061440622,3.5427292369
C,0,1.5272981758,0.0815385166,-1.0419368561
C,0,-0.6596857959,1.6735023502,0.0464944815
C,0,-0.9715188471,-0.7539380131,-1.2746517407
C,0,-1.2051006242,-0.867488862,4.5738586146
C,0,1.4074823246,-0.1188648334,4.6241669836
C,0,-0.6282120296,1.6674965842,3.5312289883
P,0,-0.6856079998,-0.8477194988,1.7524829673
P,0,1.5568513764,0.4316235313,1.7510379528
O,0,2.4852856442,0.1472373285,-1.6568534694
O,0,-1.1285420769,2.7098106128,0.0752499278
O,0,-1.6000459029,-1.2088219685,-2.1130144237
O,0,-1.9841187558,-1.4131144176,5.2007501805
O,0,2.3327947757,-0.1788527104,5.2900772091
O,0,-1.0318636537,2.7343063007,3.5155437402
O,0,-1.979234249,-1.8487197748,1.8801613447
O,0,1.6410374934,2.1105681626,1.6180531088
C,0,-2.7058157526,-2.4125156381,0.7845783447
H,0,-3.2331845264,-1.6331916631,0.2311644136
H,0,-2.0406391657,-2.95927898,0.1138321732
H,0,-3.4285082506,-3.1006732892,1.2200132626
C,0,2.4693954559,2.8071615891,2.5482870434
H,0,3.4604093302,2.3476762245,2.6253110849
H,0,2.571272124,3.8271268361,2.1790240826
H,0,2.0086797092,2.833395474,3.5418502245

$Co_2(CO)_6(POMe)_2$ P-but (C_1) BP86
0 1
Co,0,1.9100911996,0.3059480618,-0.1466796498
Co,0,-1.7969121121,0.405666323,-0.041110812
C,0,1.8607604127,2.0425330128,-0.4775498697
C,0,2.9140224334,0.3789666,1.3006129259
C,0,2.9747901578,-0.6981771696,-1.1492740098
C,0,-1.5689224603,2.1248018168,-0.3842482305
C,0,-2.6128507703,0.5492020799,1.5185148319
C,0,-3.1212749572,-0.3386277189,-0.9504563777
P,0,0.0762882166,-0.4234891609,1.2473232473
P,0,0.0180511537,-0.2981631712,-0.9720508438
O,0,1.9233971862,3.1667750937,-0.7431788173
O,0,3.529263973,0.4240731582,2.2787646657
O,0,3.6877316197,-1.3031896237,-1.8284695196
O,0,-1.5154142995,3.2494680023,-0.6483547908
O,0,-3.112724533,0.6567632271,2.5564458787
O,0,-4.0412759111,-0.7294980365,-1.5380513811
O,0,0.0377993643,-2.1369922826,1.2882503002
O,0,0.118665087,-1.6699844907,-1.8839596827
C,0,-0.0499531486,-2.6745715882,2.623228884
C,0,-0.9797419966,-2.6062212214,-1.9912147998
H,0,0.0284833864,-3.7657661534,2.522059044
H,0,0.7742608849,-2.3095951194,3.2604742846
H,0,-1.0144681153,-2.4197774841,3.0960139843
H,0,-0.6144891895,-3.4110127695,-2.641929537
H,0,-1.2343353055,-3.0033725425,-0.9988555123
H,0,-1.8571941813,-2.1289091559,-2.451876567

$Co_2(CO)_6(POMe)_2$ Rhomb (C_1) BP86
0 1
Co,0,0.0907557405,-0.0875132789,-0.0480345097
Co,0,0.0731521246,-0.0879789724,3.6026478622
C,0,1.4394132763,0.5400296319,-1.0346941051
C,0,-1.0810749088,1.2325818279,-0.08873518
C,0,-0.3723598283,-1.3679730749,-1.1890337949
C,0,-1.0558176467,-0.9506801332,4.6783375262
C,0,1.5565623445,-0.1548892138,4.6046340731
C,0,-0.548606097,1.5632233405,3.6071406745
P,0,-0.6321907753,-0.8695386375,1.7970586847
P,0,1.6097316538,0.3387343578,1.7249714507
O,0,2.3133159462,0.9570801669,-1.665129817
O,0,-1.8616983582,2.0837062098,-0.1544770958
O,0,-0.6257153534,-2.1901114466,-1.9654905151
O,0,-1.8083169789,-1.4992250778,5.3605338565
O,0,2.5236575892,-0.1768549686,5.2394297632
O,0,-0.9889768007,2.6327523995,3.6097291922
O,0,-2.0713952201,-1.6839601484,1.8642176284
O,0,1.6675972322,2.0208491196,1.567979551
C,0,-2.9250420906,-1.8973501886,0.7219272918
H,0,-3.2075482755,-0.9377480481,0.2618125695
H,0,-2.4314206919,-2.5389978694,-0.021491089
H,0,-3.8196662209,-2.4029546172,1.1078695903
C,0,2.4417171032,2.7329042475,2.553469907
H,0,3.4271484433,2.2624693111,2.7108310322
H,0,2.5777858038,3.7515509299,2.166906396
H,0,1.9001741557,2.7785775287,3.514042662

