

Decarbonylation of $P_2Co_2(CO)_6$, a Binuclear Cobalt Carbonyl Derivative of Diphosphorus¹

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Supporting Information

Table S1. The vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol , given in parentheses) of the $P_2Co_2(CO)_n$ ($n = 6, 5, 4$) complexes at the B3LYP/DZP and BP86/DZP levels.

Table S2. The Cartesian coordinates of the optimized $P_2Co_2(CO)_n$ ($n = 6, 5, 4$) structures at the B3LYP/DZP and BP86/DZP levels.

Complete Gaussian 03 reference (reference 21).

¹ This paper is dedicated to the memory of our friend Professor Ioan Silaghi-Dumitrescu (1950–2009), in recognition of his contributions to diverse areas of inorganic and computational chemistry as well as his leadership in Romanian science.

Table S1. The vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol , given in parentheses) of the $\text{P}_2\text{Co}_2(\text{CO})_n$ ($n = 6, 5, 4$) complexes at the B3LYP/DZP and BP86/DZP levels.

n	Structure	B3LYP/DZP	BP86/DZP
6	6-1S	22 (0), 52 (0), 65 (0), 67 (0), 70 (0), 82 (0), 89 (0), 92 (0), 92 (0), 103 (0), 105 (0), 105 (0), 188 (0), 241 (0), 298 (5), 307 (2), 322 (0), 363 (0), 364 (0), 408 (29), 410 (0), 423 (2), 424 (0), 454 (38), 463 (21), 474 (19), 478 (0), 480 (0), 494 (0), 521 (0), 522 (76), 529 (0), 532 (67), 547 (9), 550 (210), 581 (1), 2083 (0), 2083 (13), 2101 (804), 2106 (1387), 2117 (2089), 2156 (356)	14 (0), 44 (0), 62 (0), 64 (0), 67 (0), 79 (0), 85 (0), 88 (0), 88 (0), 97 (0), 98 (0), 99 (0), 184 (0), 237 (0), 294 (8), 308 (2), 320 (0), 359 (0), 360 (0), 407 (0), 409 (20), 420 (6), 425 (3), 474 (13), 477 (12), 482 (2), 487 (5), 491 (0), 495 (3), 528 (26), 530 (0), 531 (68), 532 (70), 549 (3), 555 (153), 563 (4), 1998 (0), 1999 (15), 2015 (745), 2019 (1197), 2039 (1552), 2069 (257)
5	5-1S	38 (0), 55 (0), 66 (0), 77 (0), 79 (0), 84 (0), 97 (0), 101 (0), 112 (0), 188 (0), 233 (0), 264 (4), 271 (1), 285 (2), 322 (0), 393 (2), 397 (0), 404 (6), 404 (0), 408 (0), 427 (0), 437 (21), 450 (67), 455 (2), 473 (0), 506 (22), 511 (29), 521 (19), 555 (42), 565 (7), 571 (84), 1924 (368), 2095 (0), 2099 (1645), 2109 (1968), 2147 (374)	27 (0), 45 (0), 52 (0), 70 (0), 73 (0), 79 (0), 79 (0), 88 (0), 96 (0), 103 (0), 180 (1), 204 (2), 283 (7), 305 (2), 318 (2), 352 (1), 388 (1), 405 (13), 416 (4), 428 (4), 470 (7), 476 (12), 483 (5), 491 (5), 492 (4), 527 (31), 530 (28), 537 (33), 545 (107), 558 (37), 572 (2), 1984 (269), 1993 (614), 2006 (666), 2021 (1677), 2053 (320)