$Co_2(CO)_6(POMe)_2$ Diphosphine (C_1) B3LYP
0 1
Co,0,2.161011374,0.0961687237,0.2533330451
Co,0,-1.9484415393,-0.0419175461,0.2791049137
C,0,3.8241004395,-0.4741512587,0.4641678326
C,0,1.4816724384,-1.3796600082,1.0368318079
C,0,2.6967135678,1.7461802307,-0.1974295021
C,0,-2.0507929839,0.8259228599,1.8170358
C,0,-3.3610514194,0.6147261419,-0.5941292999
C,0,-2.1274135421,-1.7015332173,0.8724869737
P,0,0.0714293663,0.7017807515,-0.2943069919
P,0,-0.9413213326,-0.6872661484,-1.668030163
O,0,4.8946872724,-0.8591285019,0.5288998577
O,0,1.1200300786,-2.2700413566,1.6375089299
O,0,3.0645015915,2.7972721096,-0.4161742508
O,0,-2.080894794,1.3981449637,2.8071546866
O,0,-4.3108849191,0.9799960002,-1.1167397277
O,0,-2.2933309322,-2.770646116,1.2415421903
O,0,0.0900238673,2.1873933508,-1.0723750027
O,0,-0.2061109265,-2.161299448,-1.2704779254
C,0,-0.5012709163,3.3175466254,-0.4311260942
C,0,0.7249199588,-2.6895678579,-2.212488614
H,0,-1.5719922038,3.164612767,-0.2704748799
H,0,-0.0224464104,3.5312251463,0.5308896584
H,0,-0.354359414,4.164029329,-1.1011853823
H,0,1.6798219959,-2.1501088856,-2.1578267181
H,0,0.8868887071,-3.7357516436,-1.9520137799
H,0,0.346266676,-2.6258570114,-3.2376583641

$Co_2(CO)_6(POMe)_2$ Diphosphine (C_1) BP86
0 1
Co,0,2.0862142556,-0.0154037845,0.0419154373
Co,0,-1.9622958326,-0.0428643224,0.2249347634
C,0,3.7019262621,-0.7300798746,-0.1146458494
C,0,1.4691668201,-1.2110171859,1.1864982503
C,0,2.6515056589,1.6508501767,0.0353072911
C,0,-1.9504528803,0.8265692284,1.7565737565
C,0,-3.4000144168,0.6294509631,-0.5828474366
C,0,-2.2138099029,-1.6884850065,0.8135838024
P,0,0.0330257123,0.6566445836,-0.3704399039
P,0,-1.0151404197,-0.7526165156,-1.7405085279
O,0,4.7481295594,-1.1941795587,-0.2713173225
O,0,1.1500098198,-1.8917947418,2.0630944329
O,0,3.0409762642,2.7287496916,0.1876154129
O,0,-1.9075591507,1.4014912902,2.7620799743
O,0,-4.3790019306,1.0266906909,-1.0583888531
O,0,-2.424808755,-2.7611372262,1.1930481113
O,0,0.0813440466,2.1561981438,-1.1297980637
O,0,-0.310117059,-2.2468925781,-1.3448785488
C,0,-0.5471825787,3.2818023632,-0.4860615822
C,0,0.8894761438,-2.5803802674,-2.0450609766
H,0,-1.6245269218,3.1014426702,-0.3361519003
H,0,-0.0720634301,3.5020181325,0.4846835271
H,0,-0.4072780452,4.133885047,-1.1641642897
H,0,1.7354705869,-2.0021685448,-1.6056752227
H,0,1.0701562698,-3.6542808593,-1.9003219425
H,0,0.8286059237,-2.3464225155,-3.1225553397

Table S13. The Cartesian coordinates of the optimized $Co_2(CO)_6(PNH_2)_2$ structures at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

$Co_2(CO)_6(PNH_2)_2$ Co-but (C_{2v}) B3LYP

0 1
Co,0,0.0000066475,0.0000000011,0.0000049543
Co,0,0.0000066475,-0.000000001,2.5141710455
C,0,1.2093624856,0.000000002,-1.2903707107
C,0,-1.107946642,1.350451173,-0.3418266899
C,0,-1.1079466422,-1.3504511701,-0.3418266921
C,0,1.2093624855,-0.0000000022,3.8045467106
C,0,-1.1079466421,1.3504511703,2.8560026919
C,0,-1.1079466423,-1.3504511727,2.8560026897
P,0,1.303655522,1.4383308432,1.2570880011
P,0,1.3036555218,-1.4383308433,1.2570879988
O,0,1.9568472078,0.0000000027,-2.1518432392
O,0,-1.8018067598,2.2357993021,-0.5432145698
O,0,-1.8018067601,-2.2357992989,-0.5432145735
O,0,1.9568472077,-0.0000000029,4.6660192392
O,0,-1.8018067598,2.2357992992,3.0573905732
O,0,-1.8018067602,-2.2357993018,3.0573905696
N,0,0.7465060216,3.0338817001,1.2570880024
N,0,0.7465060211,-3.0338817002,1.2570879974
H,0,-0.2075631886,3.365932475,1.2570880027
H,0,1.4385141306,3.7663380741,1.2570880031
H,0,-0.2075631892,-3.3659324749,1.2570879972
H,0,1.43851413,-3.7663380743,1.2570879969