	5-2S	33 (0), 46 (0), 57 (0), 72 (0), 78 (0), 81 (0), 84 (0), 90 (0), 101 (0), 107 (0), 180 (1), 205 (4), 285 (5), 301 (2), 318 (2), 359 (0), 384 (1), 408 (15), 422 (2), 426 (0), 455 (28), 462 (14), 467 (18), 483 (3), 490 (3), 509 (29), 524 (39), 532 (43), 546 (143), 557 (41), 594 (0), 2072 (142), 2076 (697), 2090 (1028), 2105 (2187), 2140 (387)	37 (0), 52 (0), 64 (0), 75 (0), 77 (0), 80 (0), 95 (0), 98 (0), 107 (0), 192 (0), 231 (0), 265 (0), 271 (1), 288 (4), 320 (0), 390 (4), 391 (0), 401 (5), 408 (0), 410 (1), 413 (11), 459 (7), 474 (0), 476 (24), 498 (0), 501 (18), 508 (27), 528 (9), 553 (45), 554 (23), 562 (75), 1865 (279), 2002 (0), 2006 (1417), 2020 (1663), 2053 (288)
	5-3S	22 (0), 58 (0), 61 (0), 72 (0), 76 (0), 77 (0), 90 (0), 92 (0), 92 (0), 104 (0), 184 (1), 239 (1), 277 (0), 302 (3), 309 (0), 356 (0), 371 (0), 396 (10), 410 (1), 427 (2), 441 (12), 453 (10), 457 (38), 465 (12), 484 (30), 486 (14), 505 (29), 520 (30), 522 (26), 543 (109), 579 (2), 2066 (416), 2079 (772), 2104 (1137), 2111 (1372), 2151 (542)	16 (0), 51 (0), 56 (0), 66 (0), 71 (0), 75 (0), 84 (0), 84 (0), 88 (0), 98 (0), 178 (1), 237 (1), 282 (1), 295 (1), 309 (0), 354 (0), 370 (0), 393 (2), 408 (1), 426 (7), 459 (10), 466 (2), 474 (4), 478 (13), 497 (4), 507 (27), 514 (33), 520 (36), 527 (22), 550 (67), 559 (20), 1978 (393), 1999 (291), 2016 (926), 2021 (1338), 2063 (423)
4	4-1S	39 (0), 63 (0), 73 (0), 79 (0), 91 (0), 98 (0), 104 (1), 185 (1), 220 (1), 253 (3), 275 (1), 288 (1), 318 (1), 397 (1), 404 (3), 407 (1), 421 (3), 436 (0), 449 (8), 456 (58), 463 (5), 496 (24), 514 (20), 554 (24), 572 (19), 581 (55), 1904 (412), 2089 (908), 2093 (1828), 2132 (582)	38 (0), 61 (0), 71 (0), 77 (0), 91 (0), 95 (0), 102 (0), 192 (1), 216 (1), 257 (1), 279 (1), 289 (2), 314 (1), 393 (4), 398 (2), 409 (1), 425 (1), 444 (8), 457 (2), 479 (21), 483 (5), 507 (13), 511 (22), 546 (5), 566 (26), 571 (62), 1839 (309), 1996 (1136), 2000 (1114), 2038 (524)
	4-2S	36 (0), 44 (0), 53 (0), 75 (0), 76 (0), 86 (1), 96 (0), 100 (0), 176 (0), 198 (1), 281 (6), 311 (2), 314 (2), 361 (4), 383 (1), 413 (10), 432 (1), 451 (25), 458 (14), 463 (11), 485 (3), 500 (24), 501 (35), 539 (157), 551 (13), 594 (1), 2057 (552), 2071 (953), 2089 (2545), 2121 (240)	33 (0), 43 (0), 51 (0), 74 (0), 74 (0), 85 (0), 92 (0), 97 (0), 176 (0), 195 (1), 281 (9), 311 (1), 312 (0), 359 (1), 385 (1), 412 (11), 433 (6), 469 (8), 470 (8), 476 (7), 496 (1), 520 (15), 524 (22), 541 (115), 547 (9), 575 (0), 1972 (473), 1984 (796), 2003 (1935), 2031 (178)
	4-3S	33 (0), 39 (0), 56 (0), 77 (0), 78 (0), 89 (0), 90 (1), 96 (0), 175 (0), 205 (9), 286 (1), 307 (7), 335 (4), 341 (1), 377 (0), 406 (4), 426 (1), 439 (5), 451 (18), 466 (11), 468 (22), 493 (53), 495 (0), 535 (15), 542 (147), 584 (0), 2060 (44), 2080 (1313), 2094 (2553), 2130 (315)	36 (0), 39 (0), 55 (0), 74 (0), 77 (0), 83 (0), 89 (1), 97 (0), 173 (0), 209 (4), 292 (1), 308 (10), 326 (3), 339 (1), 379 (0), 406 (3), 424 (7), 455 (6), 467 (5), 485 (3), 487 (2), 512 (3), 514 (41), 529 (3), 541 (108), 563 (1), 1972 (7), 1990 (1071), 2006 (2004), 2037 (247)

4-4S	29 (0), 55 (0), 69 (1), 71 (0), 74 (0), 83 (0), 106 (0), 109 (0), 181 (2), 202 (0), 304 (14), 326 (0), 330 (0), 360 (0), 420 (2), 427 (3), 446 (41), 446 (4), 467 (11), 488 (10), 499 (0), 515 (30), 526 (43), 535 (47), 545 (106), 575 (3), 2066 (839), 2074 (937), 2085 (1788), 2123 (397)	15 (0), 52 (0), 64 (0), 69 (0), 71 (0), 80 (0), 102 (0), 104 (0), 177 (2), 196 (0), 301 (14), 322 (0), 330 (1), 353 (0), 415 (3), 421 (6), 450 (1), 459 (24), 473 (9), 494 (1), 494 (1), 530 (34), 531 (49), 542 (96), 546 (1), 559 (9), 1984 (1124), 1987 (701), 1999 (831), 2039 (487)
4-5S	35 (0), 45 (0), 59 (0), 72 (0), 76 (0), 86 (0), 90 (0), 95 (0), 174 (2), 201 (4), 250 (0), 297 (0), 317 (3), 369 (0), 375 (0), 404 (5), 426 (1), 441 (21), 446 (15), 469 (27), 482 (9), 495 (16), 501 (31), 526 (30), 560 (65), 598 (0), 2061 (781), 2074 (647), 2092 (1756), 2132 (725)	33 (0), 44 (0), 55 (0), 69 (0), 75 (0), 83 (0), 89 (0), 93 (0), 174 (2), 207 (3), 264 (0), 302 (0), 314 (2), 360 (0), 384 (0), 408 (3), 423 (4), 457 (14), 469 (7), 482 (12), 489 (5), 508 (14), 515 (38), 528 (13), 560 (27), 574 (15), 1977 (568), 1986 (436), 2004 (1508), 2039 (520)
4-6S	33 (0), 60 (0), 69 (0), 69 (0), 83 (0), 86 (0), 90 (0), 103 (0), 184 (0), 221 (0), 274 (0), 303 (2), 312 (5), 359 (0), 403 (7), 417 (2), 429 (0), 447 (9), 456 (8), 470 (8), 477 (14), 487 (57), 509 (24), 528 (40), 540 (100), 593 (1), 2058 (782), 2080 (810), 2098 (1297), 2136 (673)	24 (0), 52 (0), 61 (0), 65 (0), 78 (0), 81 (0), 86 (0), 98 (0), 179 (0), 218 (0), 276 (1), 304 (1), 314 (3), 353 (1), 396 (2), 412 (4), 437 (1), 459 (6), 468 (3), 476 (0), 482 (5), 512 (39), 519 (22), 532 (33), 542 (77), 565 (3), 1970 (631), 1996 (705), 2010 (944), 2050 (528)
4-7S	31 (0), 68 (0), 70 (0), 70 (0), 78 (0), 79 (0), 86 (1), 102 (0), 182 (0), 240 (0), 258 (7), 297 (0), 300 (3), 328 (0), 372 (1), 403 (27), 408 (0), 426 (3), 447 (24), 453 (49), 457 (30), 469 (10), 470 (0), 498 (3), 512 (26), 588 (0), 2069 (0), 2075 (1208), 2090 (1619), 2140 (746)	17 (0), 61 (0), 61 (2), 62 (0), 73 (1), 76 (0), 76 (0), 93 (0), 177 (1), 237 (0), 270 (3), 295 (1), 305 (0), 313 (0), 369 (1), 387 (1), 409 (0), 428 (10), 469 (8), 478 (23), 481 (34), 484 (11), 496 (0), 502 (9), 507 (17), 558 (3), 1980 (0), 1997 (1370), 1998 (855), 2045 (594)

Table S2. The Cartesian coordinates of the optimized $P_2Co_2(CO)_n$ ($n = 6, 5, 4$) structures at the B3LYP/DZP and BP86/DZP levels.