$Co_2(CO)_6(PNH_2)_2$ Co-but (C_{2v}) BP86

0 1
Co,0,-0.0134907819,0.0000000011,-0.0016610004
Co,0,-0.013490782,-0.000000001,2.5158370002
C,0,1.1750743262,0.000000002,-1.299481592
C,0,-1.1090484121,1.35272758,-0.3271204036
C,0,-1.1090484123,-1.3527275772,-0.3271204058
C,0,1.1750743261,-0.0000000022,3.8136575919
C,0,-1.1090484122,1.3527275774,2.8412964056
C,0,-1.1090484124,-1.3527275798,2.8412964034
P,0,1.3167303359,1.4256060355,1.2570880011
P,0,1.3167303357,-1.4256060357,1.2570879988
O,0,1.924685837,0.0000000027,-2.1793035186
O,0,-1.8102339939,2.2521646578,-0.5308706468
O,0,-1.8102339943,-2.2521646545,-0.5308706505
O,0,1.9246858368,-0.000000003,4.6934795185
O,0,-1.810233994,2.2521646548,3.0450466502
O,0,-1.8102339943,-2.2521646575,3.0450466465
N,0,0.7728620847,3.0324620567,1.2570880024
N,0,0.7728620842,-3.0324620568,1.2570879975
H,0,-0.1879987256,3.3729167777,1.2570880027
H,0,1.4785207114,3.7640490158,1.2570880031
H,0,-0.1879987261,-3.3729167777,1.2570879971
H,0,1.4785207108,-3.764049016,1.2570879969

$Co_2(CO)_6(PNH_2)_2$ CoP-but (C_1) B3LYP

0 1
Co,0,-0.0855376145,0.0299705715,-0.0404675452
Co,0,-0.0036745593,-0.0342945957,2.7578054526
C,0,1.6039176561,-0.1441554554,0.4643476755
C,0,0.2043238966,0.9402595984,-1.5474748651
C,0,-0.5225745781,-1.6683167027,-0.398016086
C,0,0.7616695583,-1.6189069718,3.0695626942
C,0,-1.5508576841,-0.4070224294,3.5028922013
C,0,1.1407970505,1.0564421291,3.5727319651
P,0,-2.3169197208,0.7936133487,-0.0140593046
P,0,-0.8369235528,1.4499107223,1.4594465586
O,0,2.7305081014,-0.2363084587,0.6489453055
O,0,0.3884273005,1.4899905175,-2.5296654404
O,0,-0.8125182145,-2.7411629353,-0.6615371661
O,0,1.2455599011,-2.6338127651,3.2592779378
O,0,-2.4907685713,-0.5858848191,4.1344574115
O,0,1.7874812037,1.7807208018,4.1776294063
N,0,-3.2244960428,-0.4607916867,0.6947347741
N,0,-0.4433230405,3.0867403009,1.3125189192
H,0,0.5078938945,3.3791169742,1.4898086864
H,0,-1.1300676912,3.7515186938,1.6361763714
H,0,-4.1679652603,-0.2384434675,0.9802928187
H,0,-2.8110026477,-1.1971186397,1.2492896427

$Co_2(CO)_6(PNH_2)_2$ CoP-but (C_1) BP86

0 1
Co,0,-0.0852506554,0.0073992485,-0.0130201551
Co,0,-0.0080807134,0.001892356,2.7021838145
C,0,1.5760509456,-0.1627681768,0.5752612322
C,0,0.2640505277,0.9624451557,-1.4589931071
C,0,-0.4749382893,-1.659514785,-0.5143952157
C,0,0.6085470156,-1.646512663,2.926074718
C,0,-1.5036393509,-0.2378221858,3.575339461
C,0,1.1749197359,1.0231086534,3.5419909985
P,0,-2.3574236999,0.6816404018,-0.0355054817
P,0,-0.884624401,1.4705344932,1.4086665057
O,0,2.7199748844,-0.2558490846,0.7503656518
O,0,0.5127636832,1.5624507659,-2.4153103588
O,0,-0.731264537,-2.7226077888,-0.8897634502
O,0,0.9967817475,-2.7255071498,3.0814268125
O,0,-2.4154890054,-0.34479299,4.2889499284
O,0,1.86118731,1.6856409431,4.2015637292
N,0,-3.1842339376,-0.5773731154,0.7766214851
N,0,-0.497284756,3.112835115,1.2353571218
H,0,0.4421301963,3.4201886258,1.4876388018
H,0,-1.2221966121,3.780981908,1.4893915514
H,0,-4.1275943336,-0.3665195955,1.1038408594
H,0,-2.6904363695,-1.2177854008,1.4010125108