$P_2Co_2(CO)_6$ (6-1S) C_{2v} B3LYP	$P_2Co_2(CO)_6$ (6-1S) C_{2v} BP86
0 1	0 1
Co,0,0.0114755829,0.,-0.0424098373	Co,0,0.,1.2883558301,0.0118192165
Co,0,0.0114755825,0.,2.5272878371	Co,0,0.,-1.2883558301,0.0118192165
C,0,0.928888074,0.0000000003,-1.5715029022	C,0,0.,2.8048566923,-0.9023063493
O,0,1.5196727636,0.0000000005,-2.5611487774	O,0,0.,3.8087526191,-1.4985452465
C,0,-1.0564574556,-1.4431089949,-0.2901950723	C,0,-1.4291424803,1.5463388303,1.0755437865
O,0,-1.7282378888,-2.3583845188,-0.4878940214	O,0,-2.3518778201,1.7620077363,1.7566625917
C,0,-1.0564574566,1.4431089941,-0.2901950723	C,0,1.4291424803,1.5463388303,1.0755437865
O,0,-1.7282378904,2.3583845175,-0.4878940214	O,0,2.3518778201,1.7620077363,1.7566625917
C,0,0.9288880731,0.0000000003,4.0563809023	C,0,0.,-2.8048566923,-0.9023063493
O,0,1.5196727624,0.0000000005,5.0460267777	O,0,0.,-3.8087526191,-1.4985452465
C,0,-1.0564574561,-1.4431089949,2.7750730717	C,0,-1.4291424803,-1.5463388303,1.0755437865
O,0,-1.7282378894,-2.3583845188,2.9727720206	O,0,-2.3518778201,-1.7620077363,1.7566625917
C,0,-1.0564574571,1.4431089941,2.7750730717	C,0,1.4291424803,-1.5463388303,1.0755437865
O,0,-1.728237891,2.3583845175,2.9727720206	O,0,2.3518778201,-1.7620077363,1.7566625917
P,0,1.6211259119,1.0441872092,1.2424390002	P,0,1.0557924365,0.,-1.5958115483
P,0,1.6211259126,-1.0441872081,1.2424390002	P,0,-1.0557924365,0.,-1.5958115483
$P_2Co_2(CO)_5$ (5-1S) C_{2v} B3LYP	$P_2Co_2(CO)_5$ (5-1S) C_{2v} BP86
0 1	0 1
Co,0,-0.0017692879,0.0046381046,-0.0487373282	Co,0,0.0009252776,-0.0024255719,-0.0312022815
Co,0,-0.0017692888,0.0046381048,2.6102953282	Co,0,0.0009252776,-0.0024255717,2.5927602816
C,0,1.5888186574,-0.0435938435,-0.9194699574	C,0,1.5643122857,-0.042822381,-0.9175544105
C,0,-1.561218464,-1.0907004292,-0.9194699574	C,0,-1.1383554834,-1.073803277,-0.9175544105
C,0,1.5888186573,-0.043593843,3.4810279576	C,0,1.5643122856,-0.0428223805,3.4791124107
C,0,-1.561218465,-1.0907004288,3.4810279576	C,0,-1.1383554835,-1.0738032765,3.4791124107
C,0,0.4799438535,-1.2581501646,1.2807790002	C,0,0.4895199799,-1.283253528,1.2807790002
O,0,2.5869304075,-0.0647877584,-1.493412564	O,0,2.5630328913,-0.060400442,-1.5214656743
O,0,-1.886533238,-1.7712703717,-1.493412564	O,0,-1.8716292667,-1.7520815348,-1.5214656743
O,0,2.5869304073,-0.0647877578,4.0549705643	O,0,2.5630328911,-0.0604004414,4.0830236746
O,0,-1.8865332382,-1.7712703711,4.0549705643	O,0,-1.8716292669,-1.7520815342,4.0830236746
O,0,0.8996920457,-2.3585002436,1.2807790003	O,0,0.9132456632,-2.3940304123,1.2807790003
P,0,-1.5367236018,1.0639359248,1.2807789999	P,0,-1.5492040545,1.054748375,1.2807789999
P,0,0.4376958411,1.8171134887,1.2807789999	P,0,0.453124529,1.8185723791,1.2807789999
$P_2Co_2(CO)_5$ (5-2S) C_1 B3LYP	$P_2Co_2(CO)_5$ (5-2S) C_1 BP86
0 1	0 1
Co,0,1.1512863665,0.0202033722,0.0426814271	Co,0,1.15399702,0.0184747768,0.037216227
Co,0,-1.3110047789,-0.0280878092,0.2395152619	Co,0,-1.310004578,-0.0348037728,0.2517386834
C,0,2.7483501155,-0.7757118252,-0.1912633332	C,0,2.7313254725,-0.8070504634,-0.1071897315
O,0,3.7709529558,-1.28797997,-0.3361370896	O,0,3.764381034,-1.3445443493,-0.1924781246
C,0,1.3914136416,1.5850141811,-0.8233112364	C,0,1.4566750637,1.5430493624,-0.8640676241
O,0,1.5744407917,2.58306794,-1.3723738295	O,0,1.6930444882,2.5289818552,-1.443437052
C,0,1.1378475036,0.4246533083,1.7940842763	C,0,1.0958669475,0.4830823077,1.7639889848
O,0,1.1033841384,0.693508004,2.917634705	O,0,1.026750417,0.7966938962,2.8894758622
C,0,-2.9395185806,-0.7132833536,0.0895982912	C,0,-2.925580354,-0.7089352883,0.0980311314
O,0,-3.9909517821,-1.1681350913,-0.0502993673	O,0,-3.9969596865,-1.1544474422,-0.0567222074
C,0,-1.6572011993,1.727525485,0.0134421583	C,0,-1.6649998566,1.7016415185,0.0235083984
O,0,-1.8906014354,2.8404187062,-0.1800258923	O,0,-1.9207985637,2.8243693377,-0.1811865568
P,0,-0.1056587844,-1.9602533529,0.1907928672	P,0,-0.1029462951,-1.9656757965,0.1695034906
P,0,-0.1817244886,-0.8773028929,-1.5737928505	P,0,-0.1956444438,-0.8368754109,-1.5970118176