$Co_2(CO)_6(PNH_2)_2$ P-but (C_1) B3LYP

0 1
Co,0,0.1532458399,-0.1164752704,1.8817198139
Co,0,0.1761230855,-0.053679438,-1.8777956587
C,0,1.6553900819,-1.0666693776,1.7084029923
C,0,0.7802800225,1.1777089001,2.9255689789
C,0,-1.1390592121,-0.7004087576,2.9388156244
C,0,1.7475918644,-0.8932275789,-1.7047180402
C,0,0.7052002607,1.3270707076,-2.8551283571
C,0,-1.0227947759,-0.7188792521,-2.9896129189
P,0,-0.0881045255,1.4870883727,0.0571594444

$Co_2(CO)_6(PNH_2)_2$ P-but (C_1) BP86

0 1
Co,0,0.052560714,-0.272690907,1.8826076183
Co,0,0.1915656723,-0.1042677273,-1.864923438
C,0,1.2709389209,-1.5273456519,1.617472002
C,0,0.9389629348,0.7310709481,3.0427617867
C,0,-1.3704638354,-0.5598451874,2.8623064328
C,0,1.9628811884,-0.1552128942,-1.7302776828
C,0,0.5329299453,1.1508770471,-2.8683421485
C,0,-0.0877508351,-1.4873624514,-2.9195302434
P,0,0.2494725221,1.3770327223,0.0891065316

P,0,-0.7719579383,-0.6202792745,-0.0161947327
O,0,2.5870278394,-1.7259402066,1.6851604633
O,0,1.1816545719,2.033294972,3.5625101779
O,0,-1.981291722,-1.1355185457,3.5823652493
O,0,2.7351545231,-1.465401483,-1.6891995785
O,0,1.0488848227,2.2311995417,-3.4613800535
O,0,-1.8096147323,-1.1983100103,-3.6719610647
N,0,-1.629281336,2.2452659132,0.1907532639
N,0,-2.4680813541,-0.7478105813,-0.0303002822
H,0,-1.6978629932,3.138195176,-0.2779012099
H,0,-2.458027103,1.6738781259,0.0486040238
H,0,-2.9023182529,-1.0829284296,-0.8794890398
H,0,-2.9221609669,-1.0946975034,0.8036209038

P,0,-0.9011970885,-0.5713429478,-0.0422848852
O,0,2.015377922,-2.4086252456,1.5271328267
O,0,1.5185224327,1.4257492809,3.7609660682
O,0,-2.3166800952,-0.8271697894,3.4825825545
O,0,3.120275715,-0.1374226109,-1.7100713834
O,0,-0.9630697188,2.013879598,-3.5143976111
O,0,-0.2940452034,-2.4143134153,-3.5818888626
N,0,-1.1215715341,2.4069214695,0.1658635033
N,0,-2.5906690442,-0.2639499366,-0.0254171873
H,0,-1.0048852614,3.3276344273,-0.2561554646
H,0,-2.0520210301,2.0042288055,-0.0052463209
H,0,-3.1096513423,-0.6114491818,-0.8323918634
H,0,-3.0956250882,-0.4029203519,0.8511277673

$Co_2(CO)_6(PNH_2)_2$ Rhomb (C_1) B3LYP
0 1
Co,0,0.0139936546,1.8230480118,0.0143116847
Co,0,-0.16986391,-1.7411221354,0.1407324215
C,0,1.5028586698,1.6873241717,-0.9241403772
C,0,0.4661408998,2.8957460432,1.3526387395
C,0,-1.2312525509,2.8117176653,-0.8242966591
C,0,-1.4003791527,-2.7738493146,-0.6692312769
C,0,1.4372131489,-1.8415659282,-0.602827519
C,0,0.0460587909,-2.6936985597,1.6146606322
P,0,-0.1812595189,0.1104799929,1.2080012502
P,0,-0.8677992946,-0.0671868216,-1.3933428725
O,0,2.4566601172,1.5763495175,-1.5478560763
O,0,0.7763819489,3.4882407143,2.2821951486
O,0,-2.0146218451,3.4326177633,-1.3768094113
O,0,-2.1720082003,-3.4165495562,-1.2094763212
O,0,2.458932046,-1.8851931608,-1.1145184142
O,0,0.2065914901,-3.2117328336,2.6224878867
N,0,0.1106153387,0.1331637882,2.8472884483
N,0,0.0729255758,-0.3233415983,-2.8004224034
H,0,0.1402161345,-0.7015407563,3.4148634427
H,0,0.2372491952,0.9965191329,3.3561025103
H,0,1.0548314355,-0.5665043279,-2.7905527126
H,0,-0.1491069732,0.2810391918,-3.580808121

$Co_2(CO)_6(PNH_2)_2$ Rhomb (C_1) BP86
0 1
Co,0,-0.0060522185,1.8796183466,0.0228020553
Co,0,-0.1971099184,-1.7476456833,0.1371401467
C,0,1.4337112788,1.7588474029,-0.9802697898
C,0,0.4841582459,2.9218810896,1.3608371179
C,0,-1.2588152099,2.8630877088,-0.7906526741
C,0,-1.2663836347,-2.8193218317,-0.8084688831
C,0,1.4558532314,-1.8206847049,-0.4777261609
C,0,-0.1463521977,-2.6769827748,1.6300710506
P,0,-0.1650579831,0.1325176441,1.1802250353
P,0,-0.9436508551,-0.0714918043,-1.3533916684
O,0,2.3765381263,1.6686714998,-1.6503970932
O,0,0.8404050515,3.5213851782,2.28958526
O,0,-2.0552540756,3.5044670262,-1.3337104478
O,0,-1.9493920897,-3.51050372,-1.4349903466
O,0,2.5338179474,-1.8791517815,-0.8988330549
O,0,-0.0787669548,-3.2109902268,2.6584415272
N,0,0.2427220827,0.1162898987,2.8068932719
N,0,-0.0149010615,-0.3648969878,-2.7620122426
H,0,0.2819927675,-0.7352712118,3.3637889254
H,0,0.4111771808,0.9813311888,3.3175289523
H,0,0.8901865835,-0.8348727082,-2.7576735519
H,0,-0.0744492968,0.3376774513,-3.5001874294

Table S14. The Cartesian coordinates of the optimized $Co_2(CO)_6(PNMe_2)_2$ structures at the B3LYP/6-311G(d) and BP86/6-311G(d) levels.

$Co_2(CO)_6(PNMe_2)_2$ Co-but (C_2) B3LYP

0 1
Co,0,-0.02482557,1.276442459,0.2310611443
Co,0,0.02482557,-1.276442459,0.2310611443
C,0,0.2990855185,2.5009971364,-1.001386867
C,0,1.126845454,1.5161267888,1.5742626706
C,0,-1.4107853432,1.9638588861,1.1033519051
C,0,-0.2990855185,-2.5009971364,-1.001386867
C,0,1.4107853432,-1.9638588861,1.1033519051
C,0,-1.126845454,-1.5161267888,1.5742626706
P,0,1.4108248993,-0.0532345923,-1.1212869045
P,0,-1.4108248993,0.0532345923,-1.1212869045
O,0,0.4857449494,3.3487473518,-1.7433728427
O,0,1.7883945981,1.725386125,2.4826816449
O,0,-2.2520520954,2.532344022,1.6292229244
O,0,-0.4857449494,-3.3487473518,-1.7433728427
O,0,2.2520520954,-2.532344022,1.6292229244
O,0,-1.7883945981,-1.725386125,2.4826816449
N,0,3.0710086607,-0.0110513421,-0.7759391947
N,0,-3.0710086607,0.0110513421,-0.7759391947
C,0,-3.8044342879,-0.0693686769,0.4818089021
H,0,-4.5987192043,0.6850185997,0.5026185662
H,0,-4.2711229476,-1.0559825019,0.5955099563
H,0,-3.161634073,0.1016835924,1.3365077648
C,0,-3.9583183083,-0.1276205609,-1.9352547294
H,0,-4.4807117692,-1.0922805689,-1.9153242634
H,0,-4.7106786737,0.6692784356,-1.9354493226
H,0,-3.3837218997,-0.0628996552,-2.8579107247
C,0,3.8044342879,0.0693686769,0.4818089021
H,0,4.5987192043,-0.6850185997,0.5026185662
H,0,4.2711229476,1.0559825019,0.5955099563
H,0,3.161634073,-0.1016835924,1.3365077648
C,0,3.9583183083,0.1276205609,-1.9352547294
H,0,4.4807117692,1.0922805689,-1.9153242634
H,0,4.7106786737,-0.6692784356,-1.9354493226
H,0,3.3837218997,0.0628996552,-2.8579107247

$Co_2(CO)_6(PNMe_2)_2$ Co-but (C_2) BP86

0 1
Co,0,-0.0302646318,1.268706065,0.2685529317
Co,0,0.0302646318,-1.268706065,0.2685529317
C,0,0.4393465956,2.5015978419,-0.8948513262
C,0,1.0494275992,1.3782353798,1.6755668722
C,0,-1.4373759997,2.0060799546,1.0424348112
C,0,-0.4393465956,-2.5015978419,-0.8948513262
C,0,1.4373759997,-2.0060799546,1.0424348112
C,0,-1.0494275992,-1.3782353798,1.6755668722
P,0,1.387549526,-0.0706773268,-1.1359589421
P,0,-1.387549526,0.0706773268,-1.1359589421
O,0,0.7304768531,3.3742271452,-1.5980219599
O,0,1.6677800666,1.4885187186,2.6496175554
O,0,-2.3013569489,2.6225394995,1.5093522628
O,0,-0.7304768531,-3.3742271452,-1.5980219599
O,0,2.3013569489,-2.6225394995,1.5093522628
O,0,-1.6677800666,-1.4885187186,2.6496175554
N,0,3.0591337281,-0.0080885272,-0.8074794547
N,0,-3.0591337281,0.0080885272,-0.8074794547
C,0,-3.7969127407,-0.0941103874,0.4505299281
H,0,-4.6316162542,0.6291333528,0.4583929669
H,0,-4.2197990233,-1.1093284431,0.5719550222
H,0,-3.1575442904,0.1182579098,1.3110702836
C,0,-3.9248331269,-0.1708580953,-1.9828431506
H,0,-4.416813804,-1.1612995772,-1.9634019668
H,0,-4.7081502223,0.6078606793,-2.0008759689
H,0,-3.3296789504,-0.0920055511,-2.9029392293
C,0,3.7969127407,0.0941103874,0.4505299281
H,0,4.6316162542,-0.6291333528,0.4583929669
H,0,4.2197990233,1.1093284431,0.5719550222
H,0,3.1575442904,-0.1182579098,1.3110702836
C,0,3.9248331269,0.1708580953,-1.9828431506
H,0,4.416813804,1.1612995772,-1.9634019668
H,0,4.7081502223,-0.6078606793,-2.0008759689
H,0,3.3296789504,0.0920055511,-2.9029392293