$P_2Co_2(CO)_5$ (5-3S) C_s B3LYP

0 1

Co,0,0.0087100844,-0.0000000001,-0.0585419378
 Co,0,-0.0984301987,0.0000000001,2.4720407862
 C,0,0.9170727258,-0.0000000001,-1.5982036755
 O,0,1.5280029976,-0.0000000001,-2.5735928561
 C,0,-1.0094837452,-1.4832272978,-0.3349974887
 O,0,-1.6585173259,-2.4160482533,-0.5194133928
 C,0,-1.0094837456,1.4832272973,-0.3349974889
 O,0,-1.6585173266,2.4160482525,-0.5194133932
 C,0,-1.101059934,-1.4505407545,2.8448238322
 O,0,-1.761581011,-2.3746884914,3.0534813333
 C,0,-1.1010599344,1.4505407544,2.844823832
 O,0,-1.7615810117,2.3746884912,3.053481333
 P,0,1.57102991,1.0439236293,1.3124197344
 P,0,1.5710299103,-1.0439236288,1.3124197346

$P_2Co_2(CO)_4$ (4-1S) C_1 B3LYP

0 1

Co,0,-1.0782856864,0.005723695,0.2523567172
 Co,0,1.4064935271,-0.5029784361,-0.4053999816
 C,0,-2.407931167,-0.3044754521,-0.9343698635
 O,0,-3.2749336839,-0.4962002219,-1.6688424411
 C,0,-1.4594450177,1.5612720418,1.0891663484
 O,0,-1.7336995428,2.5419950128,1.6294187858
 C,0,0.1467914714,0.7469812183,-0.9847796947
 O,0,0.0918352079,1.5684385399,-1.8315750076
 C,0,2.7982676734,0.6359212389,-0.3683512925
 O,0,3.686335491,1.3651884253,-0.2669347467
 P,0,-0.1412399239,-2.080154782,0.2265816875
 P,0,0.575639308,-0.7363579061,1.668461141