$Co_2(CO)_6(PNMe_2)_2$ CoP-but (C_1) B3LYP

0 1
Co,0,0.4766782107,0.6411634763,1.177906446
Co,0,-1.3161438593,-0.840125783,-0.2722497672
C,0,-1.1507980046,0.9633800991,1.7971157673
C,0,1.2476607832,2.1998755871,1.5518253144
C,0,1.0811896756,-0.5263991406,2.4032232673
C,0,-1.6988851202,-1.9206240149,1.0849854036
C,0,-0.6565952232,-2.1085893597,-1.3111658561
C,0,-2.9383952649,-0.2380722994,-0.7191499041
P,0,2.1216393063,0.2892318908,-0.5768341563
P,0,0.0312710293,0.6689924479,-0.9723053733
O,0,-2.1250264534,1.2960705297,2.3011496309
O,0,1.754917167,3.1833034844,1.834147468
O,0,1.4627934814,-1.2140572941,3.2319262086
O,0,-1.9329796754,-2.6234317751,1.9542491643
O,0,-0.4315495251,-2.9668922479,-2.0346445287
O,0,-3.9976984552,0.0091690168,-1.0758522072
N,0,2.173739625,-1.422992209,-0.9522935716
N,0,-0.2610976597,2.0394734069,-1.9141170825
C,0,0.8318730441,2.8096704224,-2.5030636971
H,0,0.4534982763,3.3509876967,-3.374292412
H,0,1.2518241855,3.5394499353,-1.7982879933
H,0,1.6327345343,2.1478024169,-2.8273877473

$Co_2(CO)_6(PNMe_2)_2$ CoP-but (C_1) BP86

0 1
Co,0,0.4817626067,0.6278574107,1.1817246414
Co,0,-1.2769165031,-0.7837770685,-0.2626247504
C,0,-1.1760467642,0.7573247146,1.8027242476
C,0,1.0211681252,2.2822962244,1.4313225684
C,0,1.2743425012,-0.3322492377,2.4666445477
C,0,-1.3385928937,-1.9747436553,1.0376357703
C,0,-0.7686380824,-1.9459189718,-1.4742767289
C,0,-2.9483609006,-0.2312483325,-0.5606564244
P,0,2.1900967307,0.2581595223,-0.5366544754
P,0,0.0972015826,0.6979949526,-0.9828305346
O,0,-2.1374724308,1.021412274,2.4010062936
O,0,1.3670420094,3.3687329965,1.6389729338
O,0,1.8071863344,-0.860247241,3.3484778624
O,0,-1.379509679,-2.7840255741,1.8664515215
O,0,-0.5922995101,-2.7490666125,-2.2941113906
O,0,-4.0619776121,-0.0245517091,-0.8115967003
N,0,2.1513249856,-1.4469079106,-0.9499361079
N,0,-0.1877803093,2.0849727746,-1.9131702878
C,0,0.9163416717,2.9060778323,-2.4167475287
H,0,0.5997499432,3.4023960388,-3.3489079973
H,0,1.2164061799,3.6822481344,-1.687794851
H,0,1.7893785974,2.2746774567,-2.6297639651

C,0,-1.4751318089,2.8161556914,-1.6754226985
H,0,-2.2928505579,2.1675071346,-1.3685020052
H,0,-1.3251361759,3.5766205374,-0.8973410641
H,0,-1.7719101643,3.317800974,-2.5999979659
C,0,2.5150017098,-1.7142779467,-2.3469641317
H,0,3.5692053099,-1.5061380801,-2.5862323274
H,0,2.3186232069,-2.7709012732,-2.5485984991
H,0,1.8880785707,-1.1292205729,-3.0215329206
C,0,2.9208750579,-2.2735230014,-0.0265719128
H,0,4.0102555411,-2.119664887,-0.080290078
H,0,2.6026678739,-2.1011218891,0.9997126172
H,0,2.7193005481,-3.3218382284,-0.2657713426

C,0,-1.4672393704,2.7873246997,-1.7836006332
H,0,-2.2694415618,2.0758119707,-1.5490104645
H,0,-1.4315272474,3.5544043041,-0.9868766009
H,0,-1.7099658537,3.279018902,-2.7395750859
C,0,2.5160600263,-1.7560754501,-2.3381272532
H,0,3.6079767068,-1.6955444493,-2.5260027541
H,0,2.1764804313,-2.7770287364,-2.5800593686
H,0,2.0077367071,-1.0650147121,-3.0272080177
C,0,2.7035464667,-2.4031603378,0.0119966238
H,0,3.8113059295,-2.3739613105,0.0769508759
H,0,2.2918255736,-2.2159965396,1.0125461896
H,0,2.4084647985,-3.4224076142,-0.2895501106

$Co_2(CO)_6(PNMe_2)_2$ P-but (C_1) B3LYP
0 1
Co,0,-0.556122301,-0.3424160218,1.6772962489
Co,0,-0.4152043727,0.2126045799,-1.9274348469
C,0,-2.1006411706,-1.2274990229,1.3680916093
C,0,0.4594456601,-1.199203507,2.8724642661
C,0,-1.1188809175,0.9833488716,2.6773867513
C,0,-1.9440202569,-0.7343176168,-2.1093565743
C,0,0.7905353709,-0.1359882378,-3.2025500864
C,0,-1.002228518,1.7707753001,-2.4846025771
P,0,0.3434557939,-1.4467156315,-0.3778471769
P,0,0.1294885918,0.8643145425,0.0569300537
O,0,-3.0729732936,-1.812307087,1.2447197435
O,0,1.1010891436,-1.7703548296,3.629524986
O,0,-1.5019405906,1.8777926666,3.280085213
O,0,-2.8886683052,-1.346093448,-2.2941937255
O,0,1.565296473,-0.3941609086,-4.0024893359
O,0,-1.4022583759,2.79398313,-2.8024947448
N,0,2.0417111826,-1.7153445625,-0.448767474
N,0,1.3272098754,2.0257566855,0.2781607234
C,0,3.0795312796,-0.6997405866,-0.4921073115
C,0,2.4732475511,-2.9506355934,0.2062916847
C,0,1.8604996514,2.8612306923,-0.7930659447
C,0,1.926944709,2.3140035753,1.5781472886
H,0,4.0044709778,-1.1472150154,-0.8683326526
H,0,2.8020021489,0.1046279325,-1.1711453379
H,0,3.2924925826,-0.2678813163,0.4976961236
H,0,3.3592547367,-3.3459910427,-0.3004446286
H,0,2.721329778,-2.7990162397,1.2663386038
H,0,1.6842623306,-3.7015204373,0.1454954768
H,0,2.94034823,2.7045295086,-0.899665
H,0,1.3855239728,2.62346053,-1.7406300737
H,0,1.6887447306,3.9196851789,-0.5706899079
H,0,3.015344848,2.1964082656,1.526197309
H,0,1.7052997233,3.341379046,1.8861098716
H,0,1.5443867603,1.6299245993,2.3308814455

$Co_2(CO)_6(PNMe_2)_2$ P-but (C_1) BP86
0 1
Co,0,1.8237020908,-0.4524514282,-0.2712434026
Co,0,-1.8177024215,-0.344475288,-0.3630569273
C,0,1.8157881426,-1.1433315861,-1.9152731383
C,0,3.106709081,0.7699046989,-0.0988897001
C,0,2.5029405573,-1.7798822542,0.649200166
C,0,-1.8342713509,-1.1393469849,-1.9662307307
C,0,-3.0777423998,0.9113291239,-0.2635799799
C,0,-2.5189263493,-1.6311722987,0.5907325785
P,0,-0.0527472244,1.0297287325,-1.2024063917
P,0,-0.0088308004,-0.3525704535,0.783319182
O,0,1.8821655625,-1.5880644207,-2.9824116924
O,0,3.9740523573,1.5356187873,0.0033544233
O,0,2.8926963944,-2.6856390776,1.2613176841
O,0,-1.9087066638,-1.6450349704,-3.0031973233
O,0,-3.9053905249,1.721240136,-0.2115716501
O,0,-2.9366705041,-2.5135207272,1.2177002156
N,0,-0.1071441945,2.609347192,-0.5047403872
N,0,-0.0782750232,-0.0894796693,2.453613196
C,0,-0.4105692345,2.9450108521,0.8813994277
C,0,0.8344862966,3.5463047073,-1.1324242621
C,0,-1.3203812006,0.0140944869,3.2222373949
C,0,1.13007163,-0.003525598,3.2792960392
H,0,-0.7002532568,4.0075436181,0.9428502806
H,0,-1.2529544421,2.3421793713,1.2457749731
H,0,0.4610147856,2.786094181,1.5493563178
H,0,0.4146736777,4.5661651254,-1.1046905889
H,0,1.8168263038,3.5546255971,-0.6210254098
H,0,0.9941735589,3.26754059,-2.1847425645
H,0,-1.3119793566,0.9392480419,3.8250223315
H,0,-2.1847461206,0.0437745778,2.5484903693
H,0,-1.4286875182,-0.8471924247,3.9042866812
H,0,1.1264342324,0.9393684533,3.8540198349
H,0,1.1756187236,-0.8478022925,3.988928162
H,0,2.0231231918,-0.022710799,2.6432908912