$P_2Co_2(CO)_4$ (4-2S) C_2 B3LYP

0 1

Co,0,0.2585205981,-0.0309808472,0.0328721278
 Co,0,0.2585205961,0.0309808471,2.4520058718
 C,0,0.8807942885,-0.037911368,-1.6454743485
 O,0,1.3166080444,0.0066082696,-2.7138208449
 C,0,-1.128283299,1.1048893986,-0.0486985278
 O,0,-1.9795987209,1.8872178572,-0.0629761478
 C,0,0.8807942838,0.0379113668,4.1303523492
 O,0,1.3166080379,-0.0066082716,5.1986988463
 C,0,-1.1282833032,-1.104889396,2.5335765252
 O,0,-1.9795987266,-1.887217853,2.5478541437
 P,0,1.8845657627,1.0339636237,1.2840881104
 P,0,1.8845657608,-1.0339636268,1.2007898919

$P_2Co_2(CO)_4$ (4-3S) C_s B3LYP

0 1

Co,0,0.2318432443,-0.3253492435,0.0123565648
 Co,0,0.231843244,-0.3253492438,2.4725214349
 C,0,0.7991815231,0.192385714,-1.606466761
 O,0,1.2178726169,0.4812093499,-2.642039387
 C,0,-1.0274927056,-1.5515211587,-0.3678790004
 O,0,-1.8065045139,-2.362503285,-0.6309950278
 C,0,0.7991815223,0.1923857135,4.0913447609
 O,0,1.2178726157,0.4812093492,5.1269173871
 C,0,-1.0274927061,-1.551521159,2.8527569995
 O,0,-1.8065045145,-2.3625032854,3.1158730265
 P,0,1.8647352785,0.7400190939,1.2424390002
 P,0,1.770202409,-1.34277582,1.242439

$P_2Co_2(CO)_5$ (5-3S) C_s BP86

0 1

Co,0,0.2004932856,1.0082844266,0.
 Co,0,-0.5170079163,-1.4492267372,0.
 C,0,-0.1379946739,2.7441473423,0.
 O,0,-0.3834530005,3.8845945133,0.
 C,0,1.2521407419,0.9402830368,1.465103205
 O,0,1.9387353158,0.9079451701,2.4067744357
 C,0,1.2521407419,0.9402830368,-1.465103205
 O,0,1.9387353158,0.9079451701,-2.4067744357
 C,0,0.2969896147,-2.156070464,1.4273972497
 O,0,0.8634758999,-2.5981006516,2.351721912
 C,0,0.2969896147,-2.156070464,-1.4273972497
 O,0,0.8634758999,-2.5981006516,-2.351721912
 P,0,-1.6991642943,0.1995114092,-1.0593815243
 P,0,-1.6991642943,0.1995114092,1.0593815243

$P_2Co_2(CO)_4$ (4-1S) C_1 BP86

0 1

Co,0,-1.0614117152,-0.0142819749,0.2336420486
 Co,0,1.389477759,-0.4674920403,-0.4113635428
 C,0,-2.3788507636,-0.2736770828,-0.9602490145
 O,0,-3.2630712393,-0.4347160689,-1.7060198505
 C,0,-1.492588836,1.4781952581,1.1335574608
 O,0,-1.8133268784,2.435705728,1.7208584053
 C,0,0.1734311634,0.8219389878,-0.9481715793
 O,0,0.1300827484,1.7084959662,-1.7459596892
 C,0,2.7904107727,0.625856503,-0.3383656929
 O,0,3.7108489753,1.3386229656,-0.2132352342
 P,0,-0.1358594498,-2.1004660891,0.1453789327
 P,0,0.5672950466,-0.7855907318,1.6568013504

$P_2Co_2(CO)_4$ (4-2S) C_2 BP86

0 1

Co,0,0.2639899839,-0.0381856768,0.0343862155
 Co,0,0.263989982,0.0381856767,2.4504917841
 C,0,0.8748427246,-0.0289571743,-1.6328782962
 O,0,1.3090669091,0.0386735987,-2.717804552
 C,0,-1.121115656,1.0815501044,-0.0628504771
 O,0,-1.985652478,1.8717861365,-0.0960682533
 C,0,0.8748427199,0.0289571731,4.1177562969
 O,0,1.3090669025,-0.0386736008,5.2026825533
 C,0,-1.1211156601,-1.0815501018,2.5477284744
 O,0,-1.9856524837,-1.8717861323,2.5809462492
 P,0,1.8914346515,1.046121909,1.2699587166
 P,0,1.8914346495,-1.0461219122,1.2149192857