$Co_2(CO)_6(PNMe_2)_2$ Rhomb (C_1) B3LYP
0 1
Co,0,1.8233314578,-0.1342134183,0.084033505
Co,0,-1.7453660281,0.3204637054,0.0690521668
C,0,1.6401156456,-1.4871997377,1.2159017733
C,0,3.1380888218,0.7565683129,0.8640349671
C,0,2.6277421462,-0.5562433724,-1.4447789008
C,0,-3.0233829736,-0.3958253121,-0.9523421789
C,0,-1.561472585,-0.3683424844,1.7048750283
C,0,-2.6569750514,1.7747832823,0.4958446368
P,0,0.2235291978,1.2555161374,-0.0693796316
P,0,-0.3144515624,-1.2028849252,-1.0382959356
O,0,1.5908275511,-2.3901046356,1.9222436198
O,0,3.9783586834,1.3254825522,1.3951195152

$Co_2(CO)_6(PNMe_2)_2$ Rhomb (C_1) BP86
0 1
Co,0,1.8633087613,-0.1306000987,0.0136404701
Co,0,-1.7407407416,0.3124657387,0.0116222674
C,0,1.6806023039,-1.4751768059,1.1412595123
C,0,3.1690237948,0.7719807503,0.781735286
C,0,2.6543141741,-0.5923240953,-1.5042051436
C,0,-3.0175278792,-0.4728648352,-0.946058943
C,0,-1.5305417618,-0.3186586348,1.6503603718
C,0,-2.665284759,1.7635513593,0.3903281082
P,0,0.2389146628,1.238708679,-0.1520909442
P,0,-0.3198490476,-1.226540554,-1.0552742134
O,0,1.6292859473,-2.3854250702,1.8642711792
O,0,4.0333410825,1.3333483388,1.3180538181

O,0,3.1397052118,-0.8598136694,-2.4226856063	O,0,3.1780767875,-0.9261134715,-2.4845074104
O,0,-3.835749014,-0.8815992368,-1.5940849404	O,0,-3.8547073965,-1.0027415335,-1.5479238492
O,0,-1.4640315098,-0.7435022003,2.7789566049	O,0,-1.4247419065,-0.6648354354,2.7498029204
O,0,-3.2370924561,2.7064679849,0.8162020156	O,0,-3.2866109565,2.6930850613,0.6961486204
N,0,0.3702528799,2.8872122401,-0.4192025893	N,0,0.3702513572,2.9050888358,-0.4089908519
N,0,-0.618958651,-2.8002489622,-0.5090836781	N,0,-0.6455051462,-2.8137384766,-0.4894048005
C,0,-1.4389557349,-3.3003179681,0.5876981712	C,0,-1.4791620971,-3.2934447846,0.612441571
H,0,-2.2832012229,-2.6416170843,0.7726130973	H,0,-2.3131531883,-2.6076276424,0.797709116
H,0,-1.8407540781,-4.2798192072,0.310333126	H,0,-1.9035750019,-4.2738768937,0.3366477669
H,0,-0.8676757646,-3.4175070199,1.5161066009	H,0,-0.8962577453,-3.4167075218,1.5433214882
C,0,0.3227748755,-3.7982813792,-1.0199158209	C,0,0.310383351,-3.8223414146,-0.9697598137
H,0,-0.2199137204,-4.6939430942,-1.3391619394	H,0,-0.2344195612,-4.7152845262,-1.3219397919
H,0,0.8585319204,-3.4018648764,-1.8835628796	H,0,0.8906658607,-3.4205911699,-1.8137694332
H,0,1.0559314915,-4.090023432,-0.2578278993	H,0,1.0102136044,-4.1250718764,-0.1699518409
C,0,-0.679546304,3.6891805051,-1.0488955542	C,0,-0.6786736264,3.7248962999,-1.0233598179
H,0,-1.4706972221,3.0475536341,-1.4269515291	H,0,-1.4582555503,3.0858265055,-1.4540552981
H,0,-1.1053073372,4.4121711217,-0.3460431779	H,0,-1.1345070675,4.4133565606,-0.2912393303
H,0,-0.2531692222,4.2367755044,-1.8949109013	H,0,-0.2345925794,4.3225213132,-1.838011829
C,0,1.6205301897,3.6284266269,-0.2440327249	C,0,1.6076098818,3.6500863391,-0.1527600754
H,0,1.4115865955,4.5863610783,0.2417686004	H,0,1.3750895719,4.565092256,0.4188555618
H,0,2.3158980357,3.0756857449,0.3787229082	H,0,2.3109101811,3.0473919434,0.4297905434
H,0,2.0922493241,3.8263224773,-1.2127671168	H,0,2.0888682799,3.942183752,-1.1031018824

Complete Gaussian 03 reference (Reference 42)

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