$P_2Co_2(CO)_4$ (4-3S) C_s BP86

0 1

Co,0,0.1954848549,-0.2767251137,0.0031707573
 Co,0,0.1954848545,-0.276725114,2.4817072423
 C,0,0.8183196173,0.1413618158,-1.6071974672
 O,0,1.2805994359,0.3553490613,-2.6602335296
 C,0,-1.0287034379,-1.5247097072,-0.3643107229
 O,0,-1.7945357701,-2.3660262239,-0.6400383976
 C,0,0.8183196164,0.1413618153,4.0920754672
 O,0,1.2805994347,0.3553490606,5.1451115298
 C,0,-1.0287034384,-1.5247097075,2.8491887219
 O,0,-1.7945357707,-2.3660262242,3.1249163962
 P,0,1.7594135613,0.8611386167,1.2424390002
 P,0,1.762995062,-1.2539522684,1.242439

P₂Co₂(CO)₄ (4-4S) C_s B3LYP

0 1

Co,0,0.1306213399,0.0000000001,-0.1226517685
 Co,0,0.0970510553,-0.0000000006,2.3024940388
 C,0,0.917459795,0.0000000012,-1.7572382747
 O,0,1.4100904738,0.0000000019,-2.8000125043
 C,0,-0.9600679702,-1.4226840471,-0.1719925407
 O,0,-1.6726422523,-2.3338158131,-0.1884240287
 C,0,-0.9600679728,1.4226840453,-0.17199254
 O,0,-1.6726422567,2.3338158099,-0.1884240275
 C,0,0.6505602722,-0.0000000005,3.9766789669
 O,0,1.089655775,-0.0000000003,5.0466318998
 P,0,1.7172546776,1.0485517268,1.1873724361
 P,0,1.7172546795,-1.0485517243,1.1873724356

P₂Co₂(CO)₄ (4-5S) C₁ B3LYP

0 1

Co,0,1.2827699697,-0.5125912495,-0.1681652426
 Co,0,-0.9663949504,0.1904101211,0.2729432796
 C,0,2.1000408326,0.9350965522,-0.8421665967
 O,0,2.6037183189,1.8905657319,-1.2537374009
 C,0,1.7528692335,-0.6226239013,1.5613025437
 O,0,2.0062100806,-0.6375710608,2.6897902706
 C,0,-2.7402686362,0.1469483063,0.3218325045
 O,0,-3.8918639682,0.0919169791,0.3130352032
 C,0,-0.751877416,1.9788165061,0.3798817448
 O,0,-0.6101088128,3.1223716601,0.4071270982
 P,0,-0.4762219854,-2.020118336,-0.1393628716
 P,0,-0.2951349849,-0.757801717,-1.767559098

P₂Co₂(CO)₄ (4-6S) C₁ B3LYP

0 1

Co,0,0.0828033528,-0.0821845668,-0.0696839278
 Co,0,-0.0548530138,-0.0233368756,2.3507770686
 C,0,0.9111013067,0.0694200455,-1.664621888
 O,0,1.460118457,0.1768336382,-2.6714853519
 C,0,-0.8401177637,-1.6122007987,-0.353396141
 O,0,-1.4394366306,-2.5783658642,-0.545741052
 C,0,-1.0618719587,1.3099866999,-0.1193400555
 O,0,-1.812319298,2.1880108527,-0.1197508196
 C,0,-1.3245738512,-1.21084637,2.7692005692
 O,0,-2.1077081084,-2.0361924211,2.9808195559
 P,0,1.6823013017,0.9991661182,1.2750156157
 P,0,1.6601922273,-1.0674474505,1.3320284248

P₂Co₂(CO)₄ (4-7S) C_{2v} B3LYP

0 1

Co,0,0.0590155578,-0.0828716254,0.0093582666
 Co,0,0.059015559,-0.0828716268,2.4755197334
 C,0,1.8332012251,0.0004101448,-0.3714939658
 O,0,2.9688332921,0.0242030186,-0.5707803288
 C,0,-0.5998874084,-1.7322707634,-0.3714939655
 O,0,-0.9937503924,-2.7976806575,-0.5707803284
 C,0,1.8332012266,0.000410143,2.8563719641
 O,0,2.9688332939,0.0242030166,3.0556583261
 C,0,-0.5998874068,-1.7322707652,2.8563719643
 O,0,-0.9937503906,-2.7976806595,3.0556583264
 P,0,-1.7484760912,0.6650790823,1.2424390013
 P,0,-0.0567178116,1.8698347299,1.2424390011

P₂Co₂(CO)₄ (4-4S) C_s BP86

0 1

Co,0,-0.7836980128,0.6375649363,0.
 Co,0,1.4031270905,-0.442331259,0.
 C,0,-2.5841678561,0.709567406,0.
 O,0,-3.7501298571,0.7700182938,0.
 C,0,-0.3304677592,1.6267534807,1.4205473629
 O,0,-0.0125273101,2.2736049948,2.3431245926
 C,0,-0.3304677592,1.6267534807,-1.4205473629
 O,0,-0.0125273101,2.2736049948,-2.3431245926
 C,0,2.6267996135,-1.6805518415,0.
 O,0,3.3875932581,-2.5766209375,0.
 P,0,-0.3304677592,-1.3630434404,-1.0611196084
 P,0,-0.3304677592,-1.3630434404,1.0611196084

P₂Co₂(CO)₄ (4-5S) C₁ BP86

0 1

Co,0,1.2958699685,-0.5004092618,-0.1967817049
 Co,0,-0.9823047336,0.1542058345,0.3029134887
 C,0,2.1266023161,0.9578884722,-0.8098949375
 O,0,2.6482470771,1.9388349616,-1.1793998802
 C,0,1.7815925799,-0.6715163807,1.5182569373
 O,0,2.0394978675,-0.718964422,2.6600920798
 C,0,-2.7340104601,0.1123835459,0.3241475701
 O,0,-3.9030315525,0.0742619019,0.2882926492
 C,0,-0.7889546814,1.9253103305,0.440490795
 O,0,-0.670542374,3.0871946271,0.4898978405
 P,0,-0.4697170755,-2.007331318,-0.1982446831
 P,0,-0.3107198084,-0.6383811242,-1.7849305804

P₂Co₂(CO)₄ (4-6S) C₁ BP86

0 1

Co,0,0.7756325765,0.2574845882,0.0364907624
 Co,0,-1.4310576212,-0.7830909503,0.2807448968
 C,0,2.5192533541,0.2786873411,-0.3314259468
 O,0,3.6622761962,0.2735850821,-0.5674603005
 C,0,0.3051545311,1.8528065646,-0.6587457972
 O,0,0.0200326496,2.8961814194,-1.096631983
 C,0,0.8080348853,0.4018370265,1.8251687546
 O,0,0.7726930402,0.4905387469,2.9907493891
 C,0,-2.594532134,0.5407778845,0.1401959508
 O,0,-3.3127931212,1.4567129092,-0.0247732103
 P,0,0.4444792098,-2.0616578406,-0.018075902
 P,0,-0.2873172454,-0.9512872939,-1.6415614565

P₂Co₂(CO)₄ (4-7S) C_{2v} BP86

0 1

Co,0,0.0449996835,-0.0631900648,-0.0181877489
 Co,0,0.0449996848,-0.0631900661,2.503065749
 C,0,1.8014061097,-0.0064404932,-0.4103672712
 O,0,2.9530287123,-0.0045851575,-0.6107856573
 C,0,-0.5830156956,-1.7044641831,-0.410367271
 O,0,-0.9613766307,-2.7921594823,-0.6107856569
 C,0,1.8014061113,-0.006440495,2.8952452696
 O,0,2.9530287141,-0.0045851595,3.0956636546
 C,0,-0.583015694,-1.7044641849,2.8952452698
 O,0,-0.9613766289,-2.7921594843,3.0956636549
 P,0,-1.7517440121,0.6365721577,1.2424390013
 P,0,-0.0287096187,1.8636005349,1.2424390011

Complete Gaussian 03 reference (reference 21)

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